Sampling sets and quadrature formulae on the rotation group

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In this paper we construct sampling sets over the rotation group $SO(3)$. The proposed construction is based on a parameterization, which reflects the product nature $\mathbb{S}^2 \times \mathbb{S}^1$ of $SO(3)$ very well, and leads to a spherical Pythagorean-like formula in the parameter domain. We prove that by using uniformly distributed points on $\mathbb{S}^2$ and $\mathbb{S}^1$ we obtain uniformly sampling nodes on the rotation group $SO(3)$. Furthermore, quadrature formulae on $\mathbb{S}^2$ and $\mathbb{S}^1$ lead to quadratures on $SO(3)$, as well. For scattered data on $SO(3)$ we give a necessary condition on the mesh norm such that the sampling nodes possesses nonnegative quadrature weights. We propose an algorithm for computing the quadrature weights for scattered data on $SO(3)$ based on fast algorithms. We confirm our theoretical results with examples and numerical tests.

Keywords and Phrases : rotation group $SO(3)$, spherical harmonics, sampling sets, quadrature rule, scattered data

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1 Introduction

The rotation group $SO(3)$ have important applications in crystallographic texture analysis, chemical physics, molecular biology and robotics, to name but a few, cf. [1] and [7]. The efficient reconstruction of functions on the rotation group plays an important roll. Therfore the construction of sampling sets on the $SO(3)$ as well as quadrature rules on the $SO(3)$ has attracted much attention. The aim of this paper is twofold. In the first part we construct sampling sets on the rotation group $SO(3)$. Recently a method to generate uniform deterministic sampling sets was suggested by J.C. Mitchell in [12]. Here the author used the Frobenius norm to define a projective Euclidean distance metric on

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$SO(3)$, which leads to uniformity assertions. In contrast we use the natural translation invariant metric on the rotation group. The construction is based on a parameterization by a tensor product on $\mathbb{S}^2 \times \mathbb{S}^1$, where we denote as usual the two-sphere and the one-sphere by $\mathbb{S}^2$ and $\mathbb{S}^1$, respectively. Other sampling methods, based on sampling over half of the three-sphere $\mathbb{S}^3$ were suggested in [21],[7] and [6]. Our construction leads to a spherical Pythagorean-like formula in the parameter domain and furthermore we are able to construct sampling sets, which are uniformly distributed in some sense. D. Schmid was able to present a trade-off result, cf. [16], for approximation problems using positive definite basis functions on the rotation group. This work made clear that is impossible to come up with positive definite basis function that enables one to keep the estimate on the approximation error and the condition number of the associated interpolation matrix arbitrarily small simultaneously. These results reveal the importance of the distribution of the sampling points on $SO(3)$, cf. [18].

In the second part we construct quadrature rules with degree of exactness N, i.e., the integration of all polynomials $\Pi_N(SO(3))$ on $SO(3)$ is exact. In order to estimate the quality of the quadrature rules we introduce the efficiency, similar as in [10, 8] on the two-sphere, as quotient of the dimension of the polynomial space $\Pi_N(SO(3))$ of degree N and the degree of freedom, given by the number of sampling points. Based on efficient quadrature rules on the two-sphere [10, 8, 13] and the one-sphere we obtain efficient quadrature rules on the rotation group. Furthermore we obtain by our construction immediately t-designs on the rotation group from the spherical t-designs, cf. [4]. Beside the construction of quadrature rules for such special point sets, we investigate quadrature rules for scattered data. D. Schmid proved recently L^p-Marcinkiewicz-Zygmund inequalities for scattered nodes on $SO(3)$, cf. [17]. Using this result in connection with the result of H.N. Mhaskar, F.J. Narcowich and J.D. Ward [11, Proposition 4.1] one obtains a sufficient condition on the mesh norm of the sampling set such that one can construct positive quadrature rules on $SO(3)$, cf. [19, Theorem 4.27]. In contrast we give a necessary condition. For this purpose we apply a method which was used by M. Reimer and V.A. Yudin [15, Theorem 6.21] on the d-sphere. Finally we confirm our theoretical results by numerical examples. To this end, we develop an algorithm for the efficient computation of nonnegative quadrature weights for scattered nodes on $SO(3)$, which follows the method on the two-sphere given in [2]. This algorithm based on a fast algorithm for nonequispaced Fourier transforms on the rotation group [14].

The outline of this paper is as follows: Section 2 starts by introducing the necessary notation including different parameterizations on the rotation group. We utilize the natural metric on $SO(3)$ and compute the distance between two rotations in the parameterization based on the tensor product $\mathbb{S}^2 \times \mathbb{S}^1$, cf. Theorem 2.2. Furthermore we prove in Theorem 2.4 that a sampling set on the rotation group constructed from q separated sampling sets on $\mathbb{S}^2$ and $\mathbb{S}^1$, which are also uniform, leads to q separated sampling sets on $SO(3)$ which are uniform as well. In Section 3 we develop efficient quadrature formulae on the rotation group. We prove a necessary condition on the mesh norm of the sampling set on $SO(3)$ in Theorem 3.3 for the existence of positive quadrature weights. In the following Section 4 we give some special sampling sets on $SO(3)$ which result in t-designs, i.e., all quadrature weights are equal. Finally we present in Section 5 an algorithm for computing the quadrature weights for scattered data based on the fast $SO(3)$ Fourier transform [14]. We test the algorithm on various sampling sets on $SO(3)$.

2 Uniform sampling sets

Throughout this paper we use the notation

$$\mathbb{S}^2 := \{\boldsymbol{x} \in \mathbb{R}^3 \mid \|\boldsymbol{x}\|_2 = 1\}, \qquad \mathbb{S}^1 := \{\omega \in [0, 2\pi)\}$$

for the two and one dimensional sphere. Furthermore for $\boldsymbol{x} \in \mathbb{S}^2$ we make use of the parameterization in spherical coordinates

$$\boldsymbol{x} = \boldsymbol{x}(\varphi, \theta) := (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^\top, \qquad (\varphi, \theta) \in [0, 2\pi) \times [0, \pi]. \tag{2.1}$$

Now, let $SO(3) := \left\{\boldsymbol{G} \in \mathbb{R}^{3\times3} : \boldsymbol{G}^\top = \boldsymbol{G}, \det \boldsymbol{G} = 1\right\}$ denote the rotation group. This manifold can be naturally parameterized by

$$\boldsymbol{R}(\boldsymbol{r}, \alpha) := (1 - \cos(\alpha))\boldsymbol{r}\boldsymbol{r}^\top + \begin{pmatrix} \cos(\alpha) & -z\sin(\alpha) & y\sin(\alpha) \\ z\sin(\alpha) & \cos(\alpha) & -x\sin(\alpha) \\ -y\sin(\alpha) & x\sin(\alpha) & \cos(\alpha) \end{pmatrix}, \tag{2.2}$$

with rotation axis $\boldsymbol{r} = (x, y, z)^\top \in \mathbb{S}^2$ and rotation angle $\alpha \in [0, \pi]$. Besides this we also consider the parameterization in Z-Y-Z Euler angles $(\varphi, \theta, \psi) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi)$ given by

$$\boldsymbol{R}_{\text{Euler}}(\varphi, \theta, \psi) := \boldsymbol{R}(\boldsymbol{e}_z, \varphi)\boldsymbol{R}(\boldsymbol{e}_y, \theta)\boldsymbol{R}(\boldsymbol{e}_z, \psi), \tag{2.3}$$

where $\boldsymbol{e}_z := (0, 0, 1)^\top$, $\boldsymbol{e}_y := (0, 1, 0)^\top$.

Besides these parameterizations we represent a rotation $\boldsymbol{G} \in SO(3)$ as an orthonormal basis in $\mathbb{R}^3$ consisting of its columns $(\boldsymbol{g}_0, \boldsymbol{g}_1, \boldsymbol{g}_2) = \boldsymbol{G}$. In order to get all possible orthonormal bases we proceed as follows, cf. [12]. At first, we are able to choose $\boldsymbol{g}_2 \in \mathbb{S}^2$. After this we can choose $\boldsymbol{g}_0 \in \mathbb{S}^2$, which has to satisfy $\boldsymbol{g}_0^\top \boldsymbol{g}_2 = 0$. Hence, $\boldsymbol{g}_0$ lies in a great circle of $\mathbb{S}^2$. Since $\boldsymbol{g}_1$ is uniquely determined by $\boldsymbol{g}_1 = \boldsymbol{g}_2 \times \boldsymbol{g}_0$, we can identify the rotation group $SO(3)$ with the tensor product $\mathbb{S}^2 \times \mathbb{S}^1$.

