

High-dimensional approximation and sparse FFT

Toni Volkmer



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CHEMNITZ

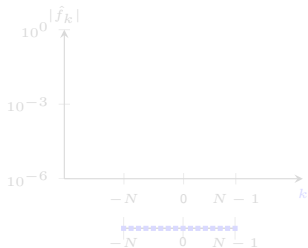
joint work with Lutz Kämmerer and Daniel Potts

supported by

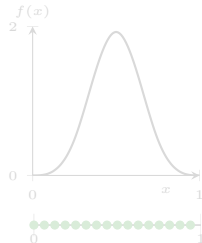


- ▶ torus $\mathbb{T} \simeq [0, 1)$, $\{e^{2\pi i k x}\}_{k \in \mathbb{Z}}$ orthonormal basis of $L_2(\mathbb{T})$
- ▶ function $f \in L_2(\mathbb{T})$, $f(x) = \sum_{k \in \mathbb{Z}} \hat{f}_k e^{2\pi i k x}$, $\hat{f}_k \in \mathbb{C}$
- ▶ smooth function $f \implies$ fast decay of Fourier coefficients \hat{f}_k
- ▶ truncated Fourier series $S_I f(x) = \sum_{k \in I} \hat{f}_k e^{2\pi i k x} \approx f(x)$
- ▶ $\hat{f}_k = \int_{\mathbb{T}} f(x) e^{-2\pi i k x} dx \approx \tilde{f}_k := \frac{1}{2N} \sum_{j=0}^{2N-1} f(x_j) e^{-2\pi i k x}$, $x_j := \frac{j}{2N}$

\implies transfer to multivariate case

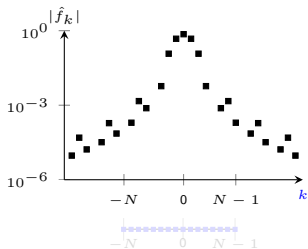


$$(\tilde{f}_k)_{k \in I} \begin{array}{c} \xleftarrow{1\text{-dim.}} \\ \xrightarrow{\text{FFT}} \end{array} (f(x_j))_{j=0}^{2N-1} \\
 \mathcal{O}(N \log N) \\
 \text{[Gau\ss 1866]} \quad \text{[Cooley, Tukey 1965]}$$

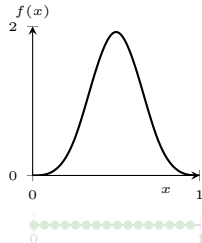


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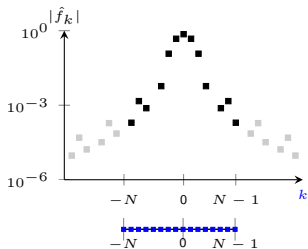


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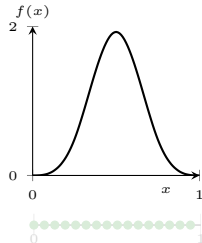
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\Rightarrow transfer to multivariate case



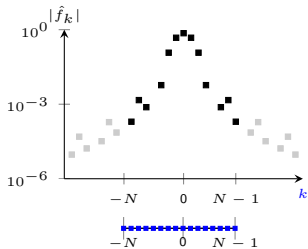
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$\mathcal{O}(N \log N)$
[Gauß 1866] [Cooley, Tukey 1965]



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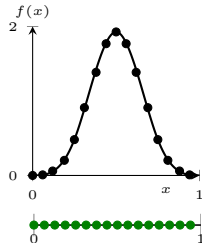
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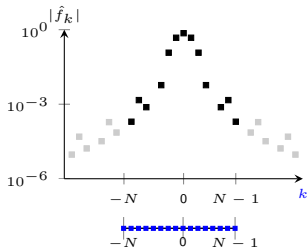
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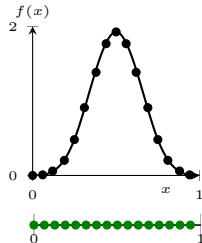
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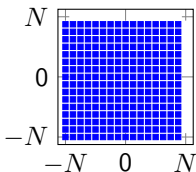
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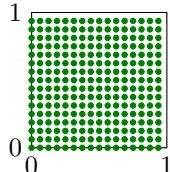
- full grid in frequency domain, **equispaced grid** in spatial domain



$$(\tilde{f}_k)_{k \in I} \xleftrightarrow[\text{FFT}]{d\text{-dim.}} (f(\mathbf{x}_j))_{j=0}^{|I|-1}$$

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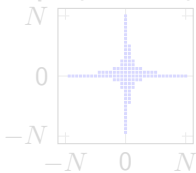
curse of dimensionality



? high-dimensional case \implies assumption: sparsity or smoothness

- hyperbolic cross in frequency domain, **sparse grid** in spatial domain

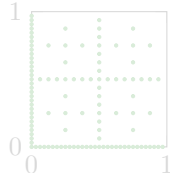
[Smolyak '63; Temlyakov '85; Baszenski, Delvos '89; Hallatschek '92; Gradinaru '07; Griebel, Hamaekers '14]



$$(\tilde{f}_k)_{k \in I} \xleftrightarrow[\text{HCFFT}]{d\text{-dim.}} (f(\mathbf{x}_j))_{j=0}^{|I|-1}$$

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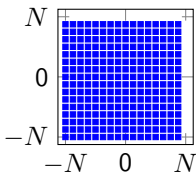
condition number of
 Fourier matrix
 [Kämmerer, Kunis '11]



? more general frequency index set $I \subset \mathbb{Z}^d$, $|I| < \infty$; different sampling set

? unknown frequency index set I / weights / function space

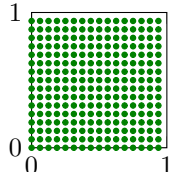
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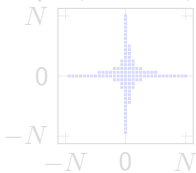
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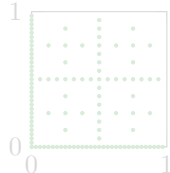
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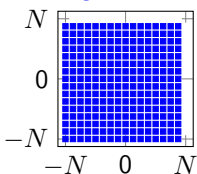
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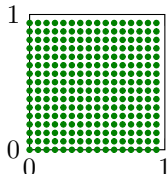
- **full grid** in frequency domain, **equispaced grid** in spatial domain



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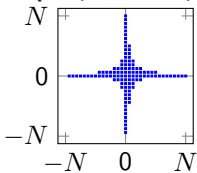
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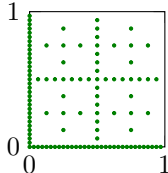
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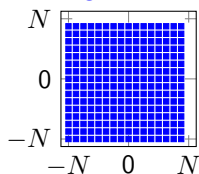
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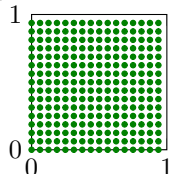
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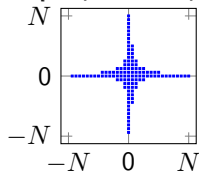
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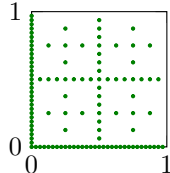
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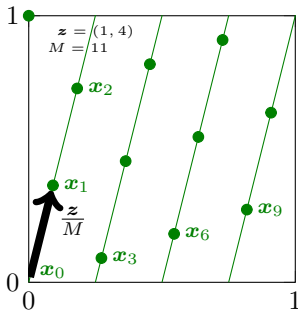


