Nonequidistant fast Fourier transform for frequencies supported on a subset of the full grid

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Road map

Introduction

- evaluation of trigonometric polynomials $f\colon \mathbb{T}^d \simeq [0,1)^d \to \mathbb{C}$,

  $$f(\boldsymbol{x}) = \sum_{\boldsymbol{j}\in\mathcal{I}_N} \hat{f}_{\boldsymbol{j}}\, \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{j}\boldsymbol{x}},\ \hat{f}_{\boldsymbol{j}} \in \mathbb{C},\ \mathcal{I}_N \subset \mathbb{Z}^d \cap [-N,N]^d, N \in \mathbb{N},$$

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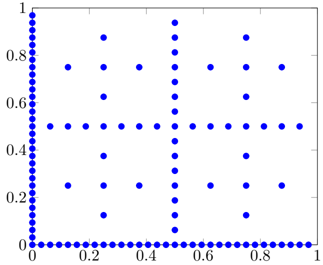
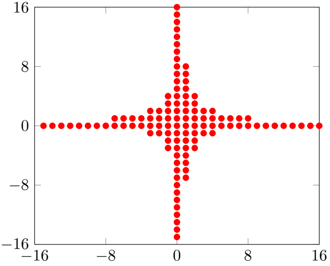
    - Taylor expansion based NFFT (Anderson, Dahleh 1996; Kunis 2008)
    for arbitrary $\boldsymbol{y}_\ell \in \mathbb{T}^d$,
    arithmetic complexity $\mathcal{O}(|\log\epsilon|^d\, L + |\log\epsilon|^d\, N^d \log N)$

Introduction

- nonequispaced hyperbolic cross fast Fourier transform
  (Döhler, Kunis, Potts 2010)
  - dyadic hyperbolic cross $\mathcal{I}_N = \tilde{H}_n^d := \cup_{\boldsymbol{j}\in\mathbb{N}_0^d, \|\boldsymbol{j}\|_1=n} \tilde{G}_{\boldsymbol{j}}$
    $\tilde{G}_{\boldsymbol{j}} := \mathbb{Z}^d \cap \times_{t=1}^d (-2^{j_t-1}, 2^{j_t-1}]$, $\|\boldsymbol{j}\|_1 = |j_1| + \ldots + |j_d|$
  - based on hyperbolic cross discrete/fast Fourier transform
    (Baszenski, Delvos 1989; Hallatschek 1992; Gradinaru 2007)
    and spline interpolation on sparse grid
  - arithmetic complexity
    $\mathcal{O}\left(|\tilde{H}_n^d| \log |\tilde{H}_n^d| + |\log \epsilon|\ |\tilde{H}_n^d| + |\log \epsilon|^d\ L\ \log |\tilde{H}_n^d|\right)$,
    $|\tilde{H}_n^d| \leq C\, n^{d-1}\, 2^n$, $C > 0$





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- method for fast approximative evaluation of

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  at arbitrary $\boldsymbol{y}_\ell \in \mathbb{T}^d$, $\ell = 0, \ldots, L-1$,
  based on FFT at nodes of rank-1 lattice of size M and
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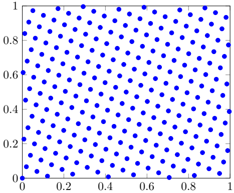
  arithmetic complexity $\mathcal{O}\left(m^d\,(L + M\log M + |\mathcal{I}_N|)\right)$



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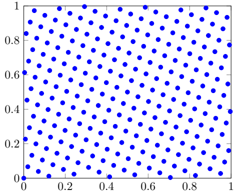
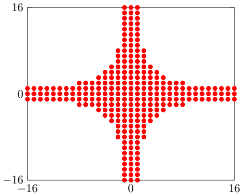
- error estimate and numerical results for
symmetric hyperbolic cross index sets
$\mathcal{I}_N = H_N^d := \{\boldsymbol{j} \in \mathbb{Z}^d \colon r(\boldsymbol{j}) \le N\}$, $r(\boldsymbol{j}) := \prod_{t=1}^d \max(1, |j_t|)$