For a better illustration we introduce the position vector of $\boldsymbol{G}$ by

$$\vec{\boldsymbol{G}} := (\boldsymbol{g}_2, \boldsymbol{g}_0) = (\boldsymbol{G}\boldsymbol{e}_z, \boldsymbol{G}\boldsymbol{e}_x),$$

where $\boldsymbol{g}_2$ is the base point on $\mathbb{S}^2$ and $\boldsymbol{g}_0$ specifies a direction in the corresponding tangent plane, cf. Figure 2.1. Furthermore, we can simply define an action on the position vector by a rotation $\boldsymbol{H}$ via

$$\boldsymbol{H}\vec{\boldsymbol{G}} := (\boldsymbol{H}\boldsymbol{g}_2, \boldsymbol{H}\boldsymbol{g}_0) = \overrightarrow{\boldsymbol{H}\boldsymbol{G}}.$$

In order to obtain a parameterization, we compose $\boldsymbol{G}$ of two successive rotations. The first rotation $\boldsymbol{R}_1$ rotates $\boldsymbol{e}_z$ to $\boldsymbol{g}_2$ along a shortest geodesic between these points in $\mathbb{S}^2$, i.e. $\boldsymbol{g}_2 = \boldsymbol{R}_1\boldsymbol{e}_z$. If we parameterize $\boldsymbol{g}_2 = \boldsymbol{x}(\varphi, \theta)$ by spherical coordinates $(\varphi, \theta) \in [0, 2\pi) \times [0, \pi]$, cf. (2.1), the rotation $\boldsymbol{R}_1$ takes the form

$$\boldsymbol{R}_1(\varphi, \theta) := \boldsymbol{R}((-\sin(\varphi), \cos(\varphi), 0)^\top, \theta).$$

We remark, if $\theta = \pi$ there are no uniquely determined geodesics. The second rotation $\boldsymbol{R}_2$ has to hold $\boldsymbol{g}_2$ fixed. One possible form is

$$\boldsymbol{R}_2(\omega) := \boldsymbol{R}(\boldsymbol{g}_2, \omega), \qquad \text{for } \omega \in [0, 2\pi),$$

where ω is uniquely determined by $\boldsymbol{g}_0 = \boldsymbol{R}_2(\boldsymbol{g}_2, \omega)\boldsymbol{R}_1(\varphi, \theta)\boldsymbol{e}_x$. Hence, we can parameterize $SO(3)$ by

$$\boldsymbol{R}_{\text{Ortho}}(\varphi, \theta, \omega) := \boldsymbol{R}_2(\omega)\boldsymbol{R}_1(\varphi, \theta), \qquad \text{for } (\varphi, \theta, \omega) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi). \tag{2.4}$$

For a more convenient notation we define

$$\begin{aligned} \boldsymbol{R}_{\text{Ortho}}(\boldsymbol{x}, \omega) &:= \boldsymbol{R}_{\text{Ortho}}(\boldsymbol{x}(\varphi, \theta), \omega) := \boldsymbol{R}_{\text{Ortho}}(\varphi, \theta, \omega) \qquad \text{and} \\ \boldsymbol{R}_{\text{Euler}}(\boldsymbol{x}, \psi) &:= \boldsymbol{R}_{\text{Euler}}(\boldsymbol{x}(\varphi, \theta), \psi) := \boldsymbol{R}_{\text{Euler}}(\varphi, \theta, \psi), \end{aligned} \tag{2.5}$$

which reflects better the character of the tensor product $\mathbb{S}^2 \times \mathbb{S}^1 \cong SO(3)$. Furthermore we have the following correspondence, which enables us to carry forward all the following assertions from one parameterization to the other.

Lemma 2.1. *For $(\varphi, \theta, \psi) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi)$ the identity*

$$\boldsymbol{R}_{\text{Euler}}(\varphi, \theta, \psi) = \boldsymbol{R}_{\text{Ortho}}(\varphi, \theta, \varphi + \psi) \tag{2.6}$$

is valid.

In the following we introduce measures to describe the quality of sampling sets on $SO(3)$. Since we can identify $SO(3)$ in a natural way with $\mathbb{S}^2 \times \mathbb{S}^1$, it should be no surprise, that this involves such measures on $\mathbb{S}^2$ and $\mathbb{S}^1$, too.

Hence, we consider finite subsets $\mathcal{X}(\mathcal{M})$ of a metric space $(\mathcal{M}, \mathrm{d}_{\mathcal{M}})$ with metric $\mathrm{d}_{\mathcal{M}}$. Then the separation distance is given by

$$q(\mathcal{X}(\mathcal{M})) := \min_{\boldsymbol{G}_i \neq \boldsymbol{G}_j \in \mathcal{X}(\mathcal{M})} \mathrm{d}_{\mathcal{M}}(\boldsymbol{G}_i, \boldsymbol{G}_j)$$

and the mesh norm by

$$\delta(\mathcal{X}(\mathcal{M})) := 2 \max_{\boldsymbol{H} \in \mathcal{M}} \min_{\boldsymbol{G}_i \in \mathcal{X}(\mathcal{M})} \mathrm{d}_{\mathcal{M}}(\boldsymbol{H}, \boldsymbol{G}_i).$$

Furthermore, we say the sampling set $\mathcal{X}(\mathcal{M})$ is uniform of order L if the condition

$$L(\mathcal{X}(\mathcal{M})) := \frac{\delta(\mathcal{X}(\mathcal{M}))}{q(\mathcal{X}(\mathcal{M}))} \leq L$$

is satisfied, where $L(\mathcal{X}(\mathcal{M}))$ denotes the uniformity of the sampling set $\mathcal{X}(\mathcal{M})$. We call a sequence of sampling sets $\{\mathcal{X}_k(\mathcal{M})\}_{k \in \mathbb{N}}$ with mesh norms $\delta(\mathcal{X}_k(\mathcal{M})) \to 0$, for $k \to \infty$, uniform of order L, if

$$\sup_{k \in \mathbb{N}} L_{\mathcal{X}_k(\mathcal{M})} \leq L.$$

Such sequences are for example required for assertions of probabilistic Marcinkiewicz-Zygmund inequalities, cf. [3, Theorem 3.5]. Furthermore these are useful for approximation problems with positive definite basis functions in order to keep the approximation error and the condition number of the corresponding interpolation matrix small, cf. [16, 18].

For $\mathcal{M} = \mathbb{S}^2$, $\mathcal{M} = \mathbb{S}^1$ the natural metrics are given by

$$\begin{aligned} \mathrm{d}_{\mathbb{S}^2}(\boldsymbol{x}_1, \boldsymbol{x}_2) &:= \arccos \boldsymbol{x}_1^\top \boldsymbol{x}_2, && \text{for } \boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{S}^2 \\ \mathrm{d}_{\mathbb{S}^1}(\omega_1, \omega_2) &:= \arccos \cos(\omega_1 - \omega_2), && \text{for } \omega_1, \omega_2 \in [0, 2\pi). \end{aligned}$$

A (left and right) translation invariant metric on $SO(3)$ is naturally given by

$$\mathrm{d}_{SO(3)}(\boldsymbol{G}_1, \boldsymbol{G}_2) := \alpha(\boldsymbol{G}_1 \boldsymbol{G}_2^\top) := \arccos \left(\frac{1}{2} (\operatorname{trace} \boldsymbol{G}_1 \boldsymbol{G}_2^\top - 1) \right), \qquad \boldsymbol{G}_1, \boldsymbol{G}_2 \in SO(3). \tag{2.7}$$

Using the parameterization (2.2) this reads as, cf. [20, p. 34],

$$\mathrm{d}_{SO(3)}(\boldsymbol{R}(\boldsymbol{r}_1, \omega_1), \boldsymbol{R}(\boldsymbol{r}_2, \omega_2)) = 2 \arccos \left(\left| \boldsymbol{r}_1^\top \boldsymbol{r}_2 \sin \frac{\omega_1}{2} \sin \frac{\omega_2}{2} + \cos \frac{\omega_1}{2} \cos \frac{\omega_2}{2} \right| \right),$$

which is related to the spherical cosine rule

$$\cos c = \cos \gamma \sin a \sin b + \cos a \cos b$$

with angle $\gamma = \mathrm{d}_{\mathbb{S}^2}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and sides $a = \omega_1/2$, $b = \omega_2/2, c = \mathrm{d}_{SO(3)}(\boldsymbol{G}_1, \boldsymbol{G}_2)/2$. In particular, if the rotation axes $\boldsymbol{r}_1, \boldsymbol{r}_2 \in \mathbb{S}^2$ are perpendicular the distance satisfies the spherical Pythagorean

$$\cos \frac{\mathrm{d}_{SO(3)}(\boldsymbol{R}(\boldsymbol{r}_1, \omega_1), \boldsymbol{R}(\boldsymbol{r}_2, \omega_2))}{2} = \left| \cos \frac{\omega_1}{2} \cos \frac{\omega_2}{2} \right|.$$

This is useful for the parameterization by $\boldsymbol{R}_{\mathrm{Ortho}}(\varphi, \theta, \omega)$, cf. equation (2.4), where the rotation axes of the consecutive rotations $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are perpendicular. There, we obtain the relation

$$\cos \frac{\alpha(\boldsymbol{R}_{\mathrm{Ortho}}(\varphi, \theta, \omega))}{2} = \left| \cos \frac{\theta}{2} \cos \frac{\omega}{2} \right|. \tag{2.8}$$

