Electronic Transactions on Numerical Analysis.
Volume 31, pp. 30-39, 2008.

ISSN 1068-9613.

ETNA
Kent State University
etna@mcs.kent.edu

STABILITY RESULTS FOR SCATTERED DATA INTERPOLATION ON THE ROTATION GROUP*

MANUEL GRÄF† AND STEFAN KUNIS†

Abstract. Fourier analysis on the rotation group $SO(3)$ expands each function into the orthogonal basis of Wigner-D functions. Recently, fast and reliable algorithms for the evaluation of finite expansion of such type, referred to as nonequispaced FFT on $SO(3)$, have become available. Here, we consider the minimal norm interpolation of given data by Wigner-D functions. We prove bounds on the conditioning of this problem which rely solely on the number of Fourier coefficients and the separation distance of the sampling nodes. The reconstruction of N^3 Fourier coefficients from M well separated samples is shown to take only $\mathcal{O}(N^3 \log^2 N + M)$ floating point operations.

Key words. Scattered data interpolation, iterative methods, FFT.

AMS subject classifications. 65T50, 65F10, 43A75, 41A05, 15A60.

1. Introduction. Scattered data interpolation and approximation on various domains is a practical problem with many important applications in science and engineering. In our particular setting, we are interested in functions defined on the rotation group $SO(3)$; cf. [24, 26]. Recent applications include protein-protein docking problems [3] and texture analysis in crystallography [25]. Given a set of measurements $(\boldsymbol{G}_j, y_j) \in SO(3) \times \mathbb{C}$, $j = 0, \ldots, M-1$, discrete least squares approximation by Wigner-D functions (similar to the complex exponentials on the circle) relies on two ingredients: a fast Fourier transform on the rotation group (see [9, 19]) and estimates on the involved condition numbers by means of Marcinkiewicz-Zygmund inequalities [6, 8, 13, 23].

On the other hand, interpolation by radial basis functions on $\mathbb{R}^d$ has become a mature tool during the last decade; see e.g. [27] and references therein. Recent generalizations to other domains include manifolds like the Euclidean spheres [10, 12, 17] or compact groups like $SO(3)$ [4, 5, 7]. Central themes in the study of such methods are their convergence rates and the conditioning of proposed solution schemes; see [21, 22] for a trade-off principle.

We are interested in the condition numbers of interpolation matrices and follow the seminal papers [1, 18] to prove explicit bounds for the extremal eigenvalues of the interpolation problem with respect to the separation distance of the sampling nodes. More specifically, the simple constraint that the polynomial degree is bounded from below by a constant multiple of the inverse separation distance turns out to be a sharp condition that allows for polynomial interpolation; cf. Theorem 3.4. Our result implies that N^3 Fourier coefficients can be computed from M well separated samples in $\mathcal{O}(N^3 \log^2 N + M)$ floating point operations; see Corollary 3.5. Moreover, Corollary 3.7 generalizes and improves a recent result [17, Theorems 2.8, 3.6] on the deterioration of the smallest eigenvalue for interpolation with minimal Sobolev norm. The proof of our main result relies on a refined version of the packing argument [5, Lemma 5.1], the construction of strongly localized polynomials on the rotation group by using a smoothness-decay principle in Fourier analysis [11, 14, 16], and a simple eigenvalue estimate by the Gershgorin circle theorem.

2. Prerequisite. Let $SO(3) := \{\boldsymbol{G} \in \mathbb{R}^{3\times 3} : \boldsymbol{G}^T\boldsymbol{G} = \boldsymbol{I}, \det \boldsymbol{G} = 1\}$ denote the (compact semisimple Lie) group of rotations in the Euclidean space $\mathbb{R}^3$; cf. [24, 26]. The parameterization of $SO(3)$ in terms of Euler angles $(\phi_1, \theta, \phi_2) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi)$

* Received November 30, 2007. Accepted July 3, 2008. Published online on October 24, 2008. Recommended by Oliver Ernst.

†Chemnitz University of Technology, Department of Mathematics, 09107 Chemnitz, Germany (`{m.graef,kunis}@mathematik.tu-chemnitz.de`)

ETNA
Kent State University
etna@mcs.kent.edu

allows the following representation of rotations

$$\boldsymbol{G} = \boldsymbol{G}(\phi_1, \theta, \phi_2) = \boldsymbol{R}_z(\phi_1)\boldsymbol{R}_y(\theta)\boldsymbol{R}_z(\phi_2),$$

where

$$\boldsymbol{R}_z(t) = \begin{bmatrix} \cos(t) & -\sin(t) & 0 \\ \sin(t) & \cos(t) & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \boldsymbol{R}_y(t) = \begin{bmatrix} \cos(t) & 0 & -\sin(t) \\ 0 & 1 & 0 \\ \sin(t) & 0 & \cos(t) \end{bmatrix}.$$

Moreover, $SO(3)$ can be identified with the three dimensional projective space such that $SO(3) \ni \boldsymbol{G} \mapsto \omega \boldsymbol{x}$ with rotation axis $\boldsymbol{x} \in \mathbb{R}^3$, i.e., $\boldsymbol{G}\boldsymbol{x} = \boldsymbol{x}$, $\|\boldsymbol{x}\| = 1$, and rotation angle $\omega \in [0, \pi]$ given by

$$\omega = \omega(\boldsymbol{G}) := \arccos \frac{\operatorname{trace}(\boldsymbol{G}) - 1}{2}.$$

