GENERALIZED SPLINES FOR RADON TRANSFORM ON COMPACT LIE GROUPS WITH APPLICATIONS TO CRYSTALLOGRAPHY

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Objective of the talk

The objective of the talk is to introduce Radon transform on compact Lie groups and to show how spline interpolation can be used for approximate inversion of such transform on general compact Lie groups.
In a particular case of the group of rotations $SO(3)$ such problem has important applications in crystallography.

The **orientation probability density function (ODF)** representing the probability law of random orientations of crystal grains by volume is a major issue.

One cannot measure ODE directly. Instead, the **pole density function (PDF)** is measured.

In *x*-ray or neuron diffraction experiments spherical intensity distributions are measured which can be interpreted in terms of spherical probability distributions of distinguished crystallographic axes.

The following people are greatly responsible for development of the corresponding mathematical theory:
Roe R (1965),
Bunge H-J (1981-1982),
Matthies S (1979),
Bernstein S and Schaeben H (2005),
Meister L and Schaeben H (2005),
S. Bernstein, R. Hielscher, H. Schaeben (2009).

The practical measurement sends a beam through the specimen coming from the direction $h \in S^2$ and measures the intensity, emitted from the specimen in the direction $r \in S^2$. One can interpret the result as the integral over all orientations $g \in SO(3)$ with $g \cdot h = r; \quad h, r \in S^2$.
The set $C_{h,r} = \{g \in SO(3) : \; g \cdot h = r; \quad h, r \in S^2\}$ of those orientations is called a great circle in $SO(3)$.

Definition

The Radon transform of a continuous complex-valued function f on $SO(3)$ is a function on $S^2 \times S^2$ which is defined by the formula

$$\mathcal{R}f(x, y) = \int_{C_{x,y}} f(g)dg. \tag{1}$$

This transform $\mathcal{R}$ can be extended to all functions in $L^2(SO(3))$.

The mathematical formulation of the problem we consider is the following: **to reconstruct a function f on $SO(3)$ from its Radon transform $\mathcal{R}f$.**
It is interesting to note that the original function f is defined on a manifold $SO(3)$ of dimension three, but the function $\mathcal{R}f$ is defined on $S^2 \times S^2$ whose dimension is four.
In this sense the information which is inherited into $\mathcal{R}f$ is redundant.
This issue was recently discussed by
V.P. Palamodov in **Reconstruction from a sampling of circle integrals in SO(3)**, Inverse Problems 26 (2010), no. 9, 095-008, 10 pp.

Every irreducible representation of $SO(3)$is unitary equivalent to a irreducible component of the quasi regular representation in $L^2(S^2)$, given by

$$T(g) : f(\xi) \mapsto f(g^{-1} \cdot x), \tag{2}$$

where $\cdot$ denotes the canonical action of $SO(3)$ on S^2. The irreducible invariant components of $L^2(S^2)$ under T are $\mathcal{H}_k = \{\mathcal{Y}_k^i, i = 1, ..., 2k+1\}$- spanned by spherical harmonics of degree k. T^k shall denote the irreducible representation, obtained by restriction of T to $\mathcal{H}_k$. The matrix coefficients of T^k are the Wigner polynomials T_{ij}^k of degree k:

$$\mathcal{Y}_k^j(g^{-1} \cdot \xi) = \sum_{i=1}^{2k+1} T_{ij}^k(g)\mathcal{Y}_k^i(\xi) T_{ij}^k(g) = \langle \mathcal{Y}_k^j(g^{-1} \cdot), \mathcal{Y}_k^i(\cdot) \rangle_{L^2(S^2)}. \tag{3}$$

We have

$$\mathcal{R}T^k_{ij}(\xi,\eta) = T^k_{i1}(\xi)\overline{T^k_{j1}(\eta)} = \frac{4\pi}{2k+1}\mathcal{Y}^i_k(\xi)\overline{\mathcal{Y}^j_k(\eta)}. \qquad (4)$$

This formula shows that range of $\mathcal{R}$ belongs to kernel of the Darboux-type operator i.e.

$$\Delta_x \mathcal{R}f(x,y) = \Delta_y \mathcal{R}f(x,y), \quad f \in L_2(SO(3)). \qquad (5)$$

Definition

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 $\Delta_x f = \Delta_y f$.

