Noncommutative Harmonic Analysis on $\mathsf{SO}(3)$

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I. Harmonic Analysis on $\mathsf{SO}(3)$

A. Representation on a Lie group

Let $f \in \mathcal{L}^2(\mathbb{R}^n)$. The (left) representation $U(g)$ of G is $\mathsf{GL}(\mathcal{L}^2(\mathbb{R}^n))$, i.e., the set of linear transformation on $\mathcal{L}^2(\mathbb{R}^n)$ defined such that

$$(U(g)f)(x) = f(g^{-1}x). \tag{1}$$

It is straightforward to show the representation is a homomorphism,

$$(U(g_1)(U(g_2)f))(x) = f(g_2^{-1}g_1^{-1}x) = (U(g_1g_2)f)(x).$$

By selecting a basis for the invariance subspaces of $\mathcal{L}^2(\mathbb{R}^n)$, $U(g)$ can be represented by a matrix, which is called a matrix representation of G.

Two matrix representations are *equivalent*, if one can obtained by a similarity transform of the other. Any representation can be transformed into a *unitary* representation by a similarity transform so that $U(g)U^*(g) = I$, or $U(g^{-1}) = U^*(g)$. A matrix representation is *reducible*, if it is equivalent to the direct sum of others, or equivalently, it can be block-diagonalized. One can redefine (1) with the group acting acting on the right side of x. Each irreducible representation acts only on the corresponding subspace, and the choice between the left action or the right action does not matter in the definition of the representation.

B. Irreducible Unitary Representation on $\mathsf{SO}(3)$

Since there is two-to-one homomorphism from $\mathsf{SU}(2)$ to $\mathsf{SO}(3)$, the representation of $\mathsf{SO}(3)$ should be a subset of those for $\mathsf{SU}(2)$, which is a set of linear transformation on $\mathcal{L}^2(\mathbb{C}^2)$. The set of homogeneous polynomials is a basis of $\mathcal{L}^2(\mathbb{C}^2)$, and one can find the matrix representation of $\mathsf{SU}(2)$ with (1), which results in generalizations of the associated Legendre function [1] that is also shown to be unitary, and irreducible. An irreducible unitary representation of $\mathsf{SO}(3)$ is constructed by taking the terms with integer indices.

The wigner-D function is another irreducible unitary representation on $\mathsf{SU}(2)$ (or $\mathsf{SO}(3)$) that is equivalent to the above representation based on the generalized associated Legendre function. Specifically, the wigner-D function is given by $D^l_{m,n}(R) \in \mathbb{C}$, where the index l is a non-negative integer, and the integer indices m, n vary in $-l \leq m, n \leq l$. When the low indices are dropped, $D^l(R)$ is considered as a square matrix where the row index (resp. the column index) corresponds to m (resp. n) varying from $-l \leq m, n \leq l$. As such $D^l(R) \in \mathbb{C}^{2l+1,2l+1}$.

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Let $(\alpha, \beta, \gamma) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi)$ be the 3-2-3 Euler angles, i.e.,

$$R(\alpha, \beta, \gamma) = \exp(\alpha\hat{e}_3)\exp(\beta\hat{e}_2)\exp(\gamma\hat{e}_3).$$

Then, $D^l_{m,n}(R(\alpha, \beta, \gamma))$ is given by

$$D^l_{m,n}(R(\alpha, \beta, \gamma)) = e^{-im\alpha} d^l_{m,n}(\beta) e^{-in\gamma},$$

where $d^l_{m,n}(\beta)$ is a real-valued wigner-d function. A recursive formulation to evaluate the wigner-d function is presented in [2].

As $D^l(R)$ is unitary, we have $D^l(R)(D^l(R))^* = I_{2l+1}$ or equivalently $(D^l(R))^{-1} = (D^l(R))^*$. Furthermore, as it is a homomorphism, $D^l(R)D^l(R^T) = I_{2l+1}$. Therefore,

$$D^l(R^T) = (D^l(R))^{-1} = (D^l(R))^*,$$
$$D^l(I_{3\times 3}) = I_{2l+1}, \quad D^l_{m,n}(R(0,0,0)) = \delta_{m,n},$$

Since $d^l(\beta) = D^l(R(0, \beta, 0))$, it follows

$$d^l(-\beta) = (d^l(\beta))^{-1} = (d^l(\beta))^T,$$
$$d^l(0) = I_{2l+1}, \quad d^l_{m,n}(0) = \delta_{m,n}.$$

