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

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joint work with L. Kämmerer and D. Potts

supported by DFG SPP 1324

Content

Introduction

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

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where the Fourier coefficients of f are given by

$$\hat{f}_{\mathbf{k}} = \int_{\mathbb{T}^d} f(\mathbf{x}) \mathrm{e}^{-2\pi \mathrm{i}\mathbf{k}\cdot\mathbf{x}} \mathrm{d}\mathbf{x}, \qquad \mathbf{k} \in \mathbb{Z}^d$$

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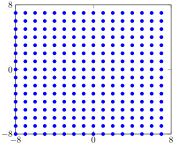
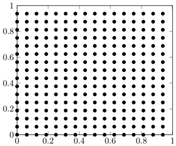
- e.g., $\mathrm{I} = \mathbb{Z}^d \cap [-N, N)^d$ full grid, $\mathbf{y}_j$ equispaced nodes



$$(\hat{p}_{\mathbf{k}})_{\mathbf{k}\in\mathrm{I}} \quad \overset{\text{d-dim}}{\underset{\text{FFT}}{\longleftrightarrow}} \quad (f(\mathbf{y}_j))_{j=0}^{|\mathrm{I}|-1}$$



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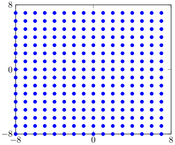

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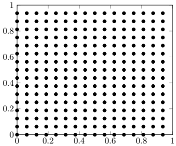
$$\mathcal{O}(N^d \log N)$$



  - problem: $|\mathrm{I}| = (2N)^d \Rightarrow$ curse of dimensionality

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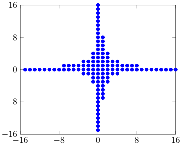

$$(\hat{p}_{\mathbf{k}})_{\mathbf{k}\in\mathrm{I}} \xleftrightarrow[\text{HCFFT}]{} (f(\mathbf{y}_j))_{j=0}^{|\mathrm{I}|-1}$$

(Baszenski, Delvos 1989; Hallatschek 1992; Gradinaru 2007; Griebel, Hamaekers 2013)

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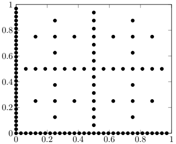

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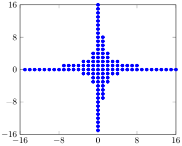

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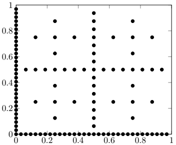

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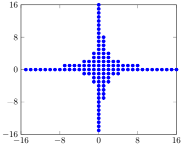

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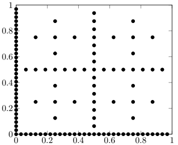

  - problem: stability (Kämmerer, Kunis 2011)
  - implementation of algorithm (HCFFT) is effortful

Introduction - Fct. Spaces $\mathcal{H}^\omega(\mathbb{T}^d)$ and Index Sets I

- Hilbert space

$$\mathcal{H}^\omega(\mathbb{T}^d) := \left\{ f \in L^2(\mathbb{T}^d) \colon \sqrt{\sum_{\mathbf{k}\in\mathbb{Z}^d} \omega(\mathbf{k})^2 |\hat{f}_{\mathbf{k}}|^2} < \infty \right\}$$

  where $\omega \colon \mathbb{Z}^d \to [1,\infty]$ is weight function

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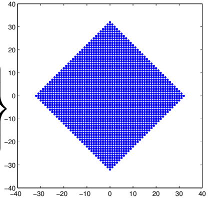

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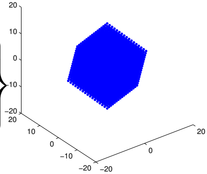

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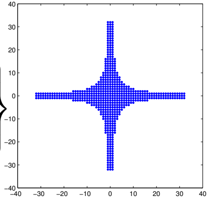

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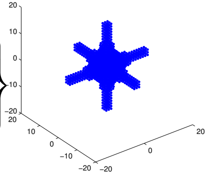

