The generalized totally geodesic Radon transform and its application to texture analysis

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SUMMARY

The generalized totally geodesic Radon transform associates the mean values over spherical tori to a function $f$ defined on $S^3 \subseteq H$, where the elements of $S^3$ are considered as quaternions representing rotations. It is introduced into the analysis of crystallographic preferred orientation and identified with the probability density function corresponding to the angle distribution function $W$. Eventually, this communication suggests a new approach to recover an approximation of $f$ from data sampling $W$. At the same time it provides additional clarification of a recently suggested method applying reproducing kernels and radial basis functions by instructive insight into its involved geometry. The focus is on the correspondence of geometrical and group features rather than on the mapping of functions and their spaces. Copyright © 2008 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The aim of this paper is to prove the equivalence of certain representations of the pole figure inversion, which are based on the totally geodesic Radon transform. Each representation raises
different aspects of the mathematical inversion problem. In particular, we will prove that in terms of the Radon transform $R$ on the unit sphere $\mathbb{S}^3 \subset \mathbb{R}^4$ and its dual transform $\tilde{R}$

$$f = \frac{1}{4\pi} (\mathcal{A} f)(\mathbf{h}, \mathbf{q}, \mathbf{h}^*; \mathbf{r}) \frac{v}{\sqrt{u^2 - v^2}} \, d\omega_2(\mathbf{h})$$

where $\mathcal{A} f$ is the so-called angle distribution function. The first part of the equation reveals the nature of any inversion formula for the Radon transform; it consists of the dual Radon transform and a differential operator. These formulae had been proven in [1]. The second part of the equation demonstrates that the inversion problem could also be considered as the inversion of an Abelian integral equation. This fact is of special interest because $\mathcal{A} f$ can be measured by experiments. Although questions about the best practical performance of numerical procedures initiated this communication, they will be pursued elsewhere. Here we focus on the mathematical basics.

The paper is organized as follows. First, we recall some geometrical objects that are the basis for the different inversion formulae of the Radon transforms; then the spherical and generalized Radon transforms are considered and their interpretation in texture analysis demonstrated. Sections 2 and 3 contain the main results of the paper. In Section 4 we consider various numerical approaches to the inversion problem and discuss their relevance to solving the Radon inversion problem in texture analysis. The paper concludes with some examples.

2. TEXTURE ANALYSIS

Texture analysis is the analysis of the statistical distribution of orientations of crystals within a specimen of polycrystalline material, which could be metals or rocks. A crystallographic orientation is a set of crystal symmetrically equivalent rotations between an individual crystal and the specimen. Patterns of crystallographic preferred orientations (‘texture’) of minerals in rocks are commonly used to infer constraints on their tectono-metamorphic history [2]. They are usually represented as pole figures (fabric diagrams) $P(\mathbf{h}, \mathbf{r})$ of specific crystal lattice planes or directions $\mathbf{h}$ as they are experimentally accessible by X-ray, neutron or synchrotron diffraction for some crystal forms. They represent the probability that a given crystallographic direction $\mathbf{h} \in \mathbb{S}^2$ (or a crystal symmetrically equivalent direction) coincides with a given specimen direction $\mathbf{r} \in \mathbb{S}^2$ subject to a random orientation $\mathbf{g} \in \text{SO}(3)$, i.e.

$$P(\mathbf{h}, \mathbf{r}) \, d\mathbf{r} = \frac{dV_{\mathbf{h}||\mathbf{r}}}{V} \geq 0$$

These pole probability density functions $P$ are projections of the orientation probability density function $f$ describing the probability by volume of crystal orientations in a representative volume of some polycrystalline specimen. Obviously, the orientation probability function $f$ is defined on the group $\text{SO}(3)$. A Radon transform based on the group $\text{SO}(3)$ is considered in [1]. In this paper we use the fact that $\text{SO}(3) \sim \mathbb{S}^3_+ \subset \mathbb{R}^3$ (upper hemisphere) and in fact, the pole probability density functions are basically provided by the one-dimensional totally geodesic Radon transform $R f$ of the orientation probability density function. In geoscience or engineering applications the practical
problem is to recover an orientation probability density function from discrete values of pole probability density functions experimentally sampled by diffraction. For this inversion the angle probability density function representing the probability that a given crystallographic direction \( h \in \mathbb{S}^2 \) encloses a given angle with a given specimen direction \( r \) is instrumental.

3. SOME GEOMETRY

In this section we give parametric representations of the geometrical objects required to compare the inversion formulae of the Radon transform and especially their relationship to the problem in texture analysis. Because of \( \mathbb{S}^3 \sim \mathbb{H}_1 \) (unit quaternions) and \( \text{SO}(3) \sim \mathbb{S}^3 \) great circles on \( \mathbb{S}^3 \) can be represented in terms of unit quaternions or by rotations \( g \in \text{SO}(3) \), which rotate \( r \in \mathbb{S}^2 \) onto \( h \in \mathbb{S}^2 \).

**Definition 1**

Let \( q_1, q_2 \in \mathbb{S}^3 \) be two orthogonal unit quaternions. The set of quaternions

\[
q(t) = q_1 \cos t + q_2 \sin t, \quad t \in [0, 2\pi)
\]

constitutes the great circle denoted by \( C(q_1, q_2) \subseteq \mathbb{S}^3 \).

If we choose for a given pair for \( h, r \in \mathbb{S}^2 \) with \( r \neq -h \)

\[
q_1 = \cos \frac{\eta}{2} + \frac{h \times r}{\|h \times r\|} \sin \frac{\eta}{2} \quad \text{and} \quad q_2 = \frac{h + r}{\|h + r\|}
\]

where \( \eta \) denotes the angle \( \angle(h, r) \) enclosed by \( h \) and \( r \), then \( q(t)hq(t)^* = r, \ t \in [0, 2\pi) \). Obviously, \( (h, r) \) and \( (-h, -r) \) define the same great circle \( C(q_1, q_2) \subseteq \mathbb{S}^3 \).

