An unified approach to scattered data approximation on $\mathbb{S}^3$ and $\mathrm{SO}(3)$

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In this paper we use the connection between the rotation group SO(3) and the three-dimensional Euclidean sphere $\mathbb{S}^3$ in order to carry over results of the three-sphere directly to the rotation group and vice versa. More precisely, these results connect properties of sampling sets and quadrature formulae on SO(3) and $\mathbb{S}^3$, respectively. Furthermore we relate Marcinkiewicz-Zygmund inequalities and conditions for the existence of positive quadrature formulae on the rotation group SO(3) to those on the three-sphere $\mathbb{S}^3$, respectively.

Keywords and Phrases : rotation group SO(3), three-sphere $\mathbb{S}^3$, quaternions, scattered data, sampling sets, quadrature formulae, Marcinkiewicz-Zygmund inequalities

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1 Introduction

Scattered data approximation on various domains is a problem with many applications in science and engineering, cf. [15, 3, 13]. Typical ingredients to treat such multivariate approximation problems are studies of scattered sampling nodes and quadrature formulae. For example D. Schmid was able to present a trade-off result, based on a paper of R. Schaback [14], for approximation problems using positive definite basis functions on the rotation group SO(3), cf. [17]. There was shown that it is impossible to come up with a 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. Another important result comes from K. Gröchenig. He investigated in [8] the problem of the reconstruction of band-limited functions from scattered sampling data and arrived on Marcinkiewicz-Zygmund type inequalities. So-called Marcinkiewicz-Zygmund inequalities provide a norm equivalence between the discrete l_p norm of the sampling values and the continuous L_p norm of the sampled function,

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where a condition on the mesh norm of the sampling set is involved. H.N. Mhaskar et al. proved in [10] such inequalities for the d-dimensional sphere $\mathbb{S}^d$ and they used them in order to derive assertions for (positive) quadrature formulae of scattered data. In later investigations such inequalities were improved and used for stability results of scattered data approximation methods as well, cf. [9, 4]. Recently, one was able to state such results of scattered data approximation on the rotation group SO(3) by using the proposed methods, we refer to [16, 6] and the dissertation of D. Schmid [18].

All the above results reveal the importance of the distribution of the sampling sets. In [7] a simple construction was proposed which leads to well distributed sampling sets on the rotation group SO(3). The same construction can also be used in order to generate quadrature formulae on the rotation group from quadratures on the two-sphere $\mathbb{S}^2$. In particular one obtains immediately t-designs on the rotation group SO(3) from t-designs on the two-sphere $\mathbb{S}^2$. In addition the authors presented a method, based on a fast algorithm for nonequispaced Fourier transforms on the rotation group SO(3), cf. [12], for the computation of nonnegative quadrature weights for scattered sampling sets on SO(3).

The aim of this paper is to consider the results on the three-sphere $\mathbb{S}^3$ and rotation group SO(3) from a common point of view. Therefore, we recapitulate the well known connection between the rotation group SO(3) and the three-sphere $\mathbb{S}^3$ by quaternions. Furthermore we show that the natural metrics, measures and polynomial spaces on these manifolds are essentially the same. From these facts we carry over assertions of sampling sets and quadrature formulae from the three-sphere $\mathbb{S}^3$ to the rotation group SO(3) and vice versa. As an application of these connections we present new proofs for the existence of nonnegative quadrature weights and Marcinkiewicz-Zygmund inequalities on the rotation group SO(3). Moreover we obtain immediately constructions of well distributed sampling sets and quadrature formulae on the three-sphere $\mathbb{S}^3$ by using the results from [7]. Therefore we are able to construct t-designs on $\mathbb{S}^3$ from t-designs on the two-sphere $\mathbb{S}^2$ and to compute in fast way nonnegative quadrature weights for antipodal scattered sampling sets on the three-sphere $\mathbb{S}^3$.

The outline of this paper is as follows. In Section 2 we introduce all necessary notations to derive an explicite isomorphism between the rotation group SO(3) and the three-dimensional projective space $\mathbb{S}^3_*$, where antipodal nodes of the three-sphere $\mathbb{S}^3$ are identified. Furthermore we show that the even polynomials on the three-sphere $\mathbb{S}^3$ correspond to the polynomials on the rotation group SO(3). With the mentioned results at hand we connect in Section 3 sampling sets and quadrature formulae on these manifolds respectively. Afterwards this connection is applied to recent results on the rotation group SO(3).

2 Quaternions and rotations

Throughout this paper we use the notation

$$\mathbb{S}^d := \{\boldsymbol{x} = (x_1, \ldots, x_{d+1}) \in \mathbb{R}^{d+1} \ : \ \|\boldsymbol{x}\|_2 = 1\}$$

for the d-sphere. The rotation group of the n-dimensional Euclidean space is denoted by

$$\mathrm{SO}(n) := \left\{ \boldsymbol{G} \in \mathbb{R}^{n\times n} : \boldsymbol{G}^\top = \boldsymbol{G}^{-1}, \det \boldsymbol{G} = 1 \right\},$$

where the group operation is given by composition. The rotation group SO(3) can be naturally parameterized by

$$\boldsymbol{R}(\boldsymbol{r},\alpha) := (1-\cos(\alpha))\boldsymbol{r}^\top \boldsymbol{r} + \begin{pmatrix} \cos(\alpha) & -z\sin(\alpha) & y\sin(\alpha) \\ z\sin(\alpha) & \cos(\alpha) & -x\sin(\alpha) \\ -y\sin(\alpha) & x\sin(\alpha) & \cos(\alpha) \end{pmatrix}, \tag{2.1}$$

with a rotation axis $\boldsymbol{r} = (x,y,z) \in \mathbb{S}^2$ and a rotation angle $\alpha \in [0,\pi]$. In the following we introduce the space of unit quaternions, which establishes the connection of the three-sphere $\mathbb{S}^3$ to the rotation group SO(3). A unit quaternion is given by