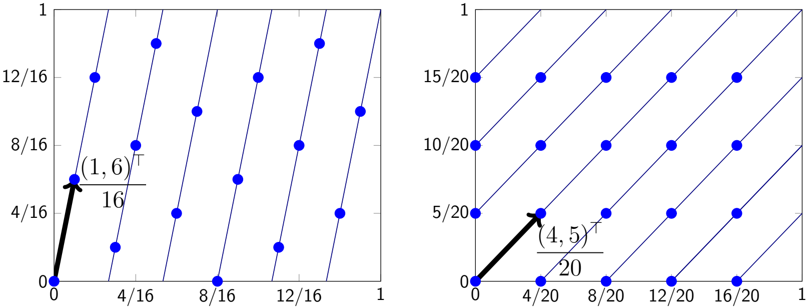


Rank-1 lattices - General

Definition (Rank-1 lattice; e.g. Sloan, Joe 1994)

Let be $\boldsymbol{z} \in \mathbb{Z}^d$ and $M \in \mathbb{N}$. We define the (integer) rank-1 lattice

$$\Lambda = \Lambda(\boldsymbol{z}, M) := \{(k\boldsymbol{z}/M) \bmod 1 : \ k = 0, \dots, M-1\} \subset \mathbb{T}^d.$$



$\boldsymbol{z} = \begin{pmatrix} 1 \\ 6 \end{pmatrix}$, $M = 16$ $\qquad$ $\boldsymbol{z} = \begin{pmatrix} 4 \\ 5 \end{pmatrix}$, $M = 20$

Rank-1 lattices - Lattice based FFT

- evaluation of multivariate function $f(\boldsymbol{x}) = \sum_{\boldsymbol{j} \in \mathcal{I}_N} \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{j} \boldsymbol{x}}$ at $\boldsymbol{x}_k = (k\boldsymbol{z}/M) \bmod 1 \in \Lambda(\boldsymbol{z}, M)$,

$$f(\boldsymbol{x}_k) = \sum_{\boldsymbol{j} \in \mathcal{I}_N} \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi \mathrm{i} k \frac{\boldsymbol{j}\boldsymbol{z}}{M}}$$

$k = 0, \ldots, M-1,$

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  $k = 0, \ldots, M-1$, by 1d DFT/FFT(M)

  (e.g. Li, Hickernell 2003; Kämmerer 2012)

  arithmetic complexity $\mathcal{O}(|\mathcal{I}_N| + M \log M)$

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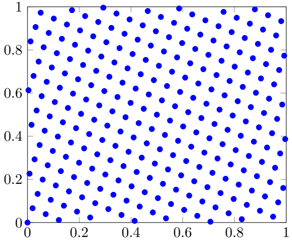

$\boldsymbol{x}_k,\ k = 0, \ldots, M-1$

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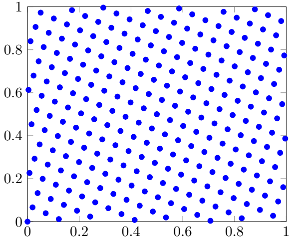

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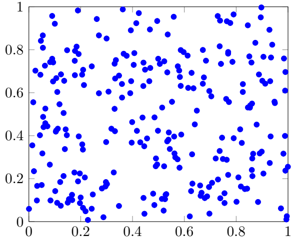

$\boldsymbol{y}_\ell,\ \ell = 0, \ldots, L-1$

Taylor and rank-1 lattice based NFFT - Method

- Let $m \in \mathbb{N}$, $\Lambda(\boldsymbol{z}, M)$ be given. Approximate $f(\boldsymbol{x}) = \sum_{\boldsymbol{j} \in \mathcal{I}_N} \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{j}\boldsymbol{x}}$ by Taylor expansion $s_m(\boldsymbol{x})$ at

$$\boldsymbol{x}_{k'} = \operatorname*{arg\,min}_{\boldsymbol{x}_k \in \Lambda(\boldsymbol{z},M)} \min_{\boldsymbol{j} \in \mathbb{Z}^d} \|\boldsymbol{x} - \boldsymbol{x}_k + \boldsymbol{j}\|_\infty$$

$$s_m(\boldsymbol{x}) \quad = \quad f(\boldsymbol{x}_{k'}) + \sum_{0 < |\boldsymbol{s}| < m} \frac{(\boldsymbol{x} - \boldsymbol{x}_{k'})^{\boldsymbol{s}}}{\boldsymbol{s}!} \, (D^{\boldsymbol{s}} f)(\boldsymbol{x}_{k'})$$