Theorem 2.2. *The distance between two rotations, cf.* (2.5),

$$\begin{aligned} \boldsymbol{G}_1 &:= \boldsymbol{R}_{\mathrm{Ortho}}(\boldsymbol{x}(\varphi_1, \theta_1), \omega_1) = \boldsymbol{R}_2(\omega_1) \boldsymbol{R}_1(\varphi_1, \theta_1), \\ \boldsymbol{G}_2 &:= \boldsymbol{R}_{\mathrm{Ortho}}(\boldsymbol{x}(\varphi_2, \theta_2), \omega_2) = \boldsymbol{R}_2(\omega_2) \boldsymbol{R}_2(\varphi_2, \theta_2) \end{aligned}$$

satisfies

$$\mathrm{d}_{SO(3)}(\boldsymbol{G}_1, \boldsymbol{G}_2) = 2 \arccos \left| \cos \frac{\mathrm{d}_{\mathbb{S}^2}(\boldsymbol{x}(\varphi_1, \theta_1), \boldsymbol{x}(\varphi_2, \theta_2))}{2} \cos \frac{\omega_2 - \omega_1 - A}{2} \right|, \tag{2.9}$$

where A is the area of the spherical triangle Δ spanned by the points

$$\boldsymbol{e}_z,\ \boldsymbol{x}(\varphi_1, \theta_1) = \boldsymbol{G}_1 \boldsymbol{e}_z,\ \boldsymbol{x}(\varphi_2, \theta_2) = \boldsymbol{G}_2 \boldsymbol{e}_z,$$

and sides

$$s_1 := \{\boldsymbol{R}_1(\varphi_1, t)\boldsymbol{e}_z \mid t \in [0, \theta_1]\},$$
$$s_2 := \{\boldsymbol{R}_1(\varphi_2, t)\boldsymbol{e}_z \mid t \in [0, \theta_2]\}$$

with interior angle $\alpha := \varphi_2 - \varphi_1$ *at* $\boldsymbol{e}_z$*. If it is* $\boldsymbol{x}(\varphi_1, \theta_1) = -\boldsymbol{x}(\varphi_2, \theta_2)$*, then the triangle* Δ*, respectively the area* A*, is not uniquely determined.*

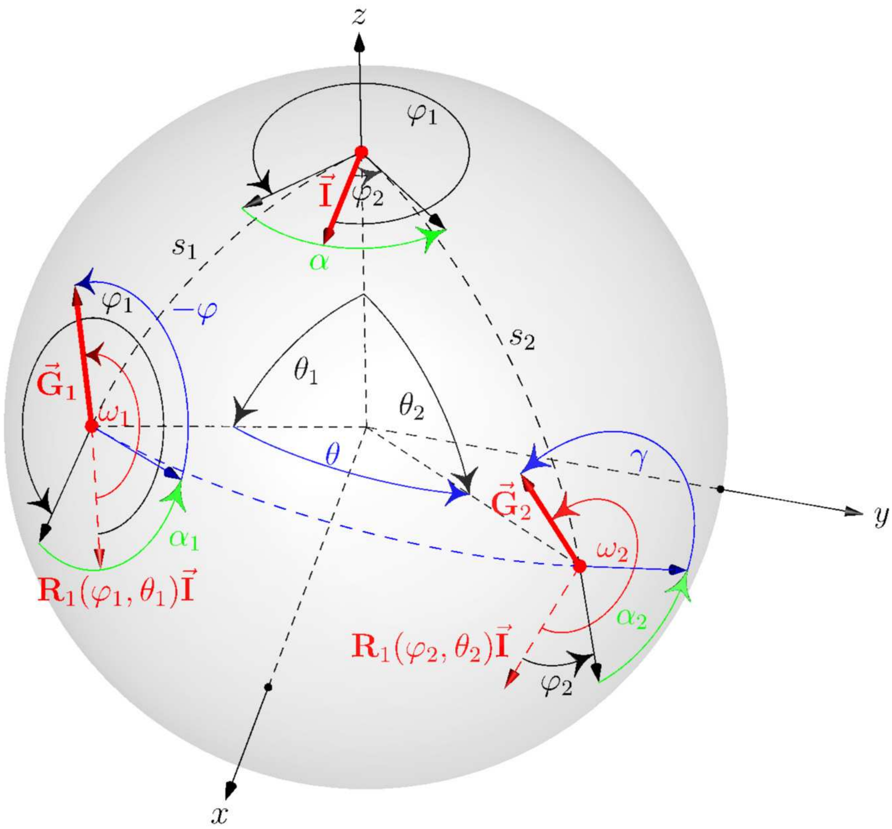

Figure 2.1: Relations between the rotations $\boldsymbol{R}_{\text{Ortho}}(\varphi_1, \theta_1, \omega_1) = \boldsymbol{R}_2(\omega_1)\boldsymbol{R}_1(\varphi_1, \theta_1)$ and $\boldsymbol{R}_{\text{Ortho}}(\varphi_2, \theta_2, \omega_2) = \boldsymbol{R}_2(\omega_2)\boldsymbol{R}_1(\varphi_2, \theta_2)$ in terms of spherical trigonometry, by the corresponding position vectors $\vec{\boldsymbol{G}}_1$ and $\vec{\boldsymbol{G}}_2$.

Proof. By equation (2.8) we have to specify the angles θ and ω of the rotation, cf. (2.4),

$$\boldsymbol{R}_{\text{Ortho}}(\varphi, \theta, \omega) = \boldsymbol{R}_{\text{Ortho}}(\varphi_1, \theta_1, \omega_1)\boldsymbol{R}_{\text{Ortho}}^{\top}(\varphi_2, \theta_2, \omega_2).$$

Therefore, in Figure 2.1 we illustrate the position vectors

$$\vec{\boldsymbol{I}}, \qquad \vec{\boldsymbol{G}}_1 = \boldsymbol{R}_2(\omega_1)\boldsymbol{R}_1(\varphi_1, \theta_1)\vec{\boldsymbol{I}}, \qquad \vec{\boldsymbol{G}}_2 = \boldsymbol{R}_2(\omega_2)\boldsymbol{R}_1(\varphi_2, \theta_2)\vec{\boldsymbol{I}}.$$

Then, we regard the rotation $\boldsymbol{G}_2\boldsymbol{G}_1^{\top}$ as the action on $\vec{\boldsymbol{G}}_1$, which results in $\vec{\boldsymbol{G}}_2 = \boldsymbol{G}_2\boldsymbol{G}_1^{\top}\vec{\boldsymbol{G}}_1$. Hence, the rotation angle θ of $\boldsymbol{R}_{\text{Ortho}}(\varphi, \theta, \omega)$ is simply the spherical distance $\mathrm{d}_{\mathbb{S}^2}(\boldsymbol{G}_1\boldsymbol{e}_z, \boldsymbol{G}_2\boldsymbol{e}_z)$ between the base points of $\vec{\boldsymbol{G}}_1$ and $\vec{\boldsymbol{G}}_2$. We remark if $\theta = \pi$ there are no unique geodesics from one base point to the other. But since the distance of the rotations $\boldsymbol{G}_1$ and $\boldsymbol{G}_2$ are already π, there is no need to specify ω. Of course, in this case ω depends on the chosen geodesic, hence on the angle φ.

If we define α_1 and α_2 to be the adjacent and opposite angle of the interior angle of the triangle Δ at the base point of $\vec{\boldsymbol{G}}_1$ and $\vec{\boldsymbol{G}}_2$, respectively, we obtain

$$\omega = \gamma - (-\varphi) = (\omega_2 - \varphi_2 - \alpha_2) - (\omega_1 - \varphi_1 - \alpha_1) = \omega_2 - \omega_1 - (\alpha_2 - \alpha_1 + \alpha).$$

The assertion (2.9) follows, since the angles α_1, α_2 and α are related to the area A of the triangle Δ. For example, if $\sin(\varphi_2 - \varphi_1) \geq 0$ we can express the area A by the spherical excess E, of the spherical triangle spanned by the base points of $\vec{\boldsymbol{I}}$, $\vec{\boldsymbol{G}}_1$, $\vec{\boldsymbol{G}}_2$, via

$$A = E = \alpha_2 - \alpha_1 + \alpha.$$

The other cases, where $\sin(\varphi_2 - \varphi_1) \leq 0$ or $\boldsymbol{x}(\varphi_i, \theta_i) = -\boldsymbol{e}_z$, $i \in \{1, 2\}$, follow similarly. ■

By virtue of the Pythagorean-like relation of Theorem 2.2 we obtain uniform sampling sets on $SO(3)$ easily, if we use uniform sampling sets on $\mathbb{S}^2$ and $\mathbb{S}^1$. For this we need the following Lemma.