$$\boldsymbol{q} := (s, \boldsymbol{v}) \in \mathbb{S}^3,$$

which consists of a scalar part $s \in \mathbb{R}$ and a vector part $\boldsymbol{v} \in \mathbb{R}^3$. Via the multiplication formula

$$\boldsymbol{q}_1 \cdot \boldsymbol{q}_2 := \left(s_1 s_2 - \boldsymbol{v}_1 \boldsymbol{v}_2^\top, s_1 \boldsymbol{v}_2 + s_2 \boldsymbol{v}_1 + (\boldsymbol{v}_1 \times \boldsymbol{v}_2) \right), \quad \boldsymbol{q}_1 = (s_1, \boldsymbol{v}_1), \boldsymbol{q}_2 = (s_2, \boldsymbol{v}_2) \in \mathbb{S}^3$$

one easily checks that the space of the unit quaternions $\mathrm{Sp}(1) := (\mathbb{S}^3, \cdot)$ is a group, the so-called one-dimensional symplectic group. The inverse element of $\boldsymbol{q} = (s, \boldsymbol{v})$ is the conjugated quaternion

$$\overline{\boldsymbol{q}} := (s, -\boldsymbol{v}).$$

Now, the connection of a unit quaternion $\boldsymbol{q} \in \mathrm{Sp}(1)$ to a rotation $\boldsymbol{G} \in \mathrm{SO}(3)$ is given by the following operation. For a vector $\boldsymbol{p} \in \mathbb{S}^2$ we define the action of a unit quaternion $\boldsymbol{q} \in \mathrm{Sp}(1)$ by

$$\boldsymbol{p}(\boldsymbol{q}) := \boldsymbol{q} \cdot (0, \boldsymbol{p}) \cdot \overline{\boldsymbol{q}}. \tag{2.2}$$

If we parameterize a quaternion $\boldsymbol{q}$ by an axis $\boldsymbol{r} = (x,y,z) \in \mathbb{S}^2$ and an angle $\alpha \in [0,\pi]$ due to

$$\boldsymbol{q}(\boldsymbol{r},\alpha) := \left(\cos\frac{\alpha}{2}, \sin\frac{\alpha}{2}\boldsymbol{r} \right) \tag{2.3}$$

we obtain the identity

$$(0, \boldsymbol{p}\boldsymbol{R}(\boldsymbol{r},\alpha)) = \boldsymbol{p}(\boldsymbol{q}(\boldsymbol{r},\alpha)), \qquad \boldsymbol{p} \in \mathbb{S}^2. \tag{2.4}$$

Form this observation we call $\boldsymbol{G} := \boldsymbol{R}(\boldsymbol{r},\alpha)$ the corresponding rotation of the quaternion $\boldsymbol{q} = \boldsymbol{q}(\boldsymbol{r},\alpha)$. Since the quaternion multiplication is associative it follows immediately that the quaternion multiplication of two unit quaternions $\boldsymbol{q}_1, \boldsymbol{q}_2 \in \mathrm{Sp}(1)$ is consistent with the composition of the corresponding rotations $\boldsymbol{G}_1, \boldsymbol{G}_2 \in \mathrm{SO}(3)$, i.e.,

$$(0, \boldsymbol{p}\boldsymbol{G}_1\boldsymbol{G}_2) = \boldsymbol{p}(\boldsymbol{q}_2 \cdot \boldsymbol{q}_1), \qquad \boldsymbol{p} \in \mathbb{S}^2.$$

By definition (2.3) the quaternion $\boldsymbol{q}(\boldsymbol{r},\alpha) = (s, \boldsymbol{v})$ is in the upper hemisphere of $\mathbb{S}^3$, i.e., $s \geq 0$. Since $\boldsymbol{q}$ and $-\boldsymbol{q}$ corresponds by (2.2) and (2.4) to the same rotation one obtains that $\mathbb{S}^3$ is a double cover of SO(3), cf. [2, Chap. III, Sect. 10]. So it is convenient to pass to the quotient space $\mathbb{S}^3_* := \mathbb{S}^3/\{1,-1\}$, where we identify antipodal quaternions. This space is also known as the three-dimensional projective space. With it we obtain an isomorphism

$$\boldsymbol{q}_* : \mathrm{SO}(3) \to \mathbb{S}^3_*, \qquad \boldsymbol{q}_*(\boldsymbol{R}(\boldsymbol{r},\alpha)) := \{\pm \boldsymbol{q}(\boldsymbol{r},\alpha)\} = \{-\boldsymbol{q}(\boldsymbol{r},\alpha), \boldsymbol{q}(\boldsymbol{r},\alpha)\}, \tag{2.5}$$

between SO(3) and the projective space $\mathbb{S}^3_*$ with the property

$$\boldsymbol{q}_*(\boldsymbol{G}_1\boldsymbol{G}_2) = \boldsymbol{q}_*(\boldsymbol{G}_2) \cdot \boldsymbol{q}_*(\boldsymbol{G}_1) := \{\pm \boldsymbol{q}_2 \cdot \boldsymbol{q}_1\}. \tag{2.6}$$

For simplicity we use a representative $\boldsymbol{x} \in \mathbb{S}^3$ to identify the corresponding element of the projective space $\mathbb{S}^3_*$ by $\boldsymbol{x}_* := \{\pm \boldsymbol{x}\}$.

