

Sparse high-dimensional FFT with applications to data mining

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joint work with Lutz Kämmerer and Daniel Potts

supported by



Content

Introduction

Multivariate trigonometric polynomials

Sparse dimension-incremental FFT

Regression and Classification

Summary

Introduction

- approximate high-dim. function $f: \mathbb{T}^d \simeq [0, 1)^d \rightarrow \mathbb{C}$ by multivariate trigonometric polynomial $p: \mathbb{T}^d \rightarrow \mathbb{C}$ with frequencies supported on $I \subset \mathbb{Z}^d$, $|I| < \infty$,

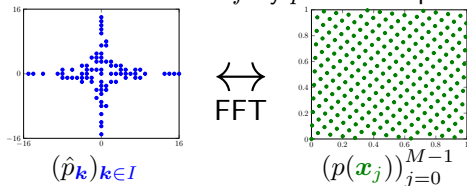
$$p(\mathbf{x}) := \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}, \quad \hat{p}_{\mathbf{k}} \in \mathbb{C}$$

Introduction

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- **arbitrary known** frequency index set $I \subset \mathbb{Z}^d$, $|I| < \infty$, rank-1 lattice nodes \mathbf{x}_j , $j = 0, \dots, M-1$
 - fast evaluation $p(\mathbf{x}_j)$, (e.g. [Li, Hickernell 03])
 - fast and exact reconstruction of $\hat{p}_{\mathbf{k}}$, $\mathbf{k} \in I$, from samples $p(\mathbf{x}_j)$, ([Kämmerer, Kunis, Potts 12] [Kämmerer 13])
 - approximate reconstruction of f by p from samples $f(\mathbf{x}_j)$

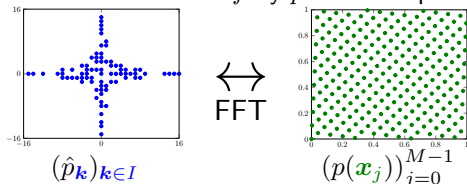


Introduction

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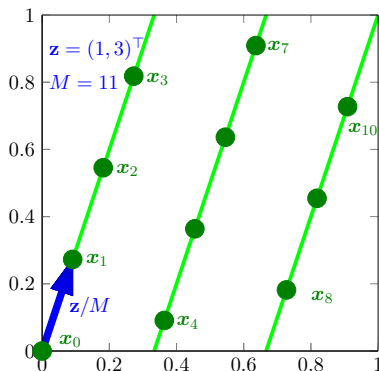


- unknown** frequency index set I ?

Trigonometric polynomials - fast evaluation

- rank-1 lattice $\text{R1L}(z, M)$: $z \in \mathbb{N}_0^d, M \in \mathbb{N}$

$$x_j = \frac{j}{M}z \bmod \mathbf{1}; j = 0, \dots, M-1$$



Korobov 59
Maisonneuve 72
Sloan & Kachoyan 84,87,90
Temlyakov 86
Lyness 89
Sloan & Joe 94
Sloan & Reztsov 01
Li & Hickernell 03

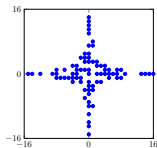
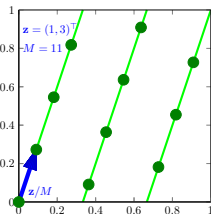
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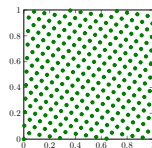
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- multivariate high-dim. trigonometric polynomial $p(\mathbf{x}) = \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$
- reformulation

$$p(\mathbf{x}_j) = \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \frac{j \mathbf{k} \cdot \mathbf{z}}{M}} = \sum_{l=0}^{M-1} \underbrace{\left(\sum_{\substack{\mathbf{k} \in I \\ \mathbf{k} \cdot \mathbf{z} \equiv l \pmod{M}} \hat{p}_{\mathbf{k}} \right)}_{\hat{g}_l} e^{2\pi i \frac{j \mathbf{k} \cdot \mathbf{z}}{M}} = \sum_{l=0}^{M-1} \hat{g}_l e^{2\pi i \frac{j l}{M}}$$



$(\hat{p}_{\mathbf{k}})_{\mathbf{k} \in I}$



$(p(\mathbf{x}_j))_{j=0}^{M-1}$

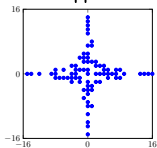
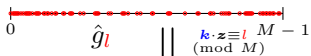
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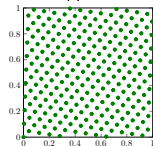
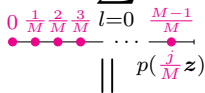
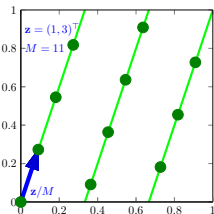
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$$(\hat{p}_{\mathbf{k}})_{\mathbf{k} \in I}$$

1-dim
 $\xrightarrow{\text{FFT}}$

$$\mathcal{O}(M \log M + d|I|)$$



$$(p(\mathbf{x}_j))_{j=0}^{M-1}$$

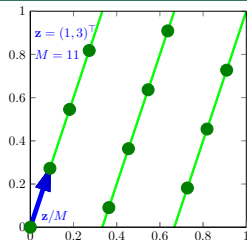
Trigonometric polynomials - fast reconstruction

- rank-1 lattice $\text{R1L}(\mathbf{z}, M)$: $\mathbf{z} \in \mathbb{N}_0^d, M \in \mathbb{N}$

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- reconstruction of Fourier coefficients $\hat{p}_{\mathbf{k}}$ of multivariate trigonometric polynomial

$$p(\mathbf{x}) = \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$$



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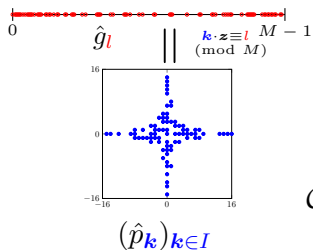
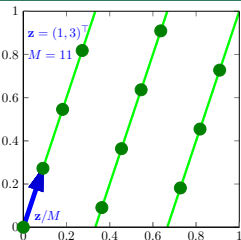
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⇒ **Definition** reconstructing R1L(z, M, I) for I :