Now we define Sobolev spaces on $SO(3)$.

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

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

Theorem

(Range description) For any $t \geq 0$ *the Radon transform on* $SO(3)$ *is an invertible mapping*

$$\mathcal{R} : H_t(SO(3)) \to H^{\Delta}_{t+\frac{1}{2}}(S^2 \times S^2). \tag{6}$$

Theorem

(Reconstruction formula) Let

$$f(x,y) = \sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} \widehat{f}(k,i,j) \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} \in H_{\frac{1}{2}}^{\Delta}(S^2 \times S^2) \qquad (7)$$

be the result of a Radon transform. Then the pre-image $g \in L^2(SO(3))$ is given by

$$g = \sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} \frac{(2k+1)}{4\pi} f\widehat{(k,i,j)} T_{ij}^k.$$

Definition

Let $\mathcal{H}$ be a closed subgroup of the compact Lie group $\mathcal{G}$. The Radon transform of a continuous function $f \in C(\mathcal{G})$ is defined by

$$\mathcal{R}f(x,y) = \int_{\mathcal{H}} f(xhy^{-1})dh, \quad x, y \in \mathcal{G}, \tag{8}$$

where dh here is the normalized Haar measure on $\mathcal{H}$.

Theorem

The following statements hold:
1) The Radon transform $\mathcal{R}$ maps functions over $\mathcal{G}$ to functions over $\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H}$.
2) If $\mathcal{H}$ is the subgroup of $\mathcal{G}$, determining the Radon transform on $\mathcal{G}$ and if $\widehat{\mathcal{G}_1} \subset \widehat{\mathcal{G}}$ is the set of irreducible representations with respect to $\mathcal{H}$, then for $f \in C^\infty(\mathcal{G})$ the following Parseval equality holds

$$\|\mathcal{R}f\|^2_{L^2(\mathcal{G}/\mathcal{H}\times\mathcal{G}/\mathcal{H})} = \sum_{\pi\in\widehat{\mathcal{G}_1}} rank(\pi_{\mathcal{H}})\|\widehat{f}(\pi)\|^2_{HS}. \tag{9}$$

In our approach to approximate inversion of the Radon transform we consider inversion as an interpolation problem. Namely, if f is a function on a compact Riemannian manifold M and a set of integrals of f over a finite family $\mathcal{M} = \{\mathcal{M}\nu\}_1^N$ of submanifolds is given, we find a "smoothest" function which has the same set of integrals as f over submanifolds from the family $\mathcal{M}$.

We consider a compact Riemannian manifold M without boundary. Let $\mathcal{L}$ be a differential of order two elliptic operator which is self-adjoint and negatively semi-definite in the space $L_2(M)$ constructed using a Riemannian density dx. The spectrum of such operator always contains $\lambda_0 = 0$. In order to have an invertible operator we will work with $I - \mathcal{L}$, where I is the identity operator in $L_2(M)$.

For a given finite family of pairwise different submanifolds $\{M_\nu\}_1^N$ consider the following family of distributions

$$F_\nu(f) = \int_{M_\nu} f \tag{10}$$

which are well defined at least for functions in $H_{\varepsilon+d/2}(M),\ \varepsilon > 0$.
In particular, if $M_\nu = x_\nu \in M$, then every F_ν is a Dirac measure $\delta_{x_\nu}\ \nu = 1, ..., N,\ x_\nu \in M$.
Note that distributions F_ν belong to $H_{-\varepsilon-d/2}(M)$ for any $\varepsilon > 0$.

Variational Problem

Given a sequence of complex numbers $v = \{v_\nu\}$, $\nu = 1, 2, ..., N$, *and a* $t > d/2$ *we consider the following variational problem:*

Find a function u *from the space* $H_t(M)$ *which has the following properties:*

1. $F_\nu(u) = v_\nu, \nu = 1, 2, ..., N, v = \{v_\nu\}$,
2. u *minimizes functional* $u \to \|(1 - \mathcal{L})^{t/2} u\|$.