In the following we use on the three-sphere $\mathbb{S}^3$the natural geodesic metric

$$\mathrm{d}_{\mathbb{S}^3}(\boldsymbol{x}_1, \boldsymbol{x}_2) := \arccos(\boldsymbol{x}_1\boldsymbol{x}_2^\top), \qquad \boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{S}^3, \tag{2.7}$$

and the natural rotation invariant surface measure $\mu_{\mathbb{S}^3}$, with normalization $\int \mathrm{d}\mu_{\mathbb{S}^3}(\boldsymbol{x}) = 1$. These definitions induce a metric and a measure on $\mathbb{S}^3_*$, respectively. More precisely we define the metric by

$$\mathrm{d}_{\mathbb{S}^3_*}(\boldsymbol{q}_{1*}, \boldsymbol{q}_{2*}) := \min_{\substack{\boldsymbol{x}_1 = \pm \boldsymbol{q}_1, \\ \boldsymbol{x}_2 = \pm \boldsymbol{q}_2}} \mathrm{d}_{\mathbb{S}^3}(\boldsymbol{x}_1, \boldsymbol{x}_2) = \arccos |\boldsymbol{q}_1\boldsymbol{q}_2^\top|, \quad \boldsymbol{q}_{1*} = \{\pm \boldsymbol{q}_1\},\ \boldsymbol{q}_{2*} = \{\pm \boldsymbol{q}_2\} \in \mathbb{S}^3_* \tag{2.8}$$

and the measure by

$$\mu_{\mathbb{S}^3_*}(\Omega_*) = \mu_{\mathbb{S}^3}(\Omega) + \mu_{\mathbb{S}^3}(-\Omega), \qquad \Omega_* = \{\boldsymbol{x}_* \ :\ \boldsymbol{x} \in \Omega\} \subset \mathbb{S}^3_*,\ \Omega \subset \mathbb{S}^3. \tag{2.9}$$

Furthermore, the distance between two rotations $\boldsymbol{G}_1, \boldsymbol{G}_2 \in \mathrm{SO}(3)$ is naturally given by

$$\mathrm{d}_{\mathrm{SO}(3)}(\boldsymbol{G}_1, \boldsymbol{G}_2) := \alpha(\boldsymbol{G}_1\boldsymbol{G}_2^\top) := \arccos\left(\frac{1}{2}(\operatorname{trace} \boldsymbol{G}_1\boldsymbol{G}_2^\top - 1)\right), \tag{2.10}$$

where $\alpha(\boldsymbol{G})$ is the rotation angle of the rotation $\boldsymbol{G} \in \mathrm{SO}(3)$. Moreover, we use the normalized (translation invariant) Haar measure $\mu_{\mathrm{SO}(3)}$, i.e.,

$$\mu_{\mathrm{SO}(3)}(\Omega) = \mu_{\mathrm{SO}(3)}(\boldsymbol{H} \cdot \Omega), \qquad \boldsymbol{H} \in \mathrm{SO}(3),\ \Omega \subset \mathrm{SO}(3),$$

with $\int_{\mathrm{SO}(3)} \mathrm{d}\mu_{\mathrm{SO}(3)}(\boldsymbol{G}) = 1$, where $\boldsymbol{H} \cdot \Omega := \{\boldsymbol{H}\boldsymbol{G} \ :\ \boldsymbol{G} \in \Omega\}$ is the translated set.

The following Lemma 2.1 states that by virtue of the isomorphism $\boldsymbol{q}_*$, cf. (2.5), the induced metric (2.8) on the projective space $\mathbb{S}^3_*$ coincides with the metric on the rotation group SO(3), as well as the induced measure (2.9) coincides with the normalized Haar measure.

Lemma 2.1. *The isomorphism* $\boldsymbol{q}_*: \mathrm{SO}(3) \to \mathbb{S}^3_*$, *cf.* (2.5) *yields the identities*

$$\begin{aligned} \mathrm{d}_{\mathrm{SO}(3)}(\boldsymbol{G}_1, \boldsymbol{G}_2) &= 2\mathrm{d}_{\mathbb{S}^3_*}(\boldsymbol{q}_*(\boldsymbol{G}_1), \boldsymbol{q}_*(\boldsymbol{G}_2)), \quad && \boldsymbol{G}_1, \boldsymbol{G}_2 \in \mathrm{SO}(3), \\ \mu_{\mathrm{SO}(3)}(\Omega) &= \mu_{\mathbb{S}^3_*}(\boldsymbol{q}_*(\Omega)), && \Omega \subset \mathrm{SO}(3), \end{aligned} \tag{2.11}$$

where $\boldsymbol{q}_*(\Omega) := \{\boldsymbol{q}_*(\boldsymbol{G}) \ : \ \boldsymbol{G} \in \Omega\}$.

Proof. We obtain the first identity by using for $\boldsymbol{G}_1$ and $\boldsymbol{G}_2$ the parameterization with rotation axes $\boldsymbol{r}_1, \boldsymbol{r}_2 \in \mathbb{S}^2$ and rotation angles $\alpha_1, \alpha_2 \in [0, \pi]$, cf. (2.1). This yields with (2.8) the desired result

$$\begin{aligned} \mathrm{d}_{\mathrm{SO}(3)}(\boldsymbol{R}(\boldsymbol{r}_1, \alpha_1), \boldsymbol{R}(\boldsymbol{r}_2, \alpha_2)) &= 2 \arccos \left| \boldsymbol{r}_1 \boldsymbol{r}_2^\top \sin\frac{\alpha_1}{2} \sin\frac{\alpha_2}{2} + \cos\frac{\alpha_1}{2} \cos\frac{\alpha_2}{2} \right| \\ &= 2 \arccos \left| \boldsymbol{q}(\boldsymbol{r}_1, \alpha_1)\, \boldsymbol{q}(\boldsymbol{r}_2, \alpha_2)^\top \right| \\ &= 2\, \mathrm{d}_{\mathbb{S}^3_*}(\boldsymbol{q}_*(\boldsymbol{R}(\boldsymbol{r}_1, \alpha_1)), \boldsymbol{q}_*(\boldsymbol{R}(\boldsymbol{r}_2, \alpha_2))). \end{aligned}$$

In order to prove the second identity we make use of the uniqueness of the Haar measure, cf. [5, Section 2.2]. Therefore let $\boldsymbol{H} \in \mathrm{SO}(3)$ and $\Omega \subset \mathrm{SO}(3)$ be given. From equation (2.6) we infer that

$$\boldsymbol{q}_*(\boldsymbol{H} \cdot \Omega) = \{\boldsymbol{q}_*(\boldsymbol{H}) \cdot \boldsymbol{q}_*(\boldsymbol{G}) \ : \ \boldsymbol{G} \in \Omega\}.$$