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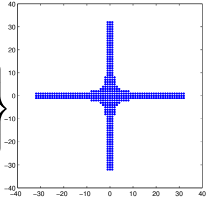

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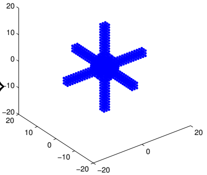

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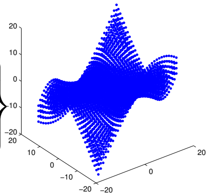

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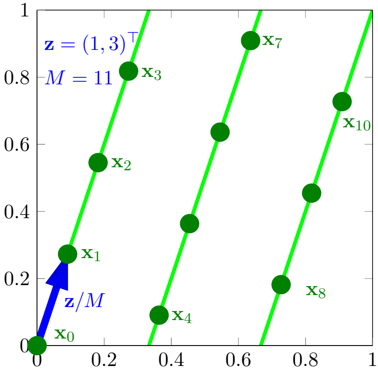
- large dimension d

Trig. polynomials - Fast evaluation at rank-1 lattices

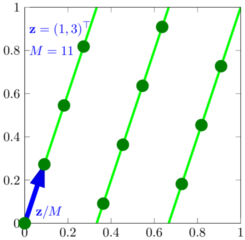
- rank-1 lattice: $\mathbf{z} \in \mathbb{N}^d, M \in \mathbb{N}$

$$\mathbf{x}_j = \frac{j}{M}\mathbf{z} \bmod \mathbf{1};\ j = 0, \ldots, M-1$$



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

Trig. polynomials - Fast evaluation at rank-1 lattices

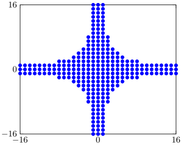


- rank-1 lattice: $\mathbf{z} \in \mathbb{N}^d, M \in \mathbb{N}$

$$\mathbf{x}_j = \frac{j}{M}\mathbf{z} \bmod \mathbf{1};\ j = 0, \ldots, M-1$$

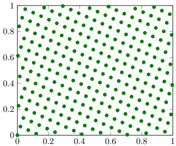
- multivariate trigonometric polynomial
  $p(\mathbf{x}) = \sum_{\mathbf{k}\in \mathrm{I}_N^d} \hat{p}_{\mathbf{k}} \mathrm{e}^{2\pi \mathrm{i} \mathbf{k}\cdot\mathbf{x}}$
- reformulation

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



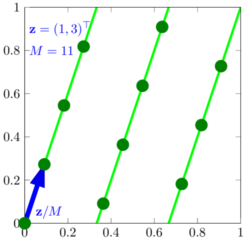
$(\hat{p}_{\mathbf{k}})_{\mathbf{k}\in I_N^d}$

$\longrightarrow$



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

Trig. polynomials - Fast evaluation at rank-1 lattices



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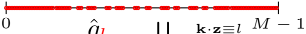
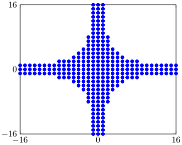


$\Big|\Big|$ $\substack{\mathbf{k}\cdot\mathbf{z}\equiv l \\ (\mathrm{mod}\ M)}$

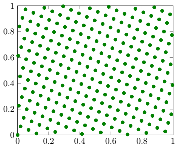


$(\hat{p}_{\mathbf{k}})_{\mathbf{k}\in I_N^d}$

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

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

$\Big|\Big|$ $p(\frac{j}{M}\mathbf{z})$



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Trig. polynomials - Fast evaluation at rank-1 lattices

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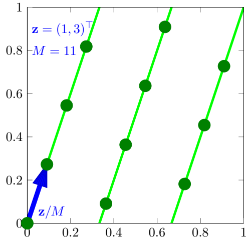