In particular, this yields the translation invariant metric

$$\mathrm{d}(\boldsymbol{G}, \boldsymbol{H}) := \omega(\boldsymbol{H}^{-1}\boldsymbol{G}).$$

Now, let a sampling set $\mathcal{X} := \{\boldsymbol{G}_j \in SO(3) : j = 0, \ldots, M-1\}$, $M \in \mathbb{N}$, be given and measure its "nonuniformity" by the separation distance

$$q_{\mathcal{X}} := \min_{0 \le j < l < M} \mathrm{d}(\boldsymbol{G}_j, \boldsymbol{G}_l).$$

The sampling set $\mathcal{X}$ is called q-separated for some $0 < q \le \pi$ if $q_{\mathcal{X}} \ge q$. Moreover, we decompose the sampling set $\mathcal{X} \subset SO(3)$ into shells

$$R_{\mathcal{X},q,m} := \{\boldsymbol{G} \in \mathcal{X} : mq \le \mathrm{d}(\boldsymbol{G}, \boldsymbol{I}) < (m+1)q\}, \qquad m \in \mathbb{N}. \tag{2.1}$$

For measurable functions $f : SO(3) \to \mathbb{C}$, the normalized Haar integral is given by

$$\int_{SO(3)} f(\boldsymbol{G}) \,\mathrm{d}\mu(\boldsymbol{G}) = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} f(\phi_1, \theta, \phi_2) \sin(\theta) \,\mathrm{d}\phi_2 \,\mathrm{d}\theta \,\mathrm{d}\phi_1.$$

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

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

In analogy to the complex exponentials $\mathrm{e}^{\mathrm{i}kx}$ on the circle, the Wigner-D functions $D_l^{k,k'}$ of degree $l \in \mathbb{N}_0$ and orders $k, k' = -l, \ldots, l$ are the key to Fourier analysis on the rotation group. First, let the space of square integrable functions on the unit sphere $f : \mathbb{S}^2 \to \mathbb{C}$ be decomposed into the mutual orthogonal spaces of spherical harmonics of degree $l \in \mathbb{N}_0$ and let $\{Y_l^k : \mathbb{S}^2 \to \mathbb{C} : k = -l, \ldots, l\}$ denote an orthonormal basis for each of them; see [15] for details. Then, the Wigner-D functions are defined pointwise by

$$D_l^{k,k'}(\boldsymbol{G}) := \int_{\mathbb{S}^2} Y_l^{k'}\left(\boldsymbol{G}^{-1}\boldsymbol{\xi}\right) \overline{Y_l^k(\boldsymbol{\xi})} \,\mathrm{d}\mu_{\mathbb{S}^2}(\boldsymbol{\xi}) \quad \text{and} \quad \int_{\mathbb{S}^2} \mathrm{d}\mu_{\mathbb{S}^2}(\boldsymbol{\xi}) = 4\pi.$$

They form an orthogonal basis of $L^2(SO(3))$, are normalized by $\|D_l^{k,k'}\|_{L^2}^2 = 1/(2l+1)$, and every $f \in L^2(SO(3))$ obeys the series expansion

$$f = \sum_{l\in\mathbb{N}_0} \sum_{k,k'=-l}^{l} \hat{f}_l^{k,k'} D_l^{k,k'}$$

with Fourier-Wigner coefficients

$$\hat{f}_l^{k,k'} = (2l+1) \int_{SO(3)} f(\boldsymbol{G})\, \overline{D_l^{k,k'}(\boldsymbol{G})}\, \mathrm{d}\mu(\boldsymbol{G}).$$

For later reference we define a family of Sobolev spaces $H_s^2 \subset L^2(SO(3))$, $s > \frac{3}{2}$, with inner product and norm

$$\langle f, g\rangle_{H_s^2} := \sum_{l\in\mathbb{N}_0} \sum_{k,k'=-l}^{l} (1+l)^{2s-1}\, \hat{f}_l^{k,k'} \overline{\hat{g}_l^{k,k'}}, \qquad \|f\|_{H_s^2} = \sqrt{\langle f, f\rangle_{H_s^2}}.$$

One of the more remarkable properties of the Wigner-D functions is the addition theorem

$$\sum_{k,k'=-l}^{l} D_l^{k,k'}(\boldsymbol{G})\, \overline{D_l^{k,k'}(\boldsymbol{H})} = U_{2l}\left(\cos \frac{\mathrm{d}(\boldsymbol{G},\boldsymbol{H})}{2}\right), \tag{2.2}$$

where $U_l(\cos\omega) = \sin((l+1)\omega)/\sin(\omega)$ denotes the l-th Chebyshev polynomial of the second kind. For a sampling set $\mathcal{X} = \{\boldsymbol{G}_j \in SO(3) : j = 0, \dots, M-1\}$, we call

$$\boldsymbol{D} = \left(D_l^{k,k'}(\boldsymbol{G}_j)\right)_{j=0,\dots,M,(l,k,k')\in J_N} \in \mathbb{C}^{M\times d_N}$$

the nonequispaced Fourier matrix on the rotation group, where

$$d_N = \frac{1}{6}(2N+1)(2N+2)(2N+3),$$
$$J_N := \{(l,k,k') \;:\; l = 0,\dots,N;\; k,k' = -l,\dots,l\}.$$

Given a vector of Fourier coefficients $\hat{\boldsymbol{f}} \in \mathbb{C}^{d_N}$ we call

$$f(\boldsymbol{G}) = \sum_{(l,k,k')\in J_N} \hat{f}_l^{k,k'} D_l^{k,k'}(\boldsymbol{G})$$

the corresponding polynomial on the rotation group and denote by $P_N(SO(3))$ the linear space of all such polynomials. Its evaluation at the sampling nodes $\mathcal{X} \subset SO(3)$ can be written in matrix vector form by $\boldsymbol{f} = (f(\boldsymbol{G}_j))_{j=0,\dots,M-1} = \boldsymbol{D}\hat{\boldsymbol{f}}$.

