Taylor and rank-1 lattice based nonequispaced fast Fourier transform

Toni Volkmer
Chemnitz University of Technology
Department of Mathematics
09107 Chemnitz, Germany
Email: toni.volkmer@mathematik.tu-chemnitz.de

Abstract—The nonequispaced fast Fourier transform (NFFT) allows the fast approximate evaluation of trigonometric polynomials with frequencies supported on full box-shaped grids at arbitrary sampling nodes. Due to the curse of dimensionality, the total number of frequencies and thus, the total arithmetic complexity can already be very large for small refinements at medium dimensions. In this paper, we present an approach for the fast approximate evaluation of trigonometric polynomials with frequencies supported on an arbitrary subset of the full grid at arbitrary sampling nodes, which is based on Taylor expansion and rank-1 lattice methods. For the special case of symmetric hyperbolic cross index sets in frequency domain, we present error estimates and numerical results.

I. INTRODUCTION

We consider the evaluation of trigonometric polynomials $f : \mathbb{T}^d := [0, 1)^d \to \mathbb{C}$,

$$f(x) = \sum_{\ell \in I_N} \hat{f}_\ell e^{-2\pi i \ell \cdot x}, \hat{f}_\ell \in \mathbb{C}, I_N \subset \mathbb{Z}^d \cap [-N, N]^d,$$  \hspace{1cm} (1)

at arbitrary sampling nodes $y_\ell \in \mathbb{T}^d$, $\ell = 0, \ldots, L - 1$. For given Fourier coefficients $\hat{f}_\ell$, the direct evaluation of the trigonometric sums $f(y_\ell)$, $\ell = 0, \ldots, L - 1$, takes $O(L |I_N|)$ arithmetic operations. Various fast methods for the approximate evaluation of the trigonometric sums $f(y_\ell)$ were developed.

In the case, when the frequency index set $I_N$ is a full grid, $I_N = G_N^d : = \mathbb{Z}^d \cap [-N, N]^d$, the nonequispaced fast Fourier transform (NFFT, see [1] and references therein) allows the fast approximate evaluation of the trigonometric polynomial $f$ at arbitrary sampling nodes $y_\ell$, $\ell = 0, \ldots, L - 1$, in $O(||\epsilon||^d L + |G_N^d| \log |G_N^d|)$ arithmetic operations, where $\epsilon$ is the approximation error. Furthermore, there exist Taylor based versions (cf. [2], [3]) with an arithmetic complexity of $O(||\epsilon||^d L + |G_N^d| \log |G_N^d|)$, which use fast Fourier transforms (FFT) for evaluating the trigonometric polynomial $f$ as well as its derivatives at equispaced nodes and approximate the trigonometric sum $f(y_\ell)$ by a Taylor expansion at the closest equispaced node. However, since the cardinality of the full grid $|G_N^d| = (2N)^d$, the total number of arithmetic operations can already be very large for small refinements $N$ at medium dimensionality (e.g. $d = 3, 4, 5$).

For dyadic hyperbolic crosses $\tilde{H}^d_n := \bigcup_{\ell \in \mathbb{N}_0^d, \sum_{j=1}^d \ell_j = n} \tilde{G}_j$, $\tilde{G}_j := \mathbb{Z}^d \cap \times_{j=1}^d (-2^{j-1}, 2^{j-1}]$, $||j||_1 = |j_1| + \ldots + |j_d|$, the nonequispaced hyperbolic cross fast Fourier transform [4] allows the fast approximate evaluation of trigonometric polynomials with frequencies supported on the index set $I_N = \tilde{H}^d_n$ at arbitrary sampling nodes $y_\ell$, $\ell = 0, \ldots, L - 1$, with an arithmetic complexity of $O \left ( |\log \epsilon|^d L \log |\tilde{H}^d_n| + |\log \epsilon| |\tilde{H}^d_n| + |\tilde{H}^d_n| \log |\tilde{H}^d_n| \right )$,

where $|\tilde{H}^d_n| \leq C n^{d-1} 2^n$ with a constant $C > 0$ depending only on $d$.