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Outline

1. Introduction
2. Fast reconstruction and approximation of multivariate periodic functions using rank-1 lattice sampling
3. Reconstructing multiple rank-1 lattices
4. High-dimensional dimension-incremental sparse FFT
5. Conclusion

- ▶ $f(\mathbf{x}) = p_I(\mathbf{x}) = \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$, arbitrary index set $I \subset \mathbb{Z}^d$, $|I| < \infty$
- ▶ rank-1 lattice $\mathbf{R1L}(\mathbf{z}, M) := \{\mathbf{x}_j := \frac{j}{M} \mathbf{z} \bmod \mathbf{1}\}_{j=0}^{M-1}$, $\mathbf{z} \in \mathbb{Z}^d$, $M \in \mathbb{N}$, as discretization in spatial domain

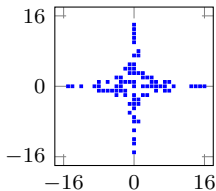


Korobov '59
 Maisonneuve '72
 Sloan & Kachoyan '84, '87, '90
 Temlyakov '86
 Lyness '89
 Sloan & Joe '94
 Sloan & Reztsov '01
 Li & Hickernell '03
 Kämmerer & Kunis & Potts '12

$$\hat{p}_{\mathbf{0}} = \int_{\mathbb{T}^d} p_I(\mathbf{x}) d\mathbf{x} \approx \sum_{j=0}^{M-1} \frac{1}{M} p_I(\mathbf{x}_j)$$

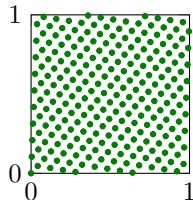
$$\hat{p}_{\mathbf{k}} = \int_{\mathbb{T}^d} p_I(\mathbf{x}) e^{-2\pi i \mathbf{k} \cdot \mathbf{x}} d\mathbf{x}, \mathbf{k} \in I$$

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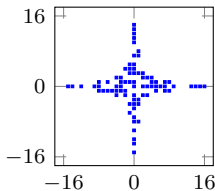


$$(\hat{p}_{\mathbf{k}})_{\mathbf{k} \in I} \xleftarrow{?} (p_I(\mathbf{x}_j))_{j=0}^{M-1}$$

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

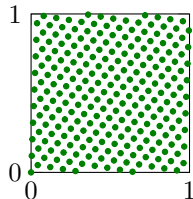


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 - ⇒ reconstruction property: [Kämmerer, Kunis, Potts '12]
 $\mathbf{k} \cdot \mathbf{z} \not\equiv \mathbf{k}' \cdot \mathbf{z} \pmod{M}$ for all $\mathbf{k}, \mathbf{k}' \in I$, $\mathbf{k} \neq \mathbf{k}'$
 - ▶ $|I| \leq M \leq |I|^2$, simple CBC construction method [Kämmerer '12]

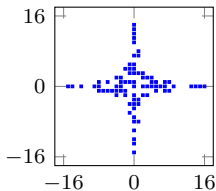


$$(\hat{p}_{\mathbf{k}})_{\mathbf{k} \in I} \xleftarrow[\text{FFT}]{\text{1-dim.}} (p_I(\mathbf{x}_j))_{j=0}^{M-1}$$

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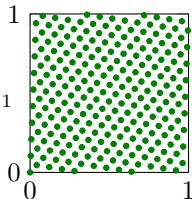


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 - ▶ $|I| \leq M \leq |I|^2$, simple CBC construction method [Kämmerer '12]
- ▶ fast approximation of $f \in L_2(\mathbb{T}^d) \cap C(\mathbb{T}^d)$, [Byrenheid, Kämmerer, Ullrich, V. '16] [V. '17]
 $f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^d} \hat{f}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$, by $S_I^{\mathbf{R1L}} f(\mathbf{x}) = \sum_{\mathbf{k} \in I} \hat{f}_{\mathbf{k}}^{\mathbf{R1L}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$

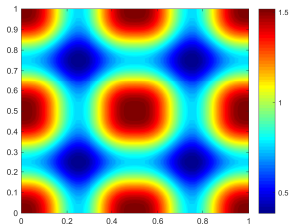
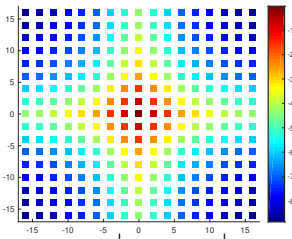
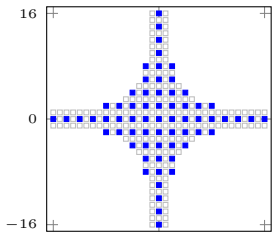


$$(\hat{f}_{\mathbf{k}}^{\mathbf{R1L}})_{\mathbf{k} \in I} \xleftarrow[\text{FFT}]{\text{1-dim.}} (f(\mathbf{x}_j))_{j=0}^{M-1}$$