**Definition 2**

Let \( q_1, q_2, q_3, q_4 \in \mathbb{S}^3 \) be four mutually orthonormal quaternions; let \( C(q_1, q_2) \) denote the circle spanned by quaternions \( q_1, q_2 \), and \( C(q_3, q_4) \) the orthogonal circle spanned by \( q_3, q_4 \). The set of quaternions

\[
q(s, t; \Theta) = (q_1 \cos s + q_2 \sin s) \cos \Theta + (q_3 \cos t + q_4 \sin t) \sin \Theta
\]

\[
\begin{align*}
s, t & \in [0, 2\pi), \quad \Theta \in [0, \pi/2] \\
(3)
\end{align*}
\]

constitutes the spherical torus denoted by \( T(C(q_1, q_2); \Theta) \subseteq \mathbb{S}^3 \) with core \( C(q_1, q_2) \).

A detailed description of the geometry can be found in [3].

3.1. Fibres

The fibre \( G(h, r) \subseteq \text{SO}(3) \) of all rotations with \( gh = r \) is represented by the circle \( C(q_1, q_2) \subseteq \mathbb{S}^3 \) spanned by unit quaternions \( q_1, q_2 \in \mathbb{S}^3 \) given in terms of \( h, r \in \mathbb{S}^2 \) by Equations (2), for example. Therefore, the notation \( C_{h,r} = C(q_1, q_2) \) is used where it is more instructive keeping in mind that \( C_{h,r} \equiv C_{h,-r} \). Thus, the major property of the circle \( C(q_1, q_2) \) is that it provides a parametric representation of the fibre \( G(h, r) \) and that it covers the fibre twice; moreover, it is uniquely characterized by the pair \( (h, r) \in \mathbb{S}^2 \times \mathbb{S}^2 \) and its antipodal symmetric \( (-h, -r) \).

More generally, the following proposition has been shown in [3].
Proposition 1
The set of all rotations mapping \( h \) on the small circle \( c(r; \rho) \subset \mathbb{S}^2 \) is equal to the set of all rotations mapping all elements of the small circle \( c(h; \rho) \) onto \( r \) and represented by the spherical torus \( T(C(q_1, q_2); \rho/2) \subset \mathbb{S}^3 \) with core \( C(q_1, q_2) \).

Thus, the torus \( T(C(q_1, q_2); \rho/2) \) consisting of all quaternions with distance \( \rho/2 \) from \( C(q_1, q_2) \) actually consists of all great circles with distance \( \rho/2 \) from \( C(q_1, q_2) \) representing all rotations mapping \( h \) on \( c(r; \rho) \) and mapping \( c(h; \rho) \) on \( r \).

The distance \( d \) of an arbitrary \( q \in \mathbb{S}^3 \) from the circle \( C(q_1, q_2) \) is given by

\[
d(q, C(q_1, q_2)) = \frac{1}{2} \arccos(qh^* \cdot r)
\]

If \( d(q, C(q_1, q_2)) = \rho \), then \( q \) and \( C \) are called \( \rho \)-incident.

Then the set of all circles \( C(p_1, p_2) \subset \mathbb{S}^3 \) with a fixed distance \( \rho/2 \) of a given \( q \in \mathbb{S}^3 \), i.e. the set of all circles tangential to the sphere \( s(q; \rho/2) \) with centre \( q \) and radius \( \rho/2 \), is characterized by

\[
\frac{\rho}{2} = d(q, C(p_1, p_2)) = \frac{1}{2} \arccos(qh^* \cdot r)
\]

where \( r \in \mathbb{S}^2 \) is uniquely defined in terms of \( h \) and \( p_1, p_2 \) by \( r := p(t)h p^*(t) \) for all \( p(t) \in C(p_1, p_2) \) and any arbitrary \( h \in \mathbb{S}^2 \), i.e. each circle \( C(p_1, p_2) \) represents all rotations mapping some \( h \in \mathbb{S}^2 \) onto an element of the small circle \( c(qh^*; \rho) \). Thus, for each \( q \in \mathbb{S}^3 \) and \( \rho \in [0, \pi) \)

\[
\left\{ C(p_1, p_2) | d(q, C(p_1, p_2)) = \frac{\rho}{2} \right\} = \bigcup_{h \in \mathbb{S}^2} \bigcup_{r \in c(qh^*; \rho)} C_{h,r}
\]

\[
= \bigcup_{h \in \mathbb{S}^2} \bigcup_{r \in c(qh^*; \rho)} C(p_1(h, r), p_2(h, r))
\]

\[
= \bigcup_{h \in \mathbb{S}^2_+} \bigcup_{r \in c(qh^*; \rho)} C(p_1(h, r), p_2(h, r))
\]

\[
= \bigcup_{h \in \mathbb{S}^2_+} T\left(C(p_1(h, r), p_2(h, r)); \frac{\rho}{2}\right)
\]

where \( \mathbb{S}^2_+ \) denotes the upper hemisphere of \( \mathbb{S}^2 \). The last equation is due to the fact that \( (h, r) \) and \( (-h, -r) \) characterize the same great circle \( C_{h,r} \equiv C_{-h, -r} \).

4. RADON TRANSFORMS

Here, we consider the totally geodesic Radon transform and the generalized Radon transform and their relationship to texture analysis. Let \( \mathcal{C} \) denote the set of all one-dimensional totally geodesic submanifolds \( C \subset \mathbb{S}^3 \). Each \( C \in \mathcal{C} \) is a 1-sphere, i.e. a great circle with centre \( C \). Each circle is characterized by a unique pair of unit vectors \( (h, r) \in \mathbb{S}^2 \times \mathbb{S}^2 \) (and equivalently by its antipodal symmetric) by virtue of \( qh^* = r \) for all \( q \in C \). Thus, referring to the quaternion representation, Equation (1) can be rewritten in a parametric form as

\[
P(h, r) = \frac{1}{8\pi} \int_{\mathcal{C} \cup \mathcal{C}^+} f(q) d\omega_1(q)
\]
where the circle $C \subset \mathbb{S}^3$ represents all rotations mapping $h \in \mathbb{S}^2$ on $r \in \mathbb{S}^2$ and where $C^\perp(q_1, q_2)$ is the orthogonal circle representing all rotations mapping $-h$ on $r$, and where $\omega_1$ denotes the usual one-dimensional circular Riemann measure.