- $\boldsymbol{x} := (x_1, \ldots, x_d)^\top$, $\boldsymbol{s} := (s_1, \ldots, s_d) \in \mathbb{N}_0^d$, $|\boldsymbol{s}| := s_1 + \ldots + s_d$, $D^{\boldsymbol{s}} f := \frac{\partial^{s_1}}{\partial {x_1}^{s_1}} \ldots \frac{\partial^{s_d}}{\partial {x_d}^{s_d}}$, $\boldsymbol{s}! := s_1! \cdot \ldots \cdot s_d!$, $\boldsymbol{x}^{\boldsymbol{s}} := {x_1}^{s_1} \cdot \ldots \cdot {x_d}^{s_d}$

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$$\begin{aligned} s_m(\boldsymbol{x}) &= f(\boldsymbol{x}_{k'}) + \sum_{0<|\boldsymbol{s}|<m} \frac{(\boldsymbol{x} - \boldsymbol{x}_{k'})^{\boldsymbol{s}}}{\boldsymbol{s}!} (D^{\boldsymbol{s}} f)(\boldsymbol{x}_{k'}) \\ &= \sum_{\boldsymbol{j} \in \mathcal{I}_N} \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{j}\boldsymbol{x}_{k'}} \\ &\quad + \sum_{0<|\boldsymbol{s}|<m} \frac{(\boldsymbol{x} - \boldsymbol{x}_{k'})^{\boldsymbol{s}}}{\boldsymbol{s}!} \sum_{\boldsymbol{j} \in \mathcal{I}_N} (-2\pi\mathrm{i}\boldsymbol{j})^{\boldsymbol{s}} \, \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{j}\boldsymbol{x}_{k'}}, \end{aligned}$$

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- For fixed $\boldsymbol{s} \in \mathbb{N}_0^d$, compute $(D^{\boldsymbol{s}} f)(\boldsymbol{x}_k) = \sum_{\boldsymbol{j} \in \mathcal{I}_N} (-2\pi \mathrm{i} \boldsymbol{j})^{\boldsymbol{s}} \, \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{j} \boldsymbol{x}_k}$ for all $\boldsymbol{x}_k \in \Lambda(\boldsymbol{z}, M)$ with 1d FFT(M) in $\mathcal{O}(M \log M + |\mathcal{I}_N|)$

Taylor and rank-1 lattice based NFFT - Method

Algorithm (Taylor and rank-1 lattice based NFFT)

Input: $\mathcal{I}_N$, $\hat{f}_{\boldsymbol{j}} \in \mathbb{C}$, $\Lambda(\boldsymbol{z}, M)$, $m \in \mathbb{N}$, $\boldsymbol{y}_\ell \in \mathbb{T}^d$, $\ell = 0, \dots, L-1$,
index $\mu_\ell \in \{0, \dots, M-1\}$ *of* $\boldsymbol{x}_{\mu_\ell} \in \Lambda(\boldsymbol{z}, M)$ *closest to* $\boldsymbol{y}_\ell$

1: Set $\tilde{s}(\boldsymbol{y}_\ell) := 0$, $\ell = 0, \dots, L-1$.
2: **for all** $\boldsymbol{s} \in \{\boldsymbol{\alpha} \in \mathbb{N}_0^d \colon 0 \le |\boldsymbol{\alpha}| \le m-1\}$ **do**
3: Compute

$$(D^{\boldsymbol{s}} f)(\boldsymbol{x}_k) = \sum_{r=0}^{M-1} \left(\sum_{\substack{\boldsymbol{j} \in \mathcal{I}_N \\ \boldsymbol{j}\boldsymbol{z} \equiv r (\mathrm{mod} M)}} (-2\pi \mathrm{i} \boldsymbol{j})^{\boldsymbol{s}} \ \hat{f}_{\boldsymbol{j}} \right) \mathrm{e}^{-2\pi \mathrm{i} \frac{kr}{M}},$$