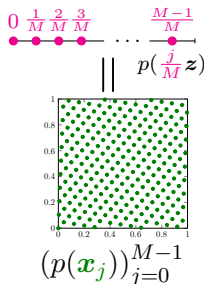
$$\mathbf{k} \cdot \mathbf{z} \not\equiv \mathbf{k}' \cdot \mathbf{z} \pmod{M} \text{ for all } \mathbf{k}, \mathbf{k}' \in I, \mathbf{k} \neq \mathbf{k}'$$

- $|I| \leq M \leq |I|^2$, CBC construction algorithm [Kämmerer 2012]



1-dim
←
iFFT

$$\mathcal{O}(M \log M + d|I|)$$



Trigonometric polynomials - fast approximation

- **fast approximation** of **high-dimensional function** $f: \mathbb{T}^d \rightarrow \mathbb{C}$
by multivariate trigonometric polynomial $p(\mathbf{x}) = \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$
from **samples** at **reconstructing rank-1 lattice** $\text{R1L}(\mathbf{z}, M, I)$



Kämmerer, L., Potts, D., Volkmer, T.

Approximation of multivariate periodic functions by trigonometric polynomials based on rank-1 lattice sampling.

J. Complexity 31, 543 – 576, 2015.



Byrenheid, G., Kämmerer, L., Ullrich, T., Volkmer, T.

Tight error bounds for rank-1 lattice sampling in spaces of hybrid mixed smoothness.

arXiv:1510.08336, Preprint, 2016.

(<http://www.tu-chemnitz.de/~tovo>)

Unknown frequency index set

until now: fast reconstruction of $p(\mathbf{x}) := \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$ or
fast approximation of function $f(\mathbf{x}) \approx p(\mathbf{x})$

- given frequency index set I
- compute $\hat{p}_{\mathbf{k}}$ from samples along reconstructing rank-1 lattice

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- search for location I of largest Fourier coefficients of f or non-zero Fourier coefficients of p
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- search domain: (possibly) large index set $\Gamma \subset \mathbb{Z}^d$, e.g., full grid $\hat{G}_N^d := \{\mathbf{k} \in \mathbb{Z}^d : \|\mathbf{k}\|_{\infty} \leq N\}$, ($|\hat{G}_{64}^{10}| \approx 1.28 \cdot 10^{21}$)

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⇒ multi-dimensional sparse FFT

Multi-dimensional sparse FFT

Various existing methods, e.g.

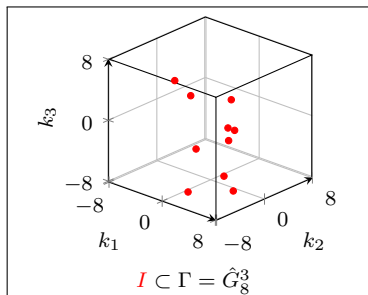
- filters [Indyk, Kapralov 14]
- Chinese remainder theorem
 - [Cuyt, Lee 08]
 - [Iwen 13]
- Prony's method
 - multiple lines [Tasche, Potts 13]
 - common ZEROS [Peter, Plonka, Schaback 15] [Kunis, Peter, Römer, von der Ohe 15]
- dimension-incremental projection
 - Zippel's Algorithm [Zippel 79] [Kaltofen, Lee 03] [Javadi Monagan 10]
 - via (reconstructing) rank-1 lattices [Potts, V. 15]
- randomized Kronecker substitution
[Arnold, Roche 14] [Arnold, Giesbrecht, Roche 15]
- (reconstructing) rank-1 lattice and 1d method
[Potts, Tasche, V. 16]

Multi-dimensional sparse FFT

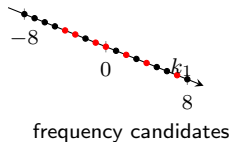
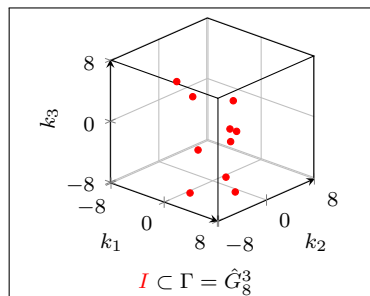
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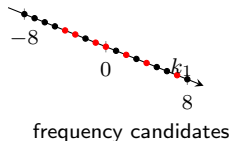
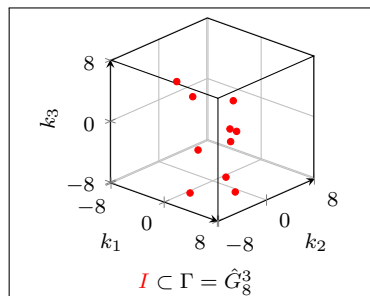
Sparse dimension-incremental FFT - method



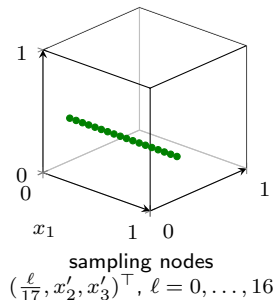
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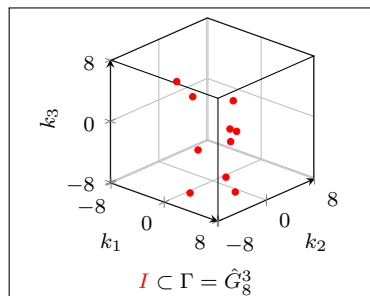
Sparse dimension-incremental FFT - method



construct
→
sampling set

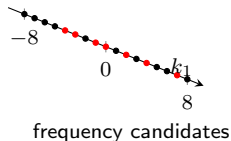


Sparse dimension-incremental FFT - method

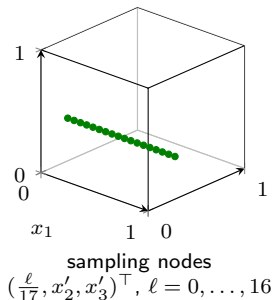


$$\hat{p}_{k_1} := \frac{1}{17} \sum_{\ell=0}^{16} p \left(\begin{pmatrix} \ell/17 \\ x'_2 \\ x'_3 \end{pmatrix} \right) e^{-2\pi i \frac{\ell k_1}{17}}$$