In what follows, we study the underdetermined interpolation of scattered data on $SO(3)$ by polynomials. Let $M < d_N$, a sampling set $\mathcal{X} = \{\boldsymbol{G}_j \in SO(3) : j = 0,\dots,M-1\}$, values $y_j \in \mathbb{C}$ for $j = 0,\dots,M-1$, and weights $\hat{w}_l > 0$ for $l = 0,\dots,N$ be given. Then, the minimal norm interpolation problem is given by

$$\min_{\hat{\boldsymbol{f}}} \sum_{(l,k,k')\in J_N} \frac{\left|\hat{f}_l^{k,k'}\right|^2}{\hat{w}_l} \qquad \text{s.t.} \qquad f(\boldsymbol{G}_j) = y_j, \quad j = 0\dots M-1. \tag{2.3}$$

3. Results. We begin with the following lemmas.

LEMMA 3.1. *Every q-separated sampling set $\mathcal{X} \subset SO(3)$ has cardinality*

$$M \leq \frac{109\pi}{2q^3}.$$

Moreover, there exists a q-separated sampling set of cardinality $M \geq 6\pi/q^3$. Given a q-separated sampling set, its decomposition into shells $R_{\mathcal{X},q,m}$ (cf. (2.1)) allows for the cardinality estimate

$$|R_{\mathcal{X},q,m}| \leq 48m^2 + 48m + 28.$$

Proof. Let $B_r(\boldsymbol{H}) := \{\boldsymbol{G} \in SO(3) : \mathrm{d}(\boldsymbol{G}, \boldsymbol{H}) \leq r\}$ denote the ball of radius $r \in (0, \pi]$ around $\boldsymbol{H} \in SO(3)$ with given measure

$$\mu\left(B_r(\boldsymbol{H})\right) = \int_{B_r(\boldsymbol{I})} \mathrm{d}\mu\left(\boldsymbol{G}\right) = \frac{2}{\pi}\int_0^r \sin^2\left(\frac{t}{2}\right)\mathrm{d}t. \tag{3.1}$$

From [5, Lemma 5.1], we know that $\mu\left(B_{q/2}(\boldsymbol{I})\right) \geq \frac{2}{\pi}\frac{q^3}{109}$ for $0 < q \leq \pi$. Since the sampling set is q-separated, we can consider all balls of radius $q/2$ with centers at the sampling nodes $\boldsymbol{G}_j$ to obtain the upper bound of the cardinality

$$M \leq \frac{\mu\left(SO(3)\right)}{\mu\left(B_{q/2}(\boldsymbol{I})\right)} \leq \frac{109\pi}{2q^3}.$$

Regarding the second claim, we presume the contrary, i.e., let a q-separated sampling set $\mathcal{X}$ with $M < 6\pi/q^3$ nodes be given. Around each node, we place a ball of radius q and obtain

$$\mu\left(SO(3)\backslash \bigcup_{j=0}^{M-1} B_q(\boldsymbol{G}_j)\right) \geq \mu\left(SO(3)\right) - \sum_{j=0}^{M-1}\mu\left(B_q(\boldsymbol{G}_j)\right) \geq 1 - M\frac{q^3}{6\pi} > 0,$$

where the estimate $\mu(B_q(\boldsymbol{G}_j)) \leq q^3/(6\pi)$ is due to $\sin(t/2) \leq t/2$ in (3.1). Hence, the set $SO(3)\backslash \bigcup_{j=0}^{M-1} B_q(\boldsymbol{G}_j)$ is not empty and there exists a point $\boldsymbol{G} \in SO(3)$ such that $\mathcal{X} \cup \{\boldsymbol{G}\}$ remains q-separated.

For the last assertion, we start by the estimate

$$\frac{n^2+1}{2}x - \frac{n^2-1}{2x} - T_n(x) = \int_x^1 \left(T_n'(t) - \frac{n^2+1}{2} - \frac{n^2-1}{2t^2}\right)\mathrm{d}t \leq 0,$$

where $x \in (0, 1]$, $n \in \mathbb{N}$ and $T_n(t) = \cos(n \arccos t)$ denotes the Chebyshev polynomials of the first kind, which derives from the upper bound $\max_{0\leq t\leq 1}|T_n'(t)| \leq n^2$. Multiplying both sides by $x\sqrt{1-x^2}$, substituting $x = \cos r$, and adding r on both sides, we get the equivalent formulation

$$r + (3n^2+4)\sin(r) - \cos(nr)\cos(r)\sin(r) \leq r + (3n^2+3)\left(\sin(r) + \frac{\sin^3(r)}{6}\right)$$

for $r \in \left[0, \frac{\pi}{2}\right]$. Truncating the power series of the arcsine, we obtain the bound $\sin(r) + \sin^3(r)/6 \leq \arcsin(\sin(r)) = r$. Bringing $(3n^2+4)\sin(r)$ to the right, dividing by $r - \sin(r)$, and setting $r = q/2$ and $n = 2m+1$ results in the assertion from the packing argument by

$$|R_{\mathcal{X},q,m}| \leq \frac{\mu\left(B_{q(m+\frac{3}{2})}(\boldsymbol{I}) \setminus B_{q(m-\frac{1}{2})}(\boldsymbol{I})\right)}{\mu\left(B_{\frac{q}{2}}(\boldsymbol{I})\right)} = 4\frac{\frac{q}{2} - \cos\left((2m+1)\frac{q}{2}\right)\cos\left(\frac{q}{2}\right)\sin\left(\frac{q}{2}\right)}{\frac{q}{2} - \sin\left(\frac{q}{2}\right)}.$$