Also,

$$(D^l_{m,n}(R(\alpha, \beta, \gamma)))^* = (-1)^{m-n} D^l_{-m,-n}(R(\alpha, \beta, \gamma)).$$

While this formulation is based on the particular 3-2-3 Euler angles, 3-1-3 Euler angles can be used without any modification, as it will be equivalent anyway [1]. Another nice feature is that $D^l_{m,n}$ is given by a product of three terms, which depend solely on each of three Euler angles. This follows directly from the use of a Gel‘fand-Tsetlin basis, i.e., a basis that respects the decomposition of the restriction to the subgroup $\mathsf{SO}(2)$ [3]. This is useful for devising fast Fourier transforms on $\mathsf{SO}(3)$. Alternatively, the wigner-D matrix is formulated in terms of quaternions and rotation matrices in [4].

We define an inner product on $\mathcal{L}^2(\mathsf{SO}(3))$ as

$$\langle f(R), g(R)\rangle = \int_{\mathsf{SO}(3)} f(R)g^*(R)dR.$$

For the 3-2-3 Euler angles, the Haar measure is written as $dR = \frac{1}{8\pi^2}\sin\beta d\alpha d\beta d\gamma$ that is normalized such that $\int_{SO} dR = 1$.

According to the Peter-Weyl theorem, the collection of the irreducible unitary representations on $\mathsf{SO}(3)$ form a complete orthogonal basis for $\mathcal{L}^2(\mathsf{SO}(3))$ over the above inner product. Specifically

$$\langle D^{l_1}_{m_1,n_1}(R), D^{l_2}_{m_2,n_2}(R)\rangle = \frac{1}{2l_1+1}\delta_{l_1,l_2}\delta_{m_1,m_2}\delta_{n_1,n_2}. \tag{2}$$

When $m_1 = m_2$ and $n_1 = n_2$, this reduces to

$$\int_0^\pi d^{l_1}_{m,n}(\beta) d^{l_2}_{m,n}(\beta)\sin\beta d\beta = \frac{2}{2l_1+1}\delta_{l_1,l_2}.$$

The various identities, symmetry relatives, and derivatives of $D^l_{m,n}$ are provided in [5]. In particular,

$$\begin{aligned}\frac{\partial}{\partial\beta}&D^l_{m,n}(\alpha,\beta,\gamma)\\&=-\frac{1}{2}\sqrt{(l+m)(l-m+1)}e^{-i\alpha}D^l_{m-1,n}(\alpha,\beta,\gamma)\\&\quad+\frac{1}{2}\sqrt{(l-m)(l+m+1)}e^{i\alpha}D^l_{m+1,n}(\alpha,\beta,\gamma).\end{aligned}\tag{3}$$

C. Character

The *character* of the representation is given by

$$\chi^l(R)=\mathrm{tr}[D^l(R)]=\sum_{m=-l}^{l}e^{-im(\alpha+\gamma)}d^l_{m,m}(\beta).$$

It is a *class function* as it is invariant under the conjugation, i.e., for any $Q\in\mathsf{SO}(3)$

$$\chi(Q^TRQ)=\mathrm{tr}[D(Q^TRQ)]=\mathrm{tr}[D(Q^T)D(R)D(Q)]=\chi(R).$$

As such, the character only depends on the rotation angle, i.e., when $R=\exp(\theta\hat{r})$ for any $r\in\mathsf{S}^2$,

$$\begin{aligned}\chi^l&(\exp(\theta\hat{r}))\\&=\chi^l(R(0,\theta,0))=\sum_{m=-l}^{l}d^l_{m,m}(\theta)\\&=\chi^l(R(\theta,0,0))=\sum_{m=-l}^{l}e^{-im\theta}=\frac{\sin(\frac{2l+1}{2}\theta)}{\sin\frac{\theta}{2}}.\end{aligned}$$