Since the quaternionic multiplication $\boldsymbol{q} \cdot \boldsymbol{x}$ of a vector $\boldsymbol{x} \in \mathbb{R}^4$ with an unit quaternion $\boldsymbol{q} \in \mathbb{S}^3$ can be considered as a linear transformation $\boldsymbol{T}\boldsymbol{x}$ with determinant $|\det \boldsymbol{T}| = 1$, we conclude that the antipodal quaternions $\boldsymbol{q}_*(\boldsymbol{H})$ represent some rotation $\boldsymbol{T} \in \mathrm{SO}(4)$ or $-\boldsymbol{T} \in \mathrm{SO}(4)$. Let without loss of generality $\boldsymbol{T} \in \mathrm{SO}(4)$, then we arrive at

$$\boldsymbol{q}_*(\boldsymbol{H} \cdot \Omega) = \{\{\pm \boldsymbol{T}\boldsymbol{x}\} \ : \ \boldsymbol{x}_* = \boldsymbol{q}_*(\boldsymbol{G}), \boldsymbol{G} \in \Omega\} =: \boldsymbol{T} \cdot \boldsymbol{q}_*(\Omega).$$

From the rotation invariance of the measure $\mu_{\mathbb{S}^3}$ on the three-sphere and the definition (2.9) we obtain the translation invariance of the induced measure

$$\mu_{\mathbb{S}^3_*}(\boldsymbol{q}_*(\boldsymbol{H} \cdot \Omega)) = \mu_{\mathbb{S}^3_*}(\boldsymbol{T} \cdot \boldsymbol{q}_*(\Omega)) = \mu_{\mathbb{S}^3_*}(\boldsymbol{q}_*(\Omega)).$$

With the normalization $1 = \mu_{\mathrm{SO}(3)}(\mathrm{SO}(3)) = \mu_{\mathbb{S}^3_*}(\mathbb{S}^3_*)$ and the uniqueness of the Haar measure we conclude that these two measures must coincide. ∎

For our considerations we introduce the harmonic spaces on $\mathbb{S}^3$ and $\mathrm{SO}(3)$. The spaces of square integrable functions are denoted by

$$\begin{aligned} L^2(\mathbb{S}^3) &:= \left\{ f : \mathbb{S}^3 \to \mathbb{C} \ : \ \int_{\mathbb{S}^3} |f(\boldsymbol{x})|^2 \mathrm{d}\mu_{\mathbb{S}^3}(\boldsymbol{x}) \right\}, \\ L^2(\mathrm{SO}(3)) &:= \left\{ f : \mathrm{SO}(3) \to \mathbb{C} \ : \ \int_{\mathrm{SO}(3)} |f(\boldsymbol{G})|^2 \mathrm{d}\mu_{\mathrm{SO}(3)}(\boldsymbol{G}) \right\}, \end{aligned}$$

where the standard orthonormal bases are given by spherical harmonics Y_l^k, $l \in \mathbb{N}_0$, $k = 0, \ldots, (l+1)^2$, and by the Wigner D-functions $D_l^{m,m'}$, $l \in \mathbb{N}_0$, $m, m' = -l, \ldots, l$, respectively. Furthermore we define for degree $l \in \mathbb{N}_0$ the harmonic spaces

$$\Gamma_l(\mathbb{S}^3) := \left\{ Y_l^k \ : \ k = 0, \ldots, (l+1)^2 \right\}, \quad \Gamma_l(\mathrm{SO}(3)) := \left\{ D_l^{m,m'} \ : \ m, m' = -l, \ldots, l \right\},$$

and

$$\Pi_N(\mathbb{S}^3) := \bigoplus_{l=0}^{N} \Gamma_l(\mathbb{S}^3), \quad \Pi_N(\mathrm{SO}(3)) := \bigoplus_{l=0}^{N} \Gamma_l(\mathrm{SO}(3)),$$

where the firsts consist of all polynomials of degree l and the latter of all polynomials of degree at most N. Additionally, for $1 \leq p < \infty$ the L^p norms of measurable functions $f : \mathbb{S}^3 \to \mathbb{C}$ and $g : \mathrm{SO}(3) \to \mathbb{C}$ are given by

$$\|f\|_p := \left(\int |f(\boldsymbol{x})|^p \mathrm{d}\mu_{\mathbb{S}^3}(\boldsymbol{x}) \right)^{\frac{1}{p}},$$

$$\|g\|_p := \left(\int |g(\boldsymbol{G})|^p \mathrm{d}\mu_{\mathrm{SO}(3)}(\boldsymbol{G}) \right)^{\frac{1}{p}}.$$

3 Sampling sets, quadratures and Marcinkiewicz-Zygmund inequalities

In the following we present three theorems which connect sampling sets, quadrature formulae and Marcinkiewicz-Zygmund inequalities on the three-sphere $\mathbb{S}^3$ to those on the rotation group SO(3), respectively.

First of all we consider finite subsets $\mathcal{X}(\mathcal{M})$ of a metric space $(\mathcal{M}, \mathrm{d}_{\mathcal{M}})$ with metric $d_{\mathcal{M}}$. In this paper the space $\mathcal{M}$ stands for the three-sphere $\mathbb{S}^3$ and the rotation group SO(3). In order to describe the quality of such a sampling set $\mathcal{X}(\mathcal{M})$ we introduce the following two parameters. The first one is the separation distance

$$q(\mathcal{X}(\mathcal{M})) := \min_{\boldsymbol{y} \neq \boldsymbol{x} \in \mathcal{X}(\mathcal{M})} \mathrm{d}_{\mathcal{M}}(\boldsymbol{x}, \boldsymbol{y}), \tag{3.1}$$

which is the minimal distance of two distinct nodes of the sampling set $\mathcal{X}(\mathcal{M})$. On the other hand the mesh norm

$$\delta(\mathcal{X}(\mathcal{M})) := 2 \max_{\boldsymbol{y} \in \mathcal{M}} \min_{\boldsymbol{x} \in \mathcal{X}(\mathcal{M})} \mathrm{d}_{\mathcal{M}}(\boldsymbol{x}, \boldsymbol{y}) \tag{3.2}$$

describes the "density" of $\mathcal{X}(\mathcal{M})$.