Equality in the above estimates holds for $q \to 0$. □

LEMMA 3.2. *The optimal interpolation problem* (2.3) *is equivalent to the normal equations of the second kind*

$$\boldsymbol{D}\hat{\boldsymbol{W}}\boldsymbol{D}^{\mathsf{H}}\tilde{\boldsymbol{f}} = \boldsymbol{y}, \qquad \hat{\boldsymbol{f}} = \hat{\boldsymbol{W}}\boldsymbol{D}^{\mathsf{H}}\tilde{\boldsymbol{f}}, \tag{3.2}$$

where $\boldsymbol{D}^{\mathsf{H}}$ *denotes the conjugate transpose of* $\boldsymbol{D}$ *and the weighting matrix is given by* $\hat{\boldsymbol{W}} := \mathrm{diag}(\tilde{\boldsymbol{w}}) \in \mathbb{R}^{d_N \times d_N}$ *for the vector*

$$\tilde{\boldsymbol{w}} = (\tilde{w}_l^{k,k'})_{(l,k,k')\in J_N}$$

with $\tilde{w}_l^{k,k'} = \hat{w}_l$, $l = 0,\ldots,N$, $|k|,|k'| \le l$.

Moreover, let the trigonometric polynomial $K_N : [-\pi,\pi] \to \mathbb{R}$ *and its corresponding interpolation matrix* $\boldsymbol{K} = (k_{i,j})_{i,j=0,\ldots,M-1}$ *be given by*

$$K_N(t) := \sum_{l=0}^{N} \hat{w}_l U_{2l}(\cos(t/2)), \qquad k_{i,j} := K_N(\mathrm{d}(\boldsymbol{G}_i, \boldsymbol{G}_j)). \tag{3.3}$$

Then, we have the identity $\boldsymbol{K} = \boldsymbol{D}\hat{\boldsymbol{W}}\boldsymbol{D}^{\mathsf{H}}$.

Proof. In matrix-vector form the optimization problem (2.3) reads as

$$\min_{\hat{\boldsymbol{f}}\in\mathbb{C}^{d_N}} \hat{\boldsymbol{f}}^{\mathsf{H}}\hat{\boldsymbol{W}}^{-1}\hat{\boldsymbol{f}} \quad \text{s.t.} \quad \boldsymbol{D}\hat{\boldsymbol{f}} = \boldsymbol{y}.$$

So the first assertion is due to [2, Theorem 1.1.2] for the matrix $\boldsymbol{D}\hat{\boldsymbol{W}}^{1/2}$. The second assertion follows from the addition theorem (2.2), i.e.,

$$\begin{aligned}(\boldsymbol{D}\hat{\boldsymbol{W}}\boldsymbol{D}^{\mathsf{H}})_{i,j} &= \sum_{l=0}^{N} \hat{w}_l \sum_{k,k'=-l}^{l} D_l^{k,k'}(\boldsymbol{G}_i)\,\overline{D_l^{k,k'}(\boldsymbol{G}_j)} \\ &= \sum_{l=0}^{N} \hat{w}_l U_{2l}\left(\cos\frac{\mathrm{d}(\boldsymbol{G}_i,\boldsymbol{G}_j)}{2}\right). \qquad \square\end{aligned}$$

Let the normalized B-spline of order $\beta \in \mathbb{N}$ be defined by

$$g_\beta : \left[-\frac{1}{2},\frac{1}{2}\right] \to \mathbb{R}, \quad g_\beta(z) := \beta N_\beta\left(\beta z + \frac{\beta}{2}\right), \quad \|g_\beta\|_{L^1} = 1,$$

with the cardinal B-spline given by

$$N_{\beta+1}(z) = \int_{z-1}^{z} N_\beta(\tau)\,\mathrm{d}\tau, \quad \beta\in\mathbb{N}, \qquad N_1(z) = \begin{cases} 1 & 0 < z < 1, \\ 0 & \text{otherwise.}\end{cases}$$

Moreover, for $N \in \mathbb{N}$ let

$$\|g_\beta\|_{1,N} := \sum_{l=-N}^{N} g_\beta\left(\frac{l}{2(N+1)}\right)$$

denote a discrete norm of g_β.

LEMMA 3.3. *Let* $N,\beta\in\mathbb{N}$, $N \ge \beta - 1 \ge 1$, *and* $B_{\beta,N}(t) = \sum_{l=0}^{N} \hat{w}_l U_{2l}(\cos(t/2))$ *with*

$$0 < \hat{w}_l := \frac{1}{\|g_\beta\|_{1,N}} \begin{cases} g_\beta\left(\frac{l}{2(N+1)}\right) - g_\beta\left(\frac{l+1}{2(N+1)}\right) & 0 \le l < N, \\ g_\beta\left(\frac{N}{2(N+1)}\right) & l = N, \end{cases} \tag{3.4}$$

ETNA
Kent State University
etna@mcs.kent.edu

be given and let $\zeta(\beta) := \sum_{l=1}^{\infty} l^{-\beta}$ denote the Riemann zeta function. Then the localization property

$$|B_{\beta,N}(t)| \le c_\beta \, |(N+1)t|^{-\beta}, \qquad c_\beta := \frac{\left(2^\beta - 1\right)\zeta(\beta)\,\beta^\beta}{2^{\beta-1} - \zeta(\beta)\,\pi^{-\beta}}, \tag{3.5}$$

holds true for $t \in (0, \pi]$, with normalization $B_{\beta,N}(0) = 1$.

