Materials Science Forum Vols. 495-497 (2005) pp 277-282
Online available since 2005/Sep/15 at www.scientific.net
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doi:10.4028/www.scientific.net/MSF.495-497.277

Common Basics of Mathematical Texture Analysis

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Keywords: X-ray diffraction, pole figure inversion, Radon transform

Abstract. In texture analysis intensities of a diffraction experiment are recorded as experimentally accessible pole figures which are modeled as a "pole figure projection" of an orientation probability density function. The recovery of the orientation density function by means of inversion of the pole figure projection has been a major issue ever since its origin as it permits the approximate numerical determination of possibly anisotropic macroscopic properties. Major publications in texture analysis have usually stressed the uniqueness of the mathematics involved in its inversion problem.
In the mathematical discipline of integral geometry the Radon transform is a favorite subject of concern. It associates mean values with respect to lower dimensional manifolds to a function defined on some multidimensional manifold. In particular, it developed methods to recover functions defined on Euclidean spaces, hyperbola and spheres, from their Radon transforms. Except for applications in medical technologies mathematicians are often not aware of other routine applications in engineering.
In our exposition on one hand we demonstrate the uniqueness of the mathematics involved but also the existence of parallel developments in texture analysis and in integral geometry which have not been aware of each other but can largely benefit of each other. More precise, the pole figure projection of texture analysis as a 1d Radon transform of the group $SO(3)$ is equivalent to the 1d Radon transform of even functions defined on the 3d sphere in 4d Euclidean space. Exploiting the geometry of the diffration experiment of texture analysis in terms of quaternions, the equivalence of the approaches as well as of its results, especially of its "inversion formulae" is proven. Thus, mathematics is proven to apply usefully to problems of advances texture analysis.

Introduction

In this paper we want to demonstrate that the pole figure inversion problem is deeply related to integral geometry and especially to the spherical Radon transform. The relationship is based on equivalent inversion formulae which might give raise to different numerical procedures. In particular, we got new inversion formulae ("back projection-type formulae") and relate them to the already known formulae. We can prove the equality of the inversion of the spherical Radon transform and the reconstruction of the even part of the orientation density function by exploration the geometry of the problem which is based on the use of quaternions.

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 $G \subset SO(3)$.

The orientation $\boldsymbol{g}$ of an individual crystal in a polycrystalline specimen is the active rotation $\boldsymbol{g} \in SO(3) : K_S \mapsto K_C$ 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,

$$\boldsymbol{g}\, K_S = K_C, \;\; \boldsymbol{g} \in SO(3)\,. \tag{1}$$

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

$$\mathbf{r}_{K_S} = \boldsymbol{g}\, \mathbf{h}_{K_C}\,. \tag{2}$$

The commonly applied convention in texture analysis (H.J. Bunge, [4]; [5]) refers to the notion of passive rotation and Eq. 2 is written in the form

$$\mathbf{h} = g\mathbf{r} \tag{3}$$

where obviously $g = \boldsymbol{g}^{-1}$. 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 $f : G \mapsto \mathbb{R}^1_+$, then

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

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 $SO(3)$ 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 $\mathcal{X}(\mathbf{h}, \mathbf{r})$ can be sampled, which represents the probability that a (fixed) crystal direction $\mathbf{h}$ or its antipodal $-\mathbf{h}$ statistically coincide with the specimen direction $\mathbf{r}$. 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

$$\mathcal{X}f(\mathbf{h}, \mathbf{r}) = \frac{1}{2}\left(P(\mathbf{h}, \mathbf{r}) + P(-\mathbf{h}, \mathbf{r})\right) \quad \text{with} \quad Pf(\mathbf{h}, \mathbf{r}) = \frac{1}{2\pi}\int_{\{g \in SO(3):\, \mathbf{h} = g\,\mathbf{r}\}} f(g)\, d\omega_g \tag{4}$$

and Pf will be called *the Radon transform in texture goniometry.*

The Angular Distribution Function We choose an arbitrary sample direction $\mathbf{y}$ as the pole of a spherical angular coordinate system. We hold the angle θ fixed and construct