For the more general case of a trigonometric polynomial $f$ from (1), we present an approach for the fast approximate evaluation at arbitrary sampling nodes $y_\ell$. This method uses one-dimensional FFTs for evaluating the trigonometric polynomial $f$ and its derivatives at nodes of a rank-1 lattice. Then, for each sampling node $y_\ell$, a Taylor expansion of degree $m - 1$, $m \in \mathbb{N}$, at a closest rank-1 lattice node is performed. This results in a total arithmetic complexity of $O(m^d (L + M \log M + |I_N|))$, where $M \in \mathbb{N}$ is the size of the rank-1 lattice.

We consider the special case of symmetric hyperbolic cross index sets $I_N = H^d_N := \{ j \in \mathbb{Z}^d : r(j) \leq N \}$ in frequency domain with refinement $N \in \mathbb{N}$, $r(j) := \prod_{j=1}^d \max(1, |j_i|)$. For this case, we show error estimates for the approximation error of the presented method. Note, that we have the inclusion $H^d_n \subset H^d_{2n-1} \subset H^d_{n+1+2d}$, see [5, Lemma 2.1].

In Section II, we give a short overview over Taylor expansion of trigonometric polynomials and define rank-1 lattices. We show that trigonometric polynomials can be evaluated at rank-1 lattice nodes using a one-dimensional FFT. The proposed method is presented in Section III as well as error estimates for the special case of symmetric hyperbolic cross index sets $I_N = H^d_N$. Results of numerical tests are presented in Section IV. Finally, we summarize the results in Section V.

II. PREREQUISITE

A. Taylor expansion

We approximate a function $f : \mathbb{T}^d \to \mathbb{C}$ by

$$f(x) \approx s_m(x) := f(a) + \sum_{1 \leq |s| < m} \frac{D^s f(a)}{s!} (x - a)^s,$$

where $m \in \mathbb{N}$, $D^s f := \frac{\partial^{s_1}}{\partial x_1^{s_1}} \ldots \frac{\partial^{s_d}}{\partial x_d^{s_d}}, x := (x_1, \ldots, x_d)^T, s := (s_1, \ldots, s_d) \in \mathbb{N}_0^d, |s| := |s_1| + \ldots + |s_d|$, $D^0 f := f$, $s! := s_1! \ldots s_d!$, $x^s := x_1^{s_1} \ldots x_d^{s_d}$. For a
trigonometric polynomial $f$ from (1), we have
$$D^s f(x) = \sum_{t \in \mathbb{Z}^d} (-2\pi i)^s f_t e^{-2\pi i t x}$$
and thus,
$$s_m(x) = \sum_{t \in \mathcal{Z}_N} f_t e^{-2\pi i t a} + \sum_{1 \leq |x| < m} \frac{(x - a)^s}{s!} \sum_{t \in \mathcal{Z}_N} (-2\pi i)^s f_t e^{-2\pi i t a} \tag{2}$$

B. Rank-1 lattice

**Definition II.1** (rank-1 lattice). Let $M \in \mathbb{N}$, $z \in \mathbb{Z}^d$. We define the rank-1 lattice $\Lambda(z, M) \subset \mathbb{T}^d$ of size $M$ with generating vector $z \in \mathbb{Z}^d$ by $\Lambda(z, M) := \{ k z \mod M \}$. 

**Definition II.2** (mesh norm). Let the metric $\mu(x, y) := \min_{k \in \mathbb{Z}^d} \| x - y - k \|_\infty$ be given for $x, y \in \mathbb{T}^d$. We define the mesh norm $\delta$ of an arbitrary point set $X \subset \mathbb{T}^d$ by $\delta := 2 \max_{x \in x \in X} \mu(x, k)$.

For an arbitrary point set $X \subset \mathbb{T}^d$ of size $|X| = M$, we have $\delta \geq 1/\sqrt{M}$, see e.g. [6, Lemma 3.1]. The following Lemma shows the existence of a rank-1 lattice $\Lambda(z, M)$ of size $M$, such that the mesh norm $\delta \leq C_d/\sqrt{M}$, where $C_d > 1$ is a constant depending only on $d$, i.e. we have $\delta \geq 1/\sqrt{M}$.

**Lemma II.3.** Let $b \in \mathbb{N}$, $b \geq 3$. Then, there exists a rank-1 lattice $\Lambda(z, M)$ of size $M = b(b+1)$ for $d = 2$ and $b^d, 2 \frac{b+1}{b-1} \leq M \leq b^d, 2 \sqrt{\frac{b-2}{b-1}}$ for $d = 3$ with generating vector $z \in \mathbb{Z}^d$, such that the mesh norm $\delta \leq C_d/\sqrt{M}$, where $C_d > 1$ is a constant depending only on $d$.