Proof. We first note that the Chebyshev polynomials of the first kind are related to the Chebyshev polynomials of the second kind by $T_l = \frac{1}{2}(U_l - U_{l-2})$, $U_{2l} = \sum_{k=0}^{l}(2-\delta_{0,k})T_{2k}$. In conjunction with (3.4), we obtain

$$\sum_{l=0}^{N} \hat{w}_l U_{2l} = \sum_{k=0}^{N}(2-\delta_{0,k})T_{2k}\sum_{l=k}^{N}\hat{w}_l = \sum_{k=0}^{N}(2-\delta_{0,k})\frac{1}{\|g_\beta\|_{1,N}}\, g_\beta\left(\frac{k}{2(N+1)}\right)T_{2k}.$$

Applying the simple equality $T_{2l}(\cos(t/2)) = \cos(2lt/2) = T_l(\cos(t))$, we arrive at

$$B_{\beta,N}(t) = \sum_{l=0}^{N}(2-\delta_{0,l})\frac{1}{\|g_\beta\|_{1,N}}\, g_\beta\left(\frac{l}{2(N+1)}\right)T_l(\cos(t))$$

from which the assertion follows by [8, Lemma 7]. □

We obtain the following result on the conditioning of the interpolation problem (2.3).

THEOREM 3.4. *Let $q > 0$ and $\mathcal{X} \subset SO(3)$ be a q-separated sampling set of cardinality $M \in \mathbb{N}$. Moreover, let $N, \beta \in \mathbb{N}$, $N \ge \beta - 1 \ge 3$ be given and define the weights $\hat{w}_k$ by (3.4) and the kernel matrix $\boldsymbol{K} \in \mathbb{R}^{M\times M}$ by (3.3). Then, the eigenvalues $\lambda_0 \le \dots \le \lambda_{M-1}$ of $\boldsymbol{K}$ satisfy $\lambda_0 \le 1 \le \lambda_{M-1}$ and*

$$|\lambda_j - 1| \le c_\beta(48\zeta(\beta-2) + 48\zeta(\beta-1) + 28\zeta(\beta))\,((N+1)q)^{-\beta} \tag{3.6}$$

for $j = 0, \dots, M-1$, where c_β is given in (3.5). In particular, the matrix $\boldsymbol{D} \in \mathbb{C}^{M\times d_N}$ has full rank M whenever $N + 1 \ge 18/q$ and this condition is optimal in the sense that there is another q-separated sampling set $\mathcal{X}' \subset SO(3)$ of cardinality M and a constant $C_1 > 0$ such that for $N + 1 \le C_1/q$ the matrix $\boldsymbol{D}'$ has rank less than M.

Proof. The first assertion follows from $\sum_{j=0}^{M-1}\lambda_j = MB_{\beta,N}(0) = M$. Moreover, the Gershgorin circle theorem yields, for every $0 \le r \le M-1$ and some $0 \le l \le M-1$, that

$$|\lambda_r - k_{l,l}| \le \sum_{\substack{j=0\\ j\ne l}}^{M-1} |B_{\beta,N}(\mathrm{d}(\boldsymbol{G}_j, \boldsymbol{G}_l))|\,.$$

Using the last assertion of Lemma 3.1 and the localization property as shown in Lemma 3.3, the assertion follows from the estimate

$$\begin{aligned}|\lambda_r - 1| &\le \sum_{m=1}^{\lfloor \pi q^{-1}\rfloor} |R_{\mathcal{X},q,m}| \max_{\boldsymbol{G}\in R_{\mathcal{X},q,m}} |B_{\beta,N}(\mathrm{d}(\boldsymbol{I},\boldsymbol{G}))| \\ &\le \sum_{m=1}^{\infty} c_\beta(48m^2 + 48m + 28)\,((N+1)mq)^{-\beta}\,.\end{aligned}$$

The last claim derives from $c_4 = 3840\pi^4/719$, i.e., we set $\beta = 4$. The optimality of this condition can be seen by applying Lemma 3.1 and using the fact that the number of Fourier

ETNA
Kent State University
etna@mcs.kent.edu

coefficients is bounded by $d_N \leq C_2 N^3$. Hence, there is a constant $C_1 > 0$ such that $N+1 \leq C_1/q$ implies $d_N < M$, and thus $\operatorname{rank}(\boldsymbol{D}') < M$. □

COROLLARY 3.5. *Under the conditions of Theorem 3.4 with $\beta = 4$, the conjugate gradient method applied to (3.2) converges linearly, i.e.,*

$$\|\hat{\boldsymbol{e}}_l\|_{\hat{\boldsymbol{W}}^{-1}} \leq 2\left(\frac{17.2}{(N+1)q}\right)^{4l} \|\hat{\boldsymbol{e}}_0\|_{\hat{\boldsymbol{W}}^{-1}},$$

where the initial error is $\hat{\boldsymbol{e}}_0 := \hat{\boldsymbol{W}}\boldsymbol{D}^{\mathsf{H}}\boldsymbol{K}^{-1}\boldsymbol{y}$ and the error associated to the l-th iterate $\hat{\boldsymbol{f}}_l$ is given by $\hat{\boldsymbol{e}}_l := \hat{\boldsymbol{f}}_l - \hat{\boldsymbol{W}}\boldsymbol{D}^{\mathsf{H}}\boldsymbol{K}^{-1}\boldsymbol{y}$.