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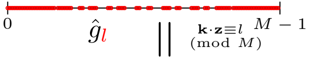
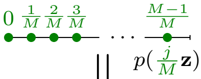
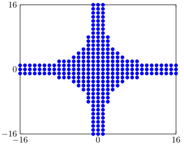


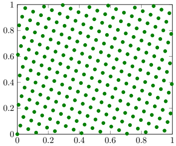




$(\hat{p}_{\mathbf{k}})_{\mathbf{k} \in I_N^d}$

? $\longleftarrow$

fast, stable, unique reconstruction



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

Trig. polynomials - Fast reconstruction

- rank-1 lattice: $\mathbf{z} \in \mathbb{N}^d, M \in \mathbb{N}$

$$\mathbf{x}_j = \frac{j}{M}\mathbf{z} \bmod \mathbf{1};\ j = 0, \ldots, M-1$$

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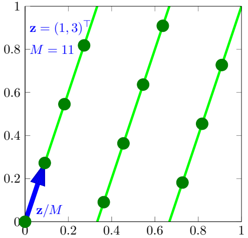

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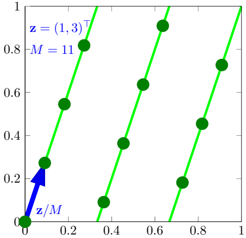

$$\hat{p}_{\mathbf{k}} = \int_{\mathbb{T}^d} p(\mathbf{x})\mathrm{e}^{-2\pi\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\mathbf{x} \approx \mathrm{Q}(p(\cdot)\mathrm{e}^{-2\pi\mathrm{i}\mathbf{k}\cdot(\cdot)}) = \underbrace{\frac{1}{M}\sum_{j=0}^{M-1} p(\mathbf{x}_j)\mathrm{e}^{-2\pi\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}}_{\hat{\tilde{p}}_{\mathbf{k}}}$$

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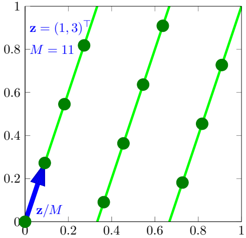

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$$\Rightarrow \ \hat{\tilde{p}}_{\mathbf{k}} = \hat{p}_{\mathbf{k}} \Leftrightarrow \mathbf{k}_1 \cdot \mathbf{z} \not\equiv \mathbf{k}_2 \cdot \mathbf{z} \pmod{M} \text{ for all } \mathbf{k}_1 \neq \mathbf{k}_2 \in \mathrm{I}_N^d$$

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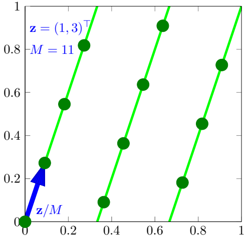

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$\Rightarrow$ Definition: reconstructing rank-1 lattice $\Lambda(\mathbf{z}, M, \mathrm{I}_N^d)$ for I_N^d,

Trig. polynomials - Fast reconstruction

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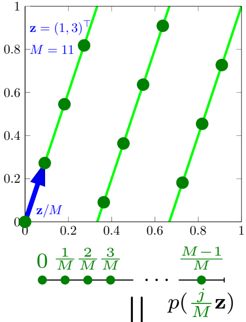
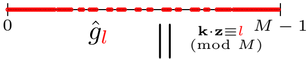
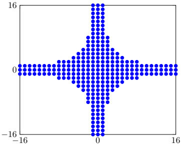


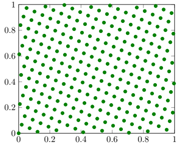




$(\hat{p}_{\mathbf{k}})_{\mathbf{k}\in I_N^d}$

$\xleftarrow[\text{iFFT}]{\text{1-dim}}$

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



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

$\Rightarrow$ Definition: reconstructing rank-1 lattice $\Lambda(\mathbf{z}, M, \mathrm{I}_N^d)$ for I_N^d, $|\mathrm{I}_N^d| \le M \le |\mathrm{I}_N^d|^2$, CBC construction algorithm (Kämmerer 2012)