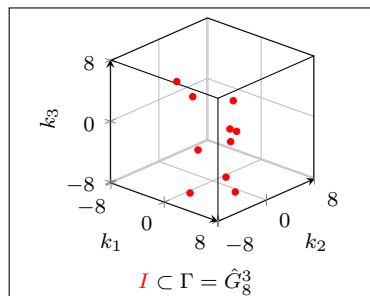
$$k_1 = -8, \dots, 8$$



1-dim
←
iFFT

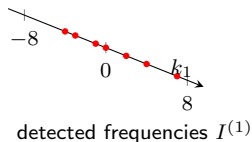


Sparse dimension-incremental FFT - method

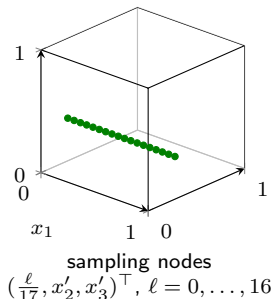


$$\begin{aligned} \hat{p}_{k_1} &:= \frac{1}{17} \sum_{\ell=0}^{16} p \left(\begin{pmatrix} \ell/17 \\ x'_2 \\ x'_3 \end{pmatrix} \right) e^{-2\pi i \frac{\ell k_1}{17}} \\ &= \sum_{\substack{(h_2, h_3) \in \{-8, \dots, 8\}^2 \\ (k_1, h_2, h_3)^\top \in \text{supp } \hat{p}}} \hat{p} \begin{pmatrix} k_1 \\ h_2 \\ h_3 \end{pmatrix} e^{2\pi i (h_2 x'_2 + h_3 x'_3)}, \end{aligned}$$

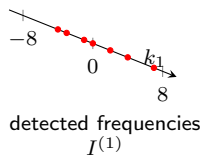
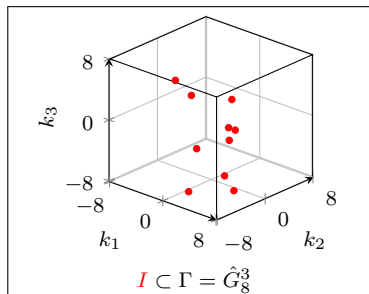
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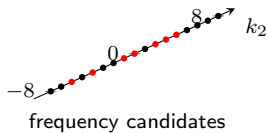
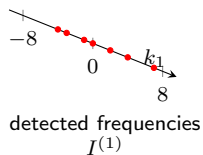
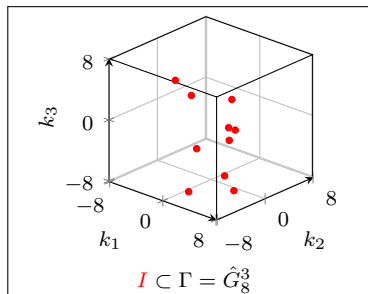
1-dim
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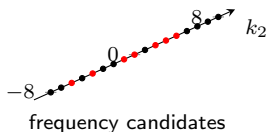
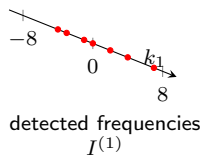
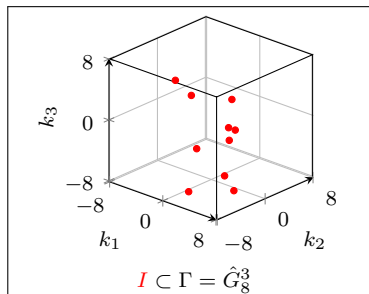
Sparse dimension-incremental FFT - method



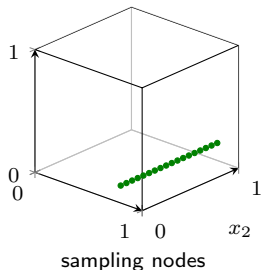
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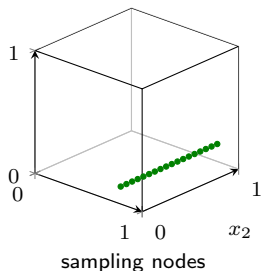
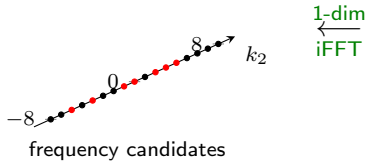
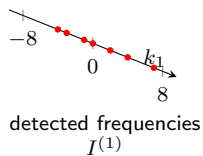
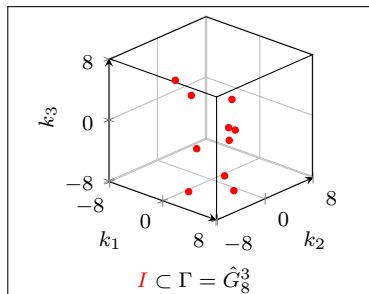
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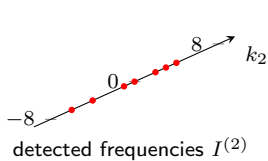
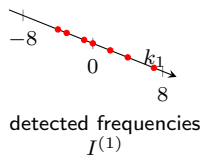
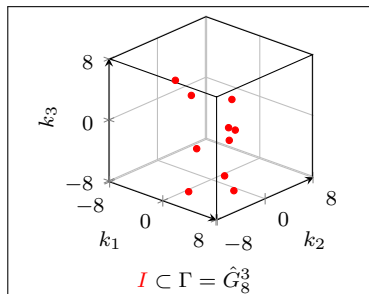
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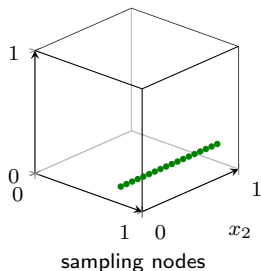
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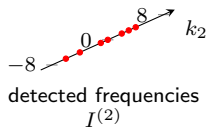
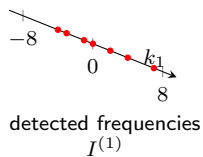
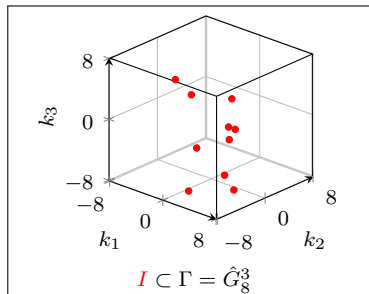
Sparse dimension-incremental FFT - method