Lemma 2.3. *For $s, t \in \left[0, \frac{\pi}{2}\right]$ the following inequality is valid*

$$\cos s \cos t \geq \cos \sqrt{s^2 + t^2}. \tag{2.10}$$

Proof. At first, we use the well known facts, that

$$\begin{aligned} &(\tan x - x)\cos x > 0, && \text{for } x \in \left(0, \frac{\pi}{2}\right), \\ &(\tan x - x)\cos x = \sin x - x\cos x \geq -x\cos x > 0, && \text{for } x \in \left(\frac{\pi}{2}, \pi\right], \end{aligned}$$

and obtain for the second derivative of $\cos\sqrt{x}$ the estimate

$$(\cos\sqrt{x})'' = \frac{\tan\sqrt{x} - \sqrt{x}}{4\sqrt{x^3}} \cos\sqrt{x} > 0, \qquad \text{for } x \in [0, \pi^2].$$

Hence, the function $\cos\sqrt{x}$ is convex for $x \in [0, \pi^2]$ and it follows for $u, v \in [0, \pi]$, by Jensen's inequality, the relation

$$\frac{1}{2}(\cos u + \cos v) = \frac{1}{2}(\cos\sqrt{u^2} + \cos\sqrt{v^2}) \geq \cos\sqrt{\frac{1}{2}(u^2 + v^2)}. \tag{2.11}$$

Now, we let $u := |s - t|$, $v = |s + t|$. Then (2.11) yields the assertion

$$\cos s \cos t = \frac{1}{2}(\cos(s-t) + \cos(s+t)) = \frac{1}{2}(\cos u + \cos v) \geq \cos\sqrt{\frac{1}{2}(u^2 + v^2)} = \cos\sqrt{s^2 + t^2},$$

by using the addition theorem. ■

Theorem 2.4. *Let the sampling sets*

$$\begin{aligned} \mathcal{X}(\mathbb{S}^2) &:= \{\boldsymbol{x}(\varphi_i,\theta_i) \mid i = 0,\dots,M_1-1\} \\ \mathcal{X}(\mathbb{S}^1) &:= \{\omega_j \mid j = 0,\dots,M_2-1\} \end{aligned}$$

of uniformity $L(\mathcal{X}(\mathbb{S}^2)), L(\mathcal{X}(\mathbb{S}^1))$ *and with separation distance* $q := q(\mathcal{X}(\mathbb{S}^2)) = q(\mathcal{X}(\mathbb{S}^1))$ *be given. Then, for arbitrary offsets* $c_i \in \mathbb{S}^1$, $i = 0,\dots,M_1-1$, *the sampling set, cf.* (2.5),

$$\mathcal{X}(SO(3)) := \{\boldsymbol{G}_{i,j} := \boldsymbol{R}_{\text{Ortho}}(\boldsymbol{x}(\varphi_i,\theta_i), \omega_j + c_i) \mid i = 0,\dots,M_1-1,\ j = 0,\dots,M_2-1\} \tag{2.12}$$

has separation distance $q(\mathcal{X}(SO(3))) = q$ *and uniformity*

$$L(\mathcal{X}(SO(3))) \le \sqrt{L(\mathcal{X}(\mathbb{S}^2))^2 + L(\mathcal{X}(\mathbb{S}^1))^2}. \tag{2.13}$$

Proof. From equation (2.9) we infer for arbitrary pairs of rotations $\boldsymbol{G}_{i,j}, \boldsymbol{G}_{k,l}$, $i,k = 0,\dots,M_1-1$, $j,l = 0,\dots,M_2-1$ the relations

$$\mathrm{d}_{SO(3)}(\boldsymbol{G}_{i,j}, \boldsymbol{G}_{k,l}) \begin{cases} = \mathrm{d}_{\mathbb{S}^1}(\omega_j, \omega_l), & i = k, \\ \ge \mathrm{d}_{\mathbb{S}^2}(\boldsymbol{x}(\varphi_i,\theta_i), \boldsymbol{x}(\varphi_k,\theta_k)), & i \ne k. \end{cases}$$

Hence we infer that the the separation distance of the sampling set $\mathcal{X}(SO(3))$ satisfies $q(\mathcal{X}(SO(3))) = q$. Furthermore we can estimate the uniformity using Theorem 2.2 by

$$\begin{aligned} L(\mathcal{X}(SO(3))) &= \frac{\delta(\mathcal{X}(SO(3)))}{q(\mathcal{X}(SO(3)))} \\ &\le \frac{4\arccos\left|\cos\frac{\delta(\mathcal{X}(\mathbb{S}^2))}{4}\cos\frac{\delta(\mathcal{X}(\mathbb{S}^1))}{4}\right|}{q(\mathcal{X}(SO(3)))} \\ &= \frac{4}{q}\arccos\left(\cos\left(\frac{q}{4}L(\mathcal{X}(\mathbb{S}^2))\right)\cos\left(\frac{q}{4}L(\mathcal{X}(\mathbb{S}^1))\right)\right). \end{aligned} \tag{2.14}$$

In order to get the desired result we use the inequality of Lemma 2.3. There, we put $s := qL(\mathcal{X}(\mathbb{S}^2))/4, t := qL(\mathcal{X}(\mathbb{S}^1))/4 \in [0,\pi/2]$ into (2.10). Now we insert (2.10) in (2.14), bearing in mind the monotony of the arccosine, and obtain the assertion

$$\begin{aligned} L(\mathcal{X}(SO(3))) &\le \frac{4}{q}\arccos\left(\cos\left(\frac{q}{4}L(\mathcal{X}(\mathbb{S}^2))\right)\cos\left(\frac{q}{4}L(\mathcal{X}(\mathbb{S}^1))\right)\right) \\ &\le \sqrt{L(\mathcal{X}(\mathbb{S}^2))^2 + L(\mathcal{X}(\mathbb{S}^1))^2}. \end{aligned}$$

■

Remark 2.5. Let the sampling set $\mathcal{X}(SO(3))$ be constructed as in Theorem 2.4.If the separation distances $q(\mathcal{X}(\mathbb{S}^2))$ and $q(\mathcal{X}(\mathbb{S}^1))$ are not equal in the construction (2.12), we obtain for $i \neq k$ that

$$\mathrm{d}_{SO(3)}(\boldsymbol{G}_{i,j}, \boldsymbol{G}_{k,l}) \geq q(\mathcal{X}(\mathbb{S}^2)),$$

but for $j \neq l$ we only obtain

$$\mathrm{d}_{SO(3)}(\boldsymbol{G}_{i,j}, \boldsymbol{G}_{k,l}) \geq \min\left(q(\mathcal{X}(\mathbb{S}^2)), q(\mathcal{X}(\mathbb{S}^2))\right).$$

□

3 Quadrature formulae

For measurable functions $f : SO(3) \to \mathbb{C}$ the normalized Haar integral reads in Euler angle parameterization as

$$\int_{SO(3)} f(\boldsymbol{G})\mathrm{d}\mu(\boldsymbol{G}) = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} f(\varphi,\theta,\psi)\sin(\theta)\mathrm{d}\psi\mathrm{d}\theta\mathrm{d}\varphi.$$

A function only depending on the rotation angle $\alpha = \alpha(\boldsymbol{G})$, cf. (2.7), is called conjugate invariant (or central) and the above integral simplifies to

$$\int_{SO(3)} f(\boldsymbol{G})\mathrm{d}\mu(\boldsymbol{G}) = \frac{2}{\pi}\int_0^{\pi} f(\alpha)\sin^2\left(\frac{\alpha}{2}\right)\mathrm{d}\alpha. \tag{3.1}$$

For the space $L^2(SO(3)) := \{f : SO(3) \to \mathbb{C} \mid \int_{SO(3)} |f(\boldsymbol{G})|^2 \,\mathrm{d}\mu(\boldsymbol{G})\}$ of square integrable functions over $SO(3)$ the standard basis is given by the Wigner D-functions $D_l^{m,n}$ of degree $l \in \mathbb{N}_0$ and orders $m, n = -l, \ldots, l$. In Euler angle parameterization these can be represented in the form

$$D_l^{m,n}(\varphi,\theta,\psi) = \mathrm{e}^{-\mathrm{i}m\varphi} d_l^{m,n}(\theta)\mathrm{e}^{-\mathrm{i}n\psi}, \tag{3.2}$$

where $d_l^{m,n}$ denote the Wigner d-functions, cf. [20, p. 76 et seqq]. Furthermore, we have the following relation to the spherical harmonics Y_l^m, cf. [20, p. 113],

$$(-1)^m\sqrt{\frac{4\pi}{2l+1}}Y_l^{-m}(\varphi,\theta) = \mathrm{e}^{-\mathrm{i}m\varphi}d_l^{m,0}(\theta). \tag{3.3}$$

Functions $f \in L^2(SO(3))$ with finite expansion in Wigner D-functions are called polynomials on $SO(3)$ and we define the space $\Pi_N(SO(3)) := \mathrm{span}\{D_l^{m,n} \mid l = 0, \ldots, N;\ m, n = -l, \ldots, l\}$ of polynomials with degree at most N with $\dim(\Pi_N(SO(3))) = d_N = (2N+1)(2N+2)(2N+3)/6$. . We say a quadrature rule

$$Q(SO(3)) := \{(\boldsymbol{G}_i, w_i) \mid i = 0, \ldots, M-1\}$$

with sampling nodes $\boldsymbol{G}_i \in SO(3)$ and quadrature weights $w_i \in \mathbb{C}$ has degree of exactness N, if for all polynomials $f \in \Pi_N(SO(3))$ the relation

$$\sum_{i=0}^{M-1} w_i f(\boldsymbol{G}_i) = \int_{SO(3)} f(\boldsymbol{G}) \mathrm{d}\mu \tag{3.4}$$

is valid. To estimate the quality of such quadrature rules we introduce, similar as on $\mathbb{S}^2$ [10, 8], the efficiency

$$E(Q(SO(3))) := \frac{(2N+1)(2N+2)(2N+3)}{24M} = \frac{d_N}{4M}, \tag{3.5}$$

and call a quadrature efficient, if $E(Q(SO(3))) \approx 1$. The idea behind this definition is, for quadrature rules with degree of exactness N we have to satisfy d_N equalities, where we can choose $4M$ free parameters, $3M$ for the coordinates of the sampling nodes and M for the weights. Moreover, we define the efficiencies

$$E(Q(\mathbb{S}^2)) := \frac{(N+1)^2}{3M_1}, \qquad E(Q(\mathbb{S}^1)) := \frac{2N+1}{2M_2} \tag{3.6}$$

for quadrature rules $Q(\mathbb{S}^2)$ and $Q(\mathbb{S}^1)$ on $\mathbb{S}^2$ and $\mathbb{S}^1$, respectively. We remark that Gauss quadrature on $\mathbb{S}^1$ is efficient with $E(Q(\mathbb{S}^1)) \to 1$ as $N \to \infty$, whereas the efficiency of the Gauss-Legendre quadrature on $\mathbb{S}^2$ is only $E(Q(\mathbb{S}^2)) \to 2/3$ as $N \to \infty$. For efficient quadratures on the sphere $\mathbb{S}^2$ we refer to [10, 8, 13]. The quadrature rule on $SO(3)$ based on the Clenshaw-Curtis quadrature, cf. [14, Section 3.5] has only an efficency $E(Q(SO(3))) \to 1/24$ as $N \to \infty$.

