

Numerical stability of nonequispaced fast Fourier transforms

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Dedicated to Franz Locher in honor of his 65th birthday

This paper presents some new results on numerical stability for multivariate fast Fourier transform of nonequispaced data (NFFT). In contrast to fast Fourier transform (of equispaced data), the NFFT is an approximate algorithm. In a worst case study, we show that both approximation error and roundoff error have a strong influence on the numerical stability of NFFT. Numerical tests confirm the theoretical estimates of numerical stability.

Key words and phrases: Fast Fourier transform, nonequispaced data, nonequispaced FFT, numerical stability, roundoff error, approximation error, sampling of trigonometric polynomials

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1 Introduction

An algorithm for the discrete Fourier transform of equispaced data with low arithmetical cost is called a *fast Fourier transform* (FFT). It is very important that a fast algorithm works stably in a floating point arithmetic. It is known (see e.g. [12, 22]) that univariate FFTs are very sensitive with respect to the accuracy of precomputation and that under certain conditions these algorithms can be remarkably stable. This result can be generalized to d -variate FFTs (see Lemma 5.2).

In this paper, we consider the fast computation of a d -variate discrete Fourier transform for nonequispaced data which is shortly called *nonequispaced fast Fourier transform* (NFFT). In recent years, the NFFT has attracted much attention [3, 5, 20, 10] as a method for the fast approximate evaluation of a d -variate trigonometric polynomial at arbitrary nodes. Let M and N be even positive integers. By I_N^d we denote the index set $\{-\frac{N}{2}, \dots, \frac{N}{2} - 1\}^d$. For given nonequispaced nodes $\mathbf{x}_j \in [-\frac{1}{2}, \frac{1}{2}]^d$ ($j \in I_M^1$) and given

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$\hat{f}_{\mathbf{k}} \in \mathbb{C}$ ($\mathbf{k} \in I_N^d$) we are interested in a fast and numerically stable computation of all values $f(\mathbf{x}_j)$ of the d -variate trigonometric polynomial

$$f(\mathbf{x}) := \sum_{\mathbf{k} \in I_N^d} \hat{f}_{\mathbf{k}} e^{-2\pi i \mathbf{k} \cdot \mathbf{x}}.$$

A direct evaluation of all values $f(\mathbf{x}_j)$ ($j \in I_M^1$) requires $\mathcal{O}(N^d M)$ arithmetical operations, too much for practical purposes. The most efficient NFFT were proposed by A. Dutt and V. Rokhlin [5] and by G. Beylkin [3]. Later, G. Steidl [20, 6] has presented a unified approach to NFFT and has improved the estimates of the approximation error. Nowadays, software of d -variate NFFT is freely available from the homepage [14].

In contrast to FFT, the NFFT is an approximate algorithm. By NFFT, we can compute only approximate values for $f(\mathbf{x}_j)$. Using oversampling, we approximate the d -variate trigonometric polynomial f by g a linear combination of translates of suitable window function φ having a good localization in the time/spatial and frequency domain. Here we choose a Gaussian or Kaiser-Bessel window function. Then the Fourier coefficients of g can be easily computed by d -variate FFT. By truncation of φ by means of a cut-off parameter, we can calculate approximate values of $f(\mathbf{x}_j)$ in a simple and fast way. Thus the d -variate NFFT with N^d input data and M output data requires $\mathcal{O}(N^d \log N + M)$ arithmetical operations.

We measure the nonuniformity of this sampling grid $\{\mathbf{x}_j \in [-\frac{1}{2}, \frac{1}{2}]^d : j \in I_M^1\}$ by a mesh norm and a separation distance. Roughly spoken, the mesh norm and the separation distance is the largest and the smallest gap between neighboring nodes, respectively. We reformulate results of K. Gröchenig [11] concerning weighted sampling of d -variate trigonometric polynomials.

In order to introduce the normwise backward stability of NFFT, we have to consider the inverse NFFT. Therefore we discuss the solvability of the linear system

$$\mathbf{A}_{M, N^d}^{(d)} \hat{\mathbf{f}} = \mathbf{f},$$

where

$$\mathbf{A}_{M, N^d}^{(d)} := (e^{-2\pi i \mathbf{k} \cdot \mathbf{x}_j})_{j \in I_M^1, \mathbf{k} \in I_N^d} \in \mathbb{C}^{M \times N^d} \quad (1.1)$$

is the nonequispaced Fourier matrix, $\hat{\mathbf{f}} := (\hat{f}_{\mathbf{k}})_{\mathbf{k} \in I_N^d} \in \mathbb{C}^{N^d}$ is an unknown vector, and $\mathbf{f} := (f_j)_{j \in I_M^1}$ is a given vector. In the case $N^d < M$, this linear system is overdetermined and nonsolvable in general. But we can find a convenient vector $\hat{\mathbf{f}}$ by weighted reconstruction, where we follow an idea of K. Gröchenig [11] and compensate the “clusters” in the sampling set by special weights. If the mesh norm of the sampling grid is smaller than $\mathcal{O}(N^{-1})$, then a weighted nonequispaced Fourier matrix is left-invertible. In the case $N^d > M$, we focus on the underdetermined and consistent linear system. We expect to interpolate the given data $f_j \in \mathbb{C}$ ($j = 0, \dots, M-1$) exactly by optimal interpolation via damping factors. If the separation distance of the sampling grid is greater than $\mathcal{O}(N^{-1})$, then a weighted nonequispaced Fourier matrix is right-invertible.

Now we are able to investigate a worst case roundoff error analysis for the d -variate NFFT. We propose a definition of normwise backward stability of the approximate

NFFT. With other words, we consider the influences of approximation error and roundoff error together. We show that under weak assumptions, the NFFT possesses a remarkable good numerical stability. The stability depends on the norm of the left inverse or right inverse of the underlying weighted nonequispaced Fourier matrix. As usual in a worst case analysis, the errors are overestimated, especially for dimensions $d > 1$. Nevertheless the theoretical results describe the right behavior of the error which is first influenced by the approximation error and later dominated by the roundoff error. This effect is demonstrated by various numerical tests for dimensions $d = 2$ and $d = 3$.

The paper is organised as follows: After introducing the necessary notations for the NFFT in the Section 2, we collect results for sampling of trigonometric polynomials in Section 3. Then in Section 4, we introduce the inverse NFFT by means of weighted reconstruction and optimal interpolation, respectively. Further we estimate the norms of a left inverse (see Theorem 4.2) and right inverse (see Theorem 4.3) of a weighted nonequispaced Fourier matrix. Finally in Section 5, we use these results in order to prove the numerical stability of the NFFT. Various numerical examples concerning the accuracy of the forward NFFT, and the reconstruction error of the inverse NFFT are presented in Section 6.

2 Nonequispaced fast Fourier transform

Let $\Pi^d := [-\frac{1}{2}, \frac{1}{2})^d$, $I_N^d := [-\frac{N}{2}, \frac{N}{2})^d \cap \mathbb{Z}^d$, where $d \in \mathbb{N}$ and $N \in 2\mathbb{N}$. In this paper, we use the notations $\mathbf{x} = (x_t)_{t=1}^d \in \mathbb{R}^d$ for a d -variate variable and $\mathbf{k} = (k_t)_{t=1}^d \in \mathbb{Z}^d$ for a d -variate index. Then we have to evaluate the 1-periodic d -variate trigonometric polynomial

$$f(\mathbf{x}) := \sum_{\mathbf{k} \in I_N^d} \hat{f}_{\mathbf{k}} e^{-2\pi i \mathbf{k} \cdot \mathbf{x}} \quad (2.1)$$

at the nodes $\mathbf{x}_j \in \Pi^d$ ($j \in I_M^1$) with $M \in 2\mathbb{N}$. For equispaced nodes $\mathbf{x}_j := \frac{j}{N}$ with $j \in I_N^d$, the values $f(\mathbf{x}_j)$ can be computed by the well-known d -variate fast Fourier transform (FFT) with only $\mathcal{O}(N^d \log N)$ arithmetical operations. Here we assume that the nodes \mathbf{x}_j ($j \in I_M^1$) are nonequispaced. We compute the values of (2.1) at the nodes \mathbf{x}_j in the following way. We introduce an *oversampling factor* $\alpha > 1$ such that $n := \alpha N$ is a power of 2. First we approximate f by

$$g(\mathbf{x}) := \sum_{\mathbf{l} \in I_n^d} g_{\mathbf{l}} \varphi(\mathbf{x} - \frac{\mathbf{l}}{n}),$$

where φ is a d -variate continuous *window function* and $g_{\mathbf{l}}$ are conveniently chosen constants. Further, φ is 1-periodic with respect to each variable. Assume that the Fourier series of φ converges uniformly. Then the Fourier series of g reads as follows

$$g(\mathbf{x}) := \sum_{\mathbf{k} \in \mathbb{Z}^d} c_{\mathbf{k}}(g) e^{-2\pi i \mathbf{k} \cdot \mathbf{x}}$$

with the corresponding Fourier coefficients

$$c_{\mathbf{k}}(g) := \int_{\Pi^d} g(\mathbf{x}) e^{2\pi i \mathbf{k} \cdot \mathbf{x}} d\mathbf{x} = \sum_{\mathbf{l} \in I_n^d} g_{\mathbf{l}} \int_{\Pi^d} \varphi(\mathbf{x} - \frac{\mathbf{l}}{n}) e^{2\pi i \mathbf{k} \cdot \mathbf{x}} d\mathbf{x} = \hat{g}_{\mathbf{k}} c_{\mathbf{k}}(\varphi)$$

with

$$\hat{g}_{\mathbf{k}} := \sum_{\mathbf{l} \in I_n^d} g_{\mathbf{l}} e^{2\pi i \mathbf{k} \cdot \mathbf{l} / n}, \quad c_{\mathbf{k}}(\varphi) := \int_{\Pi^d} \varphi(\mathbf{x}) e^{2\pi i \mathbf{k} \cdot \mathbf{x}} d\mathbf{x} \quad (\mathbf{k} \in \mathbb{Z}^d). \quad (2.2)$$

Hence we obtain that

$$\begin{aligned} g(\mathbf{x}) &= \sum_{\mathbf{k} \in \mathbb{Z}^d} \hat{g}_{\mathbf{k}} c_{\mathbf{k}}(\varphi) e^{-2\pi i \mathbf{k} \cdot \mathbf{x}} \\ &= \sum_{\mathbf{k} \in I_N^d} \hat{g}_{\mathbf{k}} c_{\mathbf{k}}(\varphi) e^{-2\pi i \mathbf{k} \cdot \mathbf{x}} + \sum_{\mathbf{r} \in \mathbb{Z}^d \setminus \{\mathbf{0}\}} \sum_{\mathbf{k} \in I_N^d} \hat{g}_{\mathbf{k}} c_{\mathbf{k} + n\mathbf{r}}(\varphi) e^{-2\pi i (\mathbf{k} + n\mathbf{r}) \cdot \mathbf{x}}. \end{aligned} \quad (2.3)$$

If the Fourier coefficients $c_{\mathbf{k}}(\varphi)$ become sufficiently small for $\mathbf{k} \in \mathbb{Z}^d \setminus I_n^d$ and if $c_{\mathbf{k}}(\varphi) \neq 0$ for all $\mathbf{k} \in I_N^d$, then we suggest by comparing (2.1) with (2.3) to set

$$\hat{g}_{\mathbf{k}} := \begin{cases} \hat{f}_{\mathbf{k}} / c_{\mathbf{k}}(\varphi) & \text{for } \mathbf{k} \in I_N^d, \\ 0 & \text{for } \mathbf{k} \in I_n^d \setminus I_N^d. \end{cases}$$

Now the values $g_{\mathbf{l}}$ can be obtained from (2.2) by the inverse d -variate reduced FFT, i.e.,

$$g_{\mathbf{l}} = n^{-d} \sum_{\mathbf{k} \in I_N^d} \hat{g}_{\mathbf{k}} e^{-2\pi i \mathbf{k} \cdot \mathbf{l} / n} \quad (\mathbf{l} \in I_n^d).$$

If φ is also localised in time/spatial such that it can be approximated by a 1-periodic d -variate function $\psi \in L_1^2(\mathbb{R}^d)$ with $\text{supp } \psi \cap \Pi^d \subset \frac{2m}{n} \Pi^d$ with $1 \leq m \ll N$, then

$$f(\mathbf{x}_j) \approx g(\mathbf{x}_j) \approx h(\mathbf{x}_j) := \sum_{\mathbf{l} \in I_{n,m}^d(\mathbf{x}_j)} g_{\mathbf{l}} \psi(\mathbf{x}_j - \frac{\mathbf{l}}{n}) \quad (j \in I_M^1) \quad (2.4)$$

with the index set $I_{n,m}^d(\mathbf{x}_j) := \{\mathbf{l} \in I_n^d : n\mathbf{x}_j - m\mathbf{1} \leq \mathbf{l} \leq n\mathbf{x}_j + m\mathbf{1}\}$. Here we have used the notation $\mathbf{1} := (1)_{t=1}^d$. For fixed \mathbf{x}_j ($j \in I_M^1$), the above sum (2.4) contains at most $(2m+1)^d$ nonzero summands. In the following, m is called *cut-off parameter*.

