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

Taeyoung Lee

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 $D^l(R) \in \mathbb{C}^{2l+1,2l+1}$.

Taeyoung Lee, Mechanical and Aerospace Engineering, George Washington University, Washington DC 20052 tylee@gwu.edu

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,

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

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 $\exp(\epsilon\hat e_3)=R(\epsilon,0,0)$,

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

Since $\exp(\epsilon\hat e_2)=R(0,\epsilon,0)$,

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

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

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

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

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

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

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

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 B if $f^l = 0$ for any $l \geq B$ in (7), or equivalently

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

The classical sampling theorem stated that the Fourier transform of a band limited function can be recovered from the sample values of the function that are chosen at a uniform grid with with a frequency that is at least twice of the band limit. Consequently, the Fourier transform of the above function can be computed from finite samples.

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

$$[\mathsf{SO(3)}]_d = \{(\alpha_{j_1},\beta_k,\gamma_{j_2}) \,|\, j_1,j_2,k \in \{0,\ldots,2B-1\}\},$$

with

$$\alpha_j = \gamma_j = \frac{\pi j}{2B}, \quad \beta_k = \frac{\pi(2k+1)}{4B}. \tag{9}$$

Define a sampling distribution of bandwidth B as

$$s(R(\alpha,\beta,\gamma)) = \sum_{j_1,k,j_2=0}^{2B-1} w_k \delta_{R(\alpha,\beta,\gamma),R(\alpha_{j_1},\beta_k,\gamma_{j_2})}, \tag{10}$$

which is the linear combination of grid points weighted by the parameter w_k. The Fourier transform of s_B is given by

$$\begin{aligned}
\bar{s}^l_{m,n} &= \langle s(R(\alpha,\beta,\gamma)), D^l_{m,n}(R)\rangle \\
&= \sum_{j_1,k,j_2=0}^{2B-1} w_k (D^l_{m,n}(R(\alpha_{j_1},\beta_k,\gamma_{j_2})))^* \\
&= \sum_{j_1=0}^{2B-1} e^{im\alpha_{j_1}} \sum_{j_2=0}^{2B-1} e^{in\gamma_{j_2}} \sum_{k=0}^{2B-1} w_k d^l_{m,n}(\beta_k).
\end{aligned}$$

For the selected grid, $\sum_{j_1=0}^{2B-1} e^{im\alpha_{j_1}} = 2B\delta_{m,0}$. Therefore,

$$\begin{aligned}
\bar{s}^l_{m,n} &= \langle s(R(\alpha,\beta,\gamma)), D^l_{m,n}(R)\rangle \\
&= \sum_{j_1,k,j_2=0}^{2B-1} w_k (D^l_{m,n}(R(\alpha_{j_1},\beta_k,\gamma_{j_2})))^* \\
&= 4B^2\delta_{m,0}\delta_{n,0} \sum_{k=0}^{2B-1} w_k d^l_{0,0}(\beta_k), \\
&= 4B^2\delta_{m,0}\delta_{n,0} \sum_{k=0}^{2B-1} w_k P_l(\beta_k),
\end{aligned}$$

where P_l is the l-th Legendre polynomial. We select the weight such that

$$\sum_{k=0}^{2B-1} w_k P_l(\beta_k) = \frac{1}{4B^2}\delta_{l,0}, \quad l = 0,\ldots 2B-1. \tag{11}$$

In [7], it is explicitly given as

$$w_k = \frac{1}{4B^3}\sin\beta_k \sum_{j=0}^{B-1} \frac{1}{2j+1}\sin((2j+1)\beta_k). \tag{12}$$

Substituting this, the Fourier transform of the sampling distribution is given by

$$\bar{s}^l_{m,n} = \delta_{m,0}\delta_{n,0}\delta_{l,0}, \quad l = 0,\ldots 2B-1. \tag{13}$$

Define $f_s(R) = f(R)s(R)$. It is straightforward to show

$$\begin{aligned}
&f_s(R(\alpha,\beta,\gamma)) \\
&= \sum_{j_1,k,j_2=0}^{2B-1} w_k f(R(\alpha_{j_1},\beta_k,\gamma_{j_2}))\delta_{R(\alpha,\beta,\gamma),R(\alpha_{j_1},\beta_k,\gamma_{j_2})},
\end{aligned}$$

and the Fourier transform is given by

$$\begin{aligned}
&(\bar{f}_s)^l_{m,n} \\
&= \sum_{j_1,k,j_2=0}^{2B-1} w_k f(R(\alpha_{j_1},\beta_k,\gamma_{j_2}))(D^l_{m,n}(R(\alpha_{j_1},\beta_k,\gamma_{j_2})))^*.
\end{aligned}$$

Next, we show that this corresponds to the Fourier coefficient of f within the band limit.