Proof. Applying the standard estimate for the convergence of the conjugate gradient method (cf. [2, p. 289]) and the estimate (3.6) yields the assertion. □

REMARK 3.6. We solve problem (3.2) by a factorized variant of conjugated gradients (CGNE, where N stands for “Normal equation” and E for “Error minimization”) [2, p. 269], where we use the nonequispaced fast Fourier transform on the rotation group [19] for fast matrix vector multiplications with $\boldsymbol{D}$ and its adjoint $\boldsymbol{D}^{\mathsf{H}}$. Note that for $(N+1)q \geq 18$ a constant number of iterations $l = \mathcal{O}(\log\varepsilon)$ suffices to decrease the error to a certain fraction $\|\hat{\boldsymbol{e}}_l\|_{\hat{\boldsymbol{W}}^{-1}}/\|\hat{\boldsymbol{e}}_0\|_{\hat{\boldsymbol{W}}^{-1}} \leq \varepsilon$. Thus, the total number of floating point operations is $\mathcal{O}((N^3\log^2 N + M)\log\varepsilon)$.

In the following we give an estimate of the smallest eigenvalue for an interpolation problem with minimal Sobolev norm. Our result generalizes [17, Theorems 2.8, 3.6] to the rotation group and improves the involved constant. Similar techniques have been used in [4, Theorem 5.1].

COROLLARY 3.7. *Let $q > 0$ and $\mathcal{X} \subset SO(3)$ be a q-separated sampling set of cardinality $M \in \mathbb{N}$. Moreover, let $s > \frac{3}{2}$ be given and consider the interpolation problem*

$$\min_{f\in H_s^2} \|f\|_{H_s^2} \qquad \text{s.t.} \qquad f(\boldsymbol{G}_j) = y_j, \quad j = 0\ldots M-1. \tag{3.7}$$

This problem is (only) mildly ill-posed in the sense that the smallest eigenvalue $\lambda_0(\boldsymbol{M})$ of the corresponding interpolation matrix

$$\boldsymbol{M} = (m_{i,j})_{i,j=0,\ldots,M-1}, \qquad m_{i,j} = \sum_{l=0}^{\infty}(1+l)^{1-2s}U_{2l}\left(\cos\frac{\mathrm{d}(\boldsymbol{G}_i,\boldsymbol{G}_j)}{2}\right), \tag{3.8}$$

satisfies

$$\lambda_0(\boldsymbol{M}) \geq \left(\frac{1}{30}\right)^{2s-2} q^{2s-3}.$$

Proof. We start with the polynomial interpolation matrix $\boldsymbol{K}$ from Theorem 3.4, with $N = \lfloor 30/q \rfloor - 1 \geq 8$ and $\beta = 4$. Due to $q \leq \pi$, the estimate (3.6) yields a smallest eigenvalue $\lambda_0(\boldsymbol{K}) \geq 2/3$. For the corresponding weights $\hat{w}_l$, $l = 0,\ldots,N$, according to (3.4) we have the formula

$$\hat{w}_l = \frac{16}{\|g_4\|_{1,N}} \begin{cases} \dfrac{2l+1}{(N+1)^2} - \dfrac{3l^2+3l+1}{(N+1)^3} & \text{for } 0 \leq l \leq \frac{N+1}{2} - 1, \\ \dfrac{1}{N+1} - \dfrac{1+2l}{(N+1)^2} + \dfrac{3l^2+3l+1}{3(N+1)^3} & \text{for } \frac{N+1}{2} \leq l \leq N, \\ \dfrac{1}{4(N+1)} - \dfrac{1}{12(N+1)^3} & \text{for } N \text{ even and } l = \lfloor \frac{N+1}{2} \rfloor. \end{cases}$$

ETNA
Kent State University
etna@mcs.kent.edu

Due to the estimate $\|g_4\|_{1,N} \geq 1.9(N+1)$ (cf. [11, Lemma 3.2]) the weights satisfy

$$\hat{w}_l \leq 10\frac{2l+1}{(N+1)^3}, \qquad l = 0, \ldots, N. \tag{3.9}$$

Now, let $\boldsymbol{c} \in \mathbb{C}^M$ be given. The assertion follows from the addition theorem (2.2) by

$$\begin{aligned}\sum_{i,j=0}^{M-1} c_i \overline{c_j} m_{i,j} &= \sum_{i,j=0}^{M-1} c_i \overline{c_j} \sum_{l=0}^{\infty} (1+l)^{1-2s} U_{2l}\left(\cos\frac{\mathrm{d}\left(\boldsymbol{G}_i, \boldsymbol{G}_j\right)}{2}\right) \qquad (3.10)\\ &= \sum_{l=0}^{\infty} (1+l)^{1-2s} \sum_{k,k'=-l}^{l} \left|\sum_{i=0}^{M-1} c_i D_l^{k,k'}\left(\boldsymbol{G}_i\right)\right|^2.\end{aligned}$$