Reconstruction of $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ - Rank-1 lattice nodes

- reconstructing rank-1 lattice $\Lambda(\mathbf{z}, M, \mathrm{I}_N^d)$:
  $\mathbf{x}_j = \frac{j}{M}\mathbf{z} \bmod \mathbf{1};\ j = 0, \ldots, M-1; \quad |\mathrm{I}_N^d| \leq M \leq |\mathrm{I}_N^d|^2$
- approximate reconstruction of the Fourier coefficients of $f \in \mathcal{H}^\omega(\mathbb{T}^d) \cap \mathcal{C}(\mathbb{T}^d)$ by applying a lattice rule

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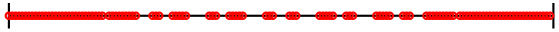
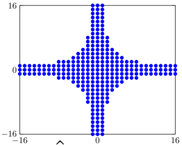


$\hat{g}_l$

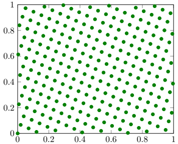
$\| \quad \mathbf{k}\cdot\mathbf{z} \equiv l \pmod{M}$



$(\hat{\tilde{f}}_{\mathbf{k}})_{\mathbf{k} \in I_N^d}$

$\xleftarrow[\text{iFFT}]{\text{1-dim}}$

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



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

Reconstruction of $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ - Rank-1 lattice nodes

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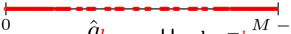
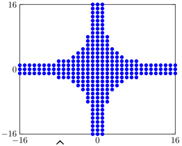


$M-1$

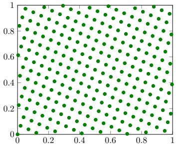
$\hat{g}_l \quad || \quad \mathbf{k}\cdot\mathbf{z} \equiv l \pmod{M}$



$(\hat{\tilde{f}}_{\mathbf{k}})_{\mathbf{k}\in I_N^d}$

1-dim $\longleftarrow$ iFFT

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



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

- approximation $\tilde{S}_{\mathrm{I}_N^d} f$ of f by $\tilde{S}_{\mathrm{I}_N^d} f(\mathbf{x}) = \sum_{\mathbf{k}\in\mathrm{I}_N^d} \hat{\tilde{f}}_{\mathbf{k}} \mathrm{e}^{2\pi\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$

Reconstruction of $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ - Error estimates

$$\underbrace{\|f - \tilde{S}_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\|}_{\text{approximation error}} \leq \underbrace{\|f - S_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\|}_{\text{truncation error}} + \underbrace{\|S_{\mathrm{I}_N^d} f - \tilde{S}_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\|}_{\text{aliasing error}}$$

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$$\|f - S_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\| \quad \leq \quad \frac{1}{N} \sqrt{\sum_{\mathbf{k} \in \mathbb{Z}^d} \omega(\mathbf{k})^2 \left| \hat{f}_{\mathbf{k}} \right|^2} = \frac{1}{N} \, \|f | \mathcal{H}^\omega(\mathbb{T}^d)\|$$

Reconstruction of $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ - Error estimates

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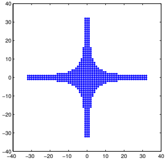
$$\|S_{\mathrm{I}_N^d} f - \tilde{S}_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\| \leq \frac{1}{N} (1 + 2\zeta(2\lambda))^{\frac{d}{2}} \cdot \sqrt{\sum_{\mathbf{k} \in \mathbb{Z}^d} \omega(\mathbf{k})^2 \left| \hat{f}_{\mathbf{k}} \right|^2 \prod_{s=1}^{d} \max(1, |k_s|)^{2\lambda}}$$

$$(\lambda > 1/2)$$

Reconstruction of $f \in \mathcal{H}^{\omega}(\mathbb{T}^d)$ - Error estimates

Example: hyperbolic cross



index set: $|\mathrm{I}_N^d| \in \mathcal{O}\left(N \log^{d-1} N\right)$

$$\mathrm{I}_N^d := \left\{ \mathbf{k} \in \mathbb{Z}^d \colon \prod_{s=1}^{d} \max(1, |k_s|) \leq N \right\}$$

weights: $\omega(\mathbf{k}) := \omega^{0,\beta}(\mathbf{k}) := \prod_{s=1}^{d} \max(1, |k_s|)^{\beta}$