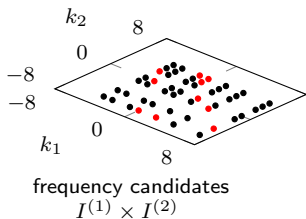
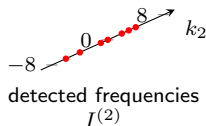
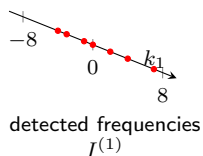
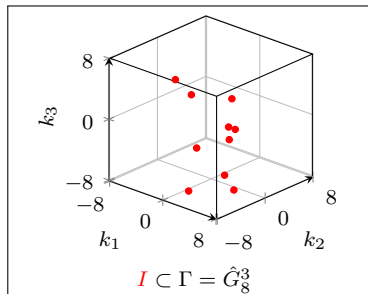
1-dim
←
iFFT



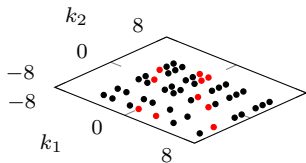
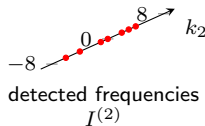
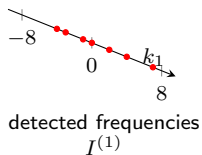
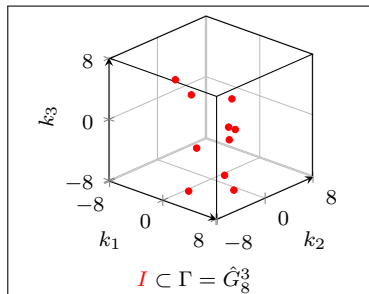
Sparse dimension-incremental FFT - method



Sparse dimension-incremental FFT - method

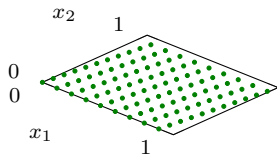


Sparse dimension-incremental FFT - method



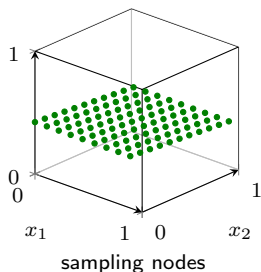
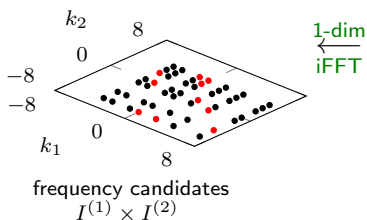
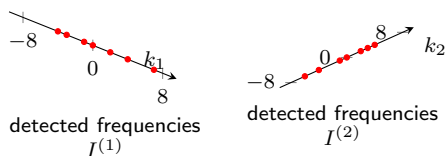
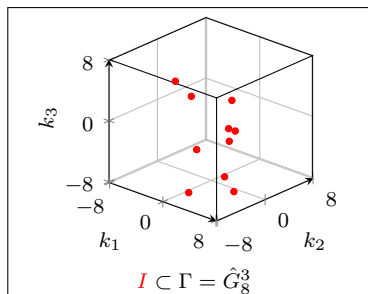
frequency candidates
 $I^{(1)} \times I^{(2)}$

reconstructing
rank-1 lattice

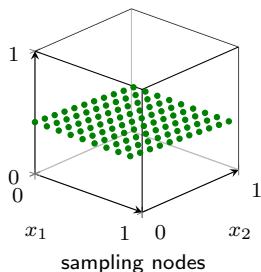
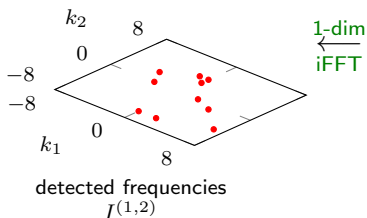
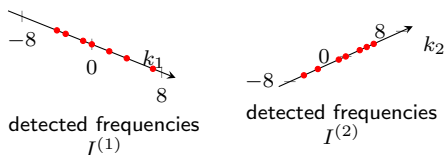
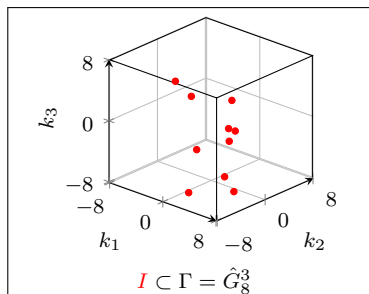


sampling nodes

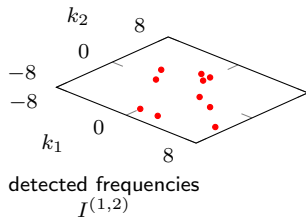
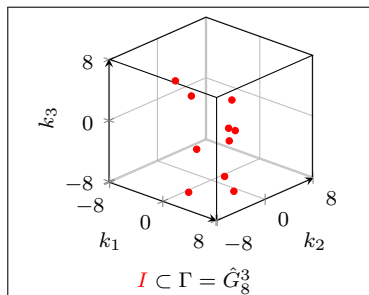
Sparse dimension-incremental FFT - method