Lemma 3.1. *For $N \in \mathbb{N}_0$, let a quadrature rule $Q(\mathbb{S}^2)$ on the sphere $\mathbb{S}^2$ with degree of exactness N by the sampling set $\mathcal{X}(\mathbb{S}^2) := \{\boldsymbol{x}(\varphi_i, \theta_i) : i = 0, \ldots, M_1 - 1\}$ with corresponding weights $w_i(\mathbb{S}^2)$, $i = 0, \ldots, M_1 - 1$, be given, i.e.,*

$$\frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} Y_k^m(\varphi, \theta) \sin(\theta) \mathrm{d}\theta \mathrm{d}\varphi = \sum_{i=0}^{M_1-1} w_i(\mathbb{S}^2) Y_k^m(\varphi_i, \theta_i), \quad 0 \le k \le N, |m| \le k. \tag{3.7}$$

Furthermore let a quadrature rule $Q(\mathbb{S}^1)$ on $\mathbb{S}^1$ with degree of exactness N by the sampling set $\mathcal{X}(\mathbb{S}^1) := \{\psi_j : j = 0, \ldots, M_2 - 1\}$ with corresponding weights $w_j(\mathbb{S}^1)$, $j = 0, \ldots, M_2 - 1$, be given, i.e.,

$$\frac{1}{2\pi} \int_0^{2\pi} \mathrm{e}^{\mathrm{i}n\psi} \mathrm{d}\psi = \sum_{j=0}^{M_2-1} w_j(\mathbb{S}^1) \mathrm{e}^{\mathrm{i}n\psi_j}, \quad |n| \le N. \tag{3.8}$$

Then, we obtain for arbitrary offsets $c_i \in \mathbb{R}$, $i = 0, \ldots, M_1 - 1$, a quadrature rule Q on the rotation group

$$\mathcal{X}(SO(3)) := \{\boldsymbol{R}_{\mathrm{Euler}}(\boldsymbol{x}(\varphi_i, \theta_i), \psi_j + c_i) : i = 0, \ldots, M_1 - 1,\ j = 0, \ldots, M_2 - 1\} \tag{3.9}$$

with corresponding weights

$$w_{i,j}(SO(3)) := w_i(\mathbb{S}^2)w_j(\mathbb{S}^1), \quad i=0,\ldots,M_1-1,\ j=0,\ldots,M_2-1. \tag{3.10}$$

That is, we integrate exactly all polynomials $f \in \Pi_N(SO(3))$ by the formula

$$\int_{SO(3)} f(\boldsymbol{G})\mathrm{d}\mu(\boldsymbol{G}) = \sum_{i=0}^{M_1-1}\sum_{j=0}^{M_2-1} w_{i,j}(SO(3)) f\left(\boldsymbol{R}_{\mathrm{Euler}}(\boldsymbol{x}(\varphi_i,\theta_i),\psi_j+c_i)\right). \tag{3.11}$$

Proof. In order to show the assertion it is sufficient to confirm equation (3.11) for all Wigner D-functions $D_l^{m,n} \in \Pi_N(SO(3))$. For $1 \le |n| \le N$, and $l = \max\{|m|, |n|\},\ldots,N$ we obtain due to the quadrature rule on $\mathbb{S}^1$ and the representation (3.2) of the Wigner D-functions the relation

$$\begin{aligned}
&\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} D_l^{m,n}(\varphi,\theta,\psi)\mathrm{d}\psi\sin(\theta)\mathrm{d}\theta\mathrm{d}\varphi\\
=&\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} \mathrm{e}^{-\mathrm{i}m\varphi} d_l^{m,n}(\theta)\sin(\theta)\mathrm{d}\theta\mathrm{d}\varphi\frac{1}{2\pi}\int_0^{2\pi}\mathrm{e}^{-\mathrm{i}n\psi}\mathrm{d}\psi\\
=&0\\
=&\sum_{i=0}^{M_1-1} w_i(\mathbb{S}^2)\mathrm{e}^{-\mathrm{i}m\varphi_i} d_l^{m,n}(\theta_i)\mathrm{e}^{-\mathrm{i}nc_i}\sum_{j=0}^{M_2-1} w_j(\mathbb{S}^1)\mathrm{e}^{-\mathrm{i}n\psi_j}\\
=&\sum_{i=0}^{M_1-1}\sum_{j=0}^{M_2-1} w_{i,j}(SO(3)) D_l^{m,n}(\varphi_i,\theta_i,c_i+\psi_j).
\end{aligned} \tag{3.12}$$

If $n=0$ we obtain for $l = |m|,\ldots,N$ due to the quadrature rule on $\mathbb{S}^1$ and $\mathbb{S}^2$ and relation (3.3) the equation

$$\begin{aligned}
&\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} D_l^{m,0}(\varphi,\theta,\psi)\mathrm{d}\psi\sin(\theta)\mathrm{d}\theta\mathrm{d}\varphi\\
=&\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}(-1)^m\sqrt{\frac{4\pi}{2l+1}}Y_l^{-m}(\varphi,\theta)\sin(\theta)\mathrm{d}\theta\mathrm{d}\varphi\frac{1}{2\pi}\int_0^{2\pi}\mathrm{e}^{0\cdot\psi}\mathrm{d}\psi\\
=&\sum_{i=0}^{M_1-1} w_i(\mathbb{S}^2)(-1)^m\sqrt{\frac{4\pi}{2l+1}}Y_l^{-m}(\varphi_i,\theta_i)\mathrm{e}^{0\cdot c_i}\sum_{j=0}^{M_2-1} w_j(\mathbb{S}^1)\mathrm{e}^{0\cdot\psi_j}\\
=&\sum_{i=0}^{M_1-1}\sum_{j=0}^{M_2-1} w_{i,j}(SO(3)) D_l^{m,0}(\varphi_i,\theta_i,c_i+\psi_j).
\end{aligned} \tag{3.13}$$

■

Remark 3.2. We note, that by constructing quadrature formulae in the way of Lemma 3.1 we can get efficient quadrature rules Q on $SO(3)$ simply by using efficient quadrature rules Q_1 and Q_2 of $\mathbb{S}^2$ and $\mathbb{S}^1$, respectively. Since, we have

$$E(Q(SO(3))) = \frac{(2N+1)(2N+2)(2N+3)}{24M_1M_2} \geq \frac{(N+1)^2}{3M_1}\frac{(2N+1)}{2M_2} = E(Q(\mathbb{S}^2))E(Q(\mathbb{S}^1)).$$

□

D. Schmid proved recently a sufficient condition on the mesh norm $\delta(\mathcal{X}(SO(3))$ such that on obtains positive quadrature rules on $SO(3)$, cf. [19, Theorem 4.27]. This result based on a L^p-Marcinkiewicz-Zygmund inequalities for scattered nodes on $SO(3)$, cf. [17] and a result of H.N. Mhaskar, F.J. Narcowich and J.D. Ward [11, Proposition 4.1]. More precisely, we can construct positive quadrature rules Q from a sampling set $\mathcal{X}(SO(3))$ if the condition

$$\delta(\mathcal{X}(SO(3)) \leq \frac{1}{924N},$$

is satisfied. It is well know that in praxis one observe a much better behavior. In contrast we proof a necessary condition and show in our numerical examples that very closed to this condition we are still able to compute positive quadrature weights, cf. Example 5.5.