$k = 0, \dots, M-1$, *using 1D FFT(M).*
4: Set $\tilde{s}(\boldsymbol{y}_\ell) := \tilde{s}(\boldsymbol{y}_\ell) + \frac{(\boldsymbol{x} - \boldsymbol{x}_{\mu_\ell})^{\boldsymbol{s}}}{\boldsymbol{s}!} (D^{\boldsymbol{s}} f)(\boldsymbol{x}_{\mu_\ell})$, $\ell = 0, \dots, L-1$.
5: **end for**

Output: $s_m(\boldsymbol{y}_\ell) := \tilde{s}(\boldsymbol{y}_\ell)$, $\ell = 0, \dots, M-1$
arithmetic complexity $\mathcal{O}\left(m^d(|\mathcal{I}_N| + M \log M + L)\right)$

Taylor and rank-1 lattice based NFFT - Method

evaluation of Taylor expansion $s_m(\boldsymbol{x})$ at $\boldsymbol{y}_\ell \in \mathbb{T}^d$, $\ell = 0, \ldots, L-1$

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- choose $M \sim |\mathcal{I}_N|$

  $\Longrightarrow \mathcal{O}\left(m^d L + m^d \, |\mathcal{I}_N| \log |\mathcal{I}_N|\right)$

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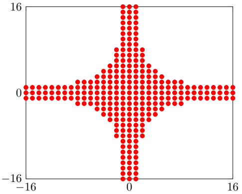
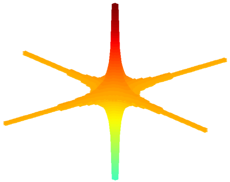
  $\Longrightarrow \mathcal{O}\left(m^d L + m^d \, |\mathcal{I}_N| \log |\mathcal{I}_N|\right)$
- for symmetric hyperbolic cross index sets

  $\mathcal{I}_N = H_N^d := \{\boldsymbol{j} \in \mathbb{Z}^d \colon r(\boldsymbol{j}) \leq N\}$, $r(\boldsymbol{j}) := \prod_{t=1}^{d} \max(1, |j_t|)$,
  $|H_N^d| \leq C \, N \log^{d-1} N$

  $\Longrightarrow \mathcal{O}(m^d L + m^d \, N \log^d N)$





Taylor and rank-1 lattice based NFFT - Error estimate

Theorem

Let a symmetric hyperbolic cross index set $\mathcal{I}_N = H_N^d$*,* $N \in \mathbb{N}$*,* $N \geq 2$*, and a trigonometric polynomial* $f(\boldsymbol{x}) := \sum_{\boldsymbol{j} \in H_N^d} \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{j}\boldsymbol{x}}$*,* $\hat{f}_{\boldsymbol{j}} \in \mathbb{C}$*, be given. Then, there exists a rank-1 lattice* $\Lambda(\boldsymbol{z}, M)$ *of size* M*,* $|H_N^d| \leq M \leq C_d \, |H_N^d|$*, such that* $R_m(\boldsymbol{x}) := f(\boldsymbol{x}) - s_m(\boldsymbol{x})$ *is bounded by*

$$|R_m(\boldsymbol{x})| < C(m,d) \, \frac{N^{(m-\alpha)_+}}{M^{m/d}} \sum_{\boldsymbol{j} \in H_N^d} |\hat{f}_{\boldsymbol{j}}| \, r(\boldsymbol{j})^\alpha$$