We decrease the right hand side by truncating to N terms and insert our "nice" weights $\hat{w}_l$:

$$\begin{aligned}\boldsymbol{c}^{\mathsf{H}} \boldsymbol{M} \boldsymbol{c} &\geq \sum_{l=0}^{N} (1+l)^{1-2s} \hat{w}_l^{-1} \hat{w}_l \sum_{k,k'=-l}^{l} \left|\sum_{i=0}^{M-1} c_i D_l^{k,k'}\left(\boldsymbol{G}_i\right)\right|^2\\ &\geq \min_{r=0,\ldots,N} (1+r)^{1-2s} \hat{w}_r^{-1} \sum_{l=0}^{N} \hat{w}_l \sum_{k,k'=-l}^{l} \left|\sum_{i=0}^{M-1} c_i D_l^{k,k'}\left(\boldsymbol{G}_i\right)\right|^2\\ &\geq \min_{r=0,\ldots,N} \frac{1}{20} \frac{(N+1)^3}{(r+1)^{2s}} \sum_{l=0}^{N} \hat{w}_l \sum_{k,k'=-l}^{l} \left|\sum_{i=0}^{M-1} c_i D_l^{k,k'}\left(\boldsymbol{G}_i\right)\right|^2\\ &\geq \frac{1}{20}(N+1)^{3-2s} \sum_{i,j=0}^{M-1} c_i \overline{c_j} k_{i,j}. \qquad (3.11)\end{aligned}$$

Finally, we use the fact that the minimal value in (3.10) is $\lambda_0(\boldsymbol{M})\|\boldsymbol{c}\|_2^2$ and the last expression in (3.11) can be bounded from below by $1/20 \cdot (q/30)^{2s-3} \cdot \lambda_0(\boldsymbol{K})\|\boldsymbol{c}\|_2^2$. ☐

REMARK 3.8. For the actual solution of the interpolation problem (3.7), we use a so-called fast summation scheme [20] for multiplication with $\boldsymbol{M} \in \mathbb{C}^{M\times M}$. Given $\varepsilon > 0$, we approximate $\boldsymbol{M} \approx \tilde{\boldsymbol{M}}$ by truncating the series in (3.8) to a polynomial degree $N \in \mathbb{N}$ such that the remainder fulfills

$$|m_{i,j} - \tilde{m}_{i,j}| = \sum_{l=N+1}^{\infty} (1+l)^{1-2s} \left|U_{2l}\left(\cos\frac{\mathrm{d}\left(\boldsymbol{G}_i, \boldsymbol{G}_j\right)}{2}\right)\right| \leq 2\int_N^{\infty} (1+l)^{2-2s}\, \mathrm{d}l \leq \varepsilon.$$

Due to the addition theorem (2.2) and the nonequispaced FFT on the rotation group [19], this yields the factorization $\tilde{\boldsymbol{M}} = \boldsymbol{D}\hat{\boldsymbol{W}}\boldsymbol{D}^{\mathsf{H}}$ which can be applied to a vector in $\mathcal{O}(N^3 \log^2 N + M)$ floating point operations. Since we ask at least for mildly ill-posed matrices $\boldsymbol{M}, \tilde{\boldsymbol{M}}$, we moreover force $N \geq \lfloor 30/q \rfloor - 1$. Thus, for q-separated sampling sets with $M \geq C_3/q^3$ nodes, the multiplication with $\tilde{\boldsymbol{M}}$ takes $\mathcal{O}(M \log^2 M)$ flops.

REMARK 3.9. As a further application of Theorem 3.4 we consider the minimal 2-norm interpolation problem

$$\min_{f \in P_N(SO(3))} \|f\|_{L^2} \qquad \text{s.t.} \qquad f\left(\boldsymbol{G}_j\right) = y_j, \quad j = 0 \ldots M-1.$$

Its corresponding interpolation matrix

$$\boldsymbol{L} \in \mathbb{C}^{M\times M}, \qquad l_{i,j} = \sum_{l=0}^{N} U_{2l}\left(\cos\frac{\mathrm{d}(\boldsymbol{G}_i, \boldsymbol{G}_j)}{2}\right),$$

has uniformly bounded condition number whenever $N \geq 18/q$ by an argument similar to Corollary 3.7. This time, we compare the interpolation matrix $\boldsymbol{L}$ with two kernel matrices $\boldsymbol{K}_1$, $\boldsymbol{K}_2$ built upon the weights $\hat{w}_{1,l_1}$, $l_1 = 0, \ldots, N$, and $\hat{w}_{2,l_2}$, $l_2 = 0, \ldots, 2N$, setting $\beta = 4$ in Theorem 3.4. The lower bound on the smallest eigenvalue follows as in (3.11) from the upper bound (3.9) on the weights $\hat{w}_{1,l_1}$, i.e.,

$$\lambda_0(\boldsymbol{L}) \geq \lambda_0(\boldsymbol{K}_1) \min_{r=0,\ldots,N} \frac{2r+1}{\hat{w}_{1,r}} \geq \frac{(N+1)^3}{10} \lambda_0(\boldsymbol{K}_1).$$

We slightly change the argument for the upper bound to

$$\sum_{l=0}^{N} (2l+1) \sum_{k,k'=-l}^{l} \left| \sum_{i=0}^{M-1} c_i D_l^{k,k'}(\boldsymbol{G}_i) \right|^2 \leq \max_{r=0,\ldots,N} \frac{2r+1}{\hat{w}_{2,r}} \sum_{l=0}^{2N} \hat{w}_{2,l} \sum_{k,k'=-l}^{l} \left| \sum_{i=0}^{M-1} c_i D_l^{k,k'}(\boldsymbol{G}_i) \right|^2 .$$

Due to $\|g_4\|_{1,2N} \leq 2.1(2N+1)$ (cf. [11, proof of Lemma 3.2]) the second set of weights fulfill $\hat{w}_{2,l_2} \geq \frac{l_2+1}{(2N+1)^3}$ for the indices $l_2 = 0, \ldots, N$, and thus

$$\lambda_{M-1}(\boldsymbol{L}) \leq 16(N+1)^3 \lambda_{M-1}(\boldsymbol{K}_2).$$

Acknowledgments. The authors thank F. Filbir, R. Hielscher, D. Potts, and D. Schmid for many fruitful discussions on the topic. This project is partially funded by Deutsche Forschungsgemeinschaft grants FI 883/3-1 and PO 711/9-1.