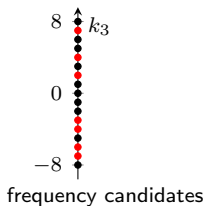
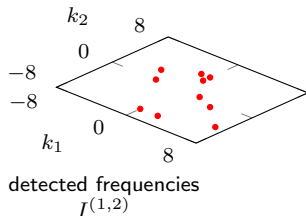
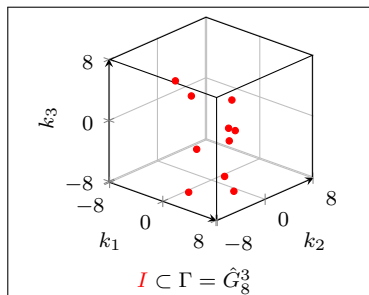
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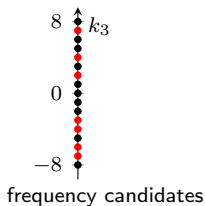
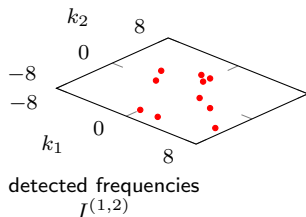
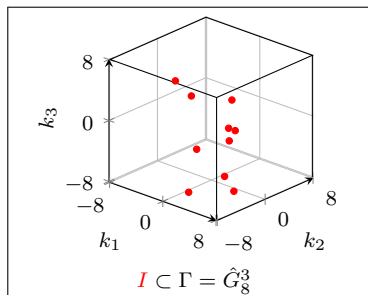
Sparse dimension-incremental FFT - method



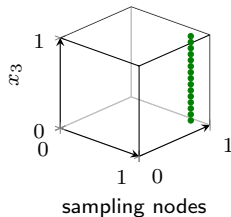
Sparse dimension-incremental FFT - method



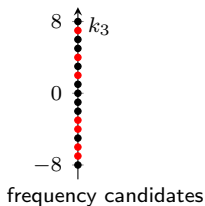
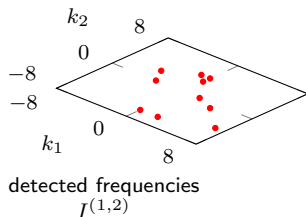
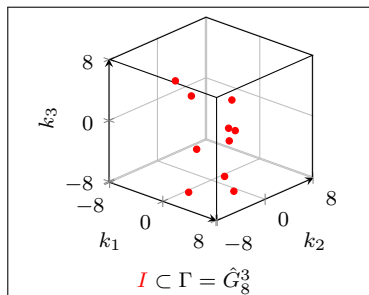
Sparse dimension-incremental FFT - method



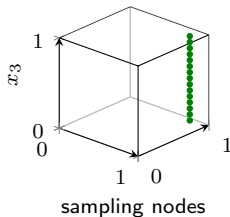
construct
→
sampling set



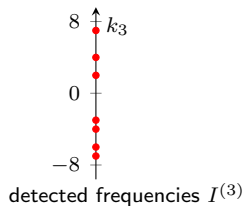
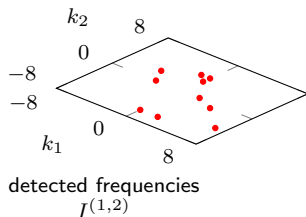
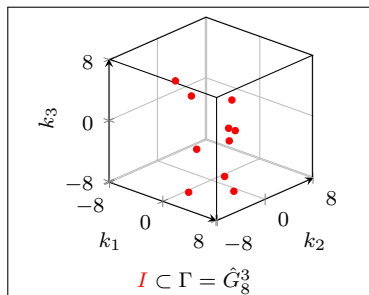
Sparse dimension-incremental FFT - method



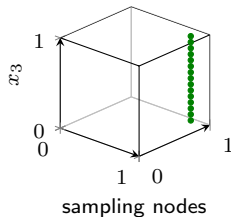
1-dim
←
iFFT



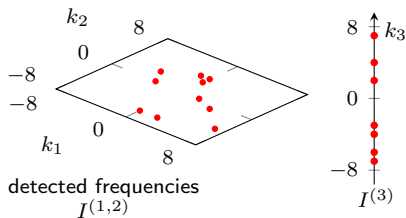
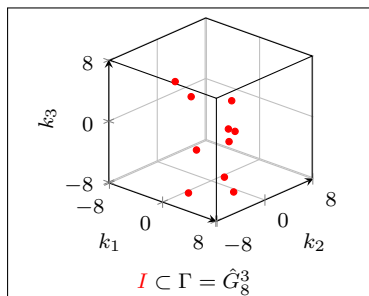
Sparse dimension-incremental FFT - method