$$Wf(\cos\theta, \mathbf{h}, \mathbf{r}) = \frac{1}{2\pi}\int_{C(\mathbf{r},\theta)} Pf(\mathbf{h}, \mathbf{r}')\, d\sigma(\mathbf{r}'), \tag{5}$$

where $C(\mathbf{r},\,\theta)$ is the small circle $\{\mathbf{r}' \in \mathbb{S}^2 : \mathbf{r}' \cdot \mathbf{r} = \cos\theta\}$. One obtains this function, if, for example, one permits the texture sample to rotate rapidly about the sample direction $\mathbf{y}$ during measurement. It thus indicates how frequently the crystal direction $\mathbf{h}$ forms the angle θ with the sample direction $\mathbf{r}$ (angle distribution function).
A special situation occurs when $\theta = \pi$. Then we have

$$Wf(-1,\,\mathbf{h},\,\mathbf{r}) = Wf(\cos\pi,\,\mathbf{h},\,\mathbf{r}) = P(\mathbf{h},\,-\mathbf{r}), \tag{6}$$

see for example [10].

Quaternions

We denote the standard orthonormal basis of $\mathbb{R}^3$ by $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$. We now define a *quaternion* as the sum

$$q = q_0 + \mathbf{q} = q_0 + \mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3.$$

To form an algebra under multiplication the following fundamental special products must be satisfied:

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1,\ \mathbf{ij} = \mathbf{k} = -\mathbf{ji},\ \mathbf{jk} = \mathbf{i} = -\mathbf{kj},\ \mathbf{ki} = \mathbf{j} = -\mathbf{ik}.$$

If $q_0 = 0$, then $q = \mathbf{q}$ is called a pure quaternion. Given two quaternions p, q their product according to the algebraic rules is given by

$$pq = p_0q_0 - \mathbf{p}\cdot\mathbf{q} + p_0\mathbf{q} + q_0\mathbf{p} + \mathbf{p}\times\mathbf{q},$$

where $\mathbf{p}\cdot\mathbf{q}$ and $\mathbf{p}\times\mathbf{q}$ represent the standard scalar and cross product in $\mathbb{R}^3$.
The quaternion $q^* = q_0 - \mathbf{q}$ is called the *conjugate* of $q = q_0 + \mathbf{q}$. The *norm* of a quaternion q, denoted by $||q||$, is the scalar defined by

$$||q|| = \sqrt{q\,q^*} = \sqrt{q^*q} = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2}$$

and is equal to norm of q in $\mathbb{R}^4$. A quaternion q with $||q|| = 1$ is called a *unit* quaternion. It is easily seen that the set of all unit quaternions form the unit sphere $\mathbb{S}^3 \subset \mathbb{R}^4$.

Basic results

Definition 1. Let q_1 and q_2 be two unit *orthogonal* quaternions. The set of quaternions

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

is called a circle in the space of unit quaternions and is denoted $C(q_1, q_2)$.

Proposition [9] *Let q_1, q_2, q_3, q_4 denote four mutually orthonormal quaternions; let $C(q_1,\,q_2)$ denote the circle of quaternions representing the rotations $g \in G(\mathbf{r},\,\mathbf{h})$, and $C(q_3,\,q_4)$ the circle representing the rotations $g \in G(-\mathbf{r},\,\mathbf{h})$. Then the spherical torus $Q(s,t;\theta) \subset \mathbb{S}^3$ defined as the set of quaternions*

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

represents all rotations mapping $\mathbf{r}$ on the small circle $C(\mathbf{h},\,2\theta) \subset \mathbb{S}^2$, $s,t,\in [0,\,2\pi)$, $\theta \in \left[0,\,\frac{\pi}{2}\right]$