For a given sampling set $\mathcal{X}(\mathcal{M}) := \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{M-1}\}$ we consider associated partitions $\mathcal{R}(\mathcal{M}) := \{\Omega_0, \ldots, \Omega_{M-1}\}$ of closed regions $\Omega_i \subset \mathcal{M}$, $i = 0, \ldots, M-1$, where we require that $\boldsymbol{x}_j$ is an interior point of Ω_j, i.e., $\boldsymbol{x}_j \in \mathring{\Omega}_j$. Moreover, the regions cover the whole space $\mathcal{M} = \bigcup_{i=0}^{M-1} \Omega_i$ and share no common interior point, i.e., $\mathring{\Omega}_j \cap \mathring{\Omega}_i = \emptyset$ for $i \neq j$. For such partitions $\mathcal{R}(\mathcal{M})$ we define the partition norm

$$\|\mathcal{R}(\mathcal{M})\| := \max_{i=0,\ldots,M-1} \max_{\boldsymbol{x}, \boldsymbol{y} \in \Omega_i} \mathrm{d}_{\mathcal{M}}(\boldsymbol{x}, \boldsymbol{y}). \tag{3.3}$$

Furthermore, we say a quadrature rule

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

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

$$\sum_{i=0}^{M-1} w_i f(\boldsymbol{x}_i) = \int_{\mathcal{M}} f(\boldsymbol{x}) \mathrm{d}_{\mathcal{M}}(\boldsymbol{x})$$

is valid.

The following Theorem 3.1 states that antipodal sampling sets on the three-sphere $\mathbb{S}^3$ can be considered as sampling sets on the rotation group and that they share the same metric properties.

Theorem 3.1. *For a sampling set* $\mathcal{X}(\mathbb{S}^3) := \{\pm\boldsymbol{x}_0, \ldots, \pm\boldsymbol{x}_{M-1}\}$ *with* $2M \geq 4$ *antipodal nodes on the three-sphere* $\mathbb{S}^3$ *and the corresponding sampling set* $\mathcal{X}(\mathrm{SO}(3)) := \{\boldsymbol{q}_*^{-1}(\boldsymbol{x}_{0*}), \ldots, \boldsymbol{q}_*^{-1}(\boldsymbol{x}_{M-1*})\}$ *with* M *nodes on the rotation group* $\mathrm{SO}(3)$ *the separation distances and mesh norms obey*

$$q(\mathcal{X}(\mathbb{S}^3)) = \frac{1}{2} q(\mathcal{X}(\mathrm{SO}(3))) \quad \textit{and} \quad \delta(\mathcal{X}(\mathbb{S}^3)) = \frac{1}{2}\delta(\mathcal{X}(\mathrm{SO}(3))),$$

respectively.

Proof. At first, we observe that the extremal nodes of the antipodal sampling set $\mathcal{X}(\mathbb{S}^3)$ in the definitions of the separation distance (3.1) and the mesh norm (3.2) occur in antipodal pairs. Hence, by the definition of the distance (2.8) we conclude for the sampling set $\mathcal{X}(\mathbb{S}^3_*) := \{\boldsymbol{x}_{0*}, \ldots, \boldsymbol{x}_{M-1*}\}$ the relations $q(\mathcal{X}(\mathbb{S}^3)) = q(\mathcal{X}(\mathbb{S}^3_*))$ and $\delta(\mathcal{X}(\mathbb{S}^3)) = \delta(\mathcal{X}(\mathbb{S}^3_*))$. So the assumption follows from Lemma 2.1. ■

A similar connection is valid for the harmonic spaces on $\mathbb{S}^3$ and SO(3), where we identify even functions on the three-sphere $\mathbb{S}^3$ with functions on the rotation group SO(3). More precisely, let $f : \mathbb{S}^3 \to \mathbb{C}$ be an even function. Then, we define the function $\tilde{f} : \mathbb{S}^3_* \to \mathbb{C}$ by

$$\tilde{f}(\boldsymbol{q}_*) := f(\pm\boldsymbol{q}), \tag{3.4}$$

where the isomorphism (2.5) yields a function $\bar{f} : \mathrm{SO}(3) \to \mathbb{C}$ by $\bar{f}(\boldsymbol{G}) = \tilde{f}(\boldsymbol{q}_*(\boldsymbol{G}))$, $\boldsymbol{G} \in \mathrm{SO}(3)$. Conversely, an arbitrarily function $\bar{f} : \mathrm{SO}(3) \to \mathbb{C}$ can be continued uniquely to an even function $f : \mathbb{S}^3 \to \mathbb{C}$.