**Proof:** In the case $d = 2$, we choose the rank-1 lattice size $M := b \cdot (b+1)$ and the generating vector $z := (b, b+1)^\top$. Since $b$ and $b+1$ are relative prime to each other, there exists a bijective mapping between the rank-1 lattice nodes $x_k := (k z \mod M)$, $k = 0, \ldots, M-1$, and the grid $(j_1/b+1, j_2/b)^\top$, $j_1 = 0, \ldots, b$ and $j_2 = 0, \ldots, b-1$. Obviously, the mesh norm $\delta = 1/b \leq \frac{1}{\sqrt{M}}$.

In the case $d = 3$, we set $v_1 := b+1$ and $v_2 := 2b$. Due to Bertrand’s postulate, there exists a prime number $p_3 \in \mathbb{N}$, $b \leq p_3 < 2b$. We choose $v_3 \in \{p_3, \ldots, v_2 - 1\}$, such that $v_3$ is relative prime to $v_1$ and $v_2$. We set the rank-1 lattice size $M := v_1 \cdot v_2 \cdot v_3$ and the generating vector $z := (v_1, v_2, v_3)^\top$. Then, the mesh norm $\delta \leq 1/v_3 \leq 1/b \leq 2/\sqrt{M}$.

Assuming that a closest rank-1 lattice node $x_{k'}$ is known for each sampling node $y_{\ell}$, the Taylor expansion $s_m(x)$ in (2) can be calculated in $O(n^d(L + M \log M + |N|))$ arithmetic operations for all sampling nodes $y_{\ell}, \ell = 0, \ldots, L-1$. For symmetric hyperbolic cross index sets $\mathcal{I}_N = H^d_N$, the evaluation of a trigonometric polynomial $g : \mathbb{T}^d \to \mathbb{C}$ supported on the frequency index set $\mathcal{I}_N \subset \mathbb{Z}^d \cap [-N,N]^d$, $g(x) := \sum_{t \in \mathcal{Z}_N} \hat{g}_t e^{-2\pi i t x}$, $\hat{g}_t \in \mathbb{C}$, at rank-1 lattice nodes $x_k \in \Lambda(z, M)$. As presented in [5], we have
$$g(x_k) = g(k z / M) = M^{-1} \sum_{j=0}^{M-1} \left( \sum_{t \in \mathcal{Z}_N} \hat{f}_t \right) e^{-2\pi i j k}$$
and the outer sum is a one-dimensional discrete Fourier transform of length $M$. Using a one-dimensional FFT, the trigonometric polynomial $g$ can be evaluated at all rank-1 lattice nodes in $O(M \log M + |\mathcal{Z}_N|)$ arithmetic operations.

Setting the Fourier coefficients $\hat{f}_t := (-2\pi i)^s \hat{f}_t$, where $\hat{f}_t$ are the Fourier coefficients of a trigonometric polynomial $f$ from (1), yields $g(x_k) = D^s f(x_k)$. Thus, for fixed $s \in \mathbb{N}_0^d$, the mixed derivatives $D^s f(x)$ of the trigonometric polynomial $f$ can be evaluated at all rank-1 lattice nodes $x_{k'}$, $k = 0, \ldots, M-1$, in $O(M \log M + |\mathcal{Z}_N|)$ arithmetic operations.

**III. NFFT based on Taylor expansion and rank-1 lattice FFT**

We approximately evaluate a trigonometric polynomial $f$ from (1) at arbitrary sampling nodes $y_{\ell} \in \mathbb{T}^d$, $\ell = 0, \ldots, L-1$, using a Taylor expansion at a closest rank-1 lattice node $x_{k'} \in \Lambda(z, M)$ for each sampling node $y_{\ell}$. For evaluating the trigonometric polynomial $f$ and its derivatives at all rank-1 lattice nodes $x_{k'} \in \Lambda(z, M)$, $k = 0, \ldots, M-1$, one-dimensional FFTs are used.