In summary, we obtain the following d -variate *nonequispaced fast Fourier transform* (NFFT) with N^d input data and M output data. This algorithm requires $\mathcal{O}(n^d \log n + m^d M)$ arithmetical operations (see [18]).

Algorithm 2.1 (d -variate NFFT)

Input: $M, N \in 2\mathbb{N}$, $m \in \mathbb{N}$, $\alpha > 1$, $n := \alpha N$, $\mathbf{x}_j \in \Pi^d$ ($j \in I_M^1$), $\hat{f}_{\mathbf{k}} \in \mathbb{C}$ ($\mathbf{k} \in I_N^d$).

1. Precompute $c_{\mathbf{k}}(\varphi)$ ($\mathbf{k} \in I_N^d$) and $\psi(\mathbf{x}_j - \frac{\mathbf{l}}{n})$ ($j \in I_M^1$, $\mathbf{l} \in I_{n,m}^d(\mathbf{x}_j)$).

2. Compute $\hat{g}_{\mathbf{k}} := \hat{f}_{\mathbf{k}}/c_{\mathbf{k}}(\varphi)$ ($\mathbf{k} \in I_N^d$).

3. Compute $g_{\mathbf{l}}$ by d -variate reduced FFT

$$g_{\mathbf{l}} := n^{-d} \sum_{\mathbf{k} \in I_N^d} \hat{g}_{\mathbf{k}} e^{-2\pi i \mathbf{k} \cdot \mathbf{l}/n} \quad (\mathbf{l} \in I_n^d).$$

4. Form

$$h(\mathbf{x}_j) := \sum_{\mathbf{l} \in I_{n,m}^d(\mathbf{x}_j)} g_{\mathbf{l}} \psi(\mathbf{x}_j - \frac{\mathbf{l}}{n}) \quad (j \in I_M^1).$$

Output: $h(\mathbf{x}_j) \approx f(\mathbf{x}_j)$ ($j \in I_M^1$). □

In contrast to FFT, the NFFT is an *approximate algorithm*. By NFFT, we can compute approximate values of $f(\mathbf{x}_j)$. The approximation error depends on the choice of the window functions φ and ψ . If the window function φ is the tensor product of 1-periodised dilated Gaussian bells with cut-off parameter m

$$\varphi(\mathbf{x}) := (\pi b)^{-d/2} \prod_{t=1}^d \left(\sum_{r_t \in \mathbb{Z}} e^{-(n(x_t+r_t))^2/b} \right),$$

if ψ is the tensor product of 1-periodised dilated truncated Gaussian bells

$$\psi(\mathbf{x}) := (\pi d)^{-d/2} \prod_{t=1}^d \sum_{r_t \in \mathbb{Z}} \chi_{[-m,m]}(n(x_t+r_t)) e^{-(n(x_t+r_t))^2/b},$$

if $\alpha \geq \frac{3}{2}$ and

$$\frac{3}{2} \leq b \leq 2\alpha m \pi^{-1} (2\alpha - 1)^{-1} \left(1 + \frac{d-1}{(2\alpha-1)^2} \right)^{-1/2},$$

then the *approximation error* can be estimated (see [6]) by

$$\left(\sum_{j \in I_M^1} |f(\mathbf{x}_j) - h(\mathbf{x}_j)|^2 \right)^{1/2} \leq M^{1/2} N^{d/2} d 2^{d+1} e^{-b\pi^2(1-\alpha^{-1})} \|\mathbf{f}\|_2. \quad (2.5)$$

Here $\chi_{[-m,m]}$ denotes the characteristic function of the interval $[-m, m]$.

If the window function φ is the tensor product of (dilated) *Kaiser-Bessel functions* φ_0 (see [13, 9]), i.e.,

$$\varphi(\mathbf{x}) = \prod_{t=1}^d \left(\sum_{r_t \in \mathbb{Z}} \varphi_0(x_t + r_t) \right),$$

where φ_0 is given by

$$\varphi_0(x_t) := \begin{cases} \frac{\sinh(b\sqrt{m^2 - n^2 x_t^2})}{\pi \sqrt{m^2 - n^2 x_t^2}} & \text{for } |x_t| \leq \frac{m}{n} \quad (b := \pi(2 - \frac{1}{\alpha})), \\ \frac{\sin(b\sqrt{n^2 x_t^2 - m^2})}{\pi \sqrt{n^2 x_t^2 - m^2}} & \text{otherwise} \end{cases}$$

with

$$c_k(\varphi_0) = \begin{cases} \frac{1}{n} I_0 \left(m \sqrt{b^2 - (2\pi k/n)^2} \right) & \text{for } k = -n \left(1 - \frac{1}{2\alpha}\right), \dots, n \left(1 - \frac{1}{2\alpha}\right), \\ 0 & \text{otherwise,} \end{cases}$$

where I_0 denotes the modified zero-order Bessel function, and if $\psi := \varphi$, then one can estimate the *approximation error* (see [6, 16])

$$\left(\sum_{j \in I_M^1} |f(\mathbf{x}_j) - h(\mathbf{x}_j)|^2 \right)^{1/2} \leq M^{1/2} N^{d/2} d 2^{d+1} \pi (m + \sqrt{m})^4 \sqrt{1 - \alpha^{-1}} e^{-2\pi m \sqrt{1 - \alpha^{-1}}} \|\hat{\mathbf{f}}\|_2 \quad (2.6)$$

with $\hat{\mathbf{f}} := (\hat{f}_{\mathbf{k}})_{\mathbf{k} \in I_N^d}$. Other possibilities are powers of sinc functions or B-splines (see e.g. [14]).

3 Sampling of trigonometric polynomials

By $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ with $M \in 2\mathbb{N}$ we denote a nonuniform sampling set of M distinct nodes. In Π^d , we introduce the metric

$$\rho(\mathbf{x}, \mathbf{y}) := \min_{\mathbf{k} \in \mathbb{Z}^d} \|\mathbf{x} - \mathbf{y} + \mathbf{k}\|_\infty \quad (\mathbf{x}, \mathbf{y} \in \Pi^d).$$

We measure the non uniformity of the given sampling set by the *mesh norm*

$$\delta := 2 \max_{\mathbf{x} \in \Pi^d} \min_{j \in I_M^1} \rho(\mathbf{x}_j, \mathbf{x}) \in (0, 1]$$

and the *separation distance*

$$q := \min_{j, l \in I_M^1, j \neq l} \rho(\mathbf{x}_j, \mathbf{x}_l) \in (0, \frac{1}{2}].$$

We might interpret the mesh norm δ and the separation distance q as the largest and the smallest gap between neighboring nodes, respectively. Note that

$$\delta = \inf \left\{ s \in (0, 1] : \bigcup_{j \in I_M^1} B(\mathbf{x}_j, s) = [-\frac{1}{2}, \frac{1}{2}]^d \right\}$$

with $B(\mathbf{x}_j, s) := \{\mathbf{x} \in [-\frac{1}{2}, \frac{1}{2}]^d : \rho(\mathbf{x}, \mathbf{x}_j) \leq \frac{s}{2}\}$ (see [2]). We have the following obvious relation between the separation distance q , the mesh norm δ and the number of sampling points M .

Lemma 3.1 *Let $M \in 2\mathbb{N}$ and $d \in \mathbb{N}$. Let $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ be an arbitrary sampling set with M distinct nodes. Then*

$$0 < q \leq M^{-1/d} \leq \delta \leq 1.$$

Proof: 1. Let $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ be an arbitrary sampling set. Assume that $\delta < M^{-1/d}$ and choose one s with $\delta < s < M^{-1/d}$. Consider to each node \mathbf{x}_j its surrounding cube $B(\mathbf{x}_j, s)$ with side length s . Then the sum of the measures of these cubes fulfils the inequality

$$\sum_{j \in I_M^1} m(B(\mathbf{x}_j, s)) = M s^d < M (M^{-1/d})^d = 1.$$

This contradicts to the fact that $\bigcup_{j \in I_M^1} B(\mathbf{x}_j, s) \supset \Pi^d$. Hence $M^{-1/d} \leq \delta \leq 1$.

2. Assume that $q > M^{-1/d}$. Then the sum of the measures of all cubes $B(\mathbf{x}_j, q)$ fulfils the inequality

$$\sum_{j \in I_M^1} m(B(\mathbf{x}_j, q)) = M q^d > M (M^{-1/d})^d = 1.$$

This contradicts to the facts that $B(\mathbf{x}_j, q) \cap B(\mathbf{x}_k, q)$ for $j, k \in I_M^1$ ($j \neq k$) have no interior points and that $\bigcup_{j \in I_M^1} B(\mathbf{x}_j, q) \subseteq \Pi^d$. Therefore $0 < q \leq M^{-1/d}$. \blacksquare

The quantity δ can be interpreted as the maximum distance of any node \mathbf{x}_j to its next neighbour. Let V_j ($j \in I_M^1$) be the modified Voronoi regions

$$V_j := \{\mathbf{x} \in \Pi^d : \rho(\mathbf{x}, \mathbf{x}_j) \leq \rho(\mathbf{x}, \mathbf{x}_k) \text{ for all } k \in I_M^1 \setminus \{j\}\}$$

and let $w_j = m(V_j)$ be the Lebesgue measure of V_j . By definition, we have $V_j \cap V_k \neq \emptyset$ for $j \neq k$ and

$$\sum_{j \in I_M^1} \chi_{V_j} = \chi_{\Pi^d} \tag{3.1}$$

almost everywhere and hence $\sum_{j \in I_M^1} w_j = 1$.

By $\mathcal{P}_{N/2}$ we denote the set of all trigonometric polynomials f of the form (2.1). The parameter $N/2$ can be interpreted as the bandwidth of f . It measures the permissible amount of oscillation. By Theorem 3.2, $f \in \mathcal{P}_{N/2}$ is uniquely determined by its values $f(\mathbf{x}_j)$ ($j \in I_M^1$) and its weighted discrete norm $(\sum_{j \in I_M^1} w_j |f(\mathbf{x}_j)|^2)^{1/2}$ is equivalent to the

L_2 -norm $\|f\|_2 := \left(\int_{\Pi^d} |f(\mathbf{x})|^2 d\mathbf{x} \right)^{1/2}$. The next result is a reformulation of Theorem 5 in [11].