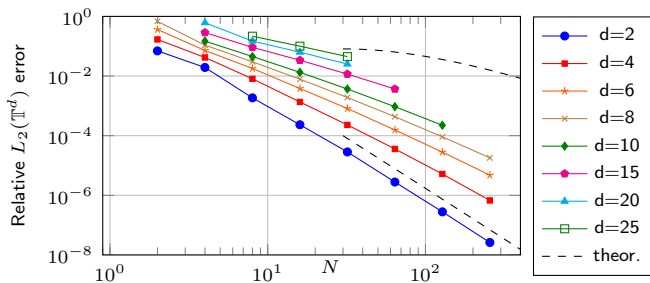
$$\mathcal{O}(M \log M + d |I|)$$



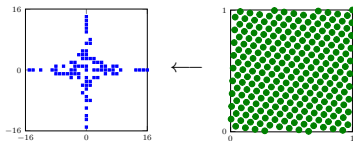
- ▶ $f(\mathbf{x}) := \prod_{s=1}^d \left(2 + \operatorname{sgn}((x_s \bmod 1) - \frac{1}{2}) \sin(2\pi x_s)^3\right)$, $f \in \mathcal{H}_{\text{mix}}^{\frac{7}{2}-\epsilon}(\mathbb{T}^d)$, $\epsilon > 0$
- ▶ $\mathcal{H}_{\text{mix}}^{\beta}(\mathbb{T}^d) := \left\{ f \in L_2 : \|f\| := \sqrt{\sum_{\mathbf{k} \in \mathbb{Z}^d} |\hat{f}_{\mathbf{k}}|^2 \prod_{s=1}^d \max(1, |k_s|)^{2\beta}} < \infty \right\}$, $\beta \geq 0$
- ▶ hyperbolic cross $I := \{\mathbf{k} \in 2\mathbb{Z}^d : \prod_{s=1}^d \max(1, |k_s|) \leq N\}$
- ▶ sparse grids: $\|f - S_I^{\text{SG}} f\|_{L_2(\mathbb{T}^d)} \lesssim N^{-\beta} \log^{\frac{d-1}{2}} N \|f\|_{\mathcal{H}_{\text{mix}}^{\beta}(\mathbb{T}^d)}$ [Sickel, Ullrich '07]
- ▶ rank-1 lattice: $\|f - S_I^{\text{R1L}} f\|_{L_2(\mathbb{T}^d)} \lesssim N^{-\beta} \log^{\frac{d-1}{2}} N \|f\|_{\mathcal{H}_{\text{mix}}^{\beta}(\mathbb{T}^d)}$
 special case of [Byrenheid, Kämmerer, Ullrich, V. '16] [V. '17]
- ▶ general approach: $\|f - S_I^{\text{R1L}} f\| \leq \|f - S_I f\| + \|S_I f - S_I^{\text{R1L}} f\|$


 $f((x_1, x_2)^{\top})$

 $\log_{10} |\hat{f}(k_1, k_2)^{\top}|$

 I

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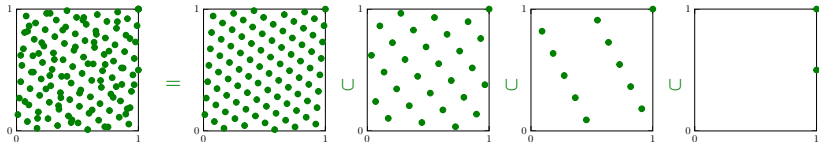


- ▶ reconstructing $\text{R1L}(z, M, I)$ has size M with $|I| \leq M \leq |I|^2$
 - ▶ number of samples: $\mathcal{O}(|I|^2)$
 - ▶ construction complexity: $\mathcal{O}(d|I|^3)$



⇒ use more than one rank-1 lattice [Kämmerer '16] [Kämmerer '17]

- ▶ perform greedy search for sequence of rank-1 lattices which reconstruct as many as possible frequencies from I



- ⇒ number of samples: $\mathcal{O}(|I| \log |I|)$,
 construction complexity: $\mathcal{O}(d|I| \log^2 |I|)$ (w.h.p.)

until now:

- ▶ fast reconstruction / approximation from samples for arbitrary **given** frequency index set $I \subset \mathbb{Z}^d$, $|I| < \infty$

next: unknown frequency index set I / weights / function space
 \Rightarrow multi-dimensional sparse FFT

- ▶ task: determine frequency index set I from samples belonging to \approx largest Fourier coefficients $\hat{f}_{\mathbf{k}}$ or to $\hat{f}_{\mathbf{k}} \neq 0$
- ▶ search domain $\Gamma \subset \mathbb{Z}^d$, e.g. full grid $\hat{G}_N^d := \{-N, -N+1, \dots, N\}^d$, $N \in \mathbb{N}$
- ▶ various existing methods, e.g., based on
 - ▶ filters [Indyk, Kapralov '14]
 - ▶ Chinese Remainder Theorem [Cuyt, Lee '08] [Iwen '13]
 - ▶ Prony's method [Tasche, Potts '13] [Peter, Plonka, Schaback '15] [Kunis, Peter, Römer, von der Ohe '15]

- ▶ **problems:** non-sparsity, implementations?, stability, many frequencies

\Rightarrow dimension-incremental sparse FFT based on rank-1 lattices [Potts, V. '15] [V. '17]
 (similar basic idea without rank-1 lattices:
 [Zippel '79] [Kaltfofen, Lee '03] [Javadi Monagan '10] [Potts, Tasche '13])

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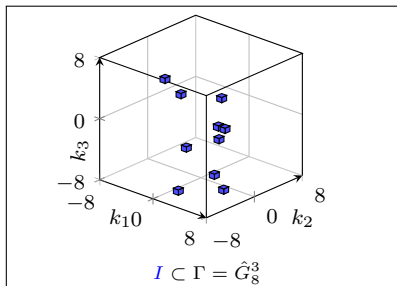
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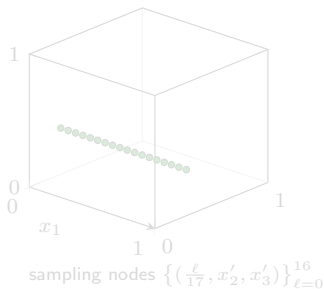
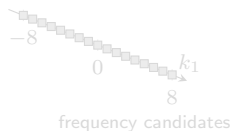
(similar basic idea without rank-1 lattices:

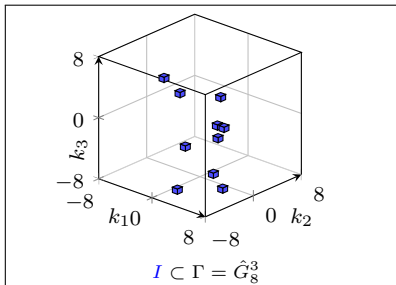
[Zippel '79] [Kaltfofen, Lee '03] [Javadi Monagan '10] [Potts, Tasche '13])



$$\hat{p}_{k_1} := \frac{1}{17} \sum_{\ell=0}^{16} p \left(\begin{pmatrix} \ell/17 \\ x_2' \\ x_3' \end{pmatrix} \right) e^{-2\pi i \frac{\ell k_1}{17}}$$

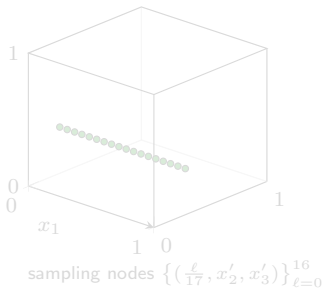
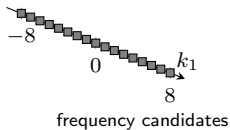
$$k_1 = -8, \dots, 8$$

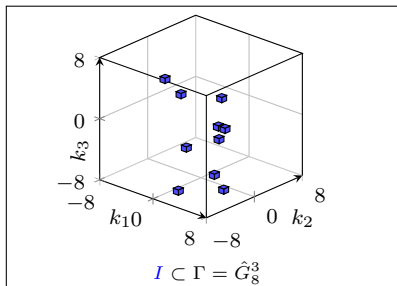




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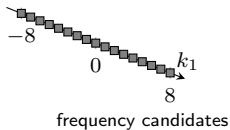
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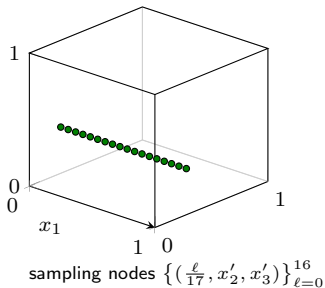