**Definition 3**

Following Helgason [4, 5]

\[
\frac{1}{2\pi} \int_C f(q) \, d\omega_1(q) = \int_C f(q) \, dm(q) = \mathcal{R} f(C)
\]

with the normalized measure $m = (1/2\pi)\omega_1$ is referred to as one-dimensional totally geodesic Radon transform of $f$ whenever $f$ is integrable on each great circle.

The Radon transform of $f$ may be represented as the convolution of $f$ with the indicator function of the great circle $C$. It associates with the function $f$ its mean values over great circles $C \in \mathbb{S}^2$. Since each great circle is uniquely characterized by a pair $(h, r) \in \mathbb{S}^2 \times \mathbb{S}^2$ and its antipodal symmetric, we also use the notation $(\mathcal{R} f)(h, r) \equiv (\mathcal{R} f)(-h, -r)$ whenever it is more instructive.

It should be noted that no distinction has been made whether $f$ refers to $\text{SO}(3)$ or $\mathbb{S}^3$, even though the form of $f$ depends on the representation of $g$; in particular, with respect to $\mathbb{S}^3$ only even functions $f$ could be orientation probability density functions as $q \in \mathbb{S}^3$ and $-q$ represent the same orientation. Then

\[
P(h, r) = \frac{1}{4} (\mathcal{R} f(C, r) + \mathcal{R} f(C, -r)) = \mathcal{R} f(h, r)
\]  

(6)

where $P(h, r)$ is also referred to as basic crystallographic X-ray transform.

Further, following Helgason [4, 5] the generalized one-dimensional totally geodesic Radon transform and the respective dual are well defined.

**Definition 4**

The generalized one-dimensional totally geodesic Radon transform of a real function $f : \mathbb{S}^3 \mapsto \mathbb{R}^3$ is defined as

\[
\mathcal{R}^{(\rho)} f(C) = \frac{1}{4\pi^2 \sin \rho} \int_{d(q, C) = \rho} f(q) \, dq
\]

The generalized Radon transform of $f$ may be represented as the convolution of $f$ with the indicator function of the torus $T$. It associates with $f$ its mean values over the torus $T(C, \rho)$ with core $C$ and radius $\rho$, Equation (3).

According to [6, 7, p. 64], a spherically generalized translation is defined as follows.

**Definition 5**

The spherically generalized translation of a real function $F \in C(\mathbb{S}^2)$ or $F \in L^p(\mathbb{S}^2)$, $1 \leq p < \infty$, is defined as

\[
\mathcal{F}_2^{(\rho)} F(r) = \frac{1}{2\pi \sqrt{1 - \cos^2 \rho}} \int_{\rho r' = \cos \rho} F(r') \, dr'
\]

where $2\pi \sqrt{1 - \cos^2 \rho}$ is the length of the circle $c(r; \rho)$ centred at $r$ with radius $\cos \rho$. 

Similarly, the spherically generalized translation of a real function \( f \in C(\mathbb{S}^3) \) or \( f \in L^p(\mathbb{S}^3), 1 \leq p < \infty \), is defined by the mean value operator

\[
\mathcal{F}_3^{(p)} f(q) = \frac{1}{A(\rho)} \int_{S_c(q^*; \rho) = \cos \rho} f(p) \, dp
\]

where \( A(\rho) \) denotes the surface area of the sphere \( s(q; \rho) \) centred at \( q \in \mathbb{S}^3 \) with radius \( \cos \rho \).

When the translation \( \mathcal{F}_2^{(p)} \) is applied to the Radon transform with respect to one of its arguments, then the geometry of rotations represented by quaternions amounts to

\[
(\mathcal{F}_2^{(p)} [Rf])(\mathbf{h}, \mathbf{r}) = \frac{1}{2\pi \sin \rho} \int_{c(\mathbf{h}, \rho)} Rf(h', \mathbf{r}) \, dh'
\]

\[
= \frac{1}{2\pi \sin \rho} \int_{c(\mathbf{r}, \rho)} Rf(h', \mathbf{r}') \, dr'
\]

\[
= \frac{1}{4\pi^2 \sin \rho} \int_{c(\mathbf{r}, \rho)} \int_{C(q_1(h', r'), q_2(h, r'))} f(q) \, d\omega_1(q) \, dr'
\]

(7)

Now, the domain of integration is just the torus \( T(C(q_1(h, r), q_2(h, r)); \rho/2) \) due to Proposition 1. Therefore, we conclude

\[
(\mathcal{F}_2^{(p)} [Rf])(\mathbf{h}, \mathbf{r}) = \frac{1}{4\pi^2 \sin \rho} \int_{T(C(q_1(h, r), q_2(h, r)); \rho/2)} f(q) \, dq
\]

(8)

\[
= \frac{1}{4\pi^2 \sin \rho} \int_{d(q, C(q_1(h, r), q_2(h, r))); \rho/2} f(q) \, dq
\]

(9)

Equation (7) is an Ásgeirsson-type mean value theorem (cf. [8, 9]) justifying the application of \( \mathcal{F}_2^{(p)} \) to \( Rf \) regardless of the order of its arguments, and Equation (8) is instrumental in the inversion of the totally geodesic Radon transform [4, 5].

Thus, we may state the following theorem.