**A. Method**

Let a frequency index set $\mathcal{I}_N \subset \mathbb{Z}^d \cap [-N,N]^d$ and a rank-1 lattice $\Lambda(z, M)$ of size $M$ be given. We replace the expansion point $a$ in (2) by a closest rank-1 lattice node $x_{k'} = \arg\min_{x \in \Lambda(z, M)} \mu(x, x_{k'})$ and obtain an approximation for the trigonometric polynomial $f(x) := \sum_{t \in \mathcal{Z}_N} \hat{f}_t e^{-2\pi i t a}$ by the Taylor expansion
$$s_m(x) = \sum_{t \in \mathcal{Z}_N} \hat{f}_t e^{-2\pi i t a_{k'}} + \sum_{1 \leq |x| < m} \frac{(x - a)^s}{s!} \sum_{t \in \mathcal{Z}_N} (-2\pi i)^s \hat{f}_t e^{-2\pi i t a_{k'}} \tag{3}$$

Assuming that a closest rank-1 lattice node $x_{k'}$ is known for each sampling node $y_{\ell}$, the Taylor expansion $s_m$ in (3) can be calculated in $O(n^d(L + M \log M + |\mathcal{Z}_N|))$ arithmetic operations for all sampling nodes $y_{\ell}, \ell = 0, \ldots, L-1$.

For symmetric hyperbolic cross index sets $\mathcal{I}_N = H^d_N$, $N \in \mathbb{N}$, $N \geq 2$, we have $|H^d_N| \leq C_{H} N \log^{-d-1} N$ for $N \geq 2$ with a constant $C_{H} > 0$, see e.g. [7]. Choosing the rank-1 lattice size $M \sim |H^d_N|$, we obtain an arithmetic complexity of $O\left(n^d(L + \log^d N)\right)$.

**B. Error estimates for symmetric hyperbolic cross index sets**

In this section, we establish error bounds for the approximation of a trigonometric polynomial $f$ from (1) by a Taylor expansion $s_m$ from (3) for symmetric hyperbolic cross index sets $\mathcal{I}_N = H^d_N$. 

\[ \text{Error bounds: } \]
Let a trigonometric polynomial \( f : \mathbb{T}^d \to \mathbb{C} \) supported on the frequency index set \( \mathcal{I}_N \), 
\[
 f(x) := \sum_{l \in \mathcal{I}_N} \hat{f}_l e^{-2\pi i l x}, \quad \hat{f}_l \in \mathbb{C}, \quad N \in \mathbb{N} \text{ be given.}
\]
Furthermore, let \( \Lambda(z, M) \) be a rank-1 lattice with mesh norm \( \delta \). Then, for the approximation of the trigonometric polynomial \( f \) by a truncated Taylor series 
\[
 s_m(x):= \sum_{|s| < m} D^{|s|} f(x) \frac{(x-x_k)^s}{s!}
\]
 of degree \( m - 1 \) from (3), where \( m \in \mathbb{N} \) and \( x_k = \arg \min_{x \in \Lambda(z, M)} \mu(x, x_k) \), the remainder \( R_m(x) := f(x) - s_m(x) \) is bounded by
\[
 |R_m(x)| < C(m, d) \delta^m N^{(m-\alpha)+} \sum_{l \in \mathcal{I}_N} |\hat{f}_l| r(l)^\alpha,
\]
where \( C(m, d) \geq 1 \) is a constant depending only on \( m \) and \( d \), \( \alpha \geq 0 \) is the smoothness parameter, \( (x)_+ := \max(0, x) \).