Theorem 3.2 (see [11]) *Let $N, M \in 2\mathbb{N}$ and $d \in \mathbb{N}$. If the mesh norm δ of $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ fulfils*

$$\delta < (\pi N d)^{-1} \log 2, \tag{3.2}$$

then for all d -variate trigonometric polynomials $f \in \mathcal{P}_{N/2}$

$$(2 - e^{\pi d N \delta}) \|f\|_2 \leq \left(\sum_{j \in I_M^1} w_j |f(\mathbf{x}_j)|^2 \right)^{1/2} \leq 2 \|f\|_2. \tag{3.3}$$

Proof: Since

$$\sum_{j \in I_M^1} w_j |f(\mathbf{x}_j)|^2 = \int_{\Pi^d} \left| \sum_{j \in I_M^1} f(\mathbf{x}_j) \chi_{V_j}(\mathbf{x}) \right|^2 d\mathbf{x},$$

we want to estimate

$$\|f - \sum_{j \in I_M^1} f(\mathbf{x}_j) \chi_{V_j}\|_2^2 = \sum_{j \in I_M^1} \int_{V_j} |f(\mathbf{x}) - f(\mathbf{x}_j)|^2 d\mathbf{x}.$$

We expand f into a Taylor series at \mathbf{x} and obtain

$$f(\mathbf{x}_j) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d} \frac{1}{\boldsymbol{\alpha}!} (\mathbf{x}_j - \mathbf{x})^{\boldsymbol{\alpha}} D^{\boldsymbol{\alpha}} f(\mathbf{x})$$

where $\boldsymbol{\alpha} = (\alpha_t)_{t=1}^d$, $|\boldsymbol{\alpha}| := \sum_{t=1}^d \alpha_t$, $\boldsymbol{\alpha}! := \prod_{t=1}^d (\alpha_t!)$, $\mathbf{x}^{\boldsymbol{\alpha}} := \prod_{t=1}^d x_t^{\alpha_t}$ and

$$D^{\boldsymbol{\alpha}} f(\mathbf{x}) := \frac{\partial^{|\boldsymbol{\alpha}|}}{\partial^{\alpha_1} x_1 \dots \partial^{\alpha_d} x_d} f(\mathbf{x})$$

are usual multi-index notations. This Taylor expansion yields the estimate

$$|f(\mathbf{x}) - f(\mathbf{x}_j)| \leq \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d \setminus \{\mathbf{0}\}} \frac{1}{\boldsymbol{\alpha}!} |\mathbf{x}_j - \mathbf{x}|^{\boldsymbol{\alpha}} |D^{\boldsymbol{\alpha}} f(\mathbf{x})|.$$

Since the sampling set $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ has the mesh norm δ , we see that $\rho(\mathbf{x}_j, \mathbf{x}) \leq \delta$ for $\mathbf{x} \in V_j$. Observing that f is 1-periodic in each variable, we obtain that for $\mathbf{x} \in V_j$

$$|f(\mathbf{x}) - f(\mathbf{x}_j)| \leq \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d \setminus \{\mathbf{0}\}} \frac{1}{\boldsymbol{\alpha}!} \delta^{|\boldsymbol{\alpha}|} |D^{\boldsymbol{\alpha}} f(\mathbf{x})|.$$

Hence by (3.1) it follows that

$$\sum_{j \in I_M^1} |f(\mathbf{x}) - f(\mathbf{x}_j)|^2 \chi_{V_j}(\mathbf{x}) \leq \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d \setminus \{\mathbf{0}\}} \left(\frac{1}{\boldsymbol{\alpha}!} \delta^{|\boldsymbol{\alpha}|} |D^{\boldsymbol{\alpha}} f(\mathbf{x})| \right)^2$$

almost everywhere. By Bernstein's inequality, the L^2 -norms of the partial derivatives of $f \in \mathcal{P}_{N/2}$ are majorised by

$$\|D^{\boldsymbol{\alpha}} f\|_2 \leq (N\pi)^{|\boldsymbol{\alpha}|} \|f\|_2.$$

Therefore

$$\begin{aligned} \|f - \sum_{j \in I_M^1} f(\mathbf{x}_j) \chi_{V_j}\|_2 &\leq \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d \setminus \{\mathbf{0}\}} \frac{1}{\boldsymbol{\alpha}!} \delta^{|\boldsymbol{\alpha}|} \|D^{\boldsymbol{\alpha}} f\|_2 \leq \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d \setminus \{\mathbf{0}\}} \frac{1}{\boldsymbol{\alpha}!} (\delta N\pi)^{|\boldsymbol{\alpha}|} \|f\|_2 \\ &= (e^{d\pi N\delta} - 1) \|f\|_2. \end{aligned}$$

Consequently we obtain that

$$(2 - e^{d\pi N\delta}) \|f\|_2 \leq \left\| \sum_{j \in I_M^1} f(\mathbf{x}_j) \chi_{V_j} \right\|_2 = \left(\sum_{j \in I_M^1} |f(\mathbf{x}_j)|^2 w_j \right)^{1/2} \leq e^{d\pi N\delta} \|f\|_2.$$

By our assumption (3.2), we see that $2 - e^{d\pi N\delta} > 0$. ■

Note that the specific choice of weights w_j is crucial for the explicit estimate. For dimensions $d \geq 1$ the estimate (3.3) is not optimal in the sense that the dependence on d is not expected. However for $d = 1$, K. Gröchenig has proved in [11] the following result: Let $N, M \in 2\mathbb{N}$. If the mesh norm δ of $\{x_j \in [-\frac{1}{2}, \frac{1}{2}] : j \in I_M^1\}$ fulfils $\delta < \frac{1}{N}$, then for all univariate trigonometric polynomials $f \in \mathcal{P}_{N/2}$

$$(1 - \delta N) \|f\|_2 \leq \left(\sum_{j \in I_M^1} |f(x_j)|^2 w_j \right)^{1/2} \leq (1 + \delta N) \|f\|_2.$$

4 Weighted reconstruction and optimal interpolation

The inverse NFFT can be introduced as follows. The reconstruction of a trigonometric polynomial $f \in \mathcal{P}_{N/2}$ from given values $f_j \in \mathbb{C}$ ($j \in I_M^1$) amounts to solving the following system of M linear equations

$$\sum_{\mathbf{k} \in I_N^d} \hat{f}_{\mathbf{k}} e^{-2\pi i \mathbf{k} \cdot \mathbf{x}_j} = f_j \quad (j \in I_M^1). \quad (4.1)$$

Now the discrete Fourier coefficients $\hat{f}_{\mathbf{k}}$ are the unknowns. Since f_j are often determined by measurements, we only know the exact values $f(\mathbf{x}_j)$ of (2.1) approximately, i.e., $f_j \approx f(\mathbf{x}_j)$ ($j \in I_M^1$). Introducing the *nonequispaced Fourier matrix* as in (1.1) and the vectors $\hat{\mathbf{f}} := (\hat{f}_{\mathbf{k}})_{\mathbf{k} \in I_N^d} \in \mathbb{C}^{N^d}$, $\mathbf{f} := (f_j)_{j \in I_M^1}$, the linear system (4.1) can be written in the form

$$\mathbf{A}_{M, N^d}^{(d)} \hat{\mathbf{f}} = \mathbf{f}. \quad (4.2)$$

For $N^d < M$, the linear system (4.2) is overdetermined and nonsolvable in general. Then a standard method is to determine the least squares solution of (4.2) with minimal norm, i.e.,

$$\min \left\{ \|\hat{\mathbf{f}}\|_2 : \hat{\mathbf{f}} \in \mathbb{C}^{N^d} \text{ with } \|\mathbf{A}_{M, N^d}^{(d)} \hat{\mathbf{f}} - \mathbf{f}\|_2 = \min \right\}.$$

This can be done by means of singular value decomposition which is very expensive and no practical way at all. In the following, we find $\hat{\mathbf{f}}$ by *weighted reconstruction*. In order to compensate the ‘‘clusters’’ in the sampling set $\{\mathbf{x}_j : j \in I_M^1\}$, it is useful to incorporate the weights $w_j = m(V_j) > 0$ ($j \in I_M^1$) into our problem. Hence we consider the *weighted reconstruction problem*

$$\|\mathbf{f} - \mathbf{A}_{M, N^d}^{(d)} \hat{\mathbf{f}}\|_{\mathbf{W}_M}^2 = \sum_{j \in I_M^1} w_j |f(\mathbf{x}_j) - f_j|^2 = \min \quad (4.3)$$

with the diagonal matrix $\mathbf{W}_M := \text{diag}(w_j)_{j \in I_M^1}$. In [11], it is proven that the minimisation problem (4.3) for $\hat{\mathbf{f}} \in \mathbb{C}^{N^d}$ is uniquely solvable under the assumptions of Theorem 3.2. Note that problem (4.3) can be solved with the weighted normal equation of first kind. Hence we introduce the *weighted multilevel Toeplitz matrix*

$$\mathbf{T}_{N^d} := (\mathbf{A}_{M,N^d}^{(d)})^H \mathbf{W}_M \mathbf{A}_{M,N^d}^{(d)} \in \mathbb{C}^{N^d \times N^d}. \quad (4.4)$$

Then the entries of \mathbf{T}_{N^d} reads as follows

$$t_{\mathbf{k},\mathbf{l}} := \sum_{j \in I_M^1} w_j e^{2\pi i \mathbf{x}_j \cdot (\mathbf{k} - \mathbf{l})} \quad (\mathbf{k}, \mathbf{l} \in I_N^d).$$

Note that the solution of (4.3) is computed iteratively by means of the conjugate gradient method in [7, 2], where the multilevel Toeplitz structure of \mathbf{T}_{N^d} is used for fast matrix vector multiplications (see also [15]).

Theorem 4.1 (see [2]) *Let $N, M \in 2\mathbb{N}$ and $d \in \mathbb{N}$. If the mesh norm δ of the sampling set $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ fulfils (3.2), then \mathbf{T}_{N^d} is positive definite and its spectrum is contained in $[(2 - e^{\pi d N \delta})^2, 4]$.*

Proof: We express the “sampled energy” $\sum_{j \in I_M^1} |f(\mathbf{x}_j)|^2 w_j$ of $f \in \mathcal{P}_{N/2}$ by the Fourier coefficients $\hat{f}_{\mathbf{k}}$ of f :

$$\begin{aligned} \sum_{j \in I_M^1} |f(\mathbf{x}_j)|^2 w_j &= \sum_{\mathbf{k} \in I_N^d} \sum_{\mathbf{l} \in I_N^d} \hat{f}_{\mathbf{k}} \bar{\hat{f}}_{\mathbf{l}} \sum_{j \in I_M^1} w_j e^{2\pi i (\mathbf{k} - \mathbf{l}) \cdot \mathbf{x}_j} = \sum_{\mathbf{k} \in I_N^d} \sum_{\mathbf{l} \in I_N^d} \hat{f}_{\mathbf{k}} \bar{\hat{f}}_{\mathbf{l}} \bar{t}_{\mathbf{k},\mathbf{l}} \\ &= \sum_{\mathbf{k} \in I_N^d} \hat{f}_{\mathbf{k}} \left(\overline{\sum_{\mathbf{l} \in I_N^d} t_{\mathbf{k},\mathbf{l}} \hat{f}_{\mathbf{l}}} \right) = \langle \hat{\mathbf{f}}, \mathbf{T}_{N^d} \hat{\mathbf{f}} \rangle. \end{aligned}$$