Theorem

The Variational Problem has a unique solution for any sequence of values $(v_1, v_2, ...v_N)$.

The solution to the Variational Problem will be called a spline and will be denoted as $s_t(v)$. The set of all solutions for a fixed set of distributions $F = \{F_\nu\}$ and a fixed t will be denoted as $S(F, t)$.

Definition

Given a function $f \in H_t(M)$ *we will say that the unique spline* s *from* $S(F, t)$ *interpolates* f *if*

$$F_\nu(f) = F_\nu(s).$$

Such spline will be denoted as $s_t(f)$.

The next Theorem gives the characteristic property of splines.

Theorem

A function $s_t(v) \in H_t(M), t > d/2$ is a solution of the Variational Problem if and only if it satisfies the following equation in the sense of distributions

$$(1 - \mathcal{L})^t s_t(v) = \sum_{\nu=1}^{N} \alpha_\nu(s_t(v))\overline{F_\nu}.$$

Definition

Generalized Green's functions E_ν^t*, defined as solutions of the following distributional equations*

$$(1-\mathcal{L})^t E_\nu^t = \overline{F_\nu}.$$

The following important fact holds

Theorem

Every spline $s_t(v)$ *is a linear combination of the generalized Green's functions*

$$s_t(v) = \sum_{\nu=1}^{N} \alpha_\nu(s_t(v)) E_\nu^t. \tag{11}$$

Let $\{(x_1, y_1), ..., (x_N, y_N)\}$ be a set of pairs of points from $SO(3)$, such that submanifolds $\mathcal{M}_\nu = x_\nu SO(2) y_\nu^{-1} \subset SO(3),\ \ \nu = 1, ..., N$, are pairwise different.
For a continuous function f on $\mathcal{G}, \quad t > 3/2$, and a vector (of measurements) $v = (v_\nu)_1^N$ where

$$v_\nu = \int_{\mathcal{M}_\nu} f,$$

the interpolating spline is given by

$$s_t(f) = \sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} c_{ij}^k(s_t(f)) T_{ij}^k = \sum_{k=0}^{\infty} trace\left(c_k(s_t(f)) T^k\right), \quad (12)$$

where T_{ij}^k are the Wigner polynomials.

The Fourier coefficients $c_k(s_t(f))$ of the solution are given by their matrix entries

$$c_{ij}^k(s_t(f)) = \frac{4\pi}{(2k+1)(1+k(k+1))^t} \sum_{\nu=1}^{N} \alpha_\nu(s_t(f)\mathcal{Y}_k^i(x_\nu)\overline{\mathcal{Y}_k^j(y_\nu)}, \tag{13}$$

where $\alpha(s_t(f)) = (\alpha_\nu(s_t(f)))_1^N \in \mathbb{R}^N$ is the solution of

$$\mathcal{B}\alpha(s_t(f)) = f, \tag{14}$$

with $\mathcal{B} = (\beta_{\nu\mu}) \in \mathbb{R}^{N \times N}$ given by

$$\beta_{\nu\mu} = \sum_{k=0}^{\infty} (1 + k(k+1))^{-t} C_k^{\frac{1}{2}}(x_\nu \cdot y_\nu) C_k^{\frac{1}{2}}(x_\mu \cdot y_\mu), \qquad (15)$$

where $C_k^{\frac{1}{2}}$ are the Gegenbauer polynomials.

Theorem

The function $s_t(f) \in H_t(SO(3))$ has the following properties:

1. $s_t(f)$ *has the prescribed set of measurements* $v = (v_\nu)_1^N$ *at points* $((x_\nu, y_\nu))_1^N$;
2. *it minimizes the functional*

$$u \to \|(1 - \Delta_{SO(3)})^{t/2} u\|;$$

3. *the solution is optimal in the sense that for every sufficiently large* $K > 0$ *it is the symmetry center of the convex bounded closed set of all functions* g *in* $H_t(SO(3))$ *with* $\|g\|_t \leq K$ *which have the same set of measurements* $v = (v_\nu)_1^N$ *at points* $\{(x_\nu, y_\nu)\}_1^N$.