Theorem 3.3. *Let the sampling set* $\mathcal{X}_N = \{\boldsymbol{G}_0, \ldots, \boldsymbol{G}_{M-1}\} \subset SO(3)$ *supports nonnegative quadrature weights* w_k, $k = 0, \ldots, M-1$, *integrating exactly all polynomials in* $\Pi_N(SO(3))$, $N \in \mathbb{N}$, *then the mesh norm satisfies*

$$\delta(\mathcal{X}_N(SO(3))) \leq \frac{4\pi}{N+2}. \tag{3.14}$$

Proof. We follow the ideas of the proof of [15, Theorem 6.21 (Reimer, Yudin)]. If there are zero weights w_k, we can delete the corresponding sampling nodes $\boldsymbol{G}_k$ and the mesh norm of the new sampling set does not decrease. Therefore we can assume that

$$w_k > 0, \ k = 0, \ldots, M-1.$$

We consider the function

$$p_N(x) := \frac{U_{N+1}^2(x)}{x^2 - \cos^2 \frac{\pi}{N+2}},$$

where $U_{N+1} \in \Pi_{N+1}([-1,1])$ is the $(N+1)$-th Chebyshev polynomial of second kind. Since $\pm\cos\frac{\pi}{N+2}$ are zeros of U_{N+1}, the function p_N is an even polynomial of degree $2N$. Hence, p_N can be expanded in even Chebyshev polynomials U_{2l}, $l = 0, \ldots, N$, and due to the addition theorem, cf. [20, p. 89],

$$U_{2l}\left(\cos\frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{H})}{2}\right) = \sum_{m,n=-l}^{l} \overline{D_l^{m,n}(\boldsymbol{G})} D_l^{m,n}(\boldsymbol{H}), \qquad \boldsymbol{G}, \boldsymbol{H} \in SO(3),$$

we infer for every $\boldsymbol{G} \in SO(3)$ that $P_N(\boldsymbol{G}, \cdot) \in \Pi_N(SO(3))$ with the kernel function

$$P_N(\boldsymbol{G},\boldsymbol{H}) := p_N\left(\cos\frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{H})}{2}\right).$$

Let $\boldsymbol{G} \in SO(3)$ be arbitrary, then we have by the orthogonality of the Chebyshev polynomials to the weight $\sqrt{1-x^2}$ the following integral, cf. (3.1),

$$\begin{aligned}\int_{SO(3)} P_N(\boldsymbol{G},\boldsymbol{H})\mathrm{d}\mu(\boldsymbol{H}) &= \frac{2}{\pi}\int_0^{\pi} p_N\left(\cos\frac{\alpha}{2}\right)\sin^2\left(\frac{\alpha}{2}\right)\mathrm{d}\alpha \\ &= \frac{2}{\pi}\int_{-1}^{1} U_{N+1}(x)\frac{U_{N+1}(x)}{x^2-\cos^2\frac{\pi}{N+2}}\sqrt{1-x^2}\mathrm{d}x = 0.\end{aligned} \tag{3.15}$$

Now, assume that the assumption (3.14) is false and we have $\delta(\mathcal{X}_N(SO(3))) > \frac{4\pi}{N+2}$. Then, there exists a $\boldsymbol{G}_M \in SO(3)$ with $\mathrm{d}(\boldsymbol{G}_M,\boldsymbol{G}_k) > \frac{2\pi}{N+2}$ for all $k=0,\dots,M-1$. Furthermore there exists a neighborhood $B_\varepsilon(\boldsymbol{G}_M) \subset SO(3)$ with $\varepsilon > 0$ such that

$$0 \le \cos\frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{G}_k)}{2} < \cos\frac{\pi}{N+2} \quad \text{for all } \boldsymbol{G} \in B_\varepsilon(\boldsymbol{G}_M) \text{ and } k=0,\dots,M-1.$$

Evaluating the integral (3.15) via the quadrature formula, we obtain for all $\boldsymbol{G} \in B_\varepsilon(\boldsymbol{G}_M)$ the relation

$$0 = \sum_{k=0}^{M-1} w_k P_N(\boldsymbol{G},\boldsymbol{G}_k) = \sum_{k=0}^{M-1} w_k \frac{U_{N+1}^2\left(\cos\frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{G}_k)}{2}\right)}{\cos^2\left(\frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{G}_k)}{2}\right)-\cos^2\frac{\pi}{N+2}},$$

which implies by using $\cos^2\left(\frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{G}_k)}{2}\right)-\cos^2\frac{\pi}{N+2} < 0 < w_k$ that

$$U_{N+1}\left(\cos\frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{G}_k)}{2}\right) = 0 \quad \text{for all } \boldsymbol{G} \in B_\varepsilon(\boldsymbol{G}_M) \text{ and } k=0,\dots,M-1. \tag{3.16}$$

In particular we have $\boldsymbol{G}_0 \neq \boldsymbol{G}_M$. So the rotation $\boldsymbol{G}_0\boldsymbol{G}_M^\top$ has a rotation axis $\boldsymbol{r} \in \mathbb{S}^2$ and we can parameterize a geodesic from $\boldsymbol{G}_M$ to $\boldsymbol{G}_0$ by

$$\boldsymbol{G}(t) := \boldsymbol{R}(\boldsymbol{r},t)\boldsymbol{G}_M,\ t \in [0,\mathrm{d}(\boldsymbol{G}_M,\boldsymbol{G}_0)]$$

with distance

$$\mathrm{d}(\boldsymbol{G}(t),\boldsymbol{G}_0) = \alpha(\boldsymbol{G}_0\boldsymbol{G}_M^\top\boldsymbol{R}(\boldsymbol{r},t)^\top) = \alpha(\boldsymbol{R}(\boldsymbol{r},\mathrm{d}(\boldsymbol{G}_M,G_0))\boldsymbol{R}(\boldsymbol{r},-t)) = \mathrm{d}(\boldsymbol{G}_M,\boldsymbol{G}_0)-t.$$

Hence for $t \in [0,\varepsilon]$ we obtain due to

$$\mathrm{d}(\boldsymbol{G}(t),\boldsymbol{G}_M) = \alpha(\boldsymbol{R}(\boldsymbol{r},t)^\top) = t$$

that $\boldsymbol{G}(t) \in B_\varepsilon(\boldsymbol{G}_M)$ and infer from (3.16) the relation

$$U_{N+1}\left(\cos\frac{\mathrm{d}(\boldsymbol{G}(t),\boldsymbol{G}_0)}{2}\right) = U_{N+1}\left(\cos\frac{\mathrm{d}(\boldsymbol{G}_M,\boldsymbol{G}_0)-t}{2}\right) = 0,\ t \in [0,\varepsilon], \tag{3.17}$$

which contradicts $U_{N+1} \not\equiv 0$. So our assumption $\delta(\mathcal{X}_N(SO(3))) > \frac{4\pi}{N+2}$ was false and (3.14) is valid. ■

In the following we consider only quadrature nodes $\mathcal{X}(SO(3))$ constructed as in Lemma 3.1. We already know from [15, Theorem 6.21] that for nonnegative quadrature weights and degree of exactness $N = 2L$ the mesh norms of the corresponding sampling sets $\mathcal{X}(\mathbb{S}^2)$ and $\mathcal{X}(\mathbb{S}^1)$ have to be bounded by

$$\delta(\mathcal{X}(\mathbb{S}^2)) \leq 2\arccos z_L, \qquad \delta(\mathcal{X}(\mathbb{S}^1)) \leq \frac{\pi}{L}, \tag{3.18}$$

where z_L is the greatest zero of the L-th Legendre polynomial P_L. We remark that these bounds are also valid for a degree of exactness $N = 2L-1$, which can be seen, if we follow the proof of [15, Theorem 6.21] line by line. In this case the bounds (3.18) are sharp, since the Gauss-Legendre quadrature grid on $\mathbb{S}^2$ has holes with diameter $2\arccos z_L$ at the poles and in the Gauss quadrature on $\mathbb{S}^1$ the nodes are equidistant with distance $\frac{\pi}{L}$. Now, we arrive at a bound on the mesh norm of the sampling set $\mathcal{X}(SO(3))$ constructed as in Lemma 3.1 from the Pythagorean-like relation of Theorem 2.2 by

$$\begin{aligned}\delta(\mathcal{X}(SO(3))) &\leq 4\arccos\left|\cos\frac{\delta(\mathcal{X}(\mathbb{S}^2))}{4}\cos\frac{\delta(\mathcal{X}(\mathbb{S}^1))}{4}\right| \\ &= 4\arccos\left(\cos\frac{\arccos z_L}{2}\cos\frac{\pi}{4L}\right).\end{aligned} \tag{3.19}$$

Furthermore, we can easily construct a sampling set $\mathcal{X}(SO(3))$ from sampling sets $\mathcal{X}(\mathbb{S}^2)$ and $\mathcal{X}(\mathbb{S}^1)$ by a suitable choice of the offsets c_i in Lemma 3.1, such that it holds equality in (3.19). For $L = 1$ the bounds of (3.19) and that of the scattered data version in Theorem 3.3 are equal. But for $L = 2$, respectively $N = 3$, the bound of (3.19), is circa 5% smaller. In order to get an asymptotic result between these to estimates, we make use of the asymptotic behavior of the zeros of the Legendre Polynomials P_L, stated in [15, Theorem 2.11]. Let $\varepsilon > 0$ be sufficiently small, then there is some $L' \in \mathbb{N}$ such that

$$j_{0,1} - \varepsilon \leq L\arccos z_L \leq j_{0,1} + \varepsilon, \qquad \text{for all } L \geq L',$$

is valid, where $j_{0,1}$ is the smallest zero of the Bessel function $J_0(x)$ of first kind. Therefore, we obtain for the quotient of the upper bounds of (3.19) and (3.14) the asymptotic behavior

$$\begin{aligned}\sqrt{1+\left(\frac{j_{0,1}-\varepsilon}{\pi}\right)^2} &= \lim_{L\to\infty}\frac{2L+1}{\pi}\arccos\left(\cos\frac{j_{0,1}-\varepsilon}{2L}\cos\frac{\pi}{4L}\right) \\ &\leq \lim_{L\to\infty}\frac{2L+1}{4\pi}\cdot 4\arccos\left(\cos\frac{\arccos z_L}{2}\cos\frac{\pi}{4L}\right) \\ &\leq \lim_{L\to\infty}\frac{2L+1}{\pi}\arccos\left(\cos\frac{j_{0,1}+\varepsilon}{2L}\cos\frac{\pi}{4L}\right) = \sqrt{1+\left(\frac{j_{0,1}+\varepsilon}{\pi}\right)^2},\end{aligned}$$

since ε was arbitrary we arrive at

$$\lim_{L\to\infty}\frac{2L+1}{4\pi}\cdot 4\arccos\left(\cos\frac{\arccos z_L}{2}\cos\frac{\pi}{4L}\right) = \sqrt{1+\left(\frac{j_{0,1}}{\pi}\right)^2} \approx 0.9143.$$

So, we conclude that the necessary condition of Theorem 3.3 is also quite sharp for grids constructed in the way of Lemma 3.1. Furthermore, in Section 5 we try to show numerically that the bound of (3.14) is best-possible for scattered data.