The matrix \mathbf{T}_{N^d} acts on \mathbb{C}^{N^d} and its entries $t_{\mathbf{k},\mathbf{l}}$ depend only on $\mathbf{k} - \mathbf{l}$. For $d = 1$, the matrix \mathbf{T}_N is therefore a Toeplitz matrix. For $d \geq 2$, \mathbf{T}_{N^d} is a block Toeplitz matrix with Toeplitz blocks. From Theorem 3.2, it follows that \mathbf{T}_{N^d} is positive definite, since by Parseval equation

$$(2 - e^{\pi d N \delta})^2 \langle \hat{\mathbf{f}}, \hat{\mathbf{f}} \rangle \leq \langle \hat{\mathbf{f}}, \mathbf{T}_{N^d} \hat{\mathbf{f}} \rangle \leq 4 \langle \hat{\mathbf{f}}, \hat{\mathbf{f}} \rangle$$

for all $\hat{\mathbf{f}} \in \mathbb{C}^{N^d}$. If the smallest and largest eigenvalues of the Hermitian matrix \mathbf{T}_{N^d} are denoted by $\lambda_{\min}(\mathbf{T}_{N^d})$ and $\lambda_{\max}(\mathbf{T}_{N^d})$, then by the variational properties of eigenvalues we infer

$$(2 - e^{\pi d N \delta})^2 \leq \lambda_{\min}(\mathbf{T}_{N^d}) \leq \lambda_{\max}(\mathbf{T}_{N^d}) \leq 4.$$

Hence the spectrum of \mathbf{T}_{N^d} is contained in $[(2 - e^{\pi d N \delta})^2, 4]$. ■

Theorem 4.2 Let $N, M \in 2\mathbb{N}$. If the mesh norm δ of the sampling set $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ fulfils (3.2), then the weighted nonequispaced Fourier matrix $\mathbf{W}_M^{1/2} \mathbf{A}_{M,N^d}^{(d)}$ is left-invertible. The spectral norm of the left inverse

$$\mathbf{L}_{N^d,M} := \mathbf{T}_{N^d}^{-1} (\mathbf{A}_{M,N^d}^{(d)})^H \mathbf{W}_M^{1/2}$$

is bounded by

$$\|\mathbf{L}_{N^d,M}\|_2 \leq (2 - e^{\pi d N \delta})^{-1}.$$

Proof: From $M^{-1/d} \leq \delta$ and (3.2), it follows that $N^d < M$. Immediately we see that

$$\mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2} \mathbf{A}_{M,N^d}^{(d)} = \mathbf{T}_{N^d}^{-1} \mathbf{T}_{N^d} = \mathbf{I}_{N^d}.$$

Therefore, $\mathbf{L}_{N^d,M}$ is a left inverse of $\mathbf{W}_M^{1/2} \mathbf{A}_{M,N^d}^{(d)}$. Since

$$(\mathbf{W}_M^{1/2} \mathbf{A}_{M,N^d}^{(d)})^H \mathbf{W}_M^{1/2} \mathbf{A}_{M,N^d}^{(d)} = \mathbf{T}_{N^d}$$

and since the spectrum of \mathbf{T}_{N^d} is contained in $[(2 - e^{\pi d N \delta})^{-2}, 4]$, the singular values of $\mathbf{W}_M^{1/2} \mathbf{A}_{M,N^d}^{(d)}$ are lying in $[(2 - e^{\pi d N \delta})^{-1}, 2]$. By singular value decomposition of the left inverse $\mathbf{L}_{N^d,M}$, it follows that the spectral norm of $\mathbf{L}_{N^d,M}$ can be estimated by

$$\|\mathbf{L}_{N^d,M}\|_2 \leq (2 - e^{\pi d N \delta})^{-1}.$$

This completes the proof. ■

In contrast, we focus now on the underdetermined and consistent linear system (4.2), i.e., we expect to interpolate the given data $f_j \in \mathbb{C}$, $j = 0, \dots, M-1$, exactly. We use the fact that the nonequispaced Fourier matrix $\mathbf{A}_{M,N^d}^{(d)}$ has full rank M for every polynomial order $\frac{N}{2} > d q^{-1}$ (see [15]). In particular, we incorporate *damping factors* $\hat{w}_{\mathbf{k}} > 0$, $\mathbf{k} \in I_N^d$, and consider the *optimal interpolation problem*

$$\|\hat{\mathbf{f}}\|_{\hat{\mathbf{W}}_{N^d}^{-1}}^2 = \sum_{\mathbf{k} \in I_N^d} (\hat{w}_{\mathbf{k}})^{-1} |\hat{f}_{\mathbf{k}}|^2 \xrightarrow{\hat{\mathbf{f}}} \min \quad \text{subject to} \quad \mathbf{A}_{M,N^d} \hat{\mathbf{f}} = \mathbf{f}, \quad (4.5)$$

where $\hat{\mathbf{W}}_{N^d} := \text{diag}(\hat{w}_{\mathbf{k}})_{\mathbf{k} \in I_N^d}$. From a result in [15] we obtain the following

Theorem 4.3 Let $N, M \in 2\mathbb{N}$. If the separation distance q of the sampling set $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$ fulfils $q > \frac{2d}{N}$, then the weighted nonequispaced Fourier matrix $\mathbf{A}_{M,N^d}^{(d)} \hat{\mathbf{W}}_{N^d}^{1/2}$ is right-invertible. The spectral norm of the right inverse

$$\mathbf{R}_{N^d,M} := \hat{\mathbf{W}}_{N^d}^{1/2} (\mathbf{A}_{M,N^d}^{(d)})^H \mathbf{K}_M^{-1}$$

with the kernel matrix $\mathbf{K}_M := \mathbf{A}_{M,N^d}^{(d)} \hat{\mathbf{W}}_{N^d} (\mathbf{A}_{M,N^d}^{(d)})^H$ is bounded by

$$\|\mathbf{R}_{N^d,M}\|_2 \leq \left(1 - \left(\frac{2d}{Nq}\right)^{d+1}\right)^{-1/2}.$$

Proof: We use the fact (see [15, Corollary 4.7]) that the eigenvalues of the kernel matrix \mathbf{K}_M obtained from the B-spline kernel of order $\beta = d + 1$ are bounded by

$$0 < 1 - \left(\frac{2d}{Nq}\right)^{d+1} \leq \lambda_{\min}(\mathbf{K}_M) \leq 1 \leq \lambda_{\max}(\mathbf{K}_M) \leq 1 + \left(\frac{2d}{Nq}\right)^{d+1}.$$

Following now the lines of the proof from Theorem 4.2, we obtain the assertion. \blacksquare

Note that problem (4.5) can be solved with the weighted normal equation of second kind.

5 Error analysis of NFFT

In the following we use Wilkinson's standard model for the binary floating point arithmetic for real numbers (see [12, p. 44]). Let \mathbb{M} denote the set of all floating point numbers. If $x \in \mathbb{R}$ is represented by the floating point number $\text{fl}(x) \in \mathbb{M}$, then $\text{fl}(x) = x(1 + \delta')$ with $|\delta'| \leq u$, where u denotes the *unit roundoff* or *machine precision* as long as we disregard underflow and overflow. For arbitrary $x_0, x_1 \in \mathbb{M}$ and any arithmetical operation $\circ \in \{+, -, \times, /\}$, the exact value $y = x_0 \circ x_1 \in \mathbb{R}$ and the computed value $\text{fl}(x_0 \circ x_1) \in \mathbb{M}$ are related by

$$\text{fl}(x_0 \circ x_1) = (x_0 \circ x_1)(1 + \delta^\circ) \quad (|\delta^\circ| \leq u). \quad (5.1)$$

In the IEEE single precision arithmetic (24 bits for the mantissa including 1 sign bit, 8 bits for the exponent), we have $u = 2^{-24} \approx 5.96 \times 10^{-8}$. Concerning the IEEE double precision arithmetic (53 bit for the mantissa including 1 sign bit, 11 bit for the exponent), we find $u = 2^{-53} \approx 1.11 \times 10^{-16}$ (see [12, p. 45]).

Since complex arithmetic is implemented using real arithmetic, we can derive the following bounds for the roundoff error of complex floating point operations.

Lemma 5.1 (see [12, p. 79], [23]) *Let $x_0, x_1 \in \mathbb{M} + i\mathbb{M}$. Then*

$$\begin{aligned} \text{fl}(x_0 + x_1) &= (x_0 + x_1)(1 + \delta^+) & (|\delta^+| \leq u), \\ \text{fl}(x_0 \times x_1) &= (x_0 \times x_1)(1 + \delta^\times) & (|\delta^\times| \leq \frac{4\sqrt{3}}{3}(u + u^2)). \end{aligned}$$

In the case $x_0 \in \mathbb{M} \cup i\mathbb{M}$ and $x_1 \in \mathbb{M} + i\mathbb{M}$, we have

$$\text{fl}(x_0 \times x_1) = (x_0 \times x_1)(1 + \delta^\times) \quad (|\delta^\times| \leq u). \quad (5.2)$$

In this section, we show that under weak assumptions the NFFT possesses a remarkable good numerical stability. But first we present a result concerning the numerical stability of the d -variate FFT.

5.1. The d -variate FFT is stable

Let

$$\mathbf{F}_{n^d}^{(d)} := n^{-d/2} \left(e^{-2\pi i \mathbf{l} \cdot \mathbf{k}/n} \right)_{\mathbf{l}, \mathbf{k} \in I_n^d}$$

be the d -variate (equispaced) Fourier matrix.

Lemma 5.2 *Let n be a power of 2. Assume that all complex n -th roots of unity are precomputed by direct call such that*

$$|e^{-2\pi i k/n} - \text{fl}(e^{-2\pi i k/n})| \leq \frac{\sqrt{2}}{2} u \quad (k = 1, \dots, n-1).$$

For arbitrary $\mathbf{x} \in (\mathbb{M} + i\mathbb{M})^{n^d}$ let $\mathbf{y} := \mathbf{F}_{n^d}^{(d)} \mathbf{x}$. Then the d -variate FFT is stable in the following sense that

$$\|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \leq (d k_n u + \mathcal{O}(u^2)) \|\mathbf{x}\|_2,$$

where $k_n = 4.01651 \log_2 n$ and $\tilde{\mathbf{y}} := \text{fl}(\mathbf{F}_{n^d}^{(d)} \mathbf{x})$.

Proof: 1. For a proof in the case $d = 1$ see [12, p. 453] or [21]. Thus the univariate Cooley–Tukey FFT is numerically stable in the following sense that for all input vectors $\mathbf{x} \in (\mathbb{M} + i\mathbb{M})^n$

$$\|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \leq (k_n u + \mathcal{O}(u^2)) \|\mathbf{x}\|_2,$$

where $\mathbf{y} := \mathbf{F}_n^{(1)} \mathbf{x} \in \mathbb{C}^n$ is the exact Fourier transformed vector and $\tilde{\mathbf{y}} := \text{fl}(\mathbf{F}_n^{(1)} \mathbf{x}) \in (\mathbb{M} + i\mathbb{M})^n$ is that vector computed by Cooley–Tukey FFT in floating point arithmetic. In [12, p. 453], k_n reads as follows $\frac{13}{2} \sqrt{2} \log_2 n \approx 9.119239 \log_2 n$. A more detailed analysis in [21] shows that $k_n = (1 + \frac{4\sqrt{3}}{3} + \frac{\sqrt{2}}{2}) \log_2 n \approx 4.01651 \log_2 n$ is also possible. 2. For shortness, we prove only the case $d = 2$. The (k_1, k_2) -th component of $\mathbf{y} = \mathbf{F}_{n^2}^{(2)} \mathbf{x}$ reads as follows

$$\begin{aligned} y_{k_1, k_2} &:= \frac{1}{n} \sum_{l_1 \in I_n^1} \sum_{l_2 \in I_n^1} e^{-2\pi i (l_1 k_1 + l_2 k_2)/n} x_{l_1, l_2} \quad (k_1, k_2 \in I_n^1) \\ &= \frac{1}{\sqrt{n}} \sum_{l_2 \in I_n^1} e^{-2\pi i l_2 k_2/n} \underbrace{\left(\frac{1}{\sqrt{n}} \sum_{l_1 \in I_n^1} e^{-2\pi i l_1 k_1/n} x_{l_1, l_2} \right)}_{=: z_{k_1, l_2}}. \end{aligned}$$