A similar result holds in the case of a general compact group $\mathcal{G}$ and its closed subgroup $\mathcal{H}$.

Theorem

Let $\{(x_1, y_1), ..., (x_N, y_N)\}$ be a set of pairs of points from $\mathcal{G}$, such that submanifolds $\mathcal{M}_\nu = x_\nu \mathcal{H} y_\nu^{-1} \subset \mathcal{G},\ \ \nu = 1, ..., N$, are pairwise different.
Given a continuous function f on $\mathcal{G}$ and a $t > \frac{1}{2} \dim \mathcal{G}$ the corresponding spline given by the formula

$$s_t = \sum_{\pi \in \widehat{\mathcal{G}}} \sum_{i,j=0}^{d_\pi} c_{ij}^\pi \pi_{ij}, \tag{16}$$

where π_{ij} are matrix entries of irreducible representations and

$$c_{ij}^\pi = (1 + \lambda_\pi^2)^{-t} \sum_{\nu=1}^{N} \alpha_\nu \pi_{ij}(x_\nu, y_\nu). \tag{17}$$

Here the coefficients $\alpha_1, ..., \alpha_N$ are solutions of the system

$$\beta_{1\mu}\alpha_1 + ... + \beta_{N\mu}\alpha_N = v_\mu, \quad \mu = 1, ..., N,$$

where entries $\beta_{\nu\mu}$ are given by

$$\beta_{\nu\mu} = \sum_{\pi \in \widehat{\mathcal{G}}} (1 + \lambda_\pi^2)^{-t} \sum_{i,j=1}^{d_\pi} \overline{\mathcal{R}(\pi_{ij}(x_\nu, y_\nu))} \mathcal{R}(\pi_{ij}(x_\mu, y_\mu)),$$

for all $1 \leq \nu,\ \mu \leq N$.

Theorem

One also has the following. The function $s_t(f) \in H_t(\mathcal{G})$ has the following properties:

1. *$s_t(f)$ has the prescribed set of measurements $v = (v_\nu)_1^N$ at points $((x_\nu, y_\nu))_1^N$;*
2. *it minimizes the functional*

$$u \to \|(1 - \Delta_{\mathcal{G}})^{t/2} u\|;$$

3. *the solution is optimal in the sense that for every sufficiently large $K > 0$ it is the symmetry center of the convex bounded closed set of all functions g in $H_t(\mathcal{G})$ with $\|g\|_t \leq K$ which have the same set of measurements $v = (v_\nu)_1^N$ at points $\{(x_\nu, y_\nu)\}_1^N$.*

Let me describe our second method in the case of $SO(3)$ and its subgroup $SO(2)$.
Remember, that in this case
if $f \in H_t(SO(3))$ then $\mathcal{R}f \in H^{\Delta}_{t+1/2}(S^2 \times S^2)$.
Also, integral of f over the circle $x_\nu SO(2) y_\nu^{-1}$ is the value of $\mathcal{R}f$ at (x_ν, y_ν).
We pick a small positive ρ and assume that the set $M_\rho = \{(x_\nu, y_\nu)\}_1^N$ is a ρ-lattice on the manifold $S^2 \times S^2$ in the sense that there exist constants $c_1,\ c_2 > 0$ such that

$$c_1 \rho \leq \max_{\nu} \min_{\nu \neq \mu} dist\left((x_\nu, y_\nu), (x_\mu, y_\mu)\right) \leq c_2 \rho$$

Using values of $\mathcal{R}f$ on the lattice M_ρ and choosing $\tau > 0$ we construct interpolating spline $s_\tau(\mathcal{R}f)$.
Let us stress that function $s_\tau(\mathcal{R}f)$ interpolates $\mathcal{R}f$ on the manifold $S^2 \times S^2$.
Our next goal is to return to $SO(3)$.
For this reason we consider orthogonal projection of $s_\tau(\mathcal{R}f)$ onto

$$Range\,\mathcal{R} = H^{\Delta}_{1/2}(S^2 \times S^2),$$

which will be denoted as $\widehat{s_\tau}(\mathcal{R}f)$.