From (13), the sampling distribution can be expanded as

$$s(R) = 1 + \sum_{l=2B}^{\infty} \sum_{m,n=-l}^{l} \bar{s}^l_{m,n} D^l_{m,n}(R).$$

Then,

$$f_s(R) = f(R) + f(R) \sum_{l=2B}^{\infty} \sum_{m,n=-l}^{l} \bar{s}^l_{m,n} D^l_{m,n}(R).$$

Since $f(R)$ can be expanded as a linear combination of D^{l_1} for $0 \leq l_1 \leq B-1$. The last term of the above equation is expanded by the product $D^{l_1}D^{l_2}$ with $0 \leq l_1 \leq B-1$ and $2B \leq l_2$. According to the Clebsch-Gordon theorem, $D^{l_1}D^{l_2}$ is a linear combination of D^{l_3} for $|l_1 - l_2| \leq l_3 \leq l_1 + l_2$. We have $\min|l_1 - l_2| = 2B - 1 - B = B + 1$. As such, f and f_s share the Fourier coefficients in the given band limit. Or equivalently,

$$\begin{aligned}
&\bar{f}^l_{m,n} \\
&= \sum_{j_1,k,j_2=0}^{2B-1} w_k f(R(\alpha_{j_1},\beta_k,\gamma_{j_2}))(D^l_{m,n}(R(\alpha_{j_1},\beta_k,\gamma_{j_2})))^*.
\end{aligned} \tag{14}$$

G. Fast Fourier Transform

The above summation can be decomposed into

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

This can be compute in the following order:

$$F^{\beta}_{l,m,n}(j_1,j_2) = \sum_{k=0}^{2B-1} w_k f(\alpha_{j_1},\beta_k,\gamma_{j_2}) d^l_{m,n}(\beta_k),$$

$$F^{\gamma}_{l,m,n}(j_1) = \sum_{j_2=0}^{2B-1} e^{in\gamma_{j_2}} F^{\beta}_{l,m,n}(j_1,j_2),$$

$$f^l_{m,n} = \sum_{j_1=0}^{2B-1} e^{im\alpha_{j_1}} F^{\gamma}_{l,m,n}(j_1).$$

References

[1] G. Chirikjian and A. Kyatkin, *Engineering applications of noncommutative harmonic analysis*. Boca Raton, FL: CRC Press, 2001.

[2] M. Blanco, M. Flórez, and M. Bermejo, "Evaluation of the rotation matrices in the basis of real spherical harmonics," *Journal of Molecular Structure*, vol. 419, pp. 19–27, 1997.

[3] D. K. Maslen and D. N. Rockmore, "Generalized FFTs - a survey of some recent results," in *Groups and Computation II*, vol. 28. American Mathematical Soc., 1997, pp. 183–287.

[4] R. Lynden-Bell and A. Stone, "Reorientational correlation functions, quaternions and wigner rotation matrices," *Molecular Simulation*, vol. 3, pp. 271–281, 1989.

[5] D. Varshalovich, A. Moskalaev, and V. Khersonskii, *Quantum Theore of Angular Momentum*. World Scientific, 1988.

[6] P. J. Kostelec and D. N. Rockmore, "FFTs on the rotation group," *Journal of Fourier analysis and applications*, vol. 14, no. 2, pp. 145–179, 2008.

[7] J. Driscoll and D. Healy, "Computing Fourier transform and convolutions on the 2-sphere," *Advances in Applied Mathematics*, vol. 15, pp. 202–250, 1994.

[8] D. Potts, J. Prestin, and A. Vollrath, "A fast Fourier algorithm on the rotation group," *Preprint A-07-06, Univ. zu Lübeck*, 2007.