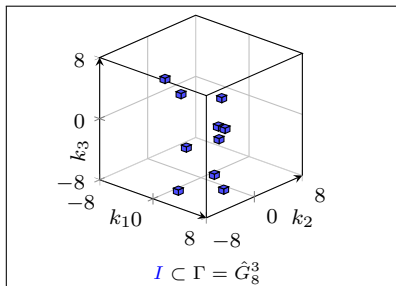
$$\hat{p}_{k_1} := \frac{1}{17} \sum_{\ell=0}^{16} p \left(\begin{pmatrix} \ell/17 \\ x'_2 \\ x'_3 \end{pmatrix} \right) e^{-2\pi i \frac{\ell k_1}{17}}$$

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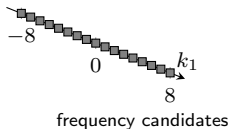
construct
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sampling set



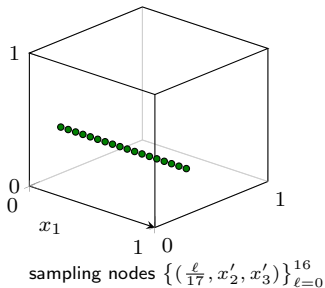


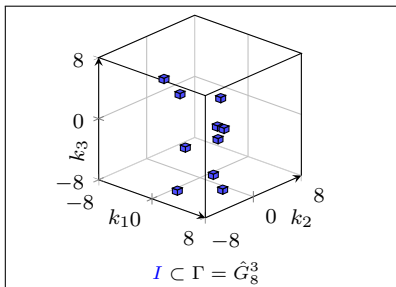
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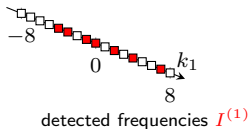
1-dim.
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FFT



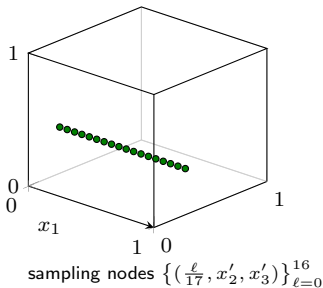


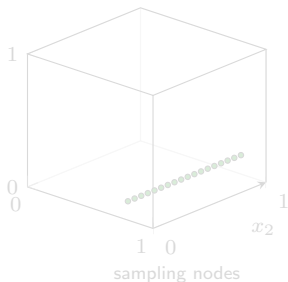
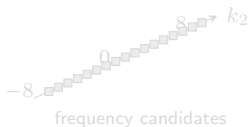
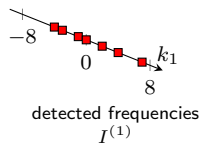
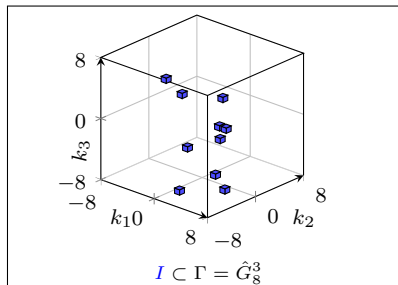
$$\begin{aligned} \hat{p}_{k_1} &:= \frac{1}{17} \sum_{\ell=0}^{16} p \left(\begin{pmatrix} \ell/17 \\ x'_2 \\ x'_3 \end{pmatrix} \right) e^{-2\pi i \frac{\ell k_1}{17}} \\ &= \sum_{\substack{(h_2, h_3) \in \{-8, \dots, 8\}^2 \\ (k_1, h_2, h_3)^\top \in \text{supp } \hat{p}}} \hat{p} \begin{pmatrix}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

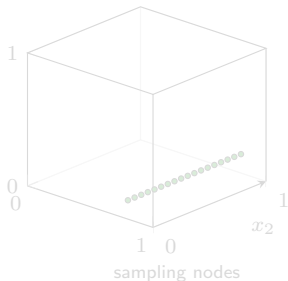
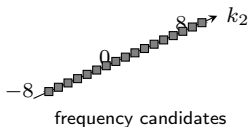
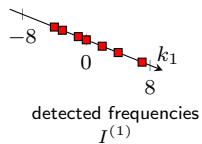
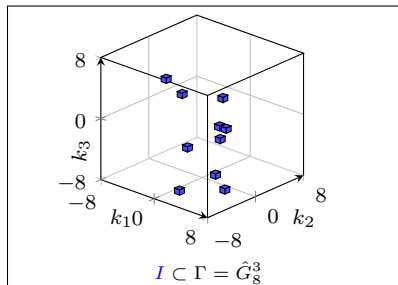
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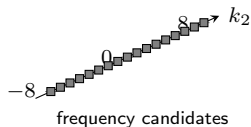
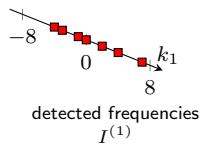
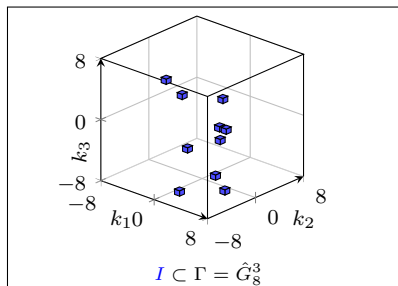


1-dim.
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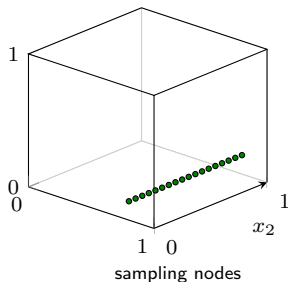


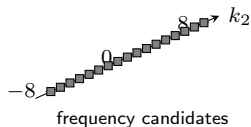
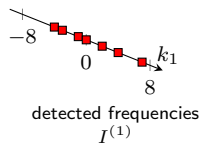
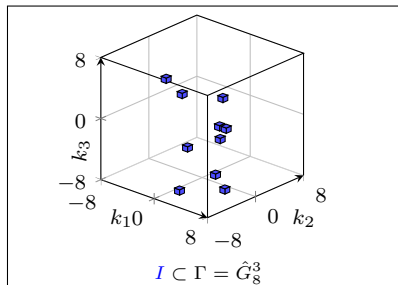




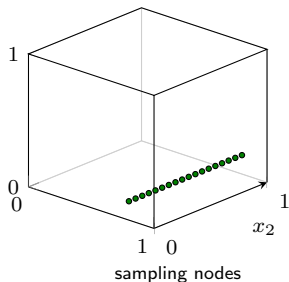


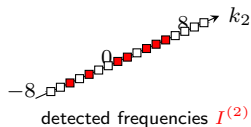
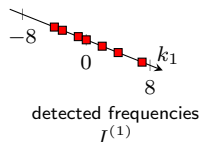
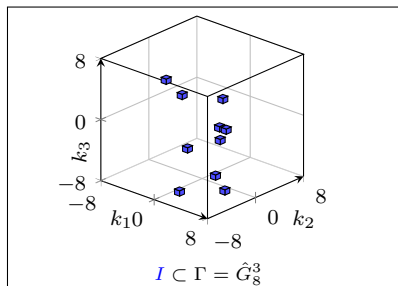
construct
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sampling set