**Proof:** Let \( \xi(t) := x_{k'} + t(x - x_{k'}) \), \( t \in [0, 1] \). The remainder \( R_m(x) \) can be written (cf. [8, Ch. 1]) in the form
\[
 R_m(x) = m \int_0^1 (1 - t)^{m-1} \sum_{|s| < m} D^{|s|} f(\xi(t)) \frac{(x-x_{k'})^s}{s!} dt.
\]
Then,
\[
 |R_m(x)| & \leq m \int_0^1 (1 - t)^{m-1} \sum_{|s| < m} |D^{|s|} f(\xi(t))| \frac{|(x-x_{k'})^s|}{s!} dt \\
 & \leq \max_{t \in [0, 1]} \sum_{|s| < m} |D^{|s|} f(\xi(t))| \frac{|(x-x_{k'})^s|}{s!} \\
 & = \max_{t \in [0, 1]} \sum_{|s| < m} \sum_{l \in \mathcal{I}_N} (-2\pi i t)^s \hat{f}_l e^{-2\pi i l(t)} \frac{|(x-x_{k'})^s|}{s!}.
\]
Since \( \mu(x, x_{k'}) \leq \delta \), we get
\[
 |R_m(x)| \leq \max_{t \in [0, 1]} \sum_{|s| < m} \left( \frac{\delta}{2} \right)^{|s|} \sum_{l \in \mathcal{I}_N} |(-2\pi i t)^s| |\hat{f}_l| e^{-2\pi i l(t)} |(x-x_{k'})^s| \\
 \leq \pi^m \delta^m \sum_{|s| < m} |\hat{f}_l| \frac{|(x-x_{k'})^s|}{s!}.
\]
Introducing weights \( r(l)^\alpha \), \( \alpha \geq 0 \), we obtain
\[
 |R_m(x)| \leq \pi^m \delta^m \sum_{|s| < m} |\hat{f}_l| r(l)^\alpha \sum_{|s| < m} \frac{|l_1|^{s_1} \ldots |l_d|^{s_d}}{r(l)^{s_d} s!} \\
 \leq \pi^m \delta^m \sum_{|s| < m} |\hat{f}_l| r(l)^\alpha \sum_{|s| < m} \frac{r(l^1)^{s_1} \ldots r(l_d)^{s_d}}{r(l)^{s_d} s!} \\
 \leq \pi^m \delta^m \max_{l \in \mathcal{I}_N} \sum_{|s| = m} \frac{r(l^1)^{s_1} \ldots r(l_d)^{s_d}}{s!} \sum_{|s| = m} N^{(m-\alpha)+} \\
 \leq \pi^m \delta^m \sum_{|s| = m} |\hat{f}_l| r(l)^\alpha \sum_{|s| = m} N^{(m-\alpha)+}.
\]
Since \( \{ s \in \mathbb{N}_0^d : |s| = m \} < (m+1)^d \), it follows that
\[
 |R_m(x)| < (m+1)^d \pi^m \delta^m N^{(m-\alpha)+} \sum_{l \in \mathcal{I}_N} |\hat{f}_l| r(l)^\alpha.
\]

**Corollary III.2.** Let a hyperbolic cross index set \( \mathcal{I}_N = H^d_N \), \( N \in \mathbb{N} \), \( N \geq 2 \), and a rank-1 lattice \( \Lambda(z, M) \) of size \( M := C_\Lambda N \log^{d-1} N \sim |H^d_N| \) for some constant \( C_\Lambda \geq 1 \) be given, where the generating vector \( z \) is chosen as in the proof of Lemma II.3. Then,
\[
 |R_m(x)| < C(m, d) (C_d)^m M^{-m/d} N^{(m-\alpha)_+} \sum_{|s| < m} |\hat{f}_l| r(l)^\alpha
\]
\[
 = C(m, d) \frac{N^{(m-\alpha)_+}}{(N \log^{d-1} N)^{m/d}} \sum_{l \in H^d_N} |\hat{f}_l| r(l)^\alpha
\]
is valid for all smoothness parameters \( \alpha \geq 0 \), where \( C_d \geq 1 \) is the constant from Lemma II.3 and \( C(m, d) > 0 \) is a constant depending only on \( m \) and \( d \).

**Proof:** From Lemma II.3, we obtain that the mesh norm \( \delta \leq C_d M^{-1/d} \). Applying Theorem III.1 and defining the constant \( C(m, d) := C(m, d) \left( C_d \sqrt{C_\Lambda}\right)^{-m} \) yields the result.

**Remark III.3.** If we choose the smoothness parameter \( \alpha \geq \frac{d-1}{m} \), Corollary III.2 guarantees a decreasing relative error 
\[
 |R_m(x)| / \left( \sum_{|l| \in H^d_N} |\hat{f}_l| r(l)^\alpha \right)
\]
for increasing refinement \( N \).

**Setting the smoothness parameter \( \alpha \) yields \( |R_m(x)| < C(m, d) (N \log^{d-1} N)^{-m/d} \sum_{|l| \in H^d_N} |\hat{f}_l| r(l)^m \).**

**IV. NUMERICAL RESULTS**

The Taylor expansion \( s_m \) in (3) was implemented in MATLAB for trigonometric polynomials \( f \) from (1) as described in Section III-A.