Hilbert space:

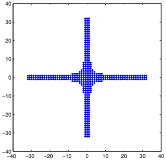
$$\mathcal{H}^{0,\beta}(\mathbb{T}^d) := \left\{ f \colon \|f|\mathcal{H}^{0,\beta}(\mathbb{T}^d)\| := \sqrt{\sum_{\mathbf{k} \in \mathbb{Z}^d} \omega^{0,\beta}(\mathbf{k})^2 |\hat{f}_{\mathbf{k}}|^2} < \infty \right\}$$

arithmetic complexity: $\mathcal{O}\left(N^2 \log^{d-1} N\right)$

error estimate: $\beta > t \geq 0$, $\lambda > 1/2$

$$\|f - \tilde{S}_{\mathrm{I}_N^d} f|\mathcal{H}^{0,t}(\mathbb{T}^d)\| \leq (1 + 2\zeta(2\lambda))^{\frac{d}{2}} N^{t-\beta} \|f|\mathcal{H}^{0,\beta+\lambda}(\mathbb{T}^d)\|$$

Reconstruction of $f \in \mathcal{H}^{\omega}(\mathbb{T}^d)$ - Error estimates



Example: energy-norm based hyperbolic cross

index set: for $0 < \alpha - r < \beta - t$, $|\mathrm{I}_N^d| \in \mathcal{O}\left(N\right)$

$$\mathrm{I}_N^d := \left\{ \mathbf{k} \in \mathbb{Z}^d \colon \max(1, \|\mathbf{k}\|_1)^{\frac{\alpha - r}{\alpha - r + \beta - t}} \prod_{s=1}^{d} \max(1, |k_s|)^{\frac{\beta - t}{\alpha - r + \beta - t}} \leq N \right\}$$

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arithmetic complexity: $\mathcal{O}\left(N^2 \log N\right)$

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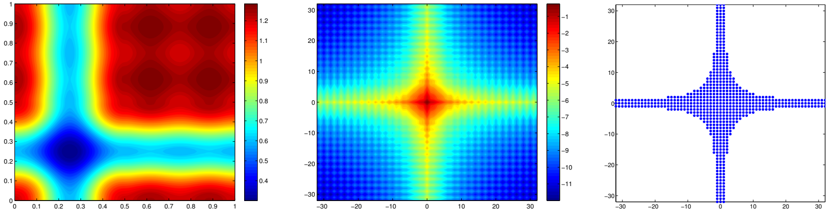
Reconstruction of $f \in \mathcal{H}^{\omega}(\mathbb{T}^d)$ - Numerical results

- function $f \in \mathcal{H}^{0,\frac{5}{2}-\epsilon}(\mathbb{T}^d)$, $\epsilon > 0$,

$$f(\mathbf{x}) := \prod_{s=1}^{d} \left(4 + \operatorname{sgn}\left(x_s - \frac{1}{2}\right) \sin\left(2\pi x_s\right)^2 + \operatorname{sgn}\left(x_s - \frac{1}{2}\right) \sin\left(2\pi x_s\right)^3\right),$$

- hyperbolic cross index set $\mathrm{I}_N^d := \left\{\mathbf{k} \in \mathbb{Z}^d \colon \prod_{s=1}^{d} \max(1, |k_s|) \leq N\right\}$



$f\left((x_1, x_2)^\top\right)$ $\log_{10}\left|\hat{f}_{(k_1,k_2)^\top}\right|$ I_N^d