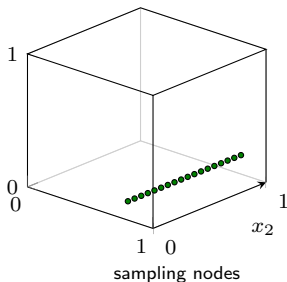


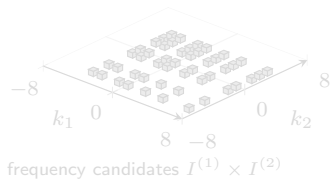
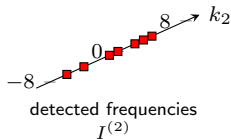
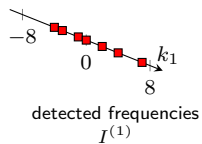
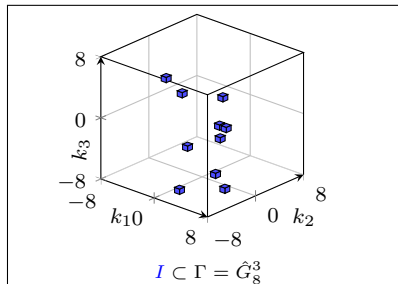
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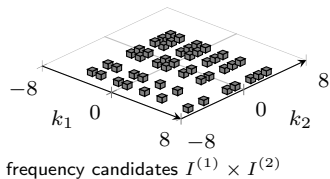
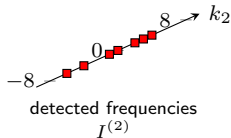
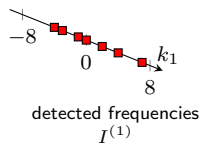
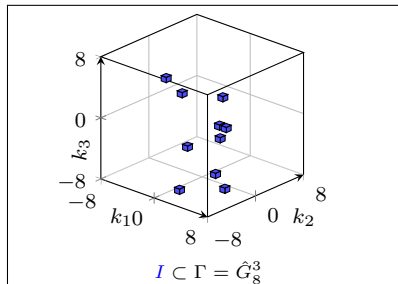


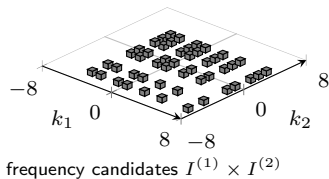
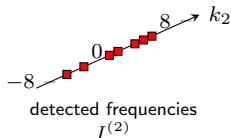
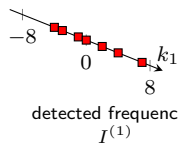
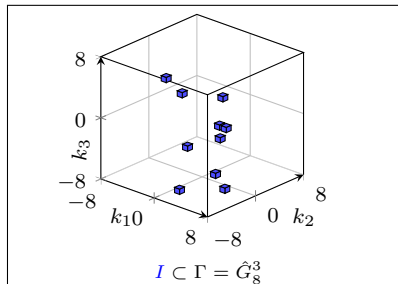


1-dim.
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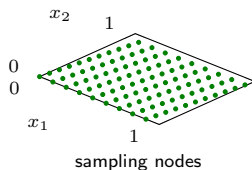


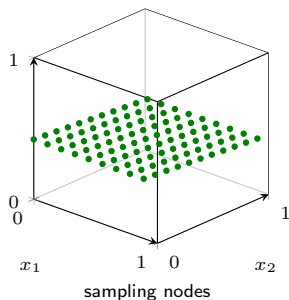
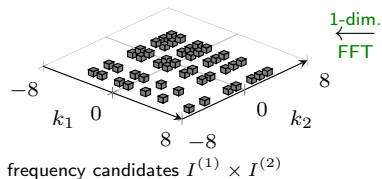
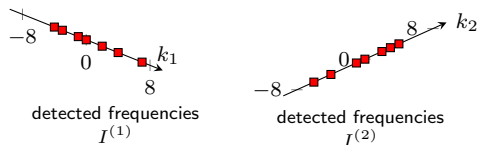
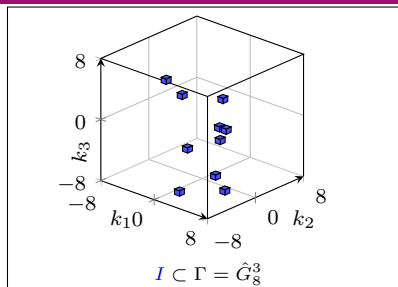


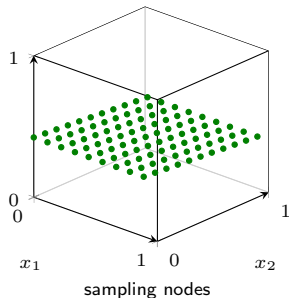
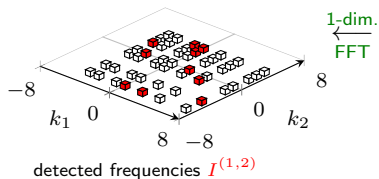
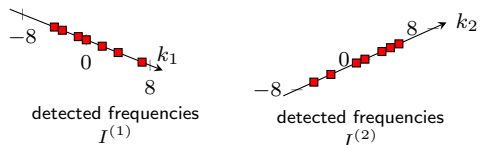
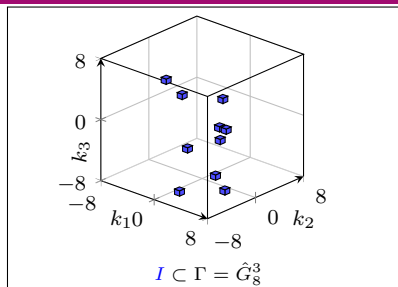


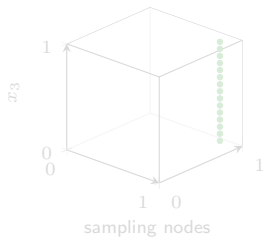
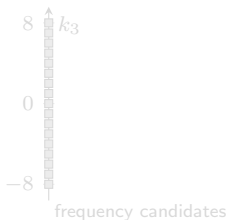
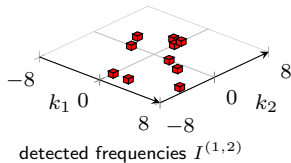
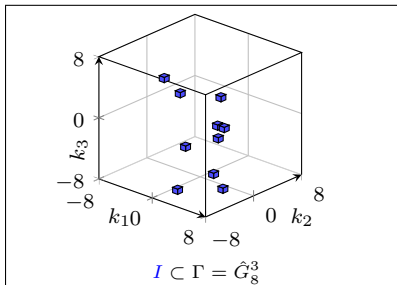