Theorem 1

The generalized one-dimensional totally geodesic Radon transform is equal to the translated totally geodesic Radon transform and it can be identified with the angle density function

\[
(\mathcal{F}_2^{(p)} [Rf])(\mathbf{h}, \mathbf{r}) = R^{(p/2)} f(C_{\mathbf{h}, \mathbf{r}}) = \mathcal{A} f(\mathbf{h}, \mathbf{r}; \rho)
\]

(10)

The angle density function \( \mathcal{A} f(\mathbf{h}, \mathbf{r}; \rho) \) has been introduced into texture analysis in [10, p. 44; 11, p. 74] (with a false normalization). According to its definition it is the mean value of the spherical pole probability density function over any small circle centred at \( \mathbf{r} \). Thus, it is the probability density that the crystallographic direction \( \mathbf{h} \) statistically encloses the angle \( \rho, 0 \leq \rho \leq \pi \), with the specimen direction \( \mathbf{r} \) given the orientation probability density function \( f \). Equation (7), i.e. the
commutation of the order of integration, has been observed without reference to Radon transforms or Ásgeirsson means and stated without proof (cf. [10, p. 47; 11, p. 76]), not to mention purely geometric arguments. Nevertheless, its central role for the inverse Radon transform was recognized in [12] by ‘rewriting’ Matthies inversion formula [13]. However, the geometrical interpretation was not recognized in the same manner as the meaning of the Darboux-type differential equation $\Delta_h R f = \Delta R f$ was polemically denied [14].

It should be noted that

$$A f(h, r; 0) = R f(h, r)$$

$$A f(h, r; \pi) = R f(h, -r)$$  \hspace{1cm} (11)

4.1. The dual totally geodesic Radon and dual generalized totally geodesic Radon transform

Following again Helgason [4, 5] we have two more definitions.

**Definition 6**

The dual one-dimensional totally geodesic Radon transform of a real continuous function $f: \mathcal{C} \to \mathbb{R}$ is defined as

$$\tilde{R} \varphi(q) = \int_{C \ni q} \varphi(C) \, d\mu(C)$$

where $\mu$ denotes the unique measure on the compact space $C \in \mathcal{C}: q \in C$, invariant under all rotations around $q$, and having total measure 1.

Thus $\tilde{R} \varphi(q)$ is the mean value of $\varphi$ over the set of circles $C \in \mathcal{C}$ passing through $q$.

**Definition 7**

The dual generalized one-dimensional totally geodesic Radon transform of a real continuous function $f: \mathcal{C} \to \mathbb{R}$ is defined as

$$\tilde{R}^{(\rho)} \varphi(q) = \int_{\{C \in \mathcal{C} : d(q, C) = \rho\}} \varphi(C) \, d\tilde{\mu}(C)$$

With the normalized measure $\tilde{\mu} = A^{-1}(\rho) \, d\mu$, $A(\rho) = 4\pi \sin^2 \rho$, it is the mean value of $\varphi$ over the set of all circles $C \in \mathcal{C}$ with distance $\rho$ from $q$.

Again, geometrical reasoning, Equations (4), (5), yields that $\tilde{R}^{(\rho)} R f(q)$ is the mean value of $R f$ over the set of all circles $C \in \mathcal{C}$ with distance $\rho$ from $q$, i.e. tangential to the sphere $s(q; \rho)$. More specifically, with the usual two-dimensional spherical Riemann measure $\omega_2$,

$$\tilde{R}^{(\rho)} R f(q) = \int_{d(q, C) = \rho} R f(C_{h, r}) \, d\tilde{\mu}(C_{h, r})$$

$$= \frac{1}{4\pi \sin(2\rho)} \int_{S^2} \int_{C(q_0 q^*, 2\rho)} R f(C_{h, r}) \, d\gamma \, d\omega_2(h)$$

$$= \frac{1}{2} \int_{S^2} A f(h, q q^*; 2\rho) \, d\omega_2(h)$$  \hspace{1cm} (12)
\[ \frac{1}{2} \int_{S^2} R^{(\rho)}(C_{h,qh^*}) \, d\omega_2(h) \]
\[ = \tilde{R} R^{(\rho)} f(q) \]  
(13)

which is instrumental for the inversion of the totally geodesic Radon transforms. In particular,
\[ \tilde{R} R f(q) = \frac{1}{2} \int_{S^2} R f(h, qh^*) \, d\omega_2(h) \]  
(14)

The previous consideration amounts to a new representation of the generalized dual Radon transform:
\[ \tilde{R}^{(\rho)} \varphi(q) = \int_{\{C \in \mathcal{C} : d(q,C) = \rho\}} \varphi(C) \, d\mu(C) \]
\[ = \int_{SO(3)} \varphi(rkr^* C_0sk^*s^*) \, dk \]

where \( dk = 1/8\pi^2 \sin \beta \, dx \, d\beta \, d\gamma \) is the invariant Haar measure on \( SO(3) \), \( C_0 \in \mathcal{C} \) a fixed great circle such that \( d(q, C_0) = \rho \) and \( q = rs^* \).

It is well known [4, 5] that

**Theorem 2**
\[ \tilde{R}^{(\rho)} \mathcal{R} f(q) = \int_{\{C \in \mathcal{C} : d(q,C) = \rho\}} \mathcal{R} f(C) \, d\tilde{\mu}(C) \]
\[ = \int_{C_0} \mathcal{F}^d(q,p) \, f(q) \, dm(p) \]  
(15)

where \( C_0 \) is a fixed great circle with distance \( d(q,C_0) = \rho \) from \( q \).