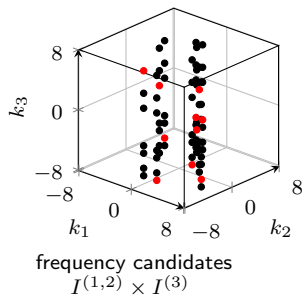
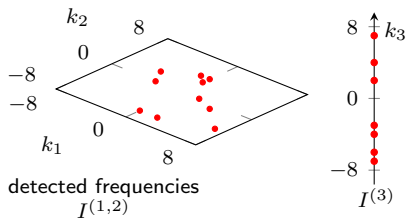
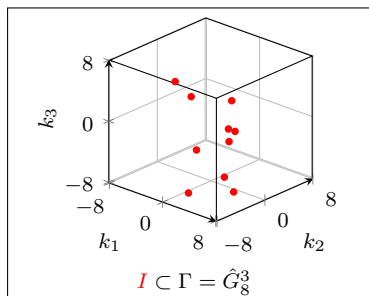
1-dim
←
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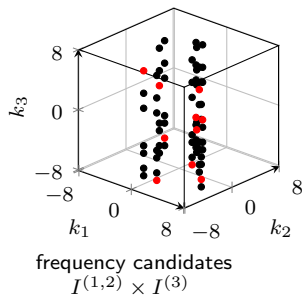
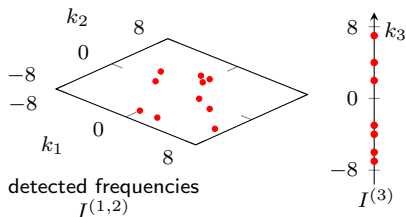
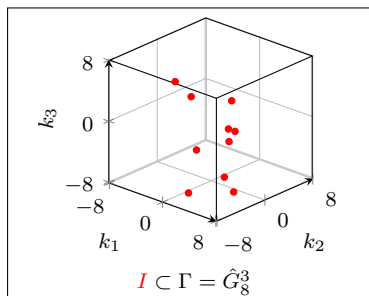
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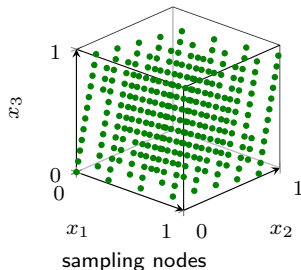
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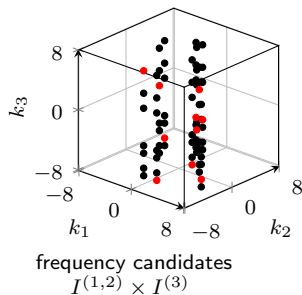
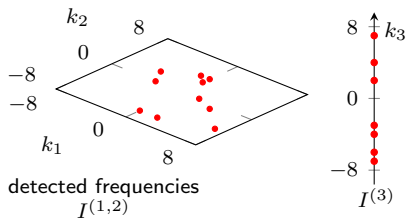
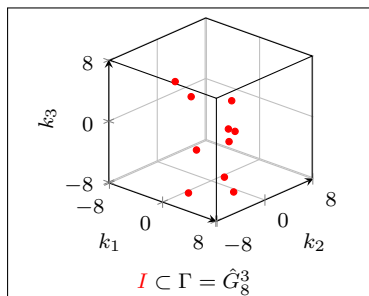
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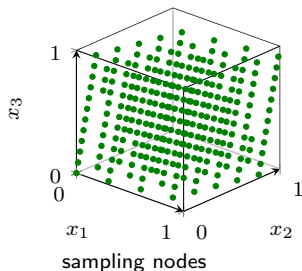
reconstructing
→
rank-1 lattice



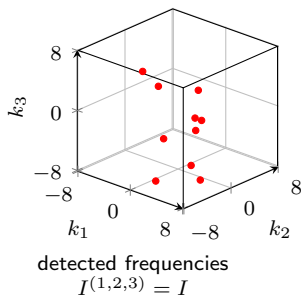
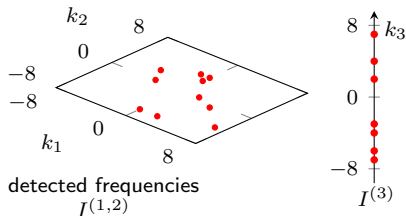
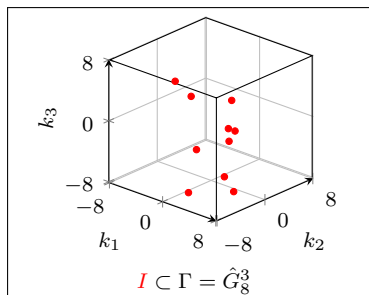
Sparse dimension-incremental FFT - method



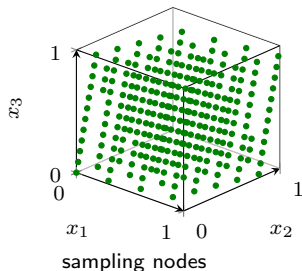
1-dim
←
iFFT



Sparse dimension-incremental FFT - method



1-dim
←
iFFT



Sparse dimension-incremental FFT - results

search domain $\Gamma = \hat{G}_N^d$ full grid, $\sqrt{N} \lesssim |I| \lesssim N^d$

- samples: $\mathcal{O}(|I|^2 \log |\Gamma|)$
- computational costs: $\mathcal{O}(d|I|^3 + |I|^2(\log |\Gamma|) \log(|I| \log |\Gamma|))$
- for arbitrary Fourier coefficients $\hat{p}_{\mathbf{k}} \in \mathbb{C}$:
probabilistic approach with several iterations
- if ($\text{Re}(\hat{p}_{\mathbf{k}})$ identical sign) AND ($\text{Im}(\hat{p}_{\mathbf{k}})$ identical sign)
then deterministic version with 1 iteration



Potts, D., Volkmer, T.

Sparse high-dimensional FFT based on rank-1 lattice sampling.

Appl. Comput. Harm. Anal. 41, 713 – 748, 2016.

(<http://www.tu-chemnitz.de/~tovo>)

Sparse dimension-incremental FFT - example

- B-spline $N_m(x) := \sum_{k \in \mathbb{Z}} C_m \operatorname{sinc}\left(\frac{\pi}{m}k\right)^m \cos(\pi k) e^{2\pi i k x}$,
 $\|N_m\|_{L^2(\mathbb{T})} = 1$, $|\hat{N}_m(k)| \sim |k|^{-m}$
- $f(\mathbf{x}) := \prod_{t \in \{1,3,8\}} N_2(x_t) + \prod_{t \in \{2,5,6,10\}} N_4(x_t) + \prod_{t \in \{4,7,9\}} N_6(x_t)$

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- full grid for $N = 64$, $d = 10$: $|\hat{G}_{64}^{10}| = 129^{10} \approx 1.28 \cdot 10^{21}$
- symmetric hyperbolic cross: $|I_{64}^{10}| = 696\,036\,321$
relative $L^2(\mathbb{T}^d)$ -error (best case) 4.1e-04