Note it means that one takes a Fourier series of $\widehat{s}_\tau(\mathcal{R}f)$ in $L_2(S^2 \times S^2)$ and leaves only terms of the following form

$$\widehat{s}_\tau(\mathcal{R}f)(\xi, \eta) = \sum_k \sum_{ij} c_{ij}^k(\mathcal{R}f; \tau)\mathcal{Y}_k^i(\xi)\overline{\mathcal{Y}_k^j(\eta)},$$

where $(\xi, \eta) \in S^2 \times S^2$.

Applying inverse $\mathcal{R}^{-1}$ we obtain that the following function which is defined on $SO(3)$

$$S_\tau(f)(\xi) = \mathcal{R}^{-1}\left(\widehat{s}_\tau(\mathcal{R}f)\right)(\xi)$$

has a representation

$$S_\tau(f)(\xi) = \sum_k \sum_{ij} \frac{2k+1}{4\pi} c_{ij}^k(\mathcal{R}f;\tau) T_{ij}^k(\xi),$$

where T_{ij}^k are Wigner functions.

Let us stress that functions $S_\tau(f)$ do not interpolate f in any sense. However, the following approximation results hold.

Theorem

If the set of points $M_\rho = \{(x_\nu, y_\nu)\} \subset S^2 \times S^2$ (which corresponds to the set of circles $x_\nu SO(2) y_\nu^{-1} \subset SO(3)$) is a ρ-lattice then for $\tau > 2$ for sufficiently smooth functions one has the estimate

$$\|(S_\tau(f) - f)\|_{L_2(SO(3))} \leq (C\rho)^\tau \|\mathcal{R}f\|_{H_\tau(S^2\times S^2)},$$

where the functions $S_\tau(f)$ constructed using only the values of $\mathcal{R}f$ on M_ρ.

Moreover, for a natural k one has uniform convergence

$$\|S_\tau(f) - f\|_{C^k(SO(3))} \leq (C\rho)^\tau \|\mathcal{R}f\|_{H_{\tau+k+2}(S^2\times S^2)}$$

for any $\tau > 2$.

For an $\omega > 0$ let us consider the space $\mathbf{E}_{\omega}(SO(3))$ of ω-bandlimited functions on $SO(3)$ i.e. the span of all Wigner functions T^k_{ij} with $k(k+1) \leq \omega$.
The Radon transform of such function is ω-bandlimited on $S^2 \times S^2$ in the sense its Fourier expansion involves only functions $\mathcal{Y}^k_i \overline{\mathcal{Y}^k_j}$ which are eigenfunctions of $\Delta_{S^2 \times S^2}$ with eigenvalue $-k(k+1)$.
Under our assumption about k the following Bernstein-type inequality holds for any function in the span of $\mathcal{Y}^k_i \overline{\mathcal{Y}^k_j}$

$$\|(1 - 2\Delta_{S^2 \times S^2})^{\tau} \mathcal{R} f\|_{L^2(S^2 \times S^2)} \leq (1 + 2\omega)^{\tau} \|\mathcal{R} f\|_{L^2(S^2 \times S^2)}$$

Theorem

(Sampling Theorem for Radon Transform) If f $\in \mathbf{E}_\omega(SO(3))$*, then for any* $\tau > o$ *and any natural k*

$$\|S_\tau(f) - f\|_{C^k(SO(3))} \leq (C\rho(1+2w))^\tau (1+2w)^{k+2}\|\mathcal{R}f\|.$$

Let us remind that the function $S_\tau(f)$ was constructed by using only the values of the Radon transform $\mathcal{R}f$ on a lattice of points on $S^2 \times S^2$. This Sampling Theorem shows that if

$$\rho < \frac{1}{\sqrt{C(1 + 2\omega)}}$$

than one can have a complete reconstruction of ω-bandlimited f when τ goes to infinity by using only the values of its Radon transform $\mathcal{R}f$ on any fixed ρ-lattice of $S^2 \times S^2$.

THANK YOU FOR COMING!!!!!!!!!!