Let a rotation matrix parameterized by spherical coordinates $(\lambda,\nu,\theta)\in[0,2\pi]\times[0,\pi]\times[0,\pi]$, where λ and ν are the polar and azimuthal angles for the axis of rotation, and θ is the angle of rotation. In these coordinate, the normalized Haar measure is given by $dR=\frac{1}{2\pi^2}\sin^2\frac{\theta}{2}\sin\nu d\lambda d\nu d\theta$. We can show the orthogonality of the character as follows

$$\begin{aligned}&\langle\chi^{l_1}(R),\chi^{l_2}(R)\rangle\\&=\frac{1}{2\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{\pi}\sin(\frac{2l_1+1}{2}\theta)\sin(\frac{2l_2+1}{2}\theta)\sin\nu d\theta d\nu d\lambda\\&=\frac{2}{\pi}\int_0^{\pi}\sin(\frac{2l_1+1}{2}\theta)\sin(\frac{2l_2+1}{2}\theta)d\theta=\delta_{l_1,l_2}.\end{aligned}$$

It has been shown that a representation $\chi(R)$ is irreducible if and only if $\|\chi(R)\|=1$. Consequently, the above orthogonality implies that $D^l(R)$ is irreducible for any l.

D. Operational Properties

Given the matrix representation $D^l(R)$, we can define a representation of $\mathfrak{so}(3)\simeq\mathbb{R}^3$ as

$$u^l(\eta)=\frac{d}{d\epsilon}\bigg|_{\epsilon=0}D^l(\exp(\epsilon\hat{\eta})),$$

where $\eta\in\mathbb{R}^3$. It satisfies

$$u^l([\eta,\zeta])=[u^l(\eta),u^l(\zeta)].$$

As it is a linear operator,

$$u^l(\sum_{i=1}^{3}\eta_ie_i)=\sum_{i=1}^{3}\eta_iu^l(e_i).$$

As such, we need to compute $u^l(e_1),u^l(e_2),u^l(e_3)\in\mathbb{C}^{(2l+1)\times(2l+1)}$ only.

Since $\exp(\epsilon\hat{e}_3)=R(\epsilon,0,0)$,

$$u^l_{m,n}(e_3)=\frac{d}{d\epsilon}\bigg|_{\epsilon=0}e^{-im\epsilon}d^l_{m,n}(0)=-im\delta_{m,n}.\tag{4}$$

Since $\exp(\epsilon\hat{e}_2)=R(0,\epsilon,0)$,

$$\begin{aligned}u^l_{m,n}(e_2)&=\frac{d}{d\epsilon}\bigg|_{\epsilon=0}D^l_{m,n}(R(0,\epsilon,0))\\&=-\frac{1}{2}\sqrt{(l+m)(l-m+1)}\delta_{m-1,n}\\&\quad+\frac{1}{2}\sqrt{(l-m)(l+m+1)}\delta_{m+1,n}\\&=-\frac{1}{2}c^l_n\delta_{m-1,n}+\frac{1}{2}c^l_{-n}\delta_{m+1,n}.\end{aligned}\tag{5}$$

with $c^l_n=\sqrt{(l-n)(l+n+1)}$, which is obtained from (3).

Last, $u^l(e_1)$ can be obtained by $u^l(e_1)=u^l(e_2\times e_3)=[u^l(e_2),u^l(e_3)]$ as

$$u^l_{m,n}(e_1)=-\frac{1}{2}ic^l_n\delta_{m-1,n}-\frac{1}{2}ic^l_{-n}\delta_{m+1,n}.\tag{6}$$

E. Fourier Transform on $\mathsf{SO}(3)$

Due to the Peter-Weyl According to the Peter-Weyl theorem, any $f\in\mathcal{L}^2(\mathsf{SO}(3))$ has the following decomposition

$$\begin{aligned}f(R(\alpha,\beta,\gamma))&=\sum_{l=0}^{\infty}\sum_{m,n=-l}^{l}(2l+1)\bar{f}^l_{m,n}D^l_{m,n}(\alpha,\beta,\gamma)\\&=\sum_{l=0}^{\infty}(2l+1)\mathrm{tr}[(\bar{f}^l)^TD^l(\alpha,\beta,\gamma)],\end{aligned}\tag{7}$$

which is the Fourier transform. From the orthogonality property (2), the Fourier parameter $\bar{f}^l_{m,n}\in\mathbb{C}$ is obtained by

$$\begin{aligned}&\bar{f}^l_{m,n}=\langle f(R),D^l_{m,n}(R)\rangle\\&=\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi}f(R(\alpha,\beta,\gamma))(D^l_{m,n}(R(\alpha,\beta,\gamma)))^*d\alpha d\beta d\gamma,\end{aligned}\tag{8}$$

which is the inverse transform. Several variations of the above definition exist. For example, in [6], $D^l_{m,n}$ is normalized such that the factor $2l+1$ does not appear. We follow the convention of [1], and the factor appears in (7).