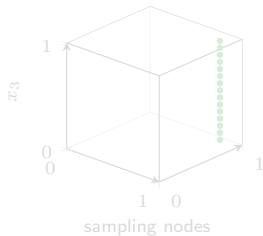
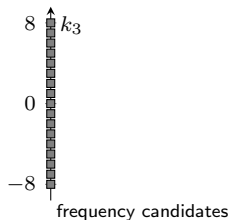
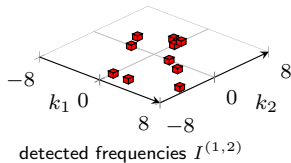
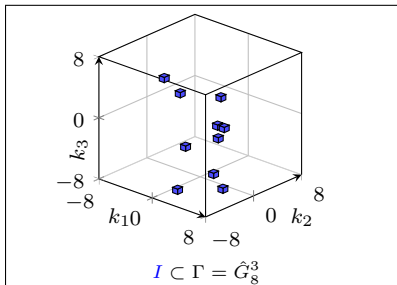
reconstructing
→
rank-1 lattice

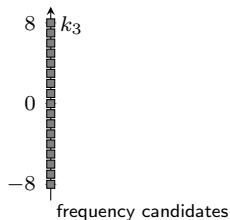
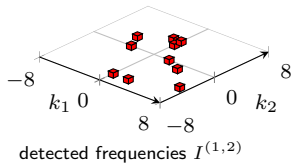
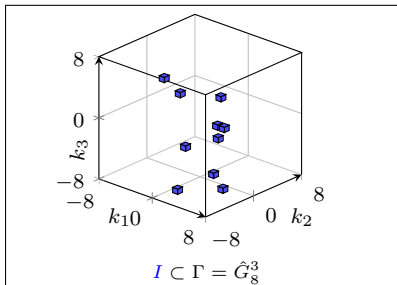




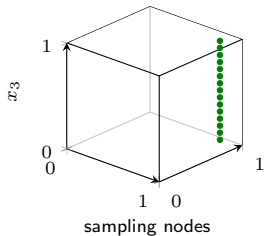


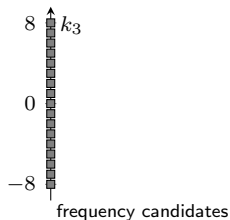
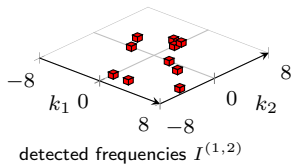
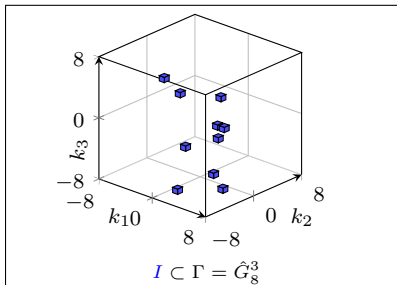




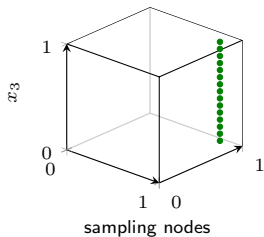


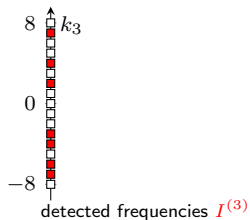
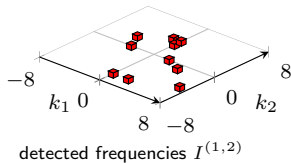
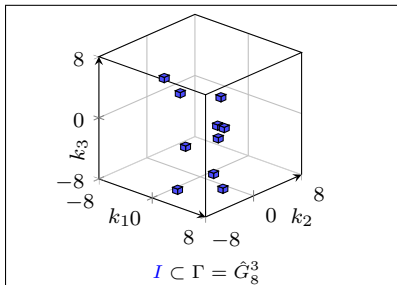
construct
→
sampling set



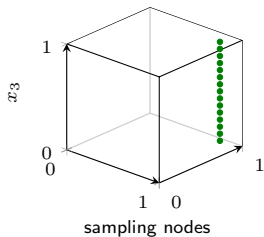


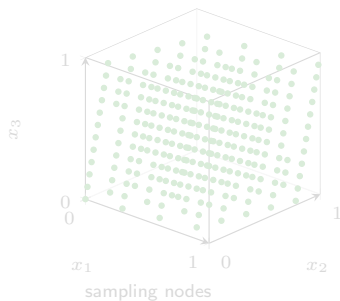
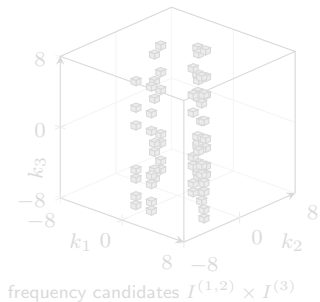
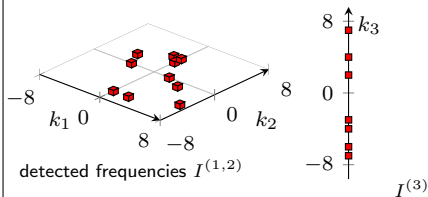
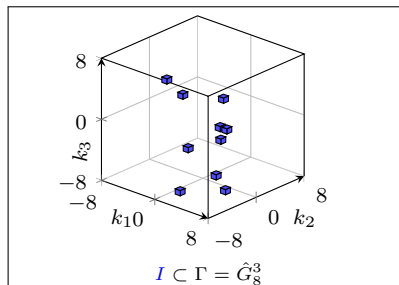
1-dim.
←
FFT

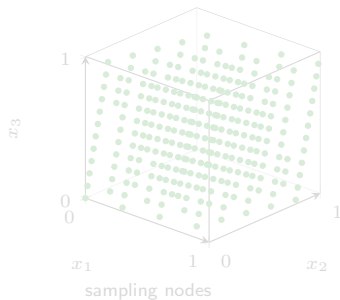
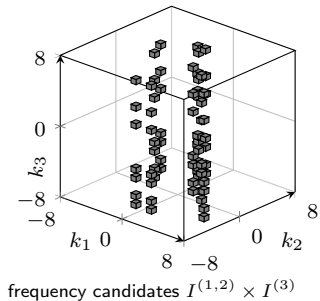
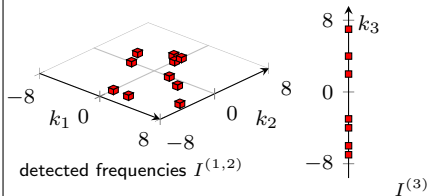
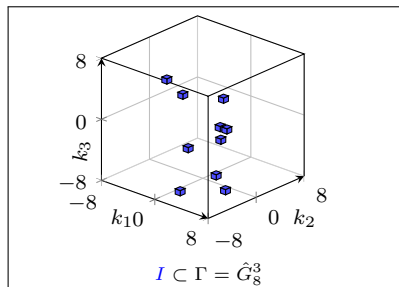