This proposition is instrumental in deriving an inversion of the Radon transform by Abel’s integrals. Here we elaborate on the special case that applies to texture analysis:
\[ \tilde{R}^{(\rho)} \mathcal{R} f(q) = \int_{\{C \in \mathcal{C} : d(q,C) = \rho\}} \mathcal{R} f(C) \, d\tilde{\mu}(C) \]
\[ = \int_{SO(3)} \mathcal{R} f(rkr^* C_0sk^*s^*) \, dk \]
\[ = \int_{C_0} \int_{SO(3)} f(rkr^* psk^*s^*) \, dk \, dm(p) \]

While \( k \) varies in \( SO(3) \), the set \( \{rkr^* psk^*s^*, k \in SO(3)\} \) is a small sphere around \( q = rs^* \) containing \( p \):
\[ d(q, rkr^* psk^*s^*) = d(rs^*, rkr^* psk^*s^*) = d(e_0, kr^* psk^*) \]
\[ = d(k^* e_0 k, r^* ps) = d(e_0, r^* ps) = d(rs^*, p) = d(q, p) \]
and \(dk = A^{-1}(\rho)\, d\tilde{q}\) is the normalized Riemann measure of the small sphere \(s(q; \rho)\) with centre \(q\) and radius \(\rho = d(q, p)\). Hence

\[
\tilde{\mathcal{R}}^{(p)} f(q) = \int_{C_0} \int_{SO(3)} f(\mathrm{rkr^*psk^*s^*})\, dk\, dm(p)
= \int_{C_0} \frac{1}{A(\rho)} \int_{s(q; \rho)} f(\tilde{q})\, d\tilde{q}\, dm(p)
= \int_{C_0} \mathcal{T}_3^{d(q, p)} f(q)\, dm(p)
\] (16)

**Remark 1**
A special situation occurs when \(f\) is a central function. Assuming that \(f\) is central with respect to \(q_0\), \(\mathcal{R} f\) is constant on the set of all great circles \(C \in \mathcal{C}\) for which \(q_0 h_C q_0^* \cdot r_C\) is constant, where \(h_C, r_C\) denote the unit vectors associated with the great circle \(C\). This is true for the set of all great circles with \(d(q_0, C) = \rho\) as they are characterized by Equation (4). Thus we can drop the outer integration and find for the right-hand side of Equation (15)

\[
\tilde{\mathcal{R}}^{(p)} f(q_0) = \mathcal{R} f(C) \quad \text{for some } C \text{ with } d(q_0, C) = \rho
\]

Moreover, in this case, \(\mathcal{T}_3^{d(q_0, p)} f(q_0) = f(q_0)\) for all \(\rho\). Thus the left-hand side of Equation (15)

\[
\int_{d(q_0, C) = \rho} \mathcal{T}_3^{d(q, p)} f(q)\, dm(p) = \mathcal{R} f(C) \quad \text{for some } C \text{ with } d(q_0, C) = \rho
\]

Parameterizing the great circle \(C_0\) by polar coordinates and assuming \(f\) even \((f(q) = f(-q))\), Equation (16) takes the form

\[
\tilde{\mathcal{R}}^{(p)} f(q) = 4 \int_0^{\pi/2} \mathcal{T}_3^{d(q, p)} f(q)\, d\tau
\] (17)

Denote by \(q_0 \in C_0\) a point with minimum distance from \(q\), i.e. \(d(q_0, q) = \rho\). Using spherical trigonometry with respect to the triangle \(qq_0p\), we obtain

\[
\cos d(q, p) = \cos d(q_0, q)\cos d(q_0, p)
\]

Fix \(q\) and set \(v = \cos d(q_0, q)\) and \(u = v\cos d(q_0, p) = \cos d(q, p)\),

\[
F(u) = \mathcal{T}_3^{d(q, p)} f(q), \quad \hat{F}(v) = \tilde{\mathcal{R}}^{(p)} f(q)
\]

Then Equation (17) becomes Abel’s integral equation

\[
\hat{F}(v) = 4 \int_0^v \frac{F(u)}{\sqrt{v^2 - u^2}}\, du
\]

which is inverted by

\[
F(u) = \frac{1}{2\pi} \frac{d}{du} \int_0^{u} \hat{F}(v) \frac{v}{\sqrt{u^2 - v^2}}\, dv
\]
Since $F(1) = \lim_{u \to 1} \sqrt[3]{\arccos u} f(q) = f(q)$, we get the following inversion formula (cf. [5])

$$f(q) = \frac{1}{2\pi} \left[ \frac{d}{du} \int_0^u \sqrt[3]{\arccos v} \mathcal{R} f(q) \frac{v}{\sqrt{u^2 - v^2}} dv \right] u=1$$

Further on, we want to introduce the notion of the angle density function $\mathcal{A} f$ and deduce Matthies’ inversion formula [13] in the terminology of [12]. Using Equation (12) we obtain

$$f(q) = \frac{1}{4\pi} \left[ \int_{S^2} \mathcal{A} f(h, q h q^*; \pi) d\omega_2(h) \right] u=1$$

$$= \frac{1}{4\pi} \left[ \int_{S^2} \mathcal{A} f(h, q h q^*; \pi) d\omega_2(h) \right] u=1$$

$$+ \int_0^s \int_{S^2} \mathcal{A} f(h, q h q^*; 2 \arccos \sqrt{s-w}) d\mathcal{h} \frac{1}{\sqrt{w}} dw \right] u=1$$

Using $d/ds.\mathcal{A} f = -d/dw(\mathcal{A} f)$ and taking into account $\mathcal{A} f(h, q h q^*; \pi) = \mathcal{R} f(h, -q h q^*)$ (cf. Equation (11)), put $2w = 1 - \cos \theta$ and $s = 1$ to obtain

$$= \frac{1}{4\pi} \left[ \int_{S^2} \mathcal{R} f(h, -q h q^*) d\omega_2(h) + 2 \int_0^\pi \int_{S^2} \mathcal{A} f(h, q h q^*; \theta) d\omega_2(h) \cos \frac{\theta}{2} d\theta \right]$$

The practical importance is that $\mathcal{A} f$ is experimentally accessible and might yield an improved inversion compared with inverting just pole intensities.