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relative $L^2(\mathbb{T}^d)$ -error (best case) 4.1e-04
- results for dimension incremental algorithm with $\Gamma = \hat{G}_{64}^{10}$:

threshold	#samples	$ I $	rel. L_2 -error
1.0e-02	254 530	491	1.4e-01
1.0e-03	2 789 050	1 121	1.1e-02
1.0e-04	17 836 042	3 013	1.7e-03
1.0e-05	82 222 438	7 163	4.7e-04

sparse dimension-incremental FFT:

- method required function f to be evaluated at arbitrary (rank-1 lattice) points
- What if sampling points $\mathbf{y}_\ell \in \mathbb{T}^d$ are given a priori?

sparse dimension-incremental FFT:

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task:

- Given a set of data $S := \{(\mathbf{y}_\ell, f_\ell)\}_{\ell=0, \dots, L-1}$
 - with nodes $\mathbf{y}_\ell \in \mathbb{T}^d$ and
 - function values $f_\ell := f(\mathbf{y}_\ell) \in \mathbb{R}$,

• determine

- frequency index set $I \subset \Gamma \subset \mathbb{Z}^d$ and
- Fourier coefficients $\hat{p}_\mathbf{k}$

of approximant $p(\mathbf{x}) := \sum_{\mathbf{k} \in I} \hat{p}_\mathbf{k} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$

Regression - dimension-incremental

ansatz: for set of data $S := \{(\mathbf{y}_\ell, f_\ell)\}_{\ell=0, \dots, L-1}$

- use regularization network approach and consider the regularized least squares problem

e.g. [Garcke, Griebel, Thess 01]

$$\frac{1}{L} \sum_{\ell=0}^{L-1} (f_\ell - p(\mathbf{y}_\ell))^2 + \lambda \Phi(p) \rightarrow \min$$

with regularization parameter $\lambda \geq 0$ and

e.g. with $\Phi(p) := \|\nabla p\|_2^2$

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$$\Rightarrow \text{solve } \left(\frac{1}{L} \mathbf{A}^* \mathbf{A} + \lambda \mathbf{C}\right) (\hat{p}_{\mathbf{k}})_{\mathbf{k} \in \Gamma} = \frac{1}{L} \mathbf{A}^* (f_\ell)_{\ell=0}^{L-1},$$

$$\mathbf{A} = (e^{2\pi i \mathbf{k} \cdot \mathbf{y}_\ell})_{\ell=0, \dots, L-1; \mathbf{k} \in \Gamma}$$

$$\mathbf{C} = (\langle \nabla e^{2\pi i \mathbf{k} \cdot \mathbf{x}}, \nabla e^{2\pi i \mathbf{h} \cdot \mathbf{x}} \rangle_2)_{\mathbf{k}, \mathbf{h} \in \Gamma} = \text{diag}((4\pi^2 \|\mathbf{k}\|_2^2)_{\mathbf{k} \in \Gamma})$$

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- combine with dimension-incremental idea

Regression - dimension-incremental

idea of the approach step-by-step:

- start with 1 attribute

Regression - dimension-incremental

idea of the approach step-by-step:

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 - keep largest Fourier coefficients
 - obtain (one-dimensional) approximant

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 - add attribute into consideration

Regression - dimension-incremental

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Regression - dimension-incremental

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- for 2nd to last attribute
 - add attribute into consideration
 - compute projected Fourier coefficients from given samples by solving the regularized least squares problem
 - keep largest Fourier coefficients
 - obtain (low dimensional) approximant
 - evaluate approximant on train / eval data set
 - if no improvement compared to previous case, then reject newly added attribute

end

Regression - example

- B-spline $N_m(x) := \sum_{k \in \mathbb{Z}} C_m \operatorname{sinc}\left(\frac{\pi}{m}k\right)^m \cos(\pi k) e^{2\pi i k x}$,
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- hyperbolic cross I_N^d for $N = 16$, $d = 10$: $|I_{16}^{10}| = 45\,548\,649$

index set I	$ I $	rel. L_2 -error (best case)
I_{16}^{10}	45 548 649	3.1e-03
$I \subset I_{16}^{10}$	2 000	4.0e-03
$I \subset I_{16}^{10}$	1 000	1.2e-02

Regression - example

- B-spline $N_m(x) := \sum_{k \in \mathbb{Z}} C_m \operatorname{sinc}\left(\frac{\pi}{m}k\right)^m \cos(\pi k) e^{2\pi i k x}$,
 $\|N_m\|_{L^2(\mathbb{T})} = 1$, $|\hat{N}_m(k)| \sim |k|^{-m}$
- $f(x) := \prod_{t \in \{1,3,8\}} N_2(x_t) + \prod_{t \in \{2,5,6,10\}} N_4(x_t) + \prod_{t \in \{4,7,9\}} N_6(x_t)$
- hyperbolic cross I_N^d for $N = 16$, $d = 10$: $|I_{16}^{10}| = 45\,548\,649$

index set I	$ I $	rel. L_2 -error (best case)
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$I \subset I_{16}^{10}$	2 000	4.0e-03
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- results for dimension incremental algorithm with $I \subset \Gamma = I_{16}^{10}$
 for **given set of data** $S := \{(\mathbf{y}_\ell, f_\ell)\}_{\ell=0, \dots, L-1}$,
 $\mathbf{C} := \operatorname{diag}\left(\left(4\pi^2 \prod_{s=1}^d \max(1, |k_s|)\right)_{\mathbf{k} \in \Gamma}\right)$

#samples L	$ I $	rel. L_2 -error
400 000	2 000	2.5e-02

Classification as regression

common approach for two-class problem:

- map classes to $f_\ell \in \{0, 1\}$ or $\in \{-1, 1\}$
- set of data $S := \{(\mathbf{y}_\ell, f_\ell)\}_{\ell=0, \dots, L-1}$
- solve the regularized least squares problem

e.g. [Garcke, Griebel, Thess 01]

$$\frac{1}{L} \sum_{\ell=0}^{L-1} (f_\ell - p(\mathbf{y}_\ell))^2 + \lambda \Phi(p) \rightarrow \min$$