for all $\alpha \geq 0$*, where* $C(m,d) > 0$ *and* $(x)_+ := \max(0, x)$*.*

Taylor and rank-1 lattice based NFFT - Error estimate

Theorem

Let a symmetric hyperbolic cross index set $\mathcal{I}_N = H_N^d$, $N \in \mathbb{N}$, $N \geq 2$, *and a trigonometric polynomial* $f(\boldsymbol{x}) := \sum_{\boldsymbol{j} \in H_N^d} \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{j}\boldsymbol{x}}$, $\hat{f}_{\boldsymbol{j}} \in \mathbb{C}$, *be given. Then, there exists a rank-1 lattice* $\Lambda(\boldsymbol{z}, M)$ *of size* M, $|H_N^d| \leq M \leq C_d \, |H_N^d|$, *such that* $R_m(\boldsymbol{x}) := f(\boldsymbol{x}) - s_m(\boldsymbol{x})$ *is bounded by*

$$|R_m(\boldsymbol{x})| < C(m,d) \, \frac{N^{(m-\alpha)_+}}{M^{m/d}} \sum_{\boldsymbol{j} \in H_N^d} |\hat{f}_{\boldsymbol{j}}| \, r(\boldsymbol{j})^\alpha$$

for all $\alpha \geq 0$, *where* $C(m,d) > 0$ *and* $(x)_+ := \max(0, x)$.

Corollary

For fixed $N \in \mathbb{N}$, $N \geq 2$, *we have* $\dfrac{\max_{\boldsymbol{x} \in \mathbb{T}^d} |R_m(\boldsymbol{x})|}{\sum_{\boldsymbol{j} \in H_N^d} |\hat{f}_{\boldsymbol{j}}| \, r(\boldsymbol{j})^\alpha} \lesssim M^{-m/d}$.

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for all $\alpha \geq 0$, *where* $C(m,d) > 0$ *and* $(x)_+ := \max(0, x)$.

Corollary

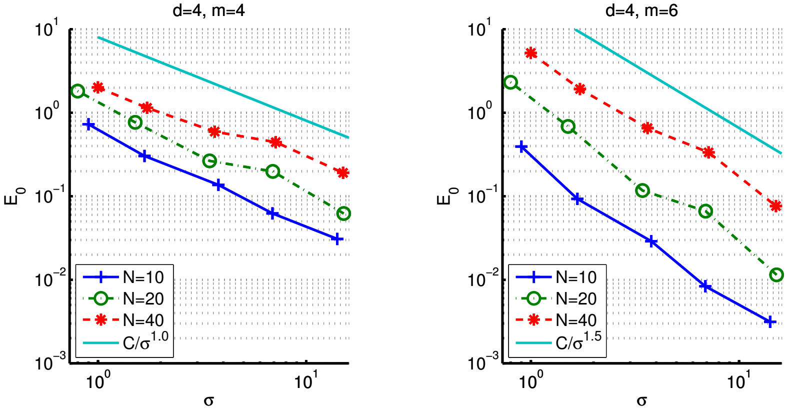
For $\alpha = m$, *we have* $\dfrac{\max_{\boldsymbol{x} \in \mathbb{T}^d} |R_m(\boldsymbol{x})|}{\sum_{\boldsymbol{j} \in H_N^d} |\hat{f}_{\boldsymbol{j}}|\, r(\boldsymbol{j})^{m}} \lesssim (N \log^{d-1} N)^{-m/d}$.

Taylor and rank-1 lattice based NFFT - Numerical Results

- Taylor and rank-1 lattice based NFFT for frequency index set $\mathcal{I}_N \subset \mathbb{Z}^d \cap [-N, N]^d$ implemented in MATLAB
- numerical tests for symmetric hyperbolic cross index set $\mathcal{I}_N = H_N^d$
- rank-1 lattice size $M \sim |H_N^d| \leq C\, N \log^{d-1} N$
- test cases $d = 2, \ldots, 4$ for Taylor expansions s_m, $m = 2, \ldots, 6$
- $L = 100\,000$ (uniformly) randomly distributed nodes $\boldsymbol{y}_\ell \in \mathbb{T}^d$, $\mathcal{Y} := \{\boldsymbol{y}_\ell\}_{\ell=0}^{L-1}$
- determination of maximum relative error