4.2. Kernels and their twofold Radon transform

The previous considerations are mainly geometric; to solve the inversion problem for the Radon transform we have also to consider appropriate function spaces such as Sobolev spaces. These Sobolev spaces are closely related to the singular value decomposition of the crystallographic X-ray transform which is defined on $\text{SO}(3)$ and maps into $S^2 \times S^2$. One of the major results in [15] may be stated as follows. Let $A = (A_t)_{t \geq 0}$ be some non-negative sequence such that the Sobolev space $\mathcal{H}(A_t, \text{SO}(3))$ defines a reproducing kernel Hilbert space, and $B_t = \sqrt{2t+1} A_t$ gives rise to another Sobolev space $\mathcal{H}(B_t, S^2 \times S^2)$, which defines a reproducing kernel Hilbert space on $S^2 \times S^2$. Moreover, the restriction of the Radon transform on $\mathcal{H}(A_t, \text{SO}(3))$ defines an isometry onto $\mathcal{H}(B_t, S^2 \times S^2)$. In particular, the reproducing kernels satisfy the equality

$$K_{S^2 \times S^2} = \mathcal{R}_2 \mathcal{R}_j \text{S} \times \text{SO}(3)$$

(18)

For instructive insight we might ask ourselves how to characterize and interpret $\mathcal{R}_2 \mathcal{R}_j K_{\text{SO}(3) \times \text{SO}(3)}$. Now let $K$ be a kernel function $K : S^3 \times S^3 \mapsto \mathbb{R}_+$. Then we may apply the Radon transform twice in the sense that we apply it once with respect to the first and once with respect to the second variable (cf. [15]), i.e.

$$\mathcal{R}_1 K(C_1) = \frac{1}{2\pi} \int_{C_1} K(p_1, p_2) d\omega_1(p_1) = F(C_1, p_2)$$
and

\[ \mathcal{R}_2[\mathcal{R}_1 K(C_1)](C_2) = \mathcal{R}_2 F(C_2) = \frac{1}{4\pi^2} \int_{C_2} \int_{C_1} K(p_1, p_2) d\omega_1(p_1) d\omega_1(p_2) = G(C_1, C_2) \]

where \( C_1 \) denotes the great circle representing all rotations mapping \( h_1 \) on \( r_1 \), and analogously \( C_2 \) with respect to \( h_2 \) and \( r_2 \).

In case the kernel \( K \) depends only on the quaternion product, i.e. \( K(p_1, p_2) = K(p^* r_2) \) as the Abel–Poisson or de la Vallée Poussin kernel does, then

\[ \mathcal{R}_2[\mathcal{R}_1 K(C_1)](C_2) = \frac{1}{4\pi^2} \int_{p_1 h_1 p_1^* = r_1} \int_{p_2 h_2 p_2^* = r_2} K(p^* p_2) d\omega_1(p_1) d\omega_1(p_2) \]

\[ = \frac{1}{4\pi^2 \sqrt{1 - (r_1 \cdot r_2)^2}} \int_{(p h_1, p^* h_2) = (r_1, r_2)} K(p) dp \]

\[ = \frac{1}{4\pi^2 \sin(\rho/2)} \int_{T(C; \rho/2)} K(p) dp = \mathcal{R}(\rho/2) K(C) \]

\[ = \mathcal{A} K(h_1, h_2; \rho) \]

with the core \( C = C_{h_1, h_2} \) and \( \rho = \arccos(r_1 \cdot r_2) \).

In case the kernel \( K \) depends only on \( \omega/2 = \arccos(Sc(p^* p_2)) \), then the function \( F \) depends only on \( \arccos(p_2 h_1 p_2^* \cdot r_1) = d(p_2, C_1) \). As a function of the variable \( p_2 \) with parameters \( h_1, r_1 \) implicitly provided by \( C_1 \), \( F \) may be referred to as fibre function. They share most of the characteristics of ridge functions initially defined in linear spaces and discussed in [16]. Then the function \( G \) depends only on \( \arccos(h_1 h_2) \) and \( \arccos(r_1 r_2) \), cf. [15].

**Theorem 3**

For a kernel function of the form \( K(p_1, p_2) = K(p^* p_2) \), the twofold application of the totally geodesic Radon transform with respect to the two components of its argument is identical with its generalized totally geodesic Radon transform, i.e. with its angle density function.

### 5. Resolution of the Inverse Crystallographic X-Ray Transform

The crystallographic X-ray transform, Equation (6), is not invertible whereas the inverse Radon transform exists under mild mathematical assumptions. In terms of harmonics on \( \text{SO}(3) \) the kernel of the crystallographic X-ray transform comprises the odd-order harmonics. The kernel of the Radon transform on \( S^3 \) consists of all odd functions; in terms of harmonics on \( S^3 \), the kernel comprises all odd order harmonics. The kernel of the crystallographic X-ray transform consists of all odd order harmonics and all harmonics of order \( 4\ell + 2, \ell = 0, 1, \ldots \). Thus, resolution of the inverse crystallographic X-ray transform requires additional modelling assumptions.
Finally, with respect to the diffraction experiment, it should be noted that
\[
\mathcal{F}^p[\mathcal{F} f](\mathbf{h}, \mathbf{r}) = \frac{1}{4} (\mathcal{R}(\rho/2) f(C) + \mathcal{R}(\rho/2) f(C^\perp))
\]
\[
= \frac{1}{4} (\mathcal{F} f(\mathbf{h}, \mathbf{r}; \rho) + \mathcal{F} f(-\mathbf{h}, \mathbf{r}; \rho))
\]
\[
= \mathcal{W} f(\mathbf{h}, \mathbf{r}; \rho)
\]
(19)

Thus, with respect to a diffraction experiment, \((\mathcal{W} f)(\mathbf{h}, \mathbf{r}; \rho)\) is at once accessible if the specimen rapidly rotates around the specimen direction \(\mathbf{r}\) during the measurements. The first experiment of this kind has been made at the texture facility of the Joint Institute for Nuclear Research at Dubna, Russia [17], and will be resumed in the future. Existing commercial or popular software packages are not capable of recovering an orientation probability density function from this novel kind of data.