Therefore, we conclude that the torus $T(q_1, q_2, q_3, q_4; \theta)$ consisting of all quaternions with distance θ from $C(q_1, q_2)$ essentially consists of all circles with distance θ from $C(q_1, q_2)$ representing all rotations $\bigcup_{\mathbf{r}' \in C(\mathbf{r}, 2\theta)} G(\mathbf{r}, \mathbf{h}')$ mapping $\mathbf{r}$ on $C(\mathbf{h}, 2\theta)$, i.e.

$$T(q_1, q_2, q_2, q_4; \theta) = \bigcup_{\mathbf{h}' \in C(\mathbf{h}, 2\theta)} C(q_1(\mathbf{h}', \mathbf{r}), q_2(\mathbf{h}', \mathbf{r})) \tag{7}$$

which has been shown to be equal to $\bigcup_{\mathbf{r}' \in C(\mathbf{r}, 2\theta)} G(\mathbf{r}', \mathbf{h})$ mapping $\mathbf{h}$ on $C(\mathbf{r}, 2\theta)$. Thus,

Theorem 2. *For each $q \in \mathbb{S}^3$ and $\theta \in [0, \pi)$*

$$\{C(p_1, p_2) : \ d(q, C(p_1, p_2)) = \theta\} = \bigcup_{\mathbf{r} \in \mathbb{S}^2} \bigcup_{\mathbf{h} \in C(q\mathbf{r}q^*, 2\theta)} C(p_1(\mathbf{h}, \mathbf{r}), p_2(\mathbf{h}, \mathbf{r})). \tag{8}$$

The inversion formulae

We rewrite formula (4) in a way such that it will turn out to be a Radon transform acting on $SO(3)$. We have

$$Pf(\mathbf{h}, \mathbf{r}) = \frac{1}{2\pi} \int_{K(\mathbf{h}, \mathbf{r})} f(g)\, d\omega_g = 4\pi \int_{SO(3)} f(g) \delta_{\mathbf{h}}(g^{-1}\mathbf{r})\, dg = 4\pi (f * \delta_{\mathbf{h}})(\mathbf{r}), \tag{9}$$

where

$$K(\mathbf{h}, \mathbf{r}) = \{g \in SO(3); \, \mathbf{r} = g \cdot \mathbf{h}\}$$

is a great circle in $SO(3)$. The representation as a convolution implies that the Radon transform must fulfil the ultra-hyperbolic equation (or Darboux equation)

$$\Delta_{\mathbb{S}^2;\mathbf{h}} (Pf)(\mathbf{h}, \mathbf{r}) = \Delta_{\mathbb{S}^2;\mathbf{r}} (Pf)(\mathbf{h}, \mathbf{r}),$$

where $\Delta_{\mathbb{S}^2;\mathbf{h}}$ denotes the Laplace-Beltrami operator with respect to the variable $\mathbf{h}$. This fact and it's importance in texture analysis had been figured out by T. I. Savyolova (cf. [12]).
It should also be mentioned that the following Ásgeirsson-type mean value property (see [1] and [11]) is an immediate consequence of the ultra-hyperbolic equation:

$$\frac{1}{2\pi} \int_{C(\mathbf{h}, \theta)} Pf(\mathbf{h}', \mathbf{r})\, d\sigma(\mathbf{h}') = \frac{1}{2\pi} \int_{C(\mathbf{r}, \theta)} Pf(\mathbf{h}, \mathbf{r}')\, d\sigma(\mathbf{r}'),$$

where $C(\mathbf{h}, \theta)$ is the small circle $\{\mathbf{h}' \in \mathbb{S}^2 : \mathbf{h}' \cdot \mathbf{h} = \cos\theta\}$. Also this result is well-known in texture analysis. It states that the integration in the pole figure leads to the same result as the integration in the inverse pole figure which was observed by H. J. Bunge (cf. [4], [5], pp. 76–77). That the Radon transform in texture analysis fulfils the ultra-hyperbolic equation implies another important fact. The manifold $\mathbb{S}^2 \times \mathbb{S}^2$ is 4d but the manifold where the Radon transform is actually living is only 3d! Which render it possible to compare the Radon transform in texture analysis with the 1d Radon transform on the 3d sphere in the Euclidean space $\mathbb{R}^4$.