Lemma 3.2. *The isomorphism* $\boldsymbol{q}_* : \mathrm{SO}(3) \to \mathbb{S}^3_*$, *cf.* (2.5), *and the definition* (3.4) *yield the following equivalence*

$$f(\cdot) \in \Gamma_{2N}(\mathbb{S}^3) \qquad \Leftrightarrow \qquad \tilde{f}(\boldsymbol{q}_*(\cdot)) \in \Gamma_N(\mathrm{SO}(3)). \tag{3.5}$$

Proof. The addition theorems, cf. [11, Theorem 2] and [19, Section 4.7 and 4.14],

$$\sum_{k=0}^{(l+1)^2} Y_l^k(\boldsymbol{x})\overline{Y_l^k(\boldsymbol{y})} = (l+1)U_l(\cos \mathrm{d}_{\mathbb{S}^3}(\boldsymbol{x},\boldsymbol{y})), \qquad \boldsymbol{x},\boldsymbol{y} \in \mathbb{S}^3,\ l \in \mathbb{N}_0,$$

$$\sum_{m,m'=-l}^{l} D_l^{m,m'}(\boldsymbol{G})\overline{D_l^{m,m'}(\boldsymbol{H})} = (2l+1)U_{2l}\left(\cos \frac{\mathrm{d}_{\mathrm{SO}(3)}(\boldsymbol{G},\boldsymbol{H})}{2}\right), \boldsymbol{G},\boldsymbol{H} \in \mathrm{SO}(3),\ l \in \mathbb{N}_0,$$

where U_n denotes the n-th Chebyshev polynomial of second kind, lead to reproducing kernels of the spaces $\Gamma_l(\mathbb{S}^3)$ and $\Gamma_l(\mathrm{SO}(3))$, respectively. Similarly as stated in [11, Theorem 3] we can express the polynomials on $\mathbb{S}^3$ and $\mathrm{SO}(3)$ by finite linear combinations of translated kernels, that is

$$\begin{aligned}\Gamma_l(\mathbb{S}^3) &= \left\{ \sum_{j=0}^{M-1} a_j U_l(\cos \mathrm{d}_{\mathbb{S}^3}(\boldsymbol{x}_j, \cdot)) \;:\; M \in \mathbb{N},\ a_j \in \mathbb{C},\ \boldsymbol{x}_j \in \mathbb{S}^3 \right\}, \\ \Gamma_l(\mathrm{SO}(3)) &= \left\{ \sum_{j=0}^{M-1} a_j U_{2l} \left(\cos \frac{\mathrm{d}_{\mathrm{SO}(3)}(\boldsymbol{G}_j, \cdot)}{2} \right) \;:\; M \in \mathbb{N},\ a_j \in \mathbb{C},\ \boldsymbol{G}_j \in \mathrm{SO}(3) \right\}.\end{aligned} \tag{3.6}$$

Now, let $f \in \Gamma_{2N}(\mathbb{S}^3)$ be given. Then, there exists $M \in \mathbb{N}$, $\boldsymbol{x}_j \in \mathbb{S}^3$ and $a_j \in \mathbb{C}$, $j = 0, \ldots, M-1$, with

$$f(\boldsymbol{x}) = \sum_{j=0}^{M-1} a_j U_{2N}(\cos \mathrm{d}_{\mathbb{S}^3}(\boldsymbol{x}_j, \boldsymbol{x})), \qquad \boldsymbol{x} \in \mathbb{S}^3,$$

and since f is even we infer from Lemma 2.1 the equation

$$\begin{aligned} f(\boldsymbol{x}) &= \sum_{j=0}^{M-1} a_j U_{2N}(\cos \mathrm{d}_{\mathbb{S}^3}(\boldsymbol{x}_j, \boldsymbol{x})) = \sum_{j=0}^{M-1} a_j U_{2N}(\cos \mathrm{d}_{\mathbb{S}^3}(\pm\boldsymbol{x}_j, \pm\boldsymbol{x})) \\ &= \sum_{j=0}^{M-1} a_j U_{2N} \left(\cos \frac{\mathrm{d}_{\mathrm{SO}(3)}\left(\boldsymbol{q}_*^{-1}(\boldsymbol{x}_{j*}), \boldsymbol{q}_*^{-1}(\boldsymbol{x}_*)\right)}{2} \right). \end{aligned}$$

Hence, it is $\tilde{f}(\boldsymbol{q}_*(\cdot)) \in \Gamma_N(\mathrm{SO}(3))$ by equation (3.6). The other direction follows similarly. ■

The above Theorem yields the following Corollary 3.3 which states an equivalence between antipodal quadrature formulae on the three-sphere $\mathbb{S}^3$ and quadrature formulae on the rotation group $\mathrm{SO}(3)$.

Corollary 3.3. A quadrature $Q(\mathbb{S}^3)$ with antipodal nodes $\mathcal{X}(\mathbb{S}^3) := \{\pm\boldsymbol{x}_0, \ldots, \pm\boldsymbol{x}_{M-1})\}$ and corresponding weights w_i, $i = 0, \ldots, M-1$, on $\mathbb{S}^3$, integrates exactly all polynomials up to degree $2N+1$, i.e.,

$$\int_{\mathbb{S}^3} f(\boldsymbol{x}) \mathrm{d}\mu_{\mathbb{S}^3}(\boldsymbol{x}) = \sum_{i=0}^{M-1} w_i (f(-\boldsymbol{x}_i) + f(\boldsymbol{x}_i)), \qquad f \in \Pi_{2N+1}(\mathbb{S}^3),$$

if and only if the quadrature $Q(\mathrm{SO}(3))$ with weights $\tilde{w}_i = 2w_i$ and nodes $\mathcal{X}(\mathrm{SO}(3)) := \{\boldsymbol{q}_*^{-1}(\boldsymbol{x}_{0*}), \ldots, \boldsymbol{q}_*^{-1}(\boldsymbol{x}_{M-1*})\}$ integrates exactly all polynomials upto degree N, that is

$$\int_{\mathrm{SO}(3)} g(\boldsymbol{G}) \mathrm{d}\mu_{\mathrm{SO}(3)}(\boldsymbol{G}) = \sum_{i=0}^{M-1} \tilde{w}_i g(\boldsymbol{q}_*^{-1}(\boldsymbol{x}_{i*})), \qquad g \in \Pi_N(\mathrm{SO}(3)).$$

Proof. For the constant functions $f \equiv 1$ and $g \equiv 1$ the assertion is trivial, since the measures are normed

$$\int_{\mathrm{SO}(3)} 1 \mathrm{d}\mu_{\mathrm{SO}(3)}(\boldsymbol{G}) = 1 = \int_{\mathbb{S}^3} 1 \mathrm{d}\mu_{\mathbb{S}^3}(\boldsymbol{x}).$$