4 Examples of t-designs

We call a set $\mathcal{X}(SO(3))$ of M sampling nodes a t-design, as in the case of $\mathbb{S}^2$ [4], if the integral of any polynomial of degree at most t over the rotation group $SO(3)$ is equal to the average value of the polynomial over the set of M nodes. By virtue of Lemma 3.1 we obtain immediately t-designs on the rotation group from t-designs on $\mathbb{S}^2$ and $\mathbb{S}^1$.

Let us consider the three dimensional rotation groups $\mathcal{X}_T, \mathcal{X}_O, \mathcal{X}_I$ of the tetrahedron, octahedron (or hexahedron) and icosahedron (or dodecahedron), respectively. The vertices of the tetrahedron, octahedron and icosahedron are given as

$$\begin{aligned}
T &:= \left\{ \boldsymbol{x}_0 := \boldsymbol{e}_z,\, \boldsymbol{x}_i := \boldsymbol{x}\left(\frac{2}{3}i\pi, \arccos -\frac{1}{3}\right) \mid i = 1,2,3 \right\}, \\
O &:= \left\{ \boldsymbol{x}_0 := \boldsymbol{e}_z,\, \boldsymbol{x}_5 := -\boldsymbol{e}_z,\, \boldsymbol{x}_i := \boldsymbol{x}\left(\frac{1}{2}i\pi, \frac{1}{2}\pi\right) \mid i = 1,\dots,4 \right\}, \\
I &:= \left\{ \boldsymbol{x}_0 := \boldsymbol{e}_z,\, \boldsymbol{x}_{11} := -\boldsymbol{e}_z,\, \boldsymbol{x}_i := \boldsymbol{x}\left(\frac{2}{5}i\pi, \arctan 2\right), \right. \\
&\qquad\qquad \left. \boldsymbol{x}_{i+5} := \boldsymbol{x}\left(\frac{2}{5}i\pi + \frac{1}{5}\pi, \pi - \arctan 2\right) \mid i = 1,\dots,5 \right\}.
\end{aligned}$$

Then, the corresponding rotation groups can be parameterized by the following tensor-like products

$$\begin{aligned}
\mathcal{X}_T &:= \left\{ \boldsymbol{R}_{\text{Ortho}}\left(\boldsymbol{x}_i, \frac{2}{3}k\pi + c_i\right) \mid \boldsymbol{x}_i \in T,\, c_i = (1-\delta_{0,i})\frac{\pi}{3};\ i = 0,\dots,3,\, k = 0,1,2 \right\}, \\
\mathcal{X}_O &:= \left\{ \boldsymbol{R}_{\text{Ortho}}\left(\boldsymbol{x}_i, \frac{1}{2}k\pi + c_i\right) \mid \boldsymbol{x}_i \in O,\, c_i = 0;\ i = 0,\dots,5,\, k = 0,\dots,3 \right\}, \\
\mathcal{X}_I &:= \left\{ \boldsymbol{R}_{\text{Ortho}}\left(\boldsymbol{x}_i, \frac{2}{5}k\pi + c_i\right) \mid \boldsymbol{x}_i \in I,\, c_i = (1-\delta_{0,i})(1-\delta_{11,i})\frac{\pi}{5}; \right. \\
&\qquad\qquad \left. i = 0,\dots,11,\, k = 0,\dots,4 \right\},
\end{aligned}$$

where the spherical coordinates of $-\boldsymbol{e}_z$ are set to $(0,\pi)$ and

$$\delta_{0,k} := \begin{cases} 1, & k = 0, \\ 0, & \text{else}, \end{cases}$$

denotes the Kronecker symbol. These sets are illustrated in Figure 4.1. Using these representations we can apply Lemma 3.1 and obtain that $\mathcal{X}_T$, $\mathcal{X}_O$ lead to quadrature formulae Q_T, Q_O of degree $N = 2$ and 3, respectively, since the vertices of these platonic solids provide spherical t-designs of the corresponding degrees, cf [4]. Hence, the quadrature rules are quite efficient with

$$E(Q_T) = \frac{35}{4 \cdot 12} \approx 0.729, \qquad E(Q_O) = \frac{84}{4 \cdot 24} = 0.875.$$

However, by applying Lemma 3.1 we obtain for the quadrature rule based on the icosahedral rotation group $\mathcal{X}_I$ only a degree of exactness $N = 4$. But one can show that $\mathcal{X}_T$ provides for equal weights w_i, $i = 0, \dots, 59$ a quadrature rule Q_I with degree of exactness $N = 5$, which results in a super-efficient quadrature formula with

$$E(Q_I) = \frac{286}{4 \cdot 60} \approx 1.19.$$

There the quadrature Q_I satisfies 286 equalities with only 60 sampling nodes.

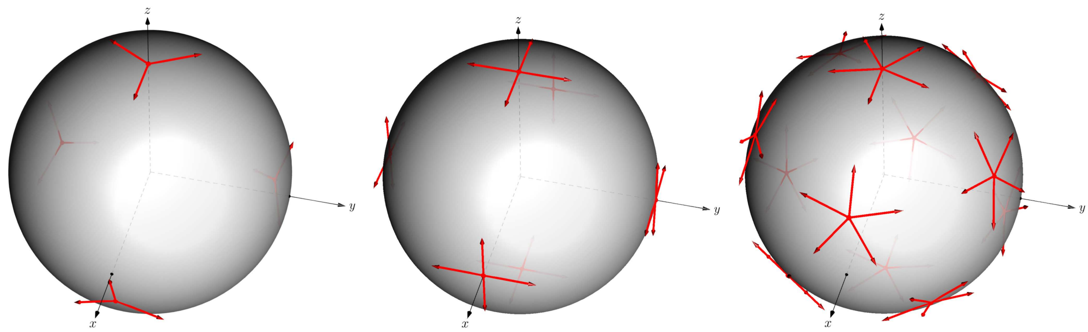

Figure 4.1: The finite rotation groups $\mathcal{X}_T$, $\mathcal{X}_O$ and $\mathcal{X}_I$, represented by position vectors of their nodes.

The bound on the mesh norm $\delta(\mathcal{X}(SO(3)))$ stated in Theorem 3.3 are actually sharp for degrees of exactness $N = 1, 2$. Since for all nodes of the 1-design

$$\mathcal{X}_A := \left\{ \boldsymbol{R}_{\text{Ortho}} \left(i\pi, \frac{\pi}{2}, j\pi + \frac{\pi}{2} \right) \mid i, j = 0, 1 \right\}$$

the identity $\boldsymbol{I} = \boldsymbol{R}_{\text{Ortho}}(0,0,0)$ has distance $\frac{2}{3}\pi$ and for all nodes of the tetrahedron rotation group $\mathcal{X}_T$ the rotation $\boldsymbol{R}_{\text{Ortho}}(0,\pi,0)$ has at least distance $\frac{\pi}{2}$.

It is likely that the sampling sets $\mathcal{X}_A$ and $\mathcal{X}_T$, $\mathcal{X}_O$, $\mathcal{X}_I$, like their pendants T, O, I on the sphere [4], are minimal 1-, 2-, 3- and 5-designs, respectively. That is, there are no corresponding t-designs with smaller cardinality.