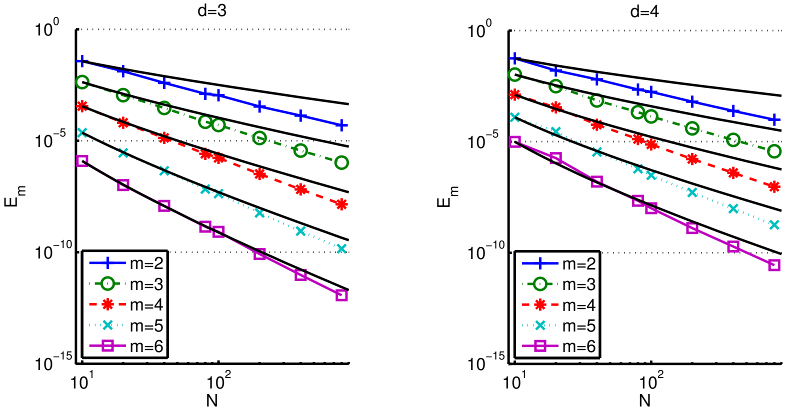
$$E_\alpha := \frac{\max\limits_{\boldsymbol{y}_\ell \in \mathcal{Y}} |R_m(\boldsymbol{y}_\ell)|}{\left(\sum_{\boldsymbol{j} \in H_N^d} |\hat{f}_{\boldsymbol{j}}|\, r(\boldsymbol{j})^\alpha\right)}$$

Taylor and rank-1 lattice based NFFT - Numerical Results



- (uniformly) random Fourier coefficients $\hat{f}_{\boldsymbol{j}} \in (0,1]/r(\boldsymbol{j})^\alpha$
- $M = \sigma\ 2|H_N^d| \leq C\,N \log^{d-1} N$, case $d=4$ for $m=4,6$
- error $E_0 := \dfrac{\max\limits_{\boldsymbol{y}_\ell \in \mathcal{Y}} |R_m(\boldsymbol{y}_\ell)|}{\sum\limits_{\boldsymbol{j}\in H_N^d} |\hat{f}_{\boldsymbol{j}}|}$ should decrease like $\sim \sigma^{-m/d}$

Taylor and rank-1 lattice based NFFT - Numerical Results



- Fourier coefficient $\hat{f}_{(N,0,\ldots,0)^\top} = 1/r(\boldsymbol{j})^\alpha$, other $\hat{f}_{\boldsymbol{j}} = 0$
- $M \approx 2|H_N^d| \leq C\, N \log^{d-1} N$, case $d = 3, 4$
- error $E_m := \dfrac{\max_{\boldsymbol{y}_\ell \in \mathcal{Y}} |R_m(\boldsymbol{y}_\ell)|}{\sum_{\boldsymbol{j} \in H_N^d} |\hat{f}_{\boldsymbol{j}}|\, r(\boldsymbol{j})^m}$ should decrease like $\sim \dfrac{1}{(N \log^{d-1} N)^{m/d}}$

Summary

- curse of dimensionality attenuated by using a (small) subset $\mathcal{I}_N$ of the full grid $\mathbb{Z}^d \cap [-N, N]^d$ in frequency domain
- algorithm for the fast approximative evaluation of trigonometric polynomials

  $$f(\boldsymbol{x}) = \sum_{\boldsymbol{j} \in \mathcal{I}_N} \hat{f}_{\boldsymbol{j}} \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{j} \boldsymbol{x}}, \; \hat{f}_{\boldsymbol{j}} \in \mathbb{C}, \; \mathcal{I}_N \subset \mathbb{Z}^d \cap [-N, N]^d, N \in \mathbb{N},$$

  at arbitrary nodes $\boldsymbol{y}_\ell \in \mathbb{T}^d$, $\ell = 0, \ldots, L-1$, presented
- error estimate for symmetric hyperbolic cross index sets $\mathcal{I}_N = H_N^d$ presented
- numerical results confirmed theoretical error estimates