5.1. Harmonic method

The harmonic series expansion of \(\mathcal{W} f\) results in a system of linear equations, which may allow a solution for the even part of the odf.

In terms of spherical harmonics, Equation (19) results in

\[
\mathcal{W} f(\mathbf{h}, \mathbf{r}; \rho) = \frac{1}{2\pi\sqrt{1-\cos^2 \rho}} \int_{c(\mathbf{r}, \rho)} \sum_{\ell=2}^{\infty} \sum_{m,n} C_{\ell}^{mn} Y_{\ell}^m(\mathbf{h}) Y_{\ell}^n(\mathbf{r}') \, d\mathbf{r}'
\]
\[
= \frac{1}{2\pi\sqrt{1-\cos^2 \rho}} \sum_{\ell=2}^{\infty} \sum_{m,n} C_{\ell}^{mn} Y_{\ell}^m(\mathbf{h}) \int_{c(\mathbf{r}, \rho)} Y_{\ell}^n(\mathbf{r}') \, d\mathbf{r}'
\]

Applying

\[
\frac{1}{2\pi\sqrt{1-\tau^2}} \int_{rr'=\tau} Y_{\ell}^n(\mathbf{r}') \, d\mathbf{r}' = P_{\ell}(\tau) Y_{\ell}^n(\mathbf{r})
\]
(cf. [7, p. 64]) with \(\tau = \cos \rho\) finally yields

\[
\mathcal{W} f(\mathbf{h}, \mathbf{r}; \rho) = \sum_{\ell=2}^{\infty} P_{\ell}(\cos \rho) \sum_{m,n} C_{\ell}^{mn} Y_{\ell}^m(\mathbf{h}) Y_{\ell}^n(\mathbf{r})
\]
(20)
(cf. [10, p. 45; 11, p. 74]).

In the case of an orientation probability function \(f(\arccos(Sc(q_0^* q)))\), which is radially symmetric with respect to a given \(q_0\), Equation (20) simplifies further to

\[
\mathcal{W} f(\mathbf{h}, \mathbf{r}; \rho) = \sum_{\ell=2}^{\infty} P_{\ell}(\cos \rho) \sum_{m,n} C_{\ell}^{mn} Y_{\ell}^m(\mathbf{h}) Y_{\ell}^n(\mathbf{r})
\]
\[
= \sum_{\ell=2}^{\infty} \frac{2\ell + 1}{4\pi} C_{\ell} P_{\ell}(\cos \rho) P_{\ell}(\cos \eta)
\]
(21)
as the Radon transform becomes a function of \(\eta = \arccos(q_0^* \mathbf{h} \mathbf{q}_0^* \cdot \mathbf{r}) = d(q_0, C)\) only, where \(C\) denotes the great circle representing all rotations mapping \(\mathbf{h}\) on \(\mathbf{r}\). It should be noted that \(\rho\) and \(\eta\) commute, i.e.

\[
\mathcal{W} f(\mathbf{h}, \mathbf{r}; \rho)|_{q_0^* \mathbf{h} \mathbf{q}_0^* \cdot \mathbf{r} = \cos \eta} = \mathcal{W} f(\mathbf{h}, \mathbf{r}; \eta)|_{q_0^* \mathbf{h} \mathbf{q}_0^* \cdot \mathbf{r} = \cos \rho}
\]

Integrating the radially symmetric totally geodesic Radon transform over a small circle with angle \(\rho\) with respect to \(\mathbf{r}\) with \(q_0^* \mathbf{h} \mathbf{q}_0^* \cdot \mathbf{r} = \cos \eta\) is equal to integrating the totally geodesic Radon transform
over a small circle with angle \( \eta \) with respect to \( r \) with \( q_0 h_0^* \cdot r = \cos \rho \). In terms of the generalized totally geodesic Radon transform, we find

**Corollary 1**

For a radially symmetric function \( f \)

\[
\mathcal{B}^{(\rho/2)} f(C_h r) |_{q_0 h_0^* \cdot r = \cos \rho} = \mathcal{A}(\eta/2) f(C_h r) |_{q_0 h_0^* \cdot r = \cos \rho}
\]

Sampling \( \mathcal{W} f(h, r; \rho) \) for discrete values of \( h, r \in S^2 \) and \( \rho \in (0, \pi/2) \) gives rise to data \( w_i = w(h_i, r_i; \rho_i) \) and a system of linear equations

\[
w_i = \sum_{\ell=2} P_\ell(\cos \rho_i) \sum_{m,n} C_{\ell m}^{\ell n} Y_{\ell m}(h_i) \Psi_{\ell n}(r_i), \quad i = 1, \ldots, I
\]

which may allow a solution for the \( C_{\ell m}^{\ell n} \)-coefficients with even \( \ell \).

5.2. **Component-fit method**

Assume that the orientation probability density function shall be modelled by the superposition of ‘components’ represented by kernels \( K_j(q_i, q) \), i.e.

\[
f(q) = \sum_j \lambda_j K_j(q_i, q) = \sum_j \lambda_j K(q_j, q)
\]

Usually in practice, we choose radially symmetric kernels that give rise to

\[
f(q) = \sum_j \lambda_j K(\arccos(Sc(q_j^* q)))
\]

Then the corresponding generalized totally geodesic Radon transform \( \mathcal{W} f \) is the superposition of the correspondingly generalized totally geodesic Radon transformed kernels \( k_j = \mathcal{W} K_j \)

\[
\mathcal{W} f(h, r; \rho) = \sum_j \lambda_j \mathcal{W} K_j(h, r; \rho) = \sum_j \lambda_j k_j(h, r; \rho)
\]

which may be fitted to the experimental data

\[
w_i \approx \sum_j \lambda_j^* k_j(h_i, r_i; \rho_i)
\]

in some sense, e.g. in the sense of a Hilbert–Sobolev norm as developed in [15, 18]. Then, an approximate orientation probability density function explaining the data is given by

\[
f(q) = \sum_j \lambda_j^* K(\arccos(Sc(q_j^* q)))
\]