For symmetric hyperbolic cross index sets \( \mathcal{I}_N = H^d_N \), numerical tests were performed. The generating vector \( z \) of each rank-1 lattice \( \Lambda(z, M) \) was chosen as in the proof of Lemma II.3. The maximum relative approximation error \( E_\alpha := \max_{y \in \mathcal{Y}} |R_m(y)| / \left( \sum_{|l| \in H^d_N} |\hat{f}_l| r(l)^\alpha \right) \) was determined using \( L = 100000 \) uniformly random sampling nodes \( y_\ell \in \mathbb{T}^d \), \( \mathcal{Y} := \{ y_\ell \}_{\ell=0}^{L-1} \).

**A. Decreasing error \( E_\alpha \) for increasing rank-1 lattice size \( M \)**

In this test case, we uniformly randomly chose the Fourier coefficients \( \hat{f}_l \in (0, 1) / r(l)^\alpha \). \( l \in \mathcal{I}_N = H^d_N \). All tests were repeated five times using different Fourier coefficients \( \hat{f}_l \) and sampling nodes \( y_\ell \). Then, the average error of these five test runs was used.

We set the rank-1 lattice size \( M := \sigma \cdot 2 |H^d_N| \) with a factor \( \sigma \geq 1/2 \). Due to Corollary III.2, the error \( E_\alpha \) should decrease at least like \( \sim \sigma^{-m/d} \) for increasing factor \( \sigma \). In tests performed for the cases \( d = 2, \ldots, 5 \) and \( m = 2, \ldots, 6 \), this behaviour could be observed. Figure 1 shows the error \( E_\alpha \) for increasing
In the four- and five-dimensional case as well as the lines (solid lines without symbols) in the cases

\[ \hat{f}_{(\pm N,0,\ldots,0)} = 1/N^{m}, \quad \hat{f}_{(0,\pm N,0,\ldots,0)} = 1/N^{m}, \ldots, \quad \hat{f}_{(0,0,\ldots,0,\pm N)} = 1/N^{m}. \]

We set the rank-1 lattice size \( M = 2\|H_N^d\| \). Test cases included Taylor expansion degrees \( m = 1, m = 2, \ldots, 6 \), and refinements up to \( N = 10^4 \) for \( d = 2 \), up to \( N = 10^5 \) for \( d = 3 \) and up to \( N = 800 \) for \( d = 4, 5 \). Remark III.3 states, that the error \( E_m \) should decrease at least like \( (N \log^{d-1} N)^{-m/d} \). In the results of the performed tests, a decrease of \( (N \log^{d-1} N)^{-m/d} \) could be observed. Figure 2 shows the results for the cases \( d = 4, 5 \).

V. Conclusion

Based on rank-1 lattice methods and Taylor expansion, we presented a method for the fast approximate evaluation of trigonometric polynomials \( f \) with frequencies supported on arbitrary index sets \( I_N \subset \mathbb{Z}^d \cap [-N,N]^d \) at arbitrary sampling nodes \( y_{\ell} \in \mathbb{T}^d, \ell = 0, \ldots, L - 1 \).

In the case of symmetric hyperbolic cross index sets \( I_N = H_N^d \) with refinement \( N \), we showed conditions which guarantee a decreasing approximation error \( |r_m(x)|/\|f\|_r(\mathbb{T}^d) \) for increasing refinement \( N \).

In particular for smoothness parameter \( \alpha = m \), a rank-1 lattice \( \Lambda(z,M) \) of size \( M \sim |H_N^d| \) exists, such that the approximation error decreases at least like \( (N \log^{d-1} N)^{-m/d} \) for increasing refinement \( N \). For such a rank-1 lattice of size \( M \sim |H_N^d| \), the total arithmetic complexity of the presented method is \( \mathcal{O}(m^dL + m^d N \log^{m/d} N) \).

The results of the numerical tests confirmed the theoretical upper bounds.

ACKNOWLEDGMENT

The author thanks Daniel Potts and Lutz Kämerer for numerous valuable discussions on the presented subject. Moreover, he gratefully acknowledges support by German Research Foundation within the project PO 711/10-2.

REFERENCES