Setting

$$\mathbf{x}_{l_2} := \left(x_{l_1, l_2} \right)_{l_1 = -\frac{n}{2}}^{\frac{n}{2}-1} \quad (l_2 \in I_n^1), \quad \mathbf{x} := \begin{pmatrix} \mathbf{x}_{-\frac{n}{2}} \\ \vdots \\ \mathbf{x}_{\frac{n}{2}-1} \end{pmatrix},$$

we compute the bivariate FFT via the known row–column method. In a first step, we calculate for each $l_2 \in I_n^1$

$$\mathbf{z}_{l_2} = \left(z_{k_1, l_2} \right)_{k_1 = -\frac{n}{2}}^{\frac{n}{2}-1} := \mathbf{F}_n^{(1)} \mathbf{x}_{l_2}$$

by univariate FFT. Then we form $\mathbf{z}'_{k_1} := \left(z_{k_1, l_2} \right)_{l_2 = -\frac{n}{2}}^{\frac{n}{2}-1}$. In a second step, we compute for each $k_1 \in I_n^1$

$$\mathbf{y}_{k_1} = \left(y_{k_1, k_2} \right)_{k_2 = -\frac{n}{2}}^{\frac{n}{2}-1} := \mathbf{F}_n^{(1)} \mathbf{z}'_{k_1}$$

and we obtain the result

$$\mathbf{y} := \begin{pmatrix} \mathbf{y}_{-\frac{n}{2}} \\ \vdots \\ \mathbf{y}_{\frac{n}{2}-1} \end{pmatrix} \in \mathbb{C}^{n^2}.$$

Now we estimate the roundoff error of the bivariate FFT. By step 1 we know that

$$\|\hat{\mathbf{z}}_{l_2} - \mathbf{z}_{l_2}\|_2^2 \leq (k_n u + \mathcal{O}(u^2))^2 \|\mathbf{x}_{l_2}\|_2^2 \quad (l_2 \in I_n^1)$$

with $k_n = 4.01651 \log_2 n$. Summation of all inequalities yields

$$\|\hat{\mathbf{z}} - \mathbf{z}\|_2^2 \leq (k_n u + \mathcal{O}(u^2))^2 \|\mathbf{x}\|_2^2, \quad (5.3)$$

where

$$\hat{\mathbf{z}}_{l_2} := \text{fl}(\mathbf{F}_n^{(1)} \mathbf{x}_{l_2}), \quad \mathbf{z} := \begin{pmatrix} \mathbf{z}_{-\frac{n}{2}} \\ \vdots \\ \mathbf{z}_{\frac{n}{2}-1} \end{pmatrix}, \quad \hat{\mathbf{z}} := \begin{pmatrix} \hat{\mathbf{z}}_{-\frac{n}{2}} \\ \vdots \\ \hat{\mathbf{z}}_{\frac{n}{2}-1} \end{pmatrix}.$$

Now we set for each $k_1 \in I_n^1$

$$\hat{\mathbf{z}}'_{k_1} := \left(\hat{\mathbf{z}}_{k_1, l_2} \right)_{l_2 = -\frac{n}{2}}^{\frac{n}{2}-1}, \quad \tilde{\mathbf{y}}_{k_1} := \mathbf{F}_n^{(1)} \hat{\mathbf{z}}'_{k_1}, \quad \hat{\mathbf{y}}_{k_1} := \text{fl}(\mathbf{F}_n^{(1)} \hat{\mathbf{z}}'_{k_1}).$$

Applying step 1 again, we can estimate that

$$\|\hat{\mathbf{y}}_{k_1} - \tilde{\mathbf{y}}_{k_1}\|_2^2 \leq (k_n u + \mathcal{O}(u^2))^2 \|\hat{\mathbf{z}}'_{k_1}\|_2^2 \quad (k_1 \in I_n^1).$$

Summation of these inequalities yields

$$\|\hat{\mathbf{y}} - \tilde{\mathbf{y}}\|_2^2 \leq (k_n u + \mathcal{O}(u^2))^2 \|\hat{\mathbf{z}}'\|_2^2 \quad (5.4)$$

with

$$\hat{\mathbf{y}} := \begin{pmatrix} \hat{\mathbf{y}}_{-\frac{n}{2}} \\ \vdots \\ \hat{\mathbf{y}}_{\frac{n}{2}-1} \end{pmatrix}, \quad \tilde{\mathbf{y}} := \begin{pmatrix} \tilde{\mathbf{y}}_{-\frac{n}{2}} \\ \vdots \\ \tilde{\mathbf{y}}_{\frac{n}{2}-1} \end{pmatrix}, \quad \hat{\mathbf{z}}' := \begin{pmatrix} \hat{\mathbf{z}}'_{-\frac{n}{2}} \\ \vdots \\ \hat{\mathbf{z}}'_{\frac{n}{2}-1} \end{pmatrix}.$$

Now by $\|\mathbf{z}\|_2 = \|\mathbf{x}\|_2$ and (5.3) it follows that

$$\|\hat{\mathbf{z}}'\|_2 = \|\hat{\mathbf{z}}\|_2 \leq \|\hat{\mathbf{z}} - \mathbf{z}\|_2 + \|\mathbf{z}\|_2 \leq (1 + k_n u + \mathcal{O}(u^2)) \|\mathbf{x}\|_2 = (1 + \mathcal{O}(u)) \|\mathbf{x}\|_2.$$

Thus by (5.4) we obtain that

$$\|\hat{\mathbf{y}} - \tilde{\mathbf{y}}\|_2 \leq (k_n u + \mathcal{O}(u^2)) (1 + \mathcal{O}(u)) \|\mathbf{x}\|_2 = (k_n u + \mathcal{O}(u^2)) \|\mathbf{x}\|_2. \quad (5.5)$$

By triangle inequality we get $\|\hat{\mathbf{y}} - \mathbf{y}\|_2 \leq \|\hat{\mathbf{y}} - \tilde{\mathbf{y}}\|_2 + \|\tilde{\mathbf{y}} - \mathbf{y}\|_2$. Now we can estimate

$$\|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \leq (k_n u + \mathcal{O}(u^2)) \|\mathbf{x}\|_2, \quad (5.6)$$

since $\tilde{\mathbf{y}}_{k_1} - \mathbf{y}_{k_1} = \mathbf{F}_n^{(1)} (\hat{\mathbf{z}}'_{k_1} - \mathbf{z}'_{k_1})$, $\mathbf{F}_n^{(1)}$ is unitary and $\|\tilde{\mathbf{y}}_{k_1} - \mathbf{y}_{k_1}\|_2^2 = \|\hat{\mathbf{z}}'_{k_1} - \mathbf{z}'_{k_1}\|_2^2$ ($k_1 \in I_n^1$). By summation of these inequalities and 1. we get

$$\|\tilde{\mathbf{y}} - \mathbf{y}\|_2^2 = \|\hat{\mathbf{z}}' - \mathbf{z}'\|_2^2 = \|\hat{\mathbf{z}} - \mathbf{z}\|_2^2 \leq (k_n u + \mathcal{O}(u^2))^2 \|\mathbf{x}\|_2^2.$$

Finally from (5.5) and (5.6) it follows the assertion for $d = 2$. ■

5.2. The d -variate NFFT is robust

The Algorithm 2.1 reads in matrix-vector notation

$$\mathbf{h} := n^{-d/2} \mathbf{B}_{M,n^d} \mathbf{F}_{n^d}^{(d)} \mathbf{D}_{n^d,N^d} \hat{\mathbf{f}} \quad (\hat{\mathbf{f}} \in (\mathbb{M} + i\mathbb{M})^{N^d}), \quad (5.7)$$

where \mathbf{B}_{M,n^d} and \mathbf{D}_{n^d,N^d} denotes sparse matrices

$$\begin{aligned} \mathbf{B}_{M,n^d} &:= \left(\psi(\mathbf{x}_j - \frac{\mathbf{l}}{n}) \right)_{j \in I_M^1, \mathbf{l} \in I_n^d}, \\ \mathbf{D}_{n^d,N^d} &:= \left(\mathbf{O}_{N^d, (n^d - N^d)/2} \mid \text{diag}(\mathbf{c}_{\mathbf{k}}(\varphi)^{-1})_{\mathbf{k} \in I_N^d} \mid \mathbf{O}_{N^d, (n^d - N^d)/2} \right) \end{aligned}$$

with the zero matrix $\mathbf{O}_{N^d, (n^d - N^d)/2}$ of size $N^d \times ((n^d - N^d)/2)$. Note that $\mathbf{h} \in \mathbb{C}^M$ is an approximation of $\mathbf{f} := \mathbf{A}_{M,N^d}^{(d)} \hat{\mathbf{f}}$.

We call an algorithm for the computation of the NFFT *robust*, if for all $\hat{\mathbf{f}} \in (\mathbb{M} + i\mathbb{M})^{N^d}$ there exist a positive constant k_N with $k_N u \ll 1$ such that

$$\|\text{fl}(\mathbf{h}) - \mathbf{h}\|_2 \leq (k_N u + \mathcal{O}(u^2)) \|\hat{\mathbf{f}}\|_2.$$

Note that for the univariate case it was proven in [18, Theorem 12.3] and [19, Theorem 5.2] that the NFFT is robust too. In the following, we show that the multivariate NFFT is robust.

Theorem 5.3 *Let $M, N \in 2\mathbb{N}$. Let $n = \alpha N$ ($\alpha > 1$) be a power of 2 and $m \in \mathbb{N}$ with $2m \ll n$ be given. Let q be the separation distance of the sampling set $\{\mathbf{x}_j : j \in I_M^1\}$. Let $\tau \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ be a nonnegative even function which decreases monotonically in $[0, \infty)$ and let*

$$\varphi_0(x) := \sum_{r \in \mathbb{Z}} \tau(n(x+r)), \quad \psi_0(x) := \sum_{r \in \mathbb{Z}} (\tau \chi_{[-m,m]})(n(x+r)) \quad (x \in \mathbb{R}).$$

Assume that φ_0 has a uniformly convergent Fourier expansion with the Fourier coefficients

$$c_k(\varphi_0) = n^{-1} \hat{\tau}\left(\frac{2\pi k}{n}\right) \quad (k \in \mathbb{Z}),$$

where $\hat{\tau}$ is the Fourier transform of τ and where $|c_k(\varphi_0)| \geq |c_{k+1}(\varphi_0)|$ for all $k \geq 0$. Let φ and ψ be the tensor products

$$\varphi(\mathbf{x}) := \varphi_0(x_1) \dots \varphi_0(x_d), \quad \psi(\mathbf{x}) := \psi_0(x_1) \dots \psi_0(x_d).$$

As φ_0 and ψ_0 , respectively, one can choose a 1-periodized dilated Gaussian bell and a 1-periodized dilated truncated Gaussian bell, respectively, for details see Section 2. If $\tilde{\mathbf{h}} = \text{fl}(\mathbf{h})$ denotes the computed vector of (5.7), then the normwise roundoff error $\|\tilde{\mathbf{h}} - \mathbf{h}\|_2$ can be estimated by

$$\|\tilde{\mathbf{h}} - \mathbf{h}\|_2 \leq (\tilde{k}_n u + \mathcal{O}(u^2)) \|\hat{\mathbf{f}}\|_2$$

for arbitrary input vector $\hat{\mathbf{f}} \in (\mathbb{M} + i\mathbb{M})^{N^d}$, where

$$\begin{aligned} \tilde{k}_n &:= n^{-d/2} \tilde{\beta} |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} ((2m+1)^d + 4.1 d \log_2 n + 3), \\ \tilde{\beta} &:= \min \left\{ \left(\frac{2m}{nq} + 1 \right)^{d/2}, M^{1/2} \right\} ((\tau(0))^2 + \|\tau\|_2^2)^{d/2}. \end{aligned}$$