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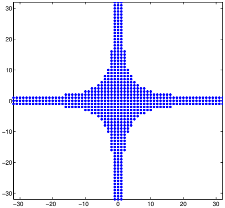
$$\|f - \tilde{S}_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\| \lesssim N^{-2+\tilde{\epsilon}} \|f | \mathcal{H}^{0,2-\tilde{\epsilon}+\lambda}(\mathbb{T}^d)\|$$



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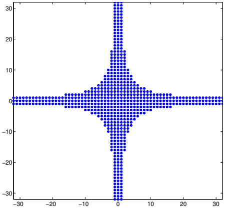
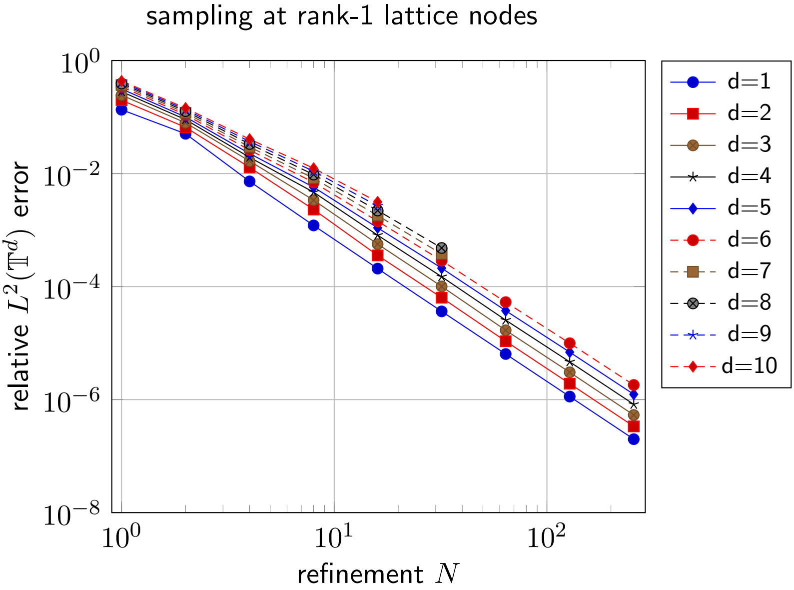


- we compute the relative $L^2(\mathbb{T}^d) = \mathcal{H}^{0,0}(\mathbb{T}^d)$
  - i.e., $\|f - \tilde{S}_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\| / \|f | L^2(\mathbb{T}^d)\|$
  - corresponds to the above error estimate with $r = t = 0$ up to a "constant" since

$$\frac{\|f - \tilde{S}_{\mathrm{I}_N^d} f | \mathcal{H}^{0,0,\gamma}(\mathbb{T}^d)\|}{\|f | \mathcal{H}^{\alpha,\beta+\lambda}(\mathbb{T}^d)\|} = \underbrace{\frac{\|f | L^2(\mathbb{T}^d)\|}{\|f | \mathcal{H}^{\alpha,\beta+\lambda}(\mathbb{T}^d)\|}}_{\le 1} \frac{\|f - \tilde{S}_{\mathrm{I}_N^d} f | L^2(\mathbb{T}^d)\|}{\|f | L^2(\mathbb{T}^d)\|}$$

Reconstruction of $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ - Numerical results