Furthermore, arbitrary odd functions f on $\mathbb{S}^3$ are integrated exactly by

$$\int_{\mathbb{S}^3} f(\boldsymbol{x}) \mathrm{d}\mu_{\mathbb{S}^3}(\boldsymbol{x}) = 0 = \sum_{i=0}^{M-1} w_i(-f(\boldsymbol{x}_i) + f(\boldsymbol{x}_i)).$$

Hence, the assertion follows by Lemma 3.2. ■

Remark 3.4. For the quadrature $Q(\mathbb{S}^3)$ with antipodal nodes we can assume without loss of generality that the weights for antipodal nodes are equal. Since, the quadrature keeps the same degree of exactness by setting $w_i = \frac{1}{2}(w_i^+ + w_i^-)$, if w_i^+, w_i^- are the weights for $\boldsymbol{x}_i$, $-\boldsymbol{x}_i$, respectively. □

For a construction of well distributed sampling sets and quadrature formulae on the rotation group SO(3) we refer to [7]. The proposed construction is based on a tensor like product of the two- and one-sphere, $\mathbb{S}^2$ and $\mathbb{S}^1$ respectively. Therefore, "nice" sampling sets and quadrature formulae on these spheres yield "nice" sampling sets and quadrature formulae on the rotation group SO(3). Hence, by Corollary 3.3 and Theorem 3.1 one obtains easily quadrature formulae and well distributed sampling sets on the three-sphere $\mathbb{S}^3$ via the isomorphism $\boldsymbol{q}_* : \mathrm{SO}(3) \to \mathbb{S}^3_*$, as well. It was also shown in [7] that the finite three dimensional rotation groups $\mathcal{X}_{\mathrm{T}}, \mathcal{X}_{\mathrm{O}}, \mathcal{X}_{\mathrm{I}}$ of the tetrahedron, octahedron (or hexahedron) and icosahedron (or dodecahedron), respectively, are t-designs on the rotation group. More precisely, they are sampling sets of quadrature formulae with equal weights for degree $N = 2, 3$ and 5, respectively. The antipodal vertices of the four-dimensional polyhedra 24-cell and 600-cell can be identified with the tetrahedral group and the icosahedral group respectively. Hence, the former statement is equivalent to the assertion that these form a 5-design and a 11-design on the three-sphere, which are well known facts, cf. [1, Example 2.8].

Moreover, the above results lead to a new proof of a necessary condition for the existence of nonnegative quadrature weights on the rotation group SO(3), cf. [7, Theorem 3.3]. We remark that the condition there is exactly the same as stated in the following Theorem 3.5.

Theorem 3.5. *Let the sampling set* $\mathcal{X}_N(\mathrm{SO}(3)) = \{\boldsymbol{G}_0, \ldots, \boldsymbol{G}_{M-1}\} \subset \mathrm{SO}(3)$ *support nonnegative quadrature weights* w_k, $k = 0, \ldots, M-1$, *integrating exactly all polynomials in* $\Pi_N(\mathrm{SO}(3))$, $N \in \mathbb{N}$, *then the mesh norm satisfies*

$$\delta(\mathcal{X}_N(\mathrm{SO}(3))) \leq \frac{4\pi}{N+2}. \tag{3.7}$$

Proof. Let $\mathcal{X}_{2N+1}(\mathbb{S}^3) := \{\pm\boldsymbol{x}_0, \ldots, \pm\boldsymbol{x}_{M-1}\}$ be the corresponding antipodal sampling set on $\mathbb{S}^3$, which supports by assumption by Corollary 3.3 nonnegative quadrature weights. Then we have the bound

$$\delta(\mathcal{X}_{2N+1}(\mathbb{S}^3)) \leq 2\arccos z_{N+1} = \frac{2\pi}{N+2},$$

where $z_{N+1} = \cos\frac{\pi}{N+2}$ is the greatest zero of the Chebyshev polynomial of second kind U_{N+1}, cf. [13, Theorem 6.21]. Actually the bound stated by Reimer is given for quadratures with degree of exactness $2N+2$, but if we follow the proof of [13, Theorem 6.21] line by line we see that this is also true for degree of exactness $2N+1$. By Theorem 3.1 the assertion follows from

$$\delta(\mathcal{X}_N(\mathrm{SO}(3))) = 2\delta(\mathcal{X}_{2N+1}(\mathbb{S}^3)) \leq \frac{4\pi}{N+2}.$$

■

Now we come to so-called Marcinkiewicz-Zygmund inequalities, which are an important tool in approximation theory, see the references [8, 10, 9, 4] to name but a few. They state the equivalence between L_p-norms of polynomials and l_p-norms of their samples under certain conditions. Such inequalities on the rotation group SO(3) were already established in [16] by using reproducing kernel techniques on the rotation group directly. Here we derive such inequalities by Marcinkiewicz-Zygmund inequalities on the three-sphere $\mathbb{S}^3$, cf. [10, 4].

Theorem 3.6. *Let $1 \leq p < \infty$ and $0 < C$ be given. Furthermore, let for arbitrary sampling sets $\mathcal{X}(\mathbb{S}^3) = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{M-1}\}$ with associated partitions $\mathcal{R}(\mathbb{S}^3) = \{\Omega_0, \ldots, \Omega_{M-1}\}$ the following Marcinkiewicz-Zygmund inequalities be valid*

$$\left(1 - N\|\mathcal{R}(\mathbb{S}^3)\|\right)\|f\|_p^p \leq \sum_{i=0}^{M-1} |f(\boldsymbol{x}_i)|^p \mu_{\mathbb{S}^3}(\Omega_i) \leq \left(1 + N\|\mathcal{R}(\mathbb{S}^3)\|\right)\|f\|_p^p, \tag{3.8}$$

for all polynomials $f \in \Pi_N(\mathbb{S}^3)$ with degree $N \leq C/\|\mathcal{R}(\mathbb{S}^3)\|$.