Proof: 1. First, we estimate the spectral norm of the sparse matrix \mathbf{D}_{n^d, N^d} . By

$$(\mathbf{D}_{n^d, N^d})^H \mathbf{D}_{n^d, N^d} = \text{diag} (|n^d c_{\mathbf{k}}(\varphi)|^{-2})_{\mathbf{k} \in I_N^d},$$

we see immediately that

$$\|\mathbf{D}_{n^d, N^d}\|_2 = \max_{\mathbf{k} \in I_N^d} \{n^{-d} |c_{\mathbf{k}}(\varphi)|^{-1}\} = n^{-d} |c_N(\varphi_0)|^{-d} = |\hat{\tau}(\frac{\pi}{\alpha})|^{-d},$$

i.e.,

$$\|\mathbf{D}_{n^d, N^d}\|_2 \leq |\hat{\tau}(\frac{\pi}{\alpha})|^{-d}. \quad (5.8)$$

2. Since ψ_0 is even, 1-periodic and monotone decreasing in $[0, \frac{1}{2}]$, we can estimate for fixed $j \in I_M^1$ that

$$n^{-1} \sum_{l \in I_n^1} \psi_0(x_j - \frac{l}{n})^2 \leq n^{-1} \psi_0(0)^2 + \int_{-1/2}^{1/2} \psi_0(x)^2 dx.$$

By definition of ψ_0 it follows that

$$\sum_{l \in I_n^1} \psi_0(x_j - \frac{l}{n})^2 \leq \tau(0)^2 + n \int_{-m/n}^{m/n} \tau(nx)^2 dx = \tau(0)^2 + \|\tau\|_2^2$$

for fixed $j \in I_M^1$. Since ψ is a tensor product, we obtain that

$$\sum_{\mathbf{l} \in I_n^d} \psi(\mathbf{x}_j - \frac{\mathbf{l}}{n})^2 \leq (\tau(0)^2 + \|\tau\|_2^2)^d \quad (5.9)$$

for fixed $j \in I_M^1$. For the sparse matrix $\mathbf{B}_{M, n^d} = (b_{j, \mathbf{l}})_{j \in I_M^1, \mathbf{l} \in I_n^d}$ with $b_{j, \mathbf{l}} := \psi(\mathbf{x}_j - \frac{\mathbf{l}}{n}) \geq 0$, the j -th component of the vector $\mathbf{B}_{M, n^d} \mathbf{y}$ with $\mathbf{y} = (y_{\mathbf{l}})_{\mathbf{l} \in I_n^d}$ reads as follows

$$(\mathbf{B}_{M, n^d} \mathbf{y})_j = \sum_{\mathbf{l} \in I_n^d} b_{j, \mathbf{l}} y_{\mathbf{l}}.$$

Let $b_{j, \mathbf{l}_r} > 0$ for $\mathbf{l}_r \in I_n^d$ ($r = 1, \dots, n_j$). By construction of ψ , we know that $n_j \leq (2m+1)^d$. By Cauchy–Schwarz inequality, we obtain for each $j \in I_M^1$

$$|(\mathbf{B}_{M, n^d} \mathbf{y})_j|^2 \leq \left(\sum_{r=1}^{n_j} b_{j, \mathbf{l}_r} |y_{\mathbf{l}_r}| \right)^2 \leq \left(\sum_{r=1}^{n_j} b_{j, \mathbf{l}_r}^2 \right) \left(\sum_{r=1}^{n_j} |y_{\mathbf{l}_r}|^2 \right).$$

Using (5.7), we can estimate

$$\sum_{r=1}^{n_j} b_{j, \mathbf{l}_r}^2 \leq \sum_{\mathbf{l} \in I_n^d} \psi(\mathbf{x}_j - \frac{\mathbf{l}}{n})^2 \leq (\tau(0)^2 + \|\tau\|_2^2)^d,$$

such that

$$|\mathbf{B}_{M,n^d}{}_j|^2 \leq (\tau(0)^2 + \|\tau\|_2^2)^d \sum_{r=1}^{n_j} |y_r|^2.$$

For each $\mathbf{l} \in I_n^d$, the cube $\frac{\mathbf{l}}{n} + [-\frac{m}{n}, \frac{m}{n}]^d$ contains at most $(\frac{2m}{nq} + 1)^d$ different nodes $\mathbf{x}_j \in \Pi^d$, since q is the separation distance of $\{\mathbf{x}_j \in \Pi^d : j \in I_M^1\}$. Therefore, each column of \mathbf{B}_{M,n^d} has at most

$$\min \left\{ \left(\frac{2m}{nq} + 1 \right)^d, M \right\}$$

non-zero entries $b_{j,\mathbf{l}}$. Consequently,

$$\|\mathbf{B}_{M,n^d} \mathbf{y}\|_2^2 = \sum_{j \in I_M^1} |(\mathbf{B}_{M,n^d} \mathbf{y})_j|^2 \leq \min \left\{ \left(\frac{2m}{nq} + 1 \right)^d, M \right\} (\tau(0)^2 + \|\tau\|_2^2)^d \|\mathbf{y}\|_2^2,$$

i.e.,

$$\|\mathbf{B}_{M,n^d}\|_2 \leq \min \left\{ \left(\frac{2m}{nq} + 1 \right)^{d/2}, M^{1/2} \right\} (\tau(0)^2 + \|\tau\|_2^2)^{d/2} =: \tilde{\beta}. \quad (5.10)$$

3. For arbitrary $\hat{\mathbf{f}} \in (\mathbb{M} + i\mathbb{M})^{N^d}$, we introduce $\mathbf{x} := \mathbf{D}_{n^d, N^d} \hat{\mathbf{f}}$ and the corresponding computed vector $\tilde{\mathbf{x}} := \text{fl}(\mathbf{D}_{n^d, N^d} \hat{\mathbf{f}})$. By Lemma 5.1 it is easy to check that

$$\|\tilde{\mathbf{x}} - \mathbf{x}\|_2 \leq u |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} \|\hat{\mathbf{f}}\|_2.$$

Now from (5.8) it follows that

$$\begin{aligned} \|\tilde{\mathbf{x}}\|_2 &\leq \|\tilde{\mathbf{x}} - \mathbf{x}\|_2 + \|\mathbf{x}\|_2 \leq \|\tilde{\mathbf{x}} - \mathbf{x}\|_2 + \|\mathbf{D}_{n^d, N^d}\|_2 \|\hat{\mathbf{f}}\|_2 \\ &\leq |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} (u + 1) \|\hat{\mathbf{f}}\|_2. \end{aligned}$$

4. Set $\mathbf{y} := \mathbf{F}_{n^d}^{(d)} \mathbf{x}$ and $\tilde{\mathbf{y}} := \text{fl}(\mathbf{F}_{n^d}^{(d)} \tilde{\mathbf{x}})$. Then we can estimate

$$\|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \leq \|\tilde{\mathbf{y}} - \mathbf{F}_{n^d}^{(d)} \tilde{\mathbf{x}}\|_2 + \|\mathbf{F}_{n^d}^{(d)} (\tilde{\mathbf{x}} - \mathbf{x})\|_2.$$

Since $\mathbf{F}_{n^d}^{(d)}$ is unitary and since the Euclidean norm is unitary invariant, we obtain by Lemma 5.2 on numerical stability of d -variate FFT that

$$\begin{aligned} \|\tilde{\mathbf{y}} - \mathbf{y}\|_2 &\leq (d k_n u + \mathcal{O}(u^2)) \|\tilde{\mathbf{x}}\|_2 + \|\tilde{\mathbf{x}} - \mathbf{x}\|_2 \\ &\leq ((d k_n + 1) u + \mathcal{O}(u^2)) |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} \|\hat{\mathbf{f}}\|_2 \end{aligned}$$

with $k_n = 4.01651 \log_2 n$, i.e.,

$$\|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \leq ((4.1 d \log_2 n + 1) u + \mathcal{O}(u^2)) |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} \|\hat{\mathbf{f}}\|_2. \quad (5.11)$$

By (5.8) and (5.11), we obtain

$$\begin{aligned} \|\tilde{\mathbf{y}}\|_2 &\leq \|\mathbf{y}\|_2 + \|\tilde{\mathbf{y}} - \mathbf{y}\|_2 = \|\mathbf{F}_{n^d}^{(d)} \mathbf{x}\|_2 + \|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \\ &= \|\mathbf{x}\|_2 + \|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \leq \|\mathbf{D}_{n^d, N^d}\|_2 \|\hat{\mathbf{f}}\|_2 + \|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \\ &\leq (|\hat{\tau}(\frac{\pi}{\alpha})|^{-d} + \mathcal{O}(u)) \|\hat{\mathbf{f}}\|_2. \end{aligned} \quad (5.12)$$

5. Now we consider the error between $\mathbf{z} := \mathbf{B}_{M,n^d} \mathbf{y}$ and $\tilde{\mathbf{z}} := \text{fl}(\mathbf{B}_{M,n^d} \tilde{\mathbf{y}})$. By (5.10) and (5.11), we obtain

$$\begin{aligned} \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 &\leq \|\tilde{\mathbf{z}} - \mathbf{B}_{M,n^d} \tilde{\mathbf{y}}\|_2 + \|\mathbf{B}_{M,n^d} (\tilde{\mathbf{y}} - \mathbf{y})\|_2 \\ &\leq \|\tilde{\mathbf{z}} - \mathbf{B}_{M,n^d} \tilde{\mathbf{y}}\|_2 + \|\mathbf{B}_{M,n^d}\|_2 \|\tilde{\mathbf{y}} - \mathbf{y}\|_2 \\ &\leq \|\tilde{\mathbf{z}} - \mathbf{B}_{M,n^d} \tilde{\mathbf{y}}\|_2 + \tilde{\beta} \left((4.1 d \log_2 n + 1) u + \mathcal{O}(u^2) \right) |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} \|\hat{\mathbf{f}}\|_2. \end{aligned}$$

Since each row of \mathbf{B}_{M,n^d} contains at most $(2m+1)^d$ nonzero entries (see step 2 of this proof), it follows by [12, p. 76] that

$$|\tilde{\mathbf{z}} - \mathbf{B}_{M,n^d} \tilde{\mathbf{y}}| \leq ((2m+1)^d u + \mathcal{O}(u^2)) \mathbf{B}_{M,n^d} |\tilde{\mathbf{y}}|$$

and consequently by (5.10) that

$$\begin{aligned} \|\tilde{\mathbf{z}} - \mathbf{B}_{M,n^d} \tilde{\mathbf{z}}\| &\leq ((2m+1)^d u + \mathcal{O}(u^2)) \|\mathbf{B}_{M,n^d}\|_2 \|\tilde{\mathbf{z}}\|_2 \\ &\leq ((2m+1)^d \tilde{\beta} u + \mathcal{O}(u^2)) \|\tilde{\mathbf{y}}\|_2 \end{aligned}$$

and hence by (5.12)

$$\|\tilde{\mathbf{z}} - \mathbf{B}_{M,n^d} \tilde{\mathbf{y}}\|_2 \leq ((2m+1)^d \tilde{\beta} |\hat{\tau}(\frac{\pi}{2})|^{-d} u + \mathcal{O}(u^2)) \|\hat{\mathbf{f}}\|_2$$

such that

$$\|\tilde{\mathbf{z}} - \mathbf{z}\|_2 \leq \tilde{\beta} |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} \left(((2m+1)^d + 4.1 d \log_2 n + 1) u + \mathcal{O}(u^2) \right) \|\hat{\mathbf{f}}\|_2. \quad (5.13)$$

By (5.8), (5.10), and (5.13), we can estimate

$$\begin{aligned} \|\tilde{\mathbf{z}}\|_2 &\leq \|\mathbf{z}\|_2 + \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 = \|\mathbf{B}_{M,n^d} \mathbf{y}\|_2 + \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 \\ &\leq \tilde{\beta} \|\mathbf{y}\|_2 + \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 \\ &= \tilde{\beta} \|\mathbf{F}_{n^d}^{(d)} \mathbf{x}\|_2 + \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 = \tilde{\beta} \|\mathbf{x}\|_2 + \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 \\ &\leq \tilde{\beta} \|\mathbf{D}_{n^d, N^d}\|_2 \|\mathbf{f}\|_2 + \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 \\ &\leq (\tilde{\beta} |\hat{\tau}(\frac{\pi}{\alpha})|^{-d} + \mathcal{O}(u)) \|\mathbf{f}\|_2. \end{aligned} \quad (5.14)$$