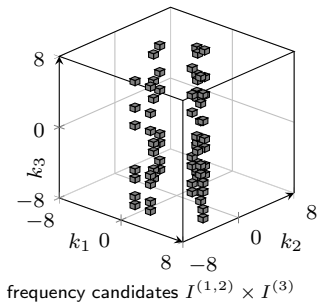
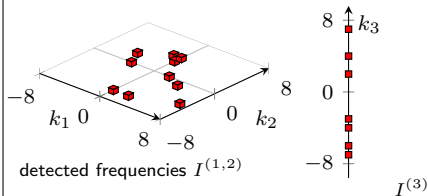
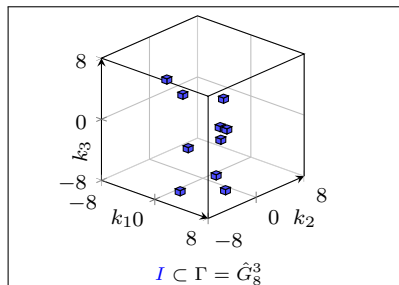


1-dim.
←
FFT

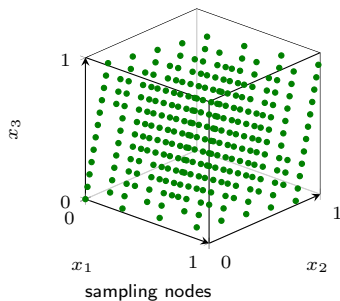


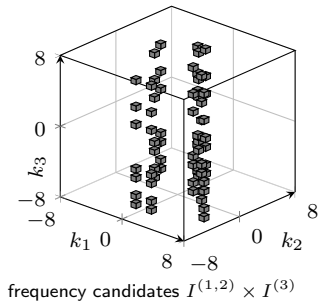
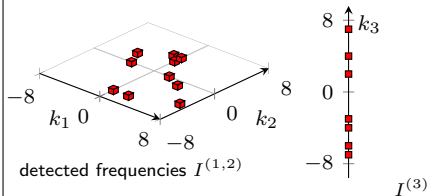
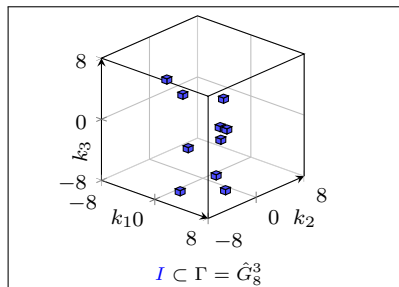




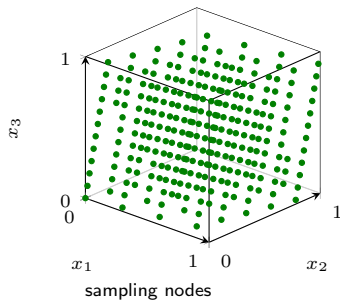


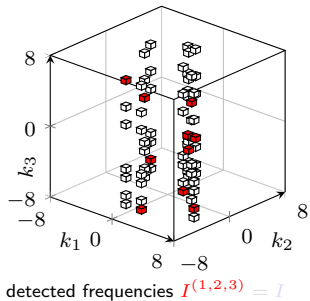
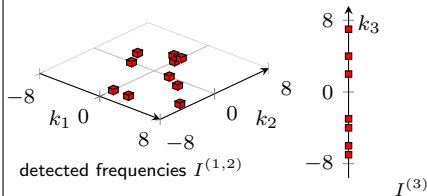
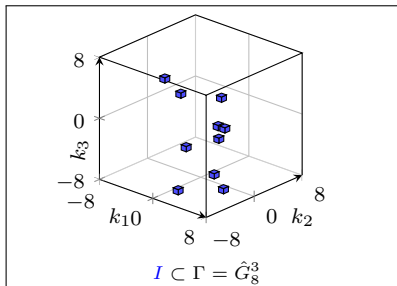
reconstructing
→
rank-1 lattice



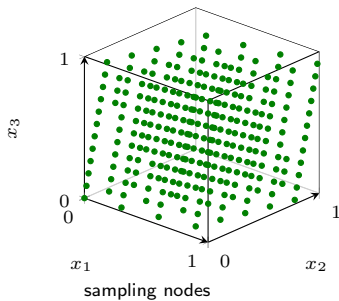


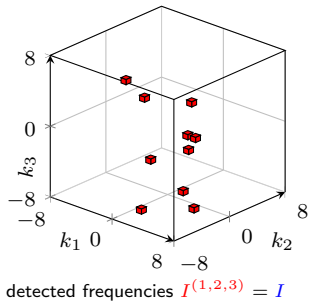
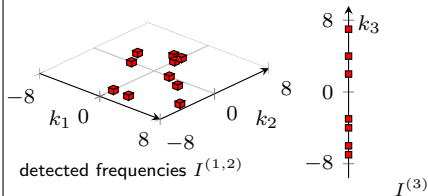
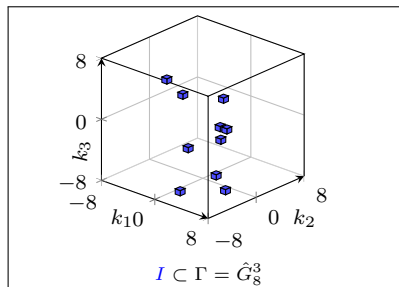
1-dim.
←
FFT



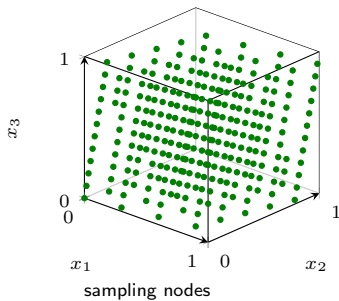


1-dim.
←
FFT





1-dim.
←
FFT

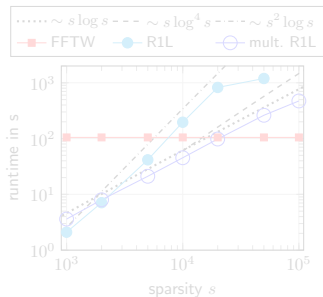
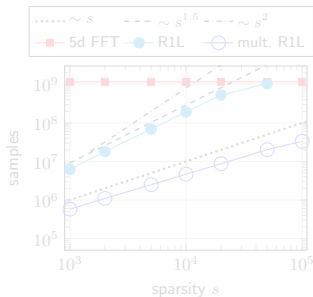


complexity of dimension-incremental sparse FFT using **rank-1 lattices**:

- ▶ sparsity $s = |I|$, search domain $\Gamma = \hat{G}_N^d := \{-N, \dots, N\}^d \supset I$,
 number of detection iterations r
 - ▶ if $(\text{Re}(\hat{p}_k))$ identical sign) AND $(\text{Im}(\hat{p}_k))$ identical sign $\Rightarrow r = 1$

	single rank-1 lattices	multiple rank-1 lattices
samples	$\mathcal{O}(dr^3 s^2 N)$	$\mathcal{O}(dr^2 s N \log^2(rsN))$
arithmetic op.	$\mathcal{O}(dr^3 s^3 + dr^3 s^2 N \log(rsN))$	$\mathcal{O}(d^2 r^2 s N \log^4(rsN))$ (w.h.p.)