Then for arbitrary sampling sets $\mathcal{X}(\mathrm{SO}(3)) = \{\boldsymbol{G}_0, \ldots, \boldsymbol{G}_{M-1}\}$ with associated partitions $\mathcal{R}(\mathrm{SO}(3)) = \{\bar{\Omega}_0, \ldots, \bar{\Omega}_{M-1}\}$ the following Marcinkiewicz-Zygmund inequalities are valid

$$(1 - N\|\mathcal{R}(\mathrm{SO}(3))\|)\|g\|_p^p \leq \sum_{i=0}^{M-1} |g(\boldsymbol{G}_i)|^p \mu_{\mathrm{SO}(3)}(\bar{\Omega}_i) \leq (1 + N\|\mathcal{R}(\mathrm{SO}(3))\|)\|g\|_p^p, \tag{3.9}$$

for all polynomials $g \in \Pi_N(\mathrm{SO}(3))$ with degree $N \leq C/\|\mathcal{R}(\mathrm{SO}(3))\|$.

Proof. Let $g \in \Pi_N(\mathrm{SO}(3))$ be given and $f \in \Pi_{2N}(\mathbb{S}^3)$ be its unique even extension on $\mathbb{S}^3$, i.e., $g(\boldsymbol{G}) = \tilde{f}(\boldsymbol{q}_*(\boldsymbol{G}))$ for $\boldsymbol{G} \in \mathrm{SO}(3)$. Furthermore, we consider to the sampling set $\mathcal{X}(\mathrm{SO}(3))$ and its associated partition $\mathcal{R}(\mathrm{SO}(3))$ the corresponding antipodal sampling set $\mathcal{X}(\mathbb{S}^3) := \{\pm\boldsymbol{x}_0, \ldots, \pm\boldsymbol{x}_{M-1}\}$ and its associated antipodal partition $\mathcal{R}(\mathbb{S}^3) := \{\pm\Omega_0, \ldots, \pm\Omega_{M-1}\}$ on the three-sphere $\mathbb{S}^3$, respectively, i.e.,

$$\boldsymbol{q}_*(\boldsymbol{G}_i) = \{\pm\boldsymbol{x}_i\}, \quad \boldsymbol{q}_*(\bar{\Omega}_i) = \{\pm\Omega_i\}, \qquad i = 0, \ldots, M-1.$$

Since the partition norm of $\mathcal{R}(\mathbb{S}^3)$ obeys the relation $\|\mathcal{R}(\mathbb{S}^3)\| = \frac{1}{2}\|\mathcal{R}(\mathrm{SO}(3))\|$, cf. Lemma 2.1 and Theorem 3.1, we obtain from the condition $N \le C/\|\mathcal{R}(\mathrm{SO}(3))\|$ that

$$2N \le 2C/\|\mathcal{R}(\mathrm{SO}(3))\| = C/\|\mathcal{R}(\mathbb{S}^3)\|.$$

Hence, by the Marcinkiewicz-Zygmund inequalities (3.8) on the three-sphere $\mathbb{S}^3$ we have

$$\begin{aligned}\left(1 - 2N\|\mathcal{R}(\mathbb{S}^3)\|\right)\|f\|_p^p \le \sum_{i=0}^{M-1} \left(|f(\boldsymbol{x}_i)|^p \mu_{\mathbb{S}^3}(\Omega_i) + |f(-\boldsymbol{x}_i)|^p \mu_{\mathbb{S}^3}(-\Omega_i)\right)\\ \le \left(1 + 2N\|\mathcal{R}(\mathbb{S}^3)\|\right)\|f\|_p^p.\end{aligned}$$

From Lemma 2.1 and definition (2.8) we infer that

$$\|f\|_p^p = \int |f(\boldsymbol{x})|^p \mathrm{d}\mu_{\mathbb{S}^3}(\boldsymbol{x}) = \int |\tilde{f}(\boldsymbol{x}_*)|^p \mathrm{d}\mu_{\mathbb{S}^3_*}(\boldsymbol{x}_*) = \int |g(\boldsymbol{G})|^p \mathrm{d}\mu_{\mathrm{SO}(3)}(\boldsymbol{G}) = \|g\|_p^p$$

and that $\mu_{\mathbb{S}^3}(\Omega_i) = \mu_{\mathbb{S}^3}(-\Omega_i) = \frac{1}{2}\mu_{\mathbb{S}^3_*}(\Omega_{i*}) = \frac{1}{2}\mu_{\mathrm{SO}(3)}(\bar{\Omega}_i)$. Thus, by using again the relations $2\|\mathcal{R}(\mathbb{S}^3)\| = \|\mathcal{R}(\mathrm{SO}(3))\|$ and $f(\pm\boldsymbol{x}_i) = g(\boldsymbol{q}_*^{-1}(\boldsymbol{x}_{i*})) = g(\boldsymbol{G}_i)$ we obtain the assertion (3.9). ■

Remark 3.7. The converse statement need not to be true, due to the missing counterpart on the rotation group SO(3) for the odd functions on the three-sphere $\mathbb{S}^3$. Hence, this approach might not lead to sharp conditions and one has to operate on the rotation group directly as proposed by D. Schmid in [16, 18]. □

4 Conclusion

In this paper we showed that in the setting of scattered data approximation the rotation group SO(3) and the three-sphere $\mathbb{S}^3$ can be treated almost equally. That is for scattered sampling nodes one obtains in the natural metrics the same values for the mesh norm and the separation distance up to a proportional factor, if we identify antipodal nodes on the three-sphere with a rotation. For the polynomial spaces we can identify even functions on the three-sphere $\mathbb{S}^3$ with functions on the rotation group SO(3). However this leads to a discrepancy in the approximation behavior for scattered data on those manifolds, since the odd functions on $\mathbb{S}^3$ lack a counter part on SO(3).

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