5 Numerical results on quadrature formulae

We shall confirm the theoretical results of Lemma 3.1 and Theorem 3.3 in the following section, where we follow the approach of [2] to compute (nonnegative) quadrature weights. Therefore we introduce for the polynomial degree N and the sampling set $\mathcal{X} := \{\boldsymbol{G}_0, \dots, \boldsymbol{G}_{M-1}\}$ the $SO(3)$ Fourier matrix

$$\boldsymbol{D} := (D_l^{m,n}(\boldsymbol{G}_i))_{i=0,\dots,M-1; l=0,\dots,N, |m|,|n| \le l} \in \mathbb{C}^{M \times d_N}. \tag{5.1}$$

Then, equation (3.4) is equivalent to the linear system of equations

$$\boldsymbol{D}^* \boldsymbol{w} = \boldsymbol{e}_0, \tag{5.2}$$

where $\boldsymbol{e}_0$ is the unit vector

$$\boldsymbol{e}_0 := (1, 0, \ldots, 0) \in \mathbb{R}^{d_N}$$

and $\boldsymbol{w}$ is the weight vector

$$\boldsymbol{w} := (w_i)_{i=0,\ldots,M-1} \in \mathbb{R}^M.$$

Since we cannot say for which degree N the equation system (5.2) is solvable, we propose the following convex optimization problem

$$\min \|\boldsymbol{D}^* \boldsymbol{w} - \boldsymbol{e}_0\|_2 \qquad \text{subject to } \boldsymbol{w} \geq \boldsymbol{0}, \tag{5.3}$$

In order to use tools for real convex optimization problems we split the $SO(3)$ Fourier matrix $\boldsymbol{D} \in \mathbb{C}^{M \times d_N}$ into its real and imaginary part. Afterwards we can eliminate some redundant equalities due to the representation (3.2) of the Wigner D functions

$$D_l^{m,n}(\varphi, \theta, \psi) = \mathrm{e}^{-\mathrm{i}m\varphi} d_l^{m,n}(\cos\theta) \mathrm{e}^{-\mathrm{i}n\psi} = d_l^{m,n}(\cos\theta) \left(\cos(m\varphi + n\psi) - \mathrm{i}\sin(m\varphi + n\psi)\right).$$

Hence, the problem (5.3) is equivalent to

$$\min \|\boldsymbol{A}\boldsymbol{w} - \boldsymbol{e}_0\|_2 \qquad \text{subject to } \boldsymbol{w} \geq \boldsymbol{0}, \tag{5.4}$$

with

$$\begin{aligned}
\boldsymbol{A} &:= \begin{pmatrix} \boldsymbol{A}_1^\top \\ \boldsymbol{A}_2^\top \end{pmatrix} \in \mathbb{R}^{d_N \times M}, \\
\boldsymbol{A}_1 &:= \mathrm{Re}\left(D_l^{m,n}(\boldsymbol{G}_i)\right)_{i=0,\ldots,M-1;\, l=0,\ldots,N, (m,n)\in I_l^1} \in \mathbb{R}^{M \times \frac{1}{3}(1+N)(3+4N+2N^2)}, \\
\boldsymbol{A}_2 &:= -\mathrm{Im}\left(D_l^{m,n}(\boldsymbol{G}_i)\right)_{i=0,\ldots,M-1;\, l=0,\ldots,N, (m,n)\in I_l^2} \in \mathbb{R}^{M \times \frac{2}{3}N(N+1)(N+2)},
\end{aligned}$$

where we use the index sets

$$\begin{aligned}
I_l^1 &:= \{(m,n) \mid m \leq 0 \leq n\} \;\cup\; \{(m,n) \mid m > 0 > n\}, \\
I_l^2 &:= \{(m,n) \mid m \leq 0 < -n\} \cup \{(m,n) \mid m > 0 \geq -n\}.
\end{aligned}$$

Recently, fast approximate algorithms for the matrix times vector multiplication with the nonequispaced $SO(3)$ Fourier matrix $\boldsymbol{D}$ and its adjoint $\boldsymbol{D}^*$ have been proposed in [14]. We use these algorithms and obtain a fast method for the matrix times vector multiplication $\boldsymbol{v} := \boldsymbol{A}\boldsymbol{w} \in \mathbb{R}^{d_N}$ based on the adjoint $SO(3)$ Fourier transform by computing $\tilde{\boldsymbol{v}} := \boldsymbol{D}^*\boldsymbol{w}$ and setting

$$\boldsymbol{v} = (v_l^{m,n})_{l=0,\ldots,N,|m|,|n|\leq l} \qquad \text{with} \qquad v_l^{m,n} := \begin{cases} \mathrm{Re}(\tilde{v}_l^{m,n}) & \text{for } (m,n) \in I_l^1, \\ \mathrm{Im}(\tilde{v}_l^{m,n}) & \text{for } (m,n) \in I_l^2. \end{cases}$$

Similarly we compute the matrix times vector multiplication $\boldsymbol{w} := \boldsymbol{A}^\top \boldsymbol{v} \in \mathbb{R}^M$ again with the $SO(3)$ Fourier transform

$$\boldsymbol{w} = \mathrm{Re}\left(\boldsymbol{D}\tilde{\boldsymbol{v}}\right) \qquad \text{after setting} \qquad \tilde{v}_l^{m,n} := \begin{cases} v_l^{m,n} & \text{for } (m,n) \in I_l^1, \\ \mathrm{i}v_l^{m,n} & \text{for } (m,n) \in I_l^2. \end{cases}$$

In both cases the arithmetical complexity is $\mathcal{O}(N^3 \log^2 N + M)$. In order to solve problem (5.3) we make use of the modified CGNR algorithm proposed in [2].

Example 5.1. We test the algorithm with the t-designs of Section 4 and some tensor products of spherical t-designs from [4] and Gauss quadratures on $\mathbb{S}^1$ of the corresponding polynomial degree N. The results are listed in Table 5.1 which confirms that our algorithm computes all weights very precisely. □

degree N	size M	$\|\boldsymbol{A}\boldsymbol{w} - \boldsymbol{e}_0\|_2$	iterations
2	12	6.656288e-11	4
3	24	1.727262e-11	6
5	60	1.439418e-11	7
13	1316	3.763450e-12	10
17	2808	1.251657e-07	21
21	5280	1.251657e-07	25

Table 5.1: Test results for N-designs.

Example 5.2. We consider very efficient quadrature formulae on $SO(3)$, obtained from efficient quadrature formulae on $\mathbb{S}^2$. There, we used the 72 nodes formula of degree $N = 14$ from McLaren [10] and some efficient formulae from Lebedev, cf. [8, 9]. The results by using the modified CGNR method are given in Table 5.2. We remark that for the formula of degree 41 we have to solve an system with 24780 variables and 98770 equations. □

degree N	size M	$\|\boldsymbol{A}\boldsymbol{w} - \boldsymbol{e}_0\|_2$	iterations
14	1080	2.721707e-12	18
29	9060	1.512788e-12	28
31	11200	1.458048e-12	29
41	24780	1.238677e-12	34

Table 5.2: Test results for very efficient quadrature formulae.

Example 5.3. Now we compute nonnegative quadrature weights for some sampling sets from [5]. The degree N in Table 5.3 is the maximal one that our algorithm achieves up to the given precision. □

Example 5.4. We consider an uniform random distribution over $SO(3)$. This is generated with the parameter $\boldsymbol{x} \in \mathbb{S}^2$ and $\boldsymbol{\omega}$ of the parameterization $\boldsymbol{R}_{\mathrm{Ortho}}(\boldsymbol{x}, \omega)$ taken from an uniform distribution over $\mathbb{S}^2$ and $\mathbb{S}^1$, respectively. Even for small polynomial degrees N we have to take many nodes to obtain positive quadrature weights. In Table 5.4 we list the results. □

name	degree N	size M	$\|\boldsymbol{Aw}-\boldsymbol{e}_0\|_2$	iterations
c600vc	9	360	1.030884e-09	17
c600vec	11	720	5.143112e-10	21
c48u27	8	648	4.707011e-11	19
c48u309	17	7416	2.502115e-13	259
c48n309	17	7416	1.388484e-13	168
c48u527	21	12648	3.539870e-13	656
c48n527	21	12648	2.790298e-13	1500
c48u8649	51	207576	3.604940e-13	929

Table 5.3: Test results for sampling sets from [5] with cardinality M and numerical maximal degree of exactness N.

degree N	size M	zero weights	$\|\boldsymbol{Aw}-\boldsymbol{e}_0\|_2$	iterations
3	200	43	3.452291e-15	390
4	400	101	5.175212e-15	560
5	700	276	7.054088e-15	1278
6	1100	329	6.532730e-15	1011
7	1700	752	1.097145e-14	1919
8	2400	768	7.805511e-15	1848
9	3200	1070	9.360416e-15	1516
10	4200	1544	1.260515e-14	2293

Table 5.4: Test results for random sampling sets with cardinality M and requested degree of exactness N.

Example 5.5. At last, we show the bound of (3.14) in Theorem 3.3 is very sharp. The results are shown in Table 5.5. There, we construct random sampling sets of cardinality M over $SO(3)$ with a hole of diameter at least $0.99 \cdot \frac{4\pi}{N+2}$ and use the proposed algorithms to compute nonnegative quadrature weights. □

degree N	size M	zero weights	$\|\boldsymbol{Aw}-\boldsymbol{e}_0\|_2$	iterations
3	6000	5775	7.488065e-14	2201
4	15000	12728	1.454949e-14	1744
5	25000	22417	3.334297e-14	4250
6	40000	35725	8.796223e-14	5405
7	55000	44686	2.957736e-14	4101

Table 5.5: Test results for random sampling sets with cardinality M and mesh norm at least $0.99 \cdot \frac{4\pi}{N+2}$ to a numerical degree of exactness N.

6 Conclusion

In this paper we constructed uniform sampling sets on the rotation group $SO(3)$ by sampling the first two Euler angles over the two-sphere $\mathbb{S}^2$ and the third over the one-sphere $\mathbb{S}^1$. The same construction scheme yields quadrature formulae with degree of exactness N from quadratures of the same degree over the spheres $\mathbb{S}^2$ and $\mathbb{S}^1$ as well. With it we easily obtained that the finite rotation groups of the Platonic solids are t-designs on $SO(3)$. We carried forward the necessary condition for the existence of positive quadrature formulae form the d-sphere to the rotation group. At the end we presented some numerical examples on the computation of nonnegative quadrature weights based on the fast $SO(3)$ Fourier transform.

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