example: $p_I(x) = \sum_{k \in I} \hat{p}_k e^{2\pi i k \cdot x}$, $I \subset \Gamma = \hat{G}_{32}^5 := \{-32, \dots, 32\}^5$, $|\Gamma| \approx 1.16 \cdot 10^9$

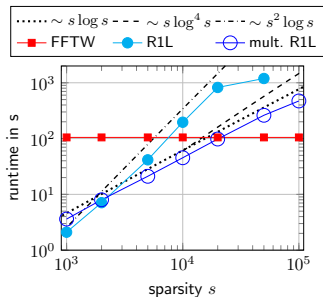
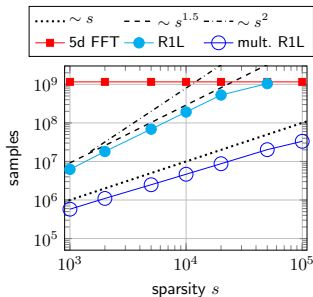


complexity of dimension-incremental sparse FFT using **rank-1 lattices**:

- ▶ sparsity $s = |I|$, search domain $\Gamma = \hat{G}_N^d := \{-N, \dots, N\}^d \supset I$,
 number of detection iterations r
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	single rank-1 lattices	multiple rank-1 lattices
samples	$\mathcal{O}(d r^3 s^2 N)$	$\mathcal{O}(d r^2 s N \log^2(rsN))$
arithmetic op.	$\mathcal{O}(d r^3 s^3 + d r^3 s^2 N \log(rsN))$	$\mathcal{O}(d^2 r^2 s N \log^4(rsN))$ (w.h.p.)

example: $p_I(\mathbf{x}) = \sum_{\mathbf{k} \in I} \hat{p}_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$, $I \subset \Gamma = \hat{G}_{32}^5 := \{-32, \dots, 32\}^5$, $|\Gamma| \approx 1.16 \cdot 10^9$



complexity of dimension-incremental sparse FFT using **rank-1 lattices**:

- ▶ sparsity $s = |I|$, search domain $\Gamma = \hat{G}_N^d := \{-N, \dots, N\}^d \supset I$,
 number of detection iterations r
 - ▶ if $(\text{Re}(\hat{p}_k))$ identical sign) AND $(\text{Im}(\hat{p}_k))$ identical sign $\Rightarrow r = 1$










	single rank-1 lattices	multiple rank-1 lattices
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arithmetic op.	$\mathcal{O}(d r^3 s^3 + d r^3 s^2 N \log(rsN))$	$\mathcal{O}(d^2 r^2 s N \log^4(rsN))$ (w.h.p.)

example:

- ▶ B-spline $N_m(x) := \sum_{k \in \mathbb{Z}} C_m \text{sinc}\left(\frac{\pi}{m} k\right)^m (-1)^k e^{2\pi i k x}$
- ▶ $f(\mathbf{x}) := \prod_{t \in \{1,3,8\}} N_2(x_t) + \prod_{t \in \{2,5,6,10\}} N_4(x_t) + \prod_{t \in \{4,7,9\}} N_6(x_t)$
- ▶ dimension-incremental method for $\Gamma = \hat{G}_{64}^{10}$: $(|\hat{G}_{64}^{10}| \approx 1.28 \cdot 10^{21})$

threshold	single rank-1 lattices			multiple rank-1 lattices		
	#samples	$ I $	rel. L_2 error	#samples	$ I $	rel. L_2 error
1.0e-02	327 689	493	1.3e-01	246 681	501	5.5e-01
1.0e-03	2 551 143	1 109	1.1e-02	1 441 455	1 205	1.1e-02
1.0e-04	17 198 228	3 009	2.0e-03	7 473 447	3 463	2.1e-03
1.0e-05	132 285 922	7 435	4.8e-04	37 056 491	11 053	4.9e-04

- ▶ multivariate periodic functions and rank-1 lattices
 - ▶ fast reconstruction of multivariate trigonometric polynomials p_I for arbitrary frequency index sets I [Kämmerer '14]
 - ▶ fast approximation [Kämmerer '14], error estimates in [Kämmerer '14] [Kämmerer, Potts, V. '15] [Byrenheid, Kämmerer, Ullrich, V. '16] [V. '17]
- ▶ similar results for multivariate non-periodic functions and rank-1 Chebyshev lattices (not in this talk) [Potts, V. '15] [V. '17]
- ▶ reconstructing multiple rank-1 lattices [Kämmerer '16] [Kämmerer '17]
 - ▶ distinct reduction of number of samples and arithmetic operations
- ▶ high-dimensional dimension-incremental sparse FFT and rank-1 lattices [Potts, V. '16] [V. '17]
 - ▶ determination of unknown frequency index set I
 - ▶ very good numerical results for high-dimensional sparse trigonometric polynomials and for high-dimensional functions (non-sparse in frequency domain)

-  L. Kämmerer. **High Dimensional Fast Fourier Transform Based on Rank-1 Lattice Sampling.** *Dissertation (PhD thesis), Faculty of Mathematics, Chemnitz University of Technology*, 2014.
-  L. Kämmerer, D. Potts and T. V. **Approximation of multivariate periodic functions by trigonometric polynomials based on rank-1 lattice sampling.** *J. Complexity*, 31:543–576, 2015.
-  L. Kämmerer, D. Potts and T. V. **Approximation of multivariate periodic functions by trigonometric polynomials based on sampling along rank-1 lattice with generating vector of Korobov form.** *J. Complexity*, 31:424–456, 2015.
-  D. Potts and T. V. **Sparse high-dimensional FFT based on rank-1 lattice sampling.** *Appl. Comput. Harmon. Anal.*, 41:713–748, 2016.
-  G. Byrenheid, L. Kämmerer, T. Ullrich and T. V. **Tight error bounds for rank-1 lattice sampling in spaces of hybrid mixed smoothness.** *Numer. Math.*, 2016, accepted.
-  L. Kämmerer. **Multiple Rank-1 Lattices as Sampling Schemes for Multivariate Trigonometric Polynomials.** *J. Fourier Anal. Appl.*, 2016.
-  L. Kämmerer. **Constructing spatial discretizations for sparse multivariate trigonometric polynomials that allow for a fast discrete Fourier transform.** *arXiv:1703.07230*, 2017.
-  T. V. **Multivariate Approximation and High-Dimensional Sparse FFT Based on Rank-1 Lattice Sampling.** *Dissertation (PhD thesis), Faculty of Mathematics, Chemnitz University of Technology*, 2017.
-  Software: MATLAB toolboxes (for single rank-1 lattices) <http://www.tu-chemnitz.de/~tovo>