- for data point \mathbf{y}
 - map approximant p to one class if $p(\mathbf{y}) \leq \text{threshold}$
 - and to the other if $p(\mathbf{y}) > \text{threshold}$

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\Rightarrow apply dimension-incremental method

Classification as regression - example

- DMC2013 data set (shopping cart cancellation)
- target attribute order $\in \{0, 1\}$
- 21 attributes
- 429 000 lines of train/eval data (split 50/50)
- 45 068 lines of test data

method	classification rate		
	train	eval	test
order := 1	0.6763	0.6758	0.6806
Decision Tree	0.7787	0.7718	0.7547
dimension incremental	0.7522	0.7519	0.7562

- **known** (arbitrary) frequency index set via **rank-1 lattices**
 - fast evaluation / reconstruction of **trigonometric polynomials**
[Li, Hickernell 03] / [Kämmerer, Kunis, Potts 12] [Kämmerer 13]
 - approximation of **periodic** functions
- **unknown** frequency index set
 - sparse dimension-incremental FFT based on **rank-1 lattices**
 -  Potts, D., Volkmer, T.
Sparse high-dimensional FFT based on rank-1 lattice sampling.
Appl. Comput. Harm. Anal. 41, 713 – 748, 2016.
(<http://www.tu-chemnitz.de/~tovo>)
- dimension-incremental method for regression / classification

Taylor and rank-1 lattice based NFFT

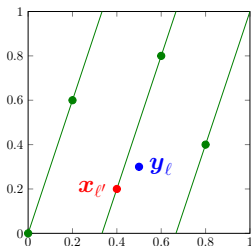
- dimension incremental method uses evaluations

$$p(\mathbf{y}_\ell) := \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{y}_\ell}, \ell = 0, \dots, L-1.$$

⇒ fast version desired

- approximate $p(\mathbf{y}_\ell)$ by Taylor expansion $s_m(\mathbf{y}_\ell)$ at closest rank-1 lattice point $\mathbf{x}_{\ell'}$,

$$s_m(\mathbf{y}_\ell) = p(\mathbf{x}_{\ell'}) + \sum_{0 < |\nu| < m} \frac{(\mathbf{y}_\ell - \mathbf{x}_{\ell'})^\nu}{\nu!} (D^\nu p)(\mathbf{x}_{\ell'})$$



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- for fixed $\boldsymbol{\nu} \in \mathbb{N}_0^d$, compute $(D^{\boldsymbol{\nu}} p)(\mathbf{x}_j)$ for all \mathbf{x}_j ,
 $j = 0, \dots, M-1$, with 1-dim FFT(M) in $\mathcal{O}(M \log M + d|I|)$

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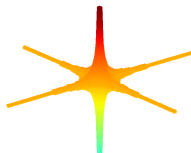
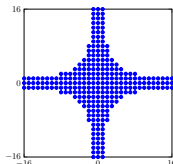
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⇒ in total $\mathcal{O}(m^d(L + M \log M + d|I|))$ arithmetic operations

Taylor and R1L based NFFT - error estimates

Lemma (V. 13)

Let $I = I_N^d$ hyperbolic cross,

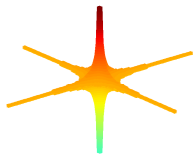
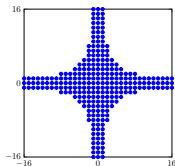


I_N^d

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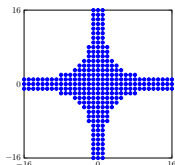


I_N^d

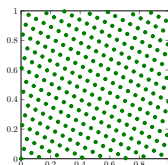
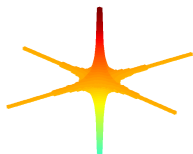
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I_N^d

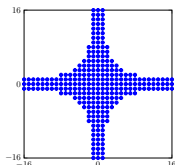


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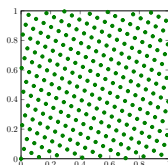
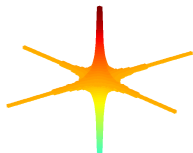
Taylor and R1L based NFFT - error estimates

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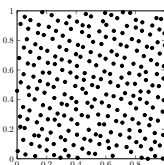
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I_N^d



R1L(\mathbf{z}, M)



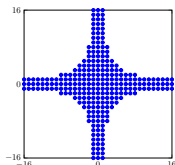
$(p(\mathbf{y}_\ell))_{\ell=0}^{L-1}$

Taylor and R1L based NFFT - error estimates

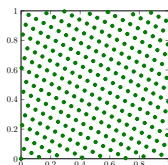
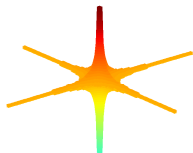
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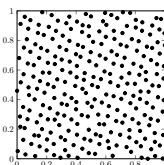
$$|(p - s_m)(\mathbf{y}_\ell)| \leq \frac{(2\pi)^m}{m!} \varepsilon^m \sum_{\mathbf{k} \in I_N^d} |\hat{p}_{\mathbf{k}}| \|\mathbf{k}\|_1^m$$



I_N^d



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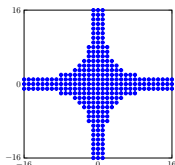
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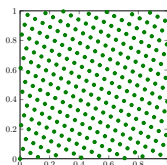
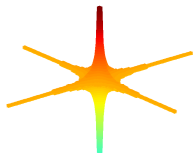
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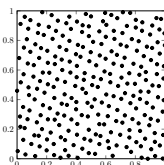
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I_N^d



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- error estimates can be generalized to other finite frequency index sets $I \subset \mathbb{Z}^d$, e.g. ℓ_1 balls, energy-based hyperbolic crosses, ...

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- decay properties of Fourier coefficients may be included