6. **EXAMPLES**

In the following we provide some formulae for the Abel–Poisson (in probability: Cauchy) and the de la Vallée Poussin kernel, their Radon transform and their twofold Radon transform.
In texture analysis the Abel–Poisson kernel is referred to as Lorentz standard function [19, p. 98; 20, p. 477], and the formulae were actually taken from there. Obviously, they were initially not related to reproducing kernels and their twofold totally geodesic Radon transform. The de la Vallée Poussin kernel has been introduced into texture analysis because its harmonic series expansion is finite [21, 22].

For the symmetrical kernel \( K(p_1, p_2) = K(p_1^* p_2) \) defined on \( \mathbb{S}^3 \times \mathbb{S}^3 \), the variable \( \omega = 2 \arccos(ac(p_1^* p_2)) \) denotes the angle of the rotation of \( p_1^* p_2 \); for the Radon transformed kernel \( \mathcal{R}_1 K(h, r, p) \) defined on \( (\mathbb{S}^2 \times \mathbb{S}^2) \times \mathbb{S}^3 \), the variable \( \eta \) denotes the angle \( \langle p h p^*, r \rangle \). The two variables \( \eta_1 \) and \( \eta_2 \) of the twofold Radon transformed kernel \( \mathcal{R}_2 \mathcal{R}_1 K(h_1, r_1, h_2, r_2) \) defined on \( (\mathbb{S}^2 \times \mathbb{S}^2) \times (\mathbb{S}^2 \times \mathbb{S}^2) \) correspond to the angles \( \langle h_1 h_2 \rangle \) and \( \langle h_2 r_2 \rangle \), respectively. The Gegenbauer and the Legendre coefficients of the kernels are denoted as \( a_\ell \).

In the list we have used the following notations for special functions: \( B \) Beta function, \( E \) complete elliptic integral, \( 2 F_1 \) hypergeometric function, and \( \Gamma \) Gamma function.

For the Abel–Poisson kernel we have

\[
a_\ell = (2\ell + 1)\kappa^{2\ell}
\]

\[
K = \frac{1}{2} \left[ \frac{1 - \kappa^2}{(1 - 2\kappa \cos(\omega/2) + \kappa^2)2} + \frac{1 - \kappa^2}{(1 + 2\kappa \cos(\omega/2) + \kappa^2)2} \right]
\]

\[
\mathcal{R}_1 K = \frac{1 - \kappa^4}{(1 - 2\kappa^2 \cos \eta + \kappa^4)^{3/2}}
\]

\[
\mathcal{R}_2 \mathcal{R}_1 K = \frac{2}{\pi (C - D) \sqrt{C + D}} E \left( \frac{2D}{C + D} \right)
\]

where \( C = 1 - 2\kappa \cos \eta_1 \cos \eta_2 + \kappa^2 \), \( D = 2\kappa \sin \eta_1 \sin \eta_2 \), \( C - D = 1 + \kappa^2 - 2\kappa \cos(\eta_1 - \eta_2) \), \( C + D = 1 + \kappa^2 - 2\kappa \cos(\eta_1 + \eta_2) \) and \( E \) denotes the elliptic integral of second kind.

Analogously, for the de la Vallée Poussin kernel

\[
a_\ell = (2B(\frac{3}{2}, \frac{3}{2} + \ell))^{-1} [S_\ell(\kappa) - S_{\ell + 1}(\kappa)]
\]

where \( S_\ell(\kappa) = \sum_{k=0}^{\ell} (-1)^k \frac{2^k}{2k} B(k + 1/2, \kappa + \ell - k + 1/2) \), and further

\[
K = \frac{B(3/2, 1/2)}{B(3/2, \kappa + 1/2)} \cos(\omega/2)^{2\kappa}
\]

\[
\mathcal{R}_1 K = (1 + \kappa) \cos(\eta/2)^{2\kappa}
\]

\[
\mathcal{R}_2 \mathcal{R}_1 K = \frac{2^{1-\kappa}}{\pi \cos \eta_1 \cos \eta_2} \frac{\Gamma(2 + \kappa)}{\Gamma(3/2 + \kappa)} \times \left( A^{1+\kappa} F_1 \left( \frac{1}{2}, 1 + \kappa, \frac{3}{2} + \kappa, \frac{A}{B} \right) - B^{1+\kappa} F_1 \left( \frac{1}{2}, 1 + \kappa, \frac{3}{2} + \kappa, \frac{B}{A} \right) \right)
\]

where \( A = 1 + \cos(\eta_1 + \eta_2) \), \( B = 1 + \cos(\eta_1 - \eta_2) \) and \( 2 F_1 \) denotes Gauss’ hypergeometric function.
7. CONCLUSIONS

The essential role of the probability density of the angle distribution for the inverse totally geodesic Radon transform has been clarified by purely geometric arguments. It is identified with the generalized totally geodesic Radon transform, which in turn is identified with the ‘spherically translated’ totally geodesic Radon transform. Of particular interest is that the twofold totally geodesic Radon transform of a symmetrical kernel function is again its corresponding angle probability density function. Practical methods of inversion in terms of harmonics or radially symmetric basis functions are sketched. Thus, our contribution is also a tribute to the late Hans–Joachim Bunge (1929–2004), who introduced the angle distribution into ‘quantitative texture analysis’. The problem whether the inversion of the generalized totally geodesic Radon transform is better conditioned than the inversion of the totally geodesic Radon transform is postponed to a future contribution as it requires a detailed analysis of the experiment to collect integral radiation intensity data.

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