The solution of Eq. (4) for $f(g)$ is called *pole figure inversion.* Several mathematical approaches to solve this equation have been proposed. A method introduced by S. Matthies, [7], [8], provides a direct inversion formula, which can be deduced for central functions on the basis of Abel's integral transformation formula, as it has been shown in [10]. Using noncommutative harmonic analysis we were able to derive more inversion formulae, one of them can be considered as an analog to the well known back projection operator in tomography. We have

$$\begin{aligned} f(g) &= 4\pi\,\check{P}(-2\Delta_{\mathbb{S}^2\times\mathbb{S}^2}+1)^{1/2}Pf \\ &= 4\pi\,(-4\Delta_{SO(3)}+1)^{1/2}\check{P}Pf \quad \text{"back projection-type formula"} \\ &= \frac{1}{4\pi}\left(\int_{\mathbb{S}^2_{\mathbf{h}}}(Pf)(\mathbf{h},\,-g\mathbf{h})\,d\mathbf{h}+2\int_{\mathbb{S}^2_{\mathbf{h}}}\int_0^{\pi}\cos\tfrac{\theta}{2}\left(\frac{d}{d\cos\theta}W(\cos\theta,\mathbf{h},g\mathbf{h})\right)d\theta\,d\mathbf{h}\right), \end{aligned} \quad (10)$$

where $W(\cos\theta,\mathbf{h},g\mathbf{h})$ denotes the angular distribution function. This formula was already obtained by S. Matthies [7], [8]. Further,

$$(\check{P}f)(g)=\int_{\mathbb{S}^2}f(g\cdot\mathbf{h},\,\mathbf{h})\,d\mathbf{h}$$

denotes the dual Radon transform in L^2-sense and $\Delta_{SO(3)}$ the Laplace operator on $SO(3)$ which coincides with the Laplace-Beltrami operator on $\mathbb{S}^3$ These facts and the proof of the inversion formulae is contained in [3], [2].

Because we now know that $g\in SO(3)$ can be identified with an unit quaternion $g\in\mathbb{S}^3$ and that the integration over great circles in $SO(3)$ is the same like the integration over great circles in $\mathbb{S}^3$ we are able to interpret (9) as a spherical Radon transform. The *one-dimensional spherical Radon transform* $\hat{f}(\xi)$ of function $f(x)$ defined on the unit sphere $\mathbb{S}^3$ (see [6]) is given by

$$\hat{f}(\xi)=\int_{\xi}f(x)\,dm(x), \quad (11)$$

where $\xi\in\Xi$ is a great circle passing through x and $dm=d\mathbb{S}^3$ is the measure given by the Riemannian structure induced by that of $\mathbb{S}^3$. The spherical Radon transform is an isomorphism for even function. Let f be an even function, then (see [6])

$$f(x)=\frac{1}{\pi}\left[\frac{d}{du^2}\int_0^u(\hat{f})^{\vee}_{\cos^{-1}(v)}(x)\,v\,(u^2-v^2)^{-1/2}\,dv\right]\Bigg|_{u=1},$$

where $(\hat{f})^{\vee}_p(x)$ is the average of the integrals of f over the great circles of $\mathbb{S}^3$ which have distance p from x. After some calculations this inversion formula gets the form

$$f(x)=\frac{1}{2\pi}\left[(\hat{f})^{\vee}_{\frac{\pi}{2}}(x)+2\int_0^{\pi}\left(\frac{d}{d\cos\theta}(\hat{f})^{\vee}_{\frac{\theta}{2}}(x)\right)\cos\frac{\theta}{2}\,d\theta\right]. \quad (12)$$

Now we compare (10) with (12). Equation (12) is equivalent to (10) if the following system of equations is fullfiled:

$$\int_{\mathbf{h}\in\mathbb{S}^2}Pf(\mathbf{h},\,-g\mathbf{h})\,d\mathbf{h}=2(\hat{f})^{\vee}_{\frac{\pi}{2}}(g), \quad (13)$$

$$\int_{\mathbf{h}\in\mathbb{S}^2}(Wf)(\cos\theta,\,\mathbf{h},\,g\mathbf{h})\,d\mathbf{h}=2(\hat{f})^{\vee}_{\frac{\theta}{2}}(g). \quad (14)$$