6. By (5.7), the final step of our NFFT algorithm is the scaling $\mathbf{h} := n^{-d/2} \mathbf{z}$, where n is a power of 2. Let $\tilde{\mathbf{h}} := \text{fl}(n^{-d/2} \tilde{\mathbf{z}})$. For even $d \log_2 n$, this scaling with a power of 2 does not produce an additional roundoff error such that $\tilde{\mathbf{h}} = n^{-d/2} \tilde{\mathbf{z}}$ and

$$\|\tilde{\mathbf{h}} - \mathbf{h}\|_2 = n^{-d/2} \|\tilde{\mathbf{z}} - \mathbf{z}\|_2.$$

For odd $d \log_2 n$, we can precompute $n^{-d/2} = 2^{-(d \log_2 n)/2}$ by $2^{-(d \log_2 n + 1)/2} \text{fl}(\sqrt{2}) \in \mathbb{M}$, where $|\text{fl}(\sqrt{2}) - \sqrt{2}| \leq u$. Then it follows from (5.2) that

$$|\tilde{\mathbf{h}} - \mathbf{h}| \leq n^{-d/2} |\tilde{\mathbf{z}} - \mathbf{z}| + n^{-d/2} |\tilde{\mathbf{z}}| (2u + \mathcal{O}(u^2))$$

and hence

$$\|\tilde{\mathbf{h}} - \mathbf{h}\|_2 \leq n^{-d/2} \|\tilde{\mathbf{z}} - \mathbf{z}\|_2 + n^{-d/2} \|\tilde{\mathbf{z}}\|_2 (2u + \mathcal{O}(u^2)).$$

The last inequality is also true for even $d \log_2 n$. By (5.13) and (5.14) we obtain the assertion and hence the multivariate NFFT is robust. \blacksquare

5.3. The d -variate NFFT is backward stable

We consider arbitrary input vectors $\hat{\mathbf{f}} \in (\mathbb{M} + i\mathbb{M})^{N^d}$, where all components of $\hat{\mathbf{f}}$ are floating point numbers. In this way, we neglect the inherent error and we essentially consider only the algorithmic one. Let $\mathbf{g} := \mathbf{A}_{M,N^d}^{(d)} \hat{\mathbf{f}}$ be the exact Fourier transformed vector. Let $\mathbf{h} := n^{-d/2} \mathbf{B}_{M,n^d} \mathbf{F}_{n^d}^{(d)} \mathbf{D}_{n^d,N^d} \hat{\mathbf{f}}$ be the exact result of the approximate NFFT Algorithm 2.1. Further, let $\tilde{\mathbf{h}} \in (\mathbb{M} + i\mathbb{M})^M$ be the output vector computed by Algorithm 2.1, using a binary floating point arithmetic with unit roundoff u . (see Figure 5.1). The weighted reconstruction problem (4.3) is solvable under the conditions of Theorem 4.2 and the matrix $\mathbf{A}_{M,N^d}^{(d)}$ has a left inverse $\mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2}$. We introduce $\Delta \hat{\mathbf{f}} \in \mathbb{C}^{N^d}$ by

$$\Delta \hat{\mathbf{f}} := \mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2} \tilde{\mathbf{h}} - \hat{\mathbf{f}}.$$

Then we say that an approximate algorithm for computing of $\mathbf{g} = \mathbf{A}_{M,N^d}^{(d)} \hat{\mathbf{f}}$ is *normwise backward stable* (see [12, p. 142]), if the scaled approximation error

$$\|\mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2}\|_2 \|\mathbf{h} - \mathbf{g}\|_2$$

is sufficiently small and if there exists a positive constant k_n with

$$\|\mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2}\|_2 k_n u \ll 1$$

such that

$$\|\Delta \hat{\mathbf{f}}\|_2 \leq (\|\mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2}\|_2 k_n u + \mathcal{O}(u^2)) \|\hat{\mathbf{f}}\|_2 + \|\mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2}\|_2 \|\mathbf{h} - \mathbf{g}\|_2.$$

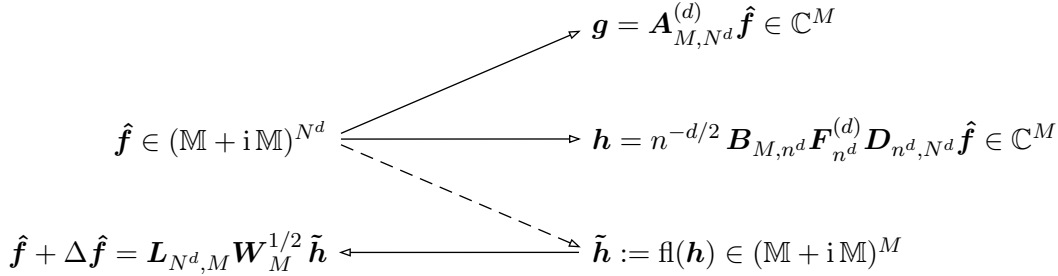


Figure 5.1: Normwise backward stability of NFFT via weighted reconstruction (4.3).

From $\hat{\mathbf{f}} = \mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2} \mathbf{A}_{M,N^d}^{(d)} \hat{\mathbf{f}}$ it follows that

$$\begin{aligned} \Delta \hat{\mathbf{f}} &= \mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2} (\tilde{\mathbf{h}} - \mathbf{A}_{M,N^d}^{(d)} \hat{\mathbf{f}}) = \mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2} (\tilde{\mathbf{h}} - \mathbf{g}) \\ &= \mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2} (\tilde{\mathbf{h}} - \mathbf{h}) + \mathbf{L}_{N^d,M} \mathbf{W}_M^{1/2} (\mathbf{h} - \mathbf{g}) \end{aligned}$$

and hence

$$\|\Delta \hat{\mathbf{f}}\|_2 \leq \|\mathbf{L}_{N^d, M} \mathbf{W}_M^{1/2}\|_2 \|\tilde{\mathbf{h}} - \mathbf{h}\|_2 + \|\mathbf{L}_{N^d, M} \mathbf{W}_M^{1/2}\|_2 \|\mathbf{h} - \mathbf{g}\|_2. \quad (5.15)$$

The approximation error $\|\mathbf{h} - \mathbf{g}\|_2$ can be estimated by (2.6) and (2.5), respectively. Under the assumptions of Theorem 4.2, we see that

$$\|\mathbf{L}_{N^d, M}\|_2 \leq (2 - e^{\pi d N \delta})^{-1}, \quad \|\mathbf{W}_M^{1/2}\|_2 \leq \max_{j \in I_M^1} \sqrt{w_j} \leq \sqrt{\delta}.$$

An estimate of $\|\tilde{\mathbf{h}} - \mathbf{h}\|_2$ is given in Theorem 5.3. Therefore we obtain immediately

Theorem 5.4 *Under the assumptions of Theorem 4.2, the weighted reconstruction problem (4.3) is solvable and the approximate NFFT Algorithm 2.1 is normwise backward stable.*

In an analogous manner, we can consider the underdetermined case, i.e., the interpolation case. The optimal interpolation problem (4.5) is solvable under the conditions of Theorem 4.3 and the matrix $\mathbf{A}_{M, N^d}^{(d)}$ has a right inverse $\hat{\mathbf{W}}_{N^d}^{1/2} \mathbf{R}_{N^d, M}$. Again we introduce $\Delta \hat{\mathbf{f}} \in \mathbb{C}^{N^d}$ by

$$\Delta \hat{\mathbf{f}} := \hat{\mathbf{W}}_{N^d}^{1/2} \mathbf{R}_{N^d, M} \tilde{\mathbf{h}} - \hat{\mathbf{f}}.$$

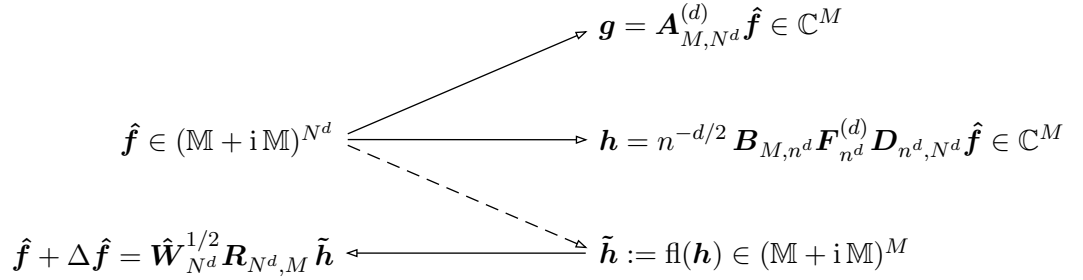


Figure 5.2: Normwise backward stability of NFFT via optimal interpolation (4.5).

See Figure 5.2. Following the lines above, we obtain by Theorem 4.3

Theorem 5.5 *Under the assumptions of Theorem 4.3, the optimal interpolation problem (4.5) is solvable and the approximate NFFT Algorithm 2.1 is normwise backward stable.*

6 Numerical examples

The following numerical examples are computed with the NFFT C-subroutine library [14], where we choose different window functions with different cut-off parameters m and

oversampling factor $\alpha = 2$. The NFFT evaluates the corresponding d -variate trigonometric polynomial (2.1) at M arbitrary nodes in $\mathcal{O}((\alpha N)^2 \log(\alpha N)^d + m^d M)$ arithmetical operations.

We start with the following numerical example, in order to confirm Theorem 5.3 by numerical results.

Example 6.1 We compute the Dirichlet kernels at $M = N^d$ random knots $\mathbf{x}_j \in [-1/2, 1/2]^d$ ($j = 0, \dots, M - 1$) by choosing $\hat{f}_{\mathbf{k}} = 1$ for $\mathbf{k} \in I_N^d$ for $d = 2$ and $d = 3$. In the bivariate case $d = 2$, we have for $\mathbf{x}_j = (x_{1j}, x_{2j}) \in [-1/2, 1/2]^2$ $j = 0, \dots, M - 1$

$$g_j = \sum_{\mathbf{k} \in I_N^2} e^{-2\pi i \mathbf{k} \cdot \mathbf{x}_j} = \frac{2(\cos(\pi N(x_{1j} + x_{2j})) - \cos(\pi N(x_{1j} - x_{2j})))}{(e^{-2\pi i x_{1j}} - 1)(e^{-2\pi i x_{2j}} - 1)}.$$

In Figure 6.1 we show the error (each is an average of 10 tests) $E := \frac{\|\mathbf{g} - \tilde{\mathbf{h}}\|_2}{\|\hat{\mathbf{f}}\|_2}$ for various cut-off parameters $m = 3, \dots, 19$, for various N and different window functions. By the triangle inequality, we can estimate

$$E = \frac{\|\mathbf{g} - \tilde{\mathbf{h}}\|_2}{\|\hat{\mathbf{f}}\|_2} \leq \frac{\|\mathbf{g} - \mathbf{h}\|_2}{\|\hat{\mathbf{f}}\|_2} + \frac{\|\mathbf{h} - \tilde{\mathbf{h}}\|_2}{\|\hat{\mathbf{f}}\|_2},$$

where the first term on the left hand side decays exponentially by (2.5) (first phase) and the second term is estimated in Theorem 5.3 (second phase). Furthermore we observe in the second phase that the constant k_n increase with increasing cut-off parameter m . Finally we present in Figure 6.1 (right) the same test in the trivariate case $d = 3$. Note that for $N = 16$ we choose $m = 3, \dots, 16$ since the NFFT requires $m \leq N$. \square

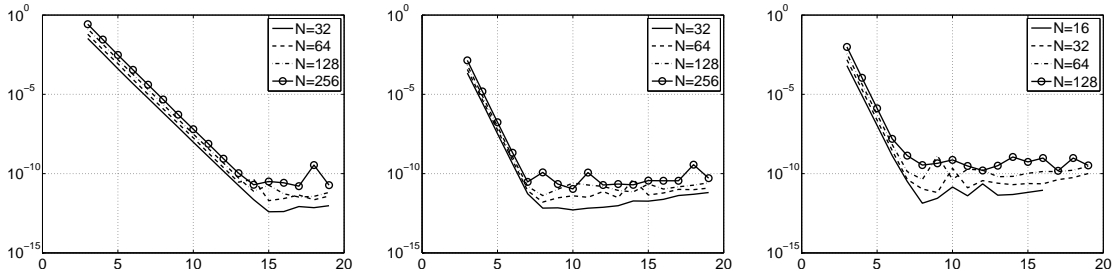


Figure 6.1: Error E with respect to various cut-off parameters $m = 3, \dots, 19$ and different N , left: Gaussian window $d = 2$, middle: Kaiser-Bessel window $d = 2$, right: Kaiser-Bessel window $d = 3$.