We also have the Plancherel theorem:

$$\langle f_1(R),f_2(R)\rangle=\sum_{l=0}^{\infty}(2l+1)\langle\bar{f}^l_1,\bar{f}^l_2\rangle,$$

with the inner product $\langle A,B\rangle=\mathrm{tr}[A^*B]$ on $A,B\in\mathbb{C}^{n\times n}$. Also,

$$\|f(R)\|^2=\sum_{l=0}^{\infty}(2l+1)\|\bar{f}^l\|^2$$

F. Sampling

A function $f \in \mathcal{L}^2(\mathsf{SO}(3))$ is called *band-limited* with the band $l_{\max}$ if $f^l = 0$ for any $l \geq l_{\max}$ in (7).

$$f(R(\alpha,\beta,\gamma)) = \sum_{l=0}^{l_{\max}} \sum_{m,n=-l}^{l} (2l+1)\bar{f}^l_{m,n} D^l_{m,n}(\alpha,\beta,\gamma).$$

The forward transform of a band-limited function is given by

$$\begin{aligned}
&\bar{f}^l_{m',n'} = \langle f(R), D^{l'}_{m',n'}(R)\rangle \\
&= \sum_{l=0}^{l_{\max}} \sum_{m,n=-l}^{l} (2l+1)\bar{f}^l_{m,n} \int_{\mathsf{SO}(3)} D^l_{m,n}(R)(D^{l'}_{m',n'}(R))^*\, dR \\
&= \sum_{l=0}^{l_{\max}} \sum_{m,n=-l}^{l} (2l+1)\bar{f}^l_{m,n} (-1)^{m'-n'} \\
&\qquad \times \int_{\mathsf{SO}(3)} D^l_{m,n}(R) D^{l'}_{-m',-n'}(R)\, dR.
\end{aligned}$$

Clebsch-Gordon formula implies that the product of D^{l_1} and D^{l_2} may be written as a linear combination of D^l with $|l_1 - l_2| \leq l \leq l_1 + l_2$. Since $0 \leq l, l' \leq l_{\max}$, the integrand of the above forward transform can be rewritten as a linear combination of D^s up to $0 \leq s \leq 2l_{\max}$. In [3], it is proposed that if a quadrature rule is selected such that the following integral for a wigner D function is evaluated exactly for $0 \leq l \leq 2l_{\max}$, the Fourier coefficients are computed exactly as well.

$$\begin{aligned}
&\int_{\mathsf{SO}(3)} D^l_{m,n}(R) dR \\
&= \frac{1}{8\pi^2} \int_0^{2\pi} e^{-im\alpha} d\alpha \int_0^{\pi} d^l_{m,n}(\beta)\sin\beta d\beta \int_0^{2\pi} e^{-in\gamma} d\gamma \\
&= \frac{1}{2}\delta_{m,0}\delta_{n,0} \int_0^{\pi} d^l_{m,n}(\beta)\sin\beta d\beta \\
&= \frac{1}{2}\delta_{m,0}\delta_{n,0} \int_0^{\pi} d^l_{0,0}(\beta)\sin\beta d\beta \\
&= \delta_{m,0}\delta_{n,0}\delta_{l,0}.
\end{aligned} \tag{9}$$

Consider the following uniform grid for $(\alpha,\beta,\gamma) \in [0, 2\pi) \times [0,\pi] \times [0, 2\pi)$:

$$[\mathsf{SO}(3)]_d = \{(\alpha_{j_1}, \beta_k, \gamma_{j_2}) \,|\, j_1, j_2, k \in \{0, \ldots, 2l_{\max}\}\},$$

with

$$\alpha_j = \gamma_j = \frac{2\pi j}{2l_{\max}+1}, \quad \beta_k = \frac{\pi k}{2l_{\max}}. \tag{10}$$