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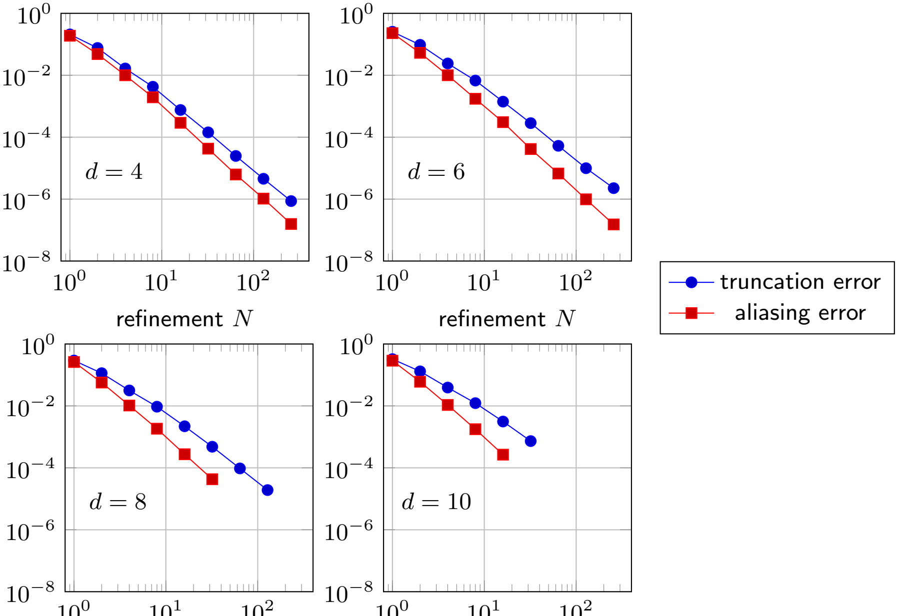

Reconstruction of $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ - Numerical results

d	N	$\lvert I_N^d \rvert$	M	$\frac{M}{\lvert I_N^d \rvert}$	rel. $L^2(\mathbb{T}^d)$ error
6	64	1 709 857	31 829 977	18.6	5.3e-05
6	128	5 137 789	192 757 285	37.5	9.9e-06
6	256	14 977 209	1 400 567 254	93.5	1.8e-06
8	8	768 609	6 027 975	7.8	9.6e-03
8	16	2 935 521	49 768 670	17.0	2.2e-03
8	32	10 665 297	359 896 131	33.7	4.8e-04
10	4	2 421 009	30 780 958	12.7	4.1e-02
10	8	10 819 089	194 144 634	17.9	1.2e-02
10	16	45 548 649	2 040 484 044	44.8	3.1e-03

Reconstruction of $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ - Improved estimates

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idea from Temlyakov 1986:

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$$\mathrm{I}_N^{d,\alpha,\beta} := \left\{ \mathbf{k} \in \mathbb{Z}^d : \max(1, \|\mathbf{k}\|_1)^{\frac{\alpha}{\alpha+\beta}} \prod_{s=1}^{d} \max(1, |k_s|)^{\frac{\beta}{\alpha+\beta}} \leq N \right\}$$

$$\|S_{\mathrm{I}_N^{d,\alpha,\beta}} f - \tilde{S}_{I_N^{d,\alpha,\beta}} f | L^2(\mathbb{T}^d)\| \leq C(d,\alpha,\beta)\, N^{-(\alpha+\beta)}\, \|f|\mathcal{H}^{\alpha,\beta}(\mathbb{T}^d)\|$$

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drawback: non-constructive proof, i.e., for sufficiently large prime M, $|I_N^{d,\alpha,\beta}| \lesssim M \lesssim |I_N^{d,\alpha,\beta}|^2$, there exists $\mathbf{z} = (1, a, a^2, \ldots, a^{d-1})^\top$ such that above error estimates are valid

Summary

approximate reconstruction of (multivariate) functions $f \in \mathcal{H}^\omega(\mathbb{T}^d)$ by sampling along rank-1 lattice nodes

- perfectly stable
- computation only uses single one-dimensional FFT + SP
- oversampling factor up to $|\mathrm{I}_N^d|$
- arithmetic complexity $\mathcal{O}\left(|\mathrm{I}_N^d|^2 \log |\mathrm{I}_N^d|\right)$
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Kämmerer, L., Potts, D., Volkmer, T.
Approximation of multivariate periodic functions by trigonometric polynomials based on sampling along rank-1 lattice with generating vector of Korobov form.
DFG-Schwerpunktprogramm 1324, Preprint 159, 2014.
(http://www.tu-chemnitz.de/~tovo)