Obviously, (13) is a special case of (14). Now, from the definition of the angular distribution function

$$\int_{\mathbb{S}^2}(Wf)(\mathbf{h},\,g\mathbf{h},\,\cos\theta)\,d\mathbf{h}=\int_{\mathbb{S}^2}\frac{1}{2\pi}\int_{C(\mathbf{h},\theta)}Pf(\mathbf{h}',\,\mathbf{r})\,d\sigma(\mathbf{h}')d\mathbf{r}$$

due to an Ásgeirsson mean-value property ([1] and [11]). Because of the relationship between the spherical torus (7) and the set of all great circles with distance $\frac{\theta}{2}$ from a point $q \in \mathbb{S}^3$ (8) we get

$$= 2\int_{T\left(q_1,q_2,q_3,q_4;\frac{\theta}{2}\right)} (\hat{f})(\xi)\, d\mu(\xi) = 2\int_{\left\{d(g,C(q_1,q_2))=\frac{\theta}{2}\right\}} \hat{f}(\xi)\, d\mu(\xi) = 2(\hat{f})^{\vee}_{\frac{\theta}{2}}(g)$$

where $d\mu$ is the average over the set of ξ at distance $\frac{\theta}{2}$ of $g \sim q$. and the validity of (13) and (14) is proven.

References

[1] L. Ásgeirsson, "Über eine Mittelwerteigenschaft von Lösungen homogener linearer partieller Differentialgleichungen zweiter Ordnung mit konstanten Koeffizienten", Ann. Math. Vol. 113, pp. 321-346, 1937.

[2] S. Bernstein, "The Radon transform in texture analysis", in: T.E. Simos and Ch. Tsitouras (eds.), *ICNAAM, International Conference on Numerical Analysis and Applied Mathematics 2004*, WILEY-VCH Verlag, Weinheim, pp. 482–485, 2004.

[3] S. Bernstein and H. Schaeben, "A one-dimensional Radon transfrom on $SO(3)$ and it's application to texture goniometry", Math. Meth. Appl. Sci., in print.

[4] H. J. Bunge, *Mathematische Methoden der Texturanalyse,* Akademie-Verlag Berlin, 1969,

[5] H. J. Bunge, *Texture Analysis in Materials Science,* Mathematical Methods, Butterworths, London, Boston, 1982.

[6] S. Helgason, *The Radon Transform,* Second Edition, Birkhäuser, 1999.

[7] S. Matthies, "On the reproducibility of the orientation distribution function of texture samples from pole figures (ghost phenomena)": Phys. Stat. Sol. (b), 92, K135–K138, 1979.

[8] S. Matthies, *Aktuelle Probleme der quantitativen Texturanalyse,* ZfK–480, Zentralinstitut für Kernforschung Rossendorf bei Dresden, ISSN 0138–2950, August 1982.

[9] L. Meister and H. Schaeben, "A concise quaternionic geometry of rotations", MMAS, Vol. 27, in print, 2004.

[10] J. Muller, C. Esling and H. J. Bunge, "An inversion formula formula expressing the texture function in terms of angular distribution functions", J. Phys. Vol. 42, pp. 161-165, 1981.

[11] D. I. Nikolayev and H. Schaeben, "Characteristics of the ultra-hyperbolic differential equation govering pole density functions", Inverse Problems Vol. 15, pp. 1603-1619, 1999.

[12] T. I. Savyolova, "Inverse formulas for orientation distribution function" in: H. J. Bunge, (ed.), *Proceedings of the 10th International Conference on Texture of Materials*, Materials Science Forum, Vol. 157–162, pp. 419–421, 1994.

Textures of Materials - ICOTOM 14
doi:10.4028/www.scientific.net/MSF.495-497

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doi:10.4028/www.scientific.net/MSF.495-497.277