Let w_k be the weight of $(\alpha_{j_1}, \beta_k, \gamma_{j_2})$ for $0 \leq k \leq 2l_{\max}$. The weighted sum of the $D^l_{m,n}$ at the selected grid is given by

$$\begin{aligned}
&\sum_{j_1,j_2,k=0}^{2l_{\max}} w_k D^l_{m,n}(R(\alpha_{j_1}, \beta_k, \gamma_{j_2})) \\
&= \sum_{j_1=0}^{2l_{\max}} e^{-im\alpha_{j_1}} \times \sum_{k=0}^{2l_{\max}} w_k d^l_{m,n}(\beta_k) \times \sum_{j_2=0}^{2l_{\max}} e^{-in\gamma_{j_2}} \\
&= (2l_{\max}+1)^2 \delta_{m,0}\delta_{n,0} \sum_{k=0}^{2l_{\max}} w_k d^l_{m,n}(\beta_k),
\end{aligned}$$

which is obtained by the property of $\alpha_{j_1}, \gamma_{j_2}$ defined in (10),

$$\sum_{j_1=0}^{2l_{\max}} e^{-im\alpha_{j_1}} = (2l_{\max}+1)\delta_{m,0}.$$

Therefore, (9) is satisfied if w_k is chosen such that

$$\sum_{k=0}^{2l_{\max}} w_k d^l_{0,0}(\beta_k) = \sum_{k=0}^{2l_{\max}} w_k P_l(\cos\beta_k) = \frac{1}{(2l_{\max}+1)^2}\delta_{l,0}, \tag{11}$$

for $0 \leq l \leq 2l_{\max}$, where $P_l(\cdot)$ is the l-th Legendre polynomial.

A similar problem has been addressed in [7], and later utilized in [6], under an alternative definition of the band-limited function and grids. In [8], the weighting parameters are chosen according to a Clenshaw-Curtis quadrature rule, but without exact transform for band-limited functions.

Here, we do not present an analytic solution to (11), but instead reformulate it into the following matrix equation.

$$Pw = \frac{1}{(2l_{\max}+1)^2} d,$$

where $P \in \mathbb{R}^{2l_{\max}+1 \times 2l_{\max}+1}$, $w, d \in \mathbb{R}^{l_{\max}+1}$ are defined such that $[P]_{lk} = P_l(\cos\beta_k)$, $[w]_k = w_k$, and $[d]_k = \delta_{k,0}$ where the row index l and the column index k are assumed to be varied from 0 to $2l_{\max}$. For the evaluation of the Legendre polynomial, we may use the following recursive relation,

$$(l+1)P_{l+1}(x) = (2l+1)xP_l(x) - lP_{l-1}(x),$$

with $P_0(x) = 1$ and $P_1(x) = x$.

Then,

$$\sum_{j_1,j_2,k=0}^{2l_{\max}} w_k D^l_{m,n}(R(\alpha_{j_1}, \beta_k, \gamma_{j_2})) = \delta_{l,0}\delta_{m,0}\delta_{n,0},$$

i.e., the weighted sum under the given grid and weight calculates (9) exactly.

Utilizing this, the Fourier transform of a band-limited function can be written as

$$f^l_{m,n} = \sum_{j_1,j_2,k=0}^{2l_{\max}} w_k f(\alpha_{j_1}, \beta_k, \gamma_{j_2})(D^l_{m,n}(R(\alpha_{j_1}, \beta_k, \gamma_{j_2})))^*.$$

G. Fast Fourier Transform

The above summation can be decomposed into

$$\begin{aligned}
f^l_{m,n} &= \sum_{j_1,j_2,k=0}^{2l_{\max}} w_k f(\alpha_{j_1}, \beta_k, \gamma_{j_2}) e^{im\alpha_{j_1}} d^l_{m,n}(\beta_k) e^{in\gamma_{j_2}} \\
&= \sum_{j_1=0}^{2l_{\max}} e^{im\alpha_{j_1}} \sum_{j_2=0}^{2l_{\max}} e^{in\gamma_{j_2}} \sum_{k}^{2l_{\max}} w_k f(\alpha_{j_1}, \beta_k, \gamma_{j_2}) d^l_{m,n}(\beta_k)
\end{aligned}$$

This can be compute in the following order:

$$F^{\beta}_{l,m,n}(j_1,j_2) = \sum_{k=0}^{2l_{\max}} w_k f(\alpha_{j_1},\beta_k,\gamma_{j_2}) d^l_{m,n}(\beta_k),$$
$$F^{\gamma}_{l,m,n}(j_1) = \sum_{j_2=0}^{2l_{\max}} e^{in\gamma_{j_2}} F^{\beta}_{l,m,n}(j_1,j_2),$$
$$f^l_{m,n} = \sum_{j_1=0}^{2l_{\max}} e^{im\alpha_{j_1}} F^{\gamma}_{l,m,n}(j_1).$$

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