In the following we provide numerical examples for the NFFT on the important linogram grid (see [17, 1, 8]). Let $d = 2$ and let $\{\mathbf{x}_1, \dots, \mathbf{x}_M\}$ be a linogram grid centered at $(0, 0)$, which is formed by concentric squares centered at $(1/2, 1/2)$ (see Figure 6.2 left). We choose $R \in 2\mathbb{N}$ and $T \in 4\mathbb{N}$ and put

$$\{\mathbf{x}_1, \dots, \mathbf{x}_M\} = \bigcup_{-R/2 \leq j \leq R/2-1} \bigcup_{-T/4 \leq t \leq T/4-1} \{\mathbf{x}_{t,j}^H, \mathbf{x}_{t,j}^V\}$$

where

$$\mathbf{x}_{t,j}^H = \left(\frac{j}{R}, \frac{4t}{T}, \frac{j}{R} \right), \quad \mathbf{x}_{t,j}^V = \left(-\frac{4t}{T}, \frac{j}{R}, \frac{j}{R} \right).$$

We take the weights $w_{t,j} = \pi|j|/(TR^2)$ and choose $T = R = 2N$. The number of points in this grid is $M = TR = 4N^2$. One can easily show that $\delta = 2/N$. Note that the assumption of Theorem 3.2 is not fulfilled, because (3.2) would require $\delta < 0.1/N$. In order to fulfil this assumption one has to chose T and R much greater. However our numerical examples show that this is not necessary. Therefore an approach for estimating the smallest eigenvalue of (1.1) based on probabilistic arguments was given in [4]. With the following numerical example we are able to explain the numerical behavior observed in [8] and confirm Theorem 5.4 by numerical results.

Example 6.2 We choose vectors randomly $\hat{\mathbf{f}} \in ([0, 1] + i[0, 1])^{1024^2}$ randomly. Then we compute by the NFFT the values $f(\mathbf{x}_j)$ of the bivariate trigonometric polynomial (2.1) on the linogram grid for $d = 2$ and $j = 0, \dots, M - 1$ with an oversampling factor $\alpha = 2$ and cut-off parameter $m = 3 : 3 : 15$, i.e., with different accuracy. In Figure 6.2 (middle) we plot the reconstruction error

$$E_2(l) := \frac{\sqrt{\sum_{\mathbf{k} \in I_N^d} |\hat{f}_{\mathbf{k}} - \hat{f}_{l,\mathbf{k}}|^2}}{\sqrt{\sum_{\mathbf{k} \in I_N^d} |\hat{f}_{\mathbf{k}}|^2}},$$

where $\hat{f}_{l,\mathbf{k}}$ denotes the \mathbf{k} -th entry of the l -th iterate within the CGNR method.

Instead of computing the left inverse $\mathbf{L}_{N^d, M} \mathbf{W}_M^{1/2}$ of $\mathbf{A}_{M, N^d}^{(d)}$, we compute an approximation of the left inverse of $n^{-d/2} \mathbf{B}_{M, n^d} \mathbf{F}_{n^d}^{(d)} \mathbf{D}_{n^d, N^d}$ by the CGNR method and denote this matrix after l CGNR steps by $\tilde{\mathbf{L}}^l \mathbf{W}_M^{1/2}$. We infer from (5.15) the estimate

$$E_2(l) \leq \|\tilde{\mathbf{L}}^l\|_2 \frac{\|\mathbf{h} - \tilde{\mathbf{h}}\|_2}{\|\hat{\mathbf{f}}\|_2} + \|\tilde{\mathbf{L}}^l - \mathbf{L}_{N^d, M} \mathbf{W}_M^{1/2}\|_2 \frac{\|\mathbf{h}\|_2}{\|\hat{\mathbf{f}}\|_2} + \|\mathbf{L}_{N^d, M} \mathbf{W}_M^{1/2}\|_2 \frac{\|\mathbf{h} - \mathbf{g}\|_2}{\|\hat{\mathbf{f}}\|_2}.$$

Our numerical results are again in perfect accordance with the theoretical results. In the first phase we observe the exponential decay of $\frac{\|\mathbf{h} - \tilde{\mathbf{h}}\|_2}{\|\hat{\mathbf{f}}\|_2}$ and in the second stage the saturation dominated by the roundoff error. By the term $\|\tilde{\mathbf{L}}^l - \mathbf{L}_{N^d, M} \mathbf{W}_M^{1/2}\|_2$ we can explain the saturation with respect to the iteration number for constant cut-off parameters m . In Figure 6.2 (middle and right) we show the reconstruction error $E_2(l)$ by using the Gaussian window function and the Kaiser-Bessel window function. We see in the saturation phase of Figure 6.2 (right) that the numerical error increase slightly with increasing m as expected for the term $\|\mathbf{h} - \tilde{\mathbf{h}}\|_2 / \|\hat{\mathbf{f}}\|_2$ (see Theorem 5.3). However we observe that the assumption (3.2) of Theorem 4.2 is too pessimistic and we observe a much better numerical behavior for greater mesh norms. \square

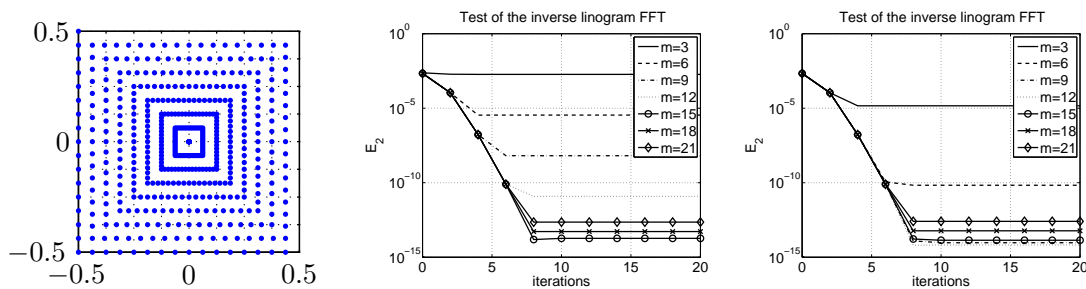


Figure 6.2: Left:linogram grid, middle and right: Reconstruction error $E_2(l)$ after l iterations for various cut-off parameters m , middle: Gaussian window, right: Kaiser-Bessel window.

References

- [1] A. Averbuch, R. Coifman, D. L. Donoho, M. Elad, and M. Israeli. Fast and accurate polar Fourier transform. *Appl. Comput. Harmon. Anal.*, 21:145 – 167, 2006.
- [2] R. F. Bass and K. Gröchenig. Random sampling of multivariate trigonometric polynomials. *SIAM J. Math. Anal.*, 36:773 – 795, 2004.
- [3] G. Beylkin. On the fast Fourier transform of functions with singularities. *Appl. Comput. Harmon. Anal.*, 2:363 – 381, 1995.
- [4] A. Böttcher, D. Potts, and D. Wenzel. A probability argument in favor of ignoring small singular values. *Operators and Matrices*, 1:31 – 43, 2007.
- [5] A. Dutt and V. Rokhlin. Fast Fourier transforms for nonequispaced data. *SIAM J. Sci. Stat. Comput.*, 14:1368 – 1393, 1993.
- [6] B. Elbel and G. Steidl. Fast Fourier transform for nonequispaced data. In C. K. Chui and L. L. Schumaker (eds.), *Approximation Theory IX*, Volume 2, pages 39 – 46, Nashville, 1998. Vanderbilt Univ. Press.
- [7] H. G. Feichtinger, K. Gröchenig, and T. Strohmer. Efficient numerical methods in non-uniform sampling theory. *Numer. Math.*, 69:423 – 440, 1995.
- [8] M. Fenn, S. Kunis, and D. Potts. On the computation of the polar FFT. *Appl. Comput. Harmon. Anal.*, 22:257 – 263, 2007.
- [9] K. Fourmont. Non equispaced fast Fourier transforms with applications to tomography. *J. Fourier Anal. Appl.*, 9:431 – 450, 2003.
- [10] L. Greengard and J.-Y. Lee. Accelerating the nonuniform fast Fourier transform. *SIAM Rev.*, 46:443 – 454, 2004.
- [11] K. Gröchenig. Reconstruction algorithms in irregular sampling. *Math. Comput.*, 59:181 – 194, 1992.

- [12] N. J. Higham. *Accuracy and Stability of Numerical Algorithms*. 2nd ed., SIAM, Philadelphia, 2002.
- [13] J. I. Jackson, C. H. Meyer, D. G. Nishimura, and A. Macovski. Selection of a convolution function for Fourier inversion using gridding. *IEEE Trans. Med. Imag.*, 10:473 – 478, 1991.
- [14] J. Keiner, S. Kunis, and D. Potts. NFFT3.0, Softwarepackage, C subroutine library. <http://www.tu-chemnitz.de/~potts/nfft>, 2006.
- [15] S. Kunis and D. Potts. Stability results for scattered data interpolation by trigonometric polynomials. *SIAM J. Sci. Comput.*, 29:1403 – 1419, 2007.
- [16] D. Potts. Schnelle Fourier-Transformationen für nichtäquidistante Daten und Anwendungen. Habilitation, Univ. Lübeck, 2003. <http://www.tu-chemnitz.de/~potts>.
- [17] D. Potts and G. Steidl. A new linogram algorithm for computerized tomography. *IMA J. Numer. Anal.*, 21:769 – 782, 2001.
- [18] D. Potts, G. Steidl, and M. Tasche. Fast Fourier transforms for nonequispaced data: A tutorial. In J. J. Benedetto and P. J. S. G. Ferreira (eds.), *Modern Sampling Theory: Mathematics and Applications*, pages 247 – 270. Birkhäuser, Boston, 2001.
- [19] D. Potts, G. Steidl, and M. Tasche. Numerical stability of fast trigonometric transforms - a worst case study. *J. Concrete Appl. Math.*, 1:1 – 36, 2003.
- [20] G. Steidl. A note on fast Fourier transforms for nonequispaced grids. *Adv. Comput. Math.*, 9:337 – 353, 1998.
- [21] M. Tasche and H. Zeuner. Roundoff error analysis for fast trigonometric transforms. In G. Anastassiou (ed.), *Handbook of Analytic-Computational Methods in Applied Mathematics*, pages 357 – 406, CRC Press, Boca Raton, 2000.
- [22] M. Tasche and H. Zeuner. Worst and average case roundoff error analysis for FFT. *BIT*, 41:563 – 581, 2001.
- [23] M. Tasche and H. Zeuner. Roundoff error analysis for the fast Fourier transform with precomputed twiddle factors. *J. Comput. Anal. Appl.*, 4:1 – 18, 2002.