REFERENCES

[1] K. BALL, *Eigenvalues of Euclidean distance matrices*, J. Approx. Theory, 68 (1992), pp. 74–82.
[2] Å. BJÖRCK, *Numerical Methods for Least Squares Problems*, SIAM, Philadelphia, USA, 1996.
[3] J. E. CASTRILLON-CANDAS, V. SIDDAVANAHALLI, AND C. BAJAJ, *Nonequispaced Fourier transforms for protein-protein docking*, ICES Report 05-44, Univ. Texas, (2005).
[4] W. ERB AND F. FILBIR, *Approximation by positive definite functions on compact groups*, Numer. Funct. Anal. Optim., in press.
[5] F. FILBIR AND D. SCHMID, *Stability results for approximation by positive definite functions on $SO(3)$*, J. Approx. Theory, 153 (2008), pp. 170–183.
[6] F. FILBIR AND W. THEMISTOCLAKIS, *Polynomial approximation on the sphere using scattered data*, Math. Nachr., 281 (2008), pp. 650–668.
[7] T. GUTZMER, *Interpolation by positive definite functions on locally compact groups with application to $SO(3)$*, Results Math., 29 (1996), pp. 69–77.
[8] J. KEINER, S. KUNIS, AND D. POTTS, *Efficient reconstruction of functions on the sphere from scattered data*, J. Fourier Anal. Appl., 13 (2007), pp. 435–458.
[9] P. J. KOSTELEC AND D. N. ROCKMORE, *FFTs on the rotation group*, J. Fourier Anal. Appl., 14 (2008), pp. 145–179.
[10] S. KUNIS, *A note on stability results for scattered data interpolation on Euclidean spheres*, Adv. Comput. Math., in press.
[11] S. KUNIS AND D. POTTS, *Stability results for scattered data interpolation by trigonometric polynomials*, SIAM J. Sci. Comput., 29 (2007), pp. 1403–1419.
[12] J. LEVESLEY, Z. LUO, AND X. SUN, *Norm estimates of interpolation matrices and their inverses associated with strictly positive definite functions*, Proc. Amer. Math. Soc., 127 (1999), pp. 2127–2134.
[13] H. N. MHASKAR, F. J. NARCOWICH, AND J. D. WARD, *Spherical Marcinkiewicz-Zygmund inequalities and positive quadrature*, Math. Comp., 70 (2001), pp. 1113–1130. Corrigendum on the positivity of the quadrature weights in 71 (2002), pp. 453–454.

ETNA
Kent State University
etna@mcs.kent.edu

[14] H. N. MHASKAR AND J. PRESTIN, *On the detection of singularities of a periodic function*, Adv. Comput. Math., 12 (2000), pp. 95–131.
[15] C. MÜLLER, *Spherical Harmonics*, Springer, Aachen, 1966.
[16] F. J. NARCOWICH, P. PETRUSHEV, AND J. D. WARD, *Localized tight frames on spheres*, SIAM J. Math. Anal., 38 (2006), pp. 574–594.
[17] F. J. NARCOWICH, N. SIVAKUMAR, AND J. D. WARD, *Stability results for scattered-data interpolation on Euclidean spheres*, Adv. Comput. Math., 8 (1998), pp. 137–163.
[18] F. J. NARCOWICH AND J. D. WARD, *Norms of inverses and condition numbers for matrices associated with scattered data*, J. Approx. Theory, 64 (1991), pp. 69–94.
[19] D. POTTS, J. PRESTIN, AND A. VOLLRATH, *A fast Fourier algorithm on the rotation group*, submitted.
[20] D. POTTS AND G. STEIDL, *Fast summation at nonequispaced knots by NFFTs*, SIAM J. Sci. Comput., 24 (2003), pp. 2013–2037.
[21] R. SCHABACK, *Error estimates and condition numbers for radial basis function interpolation*, Adv. Comput. Math., 3 (1995), pp. 251–264.
[22] D. SCHMID, *A trade-off principle in connection with the approximation by positive definite kernels*, in Approximation Theory XII: San Antonio, C. K. Chui, M. Neamtu, and L. L. Schumaker, eds., Brentwood, 2008, Nashboro Press, pp. 348–359.
[23] ———, *Marcinkiewicz-Zygmund inequalities and polynomial approximation from scattered data on $SO(3)$*, Numer. Funct. Anal. Optim., 29 (2008), pp. 855–882.
[24] D. VARSHALOVICH, A. MOSKALEV, AND V. KHERSONSKI, *Quantum Theory of Angular Momentum*, World Scientific Publishing, Singapore, 1988.
[25] K. G. V.D. BOOGAART, R. HIELSCHER, J. PRESTIN, AND H. SCHAEBEN, *Kernel-based methods for inversion of the Radon transform on $SO(3)$ and their applications to texture analysis*, J. Comput. Appl. Math., 199 (2007), pp. 122–140.
[26] N. VILENKIN, *Special Functions and the Theory of Group Representations*, Amer. Math. Soc., Providence, RI, 1968.
[27] H. WENDLAND, *Scattered Data Approximation*, Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press, Cambridge, 2005.