The uniform sparse FFT

with application to PDEs with random coefficients

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joint work with Lutz Kämmerer and Daniel Potts

Chemnitz University of Technology
Applied Functional Analysis

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Outline

General aim

Approximation (by using samples) of the solution $u(\boldsymbol{x}, \boldsymbol{y})$ of the PDE

$$\begin{aligned} -\nabla_{\boldsymbol{x}} \cdot (a(\boldsymbol{x}, \boldsymbol{y}) \nabla_{\boldsymbol{x}} u(\boldsymbol{x}, \boldsymbol{y})) &= f(\boldsymbol{x}), && \boldsymbol{x} \in D,\ \boldsymbol{y} \in D_{\boldsymbol{y}} \\ u(\boldsymbol{x}, \boldsymbol{y}) &= 0, && \forall\, \boldsymbol{x} \in \partial D,\ \boldsymbol{y} \in D_{\boldsymbol{y}}. \end{aligned}$$

spatial variable $\boldsymbol{x}$

$\boldsymbol{x} \in D \subset \mathbb{R}^{d_{\boldsymbol{x}}}$, $d_{\boldsymbol{x}} \in \{1, 2, 3\}$

random variable $\boldsymbol{y}$

$\boldsymbol{y} = (y_j)_{j=1}^{d} \in D_{\boldsymbol{y}}$, d very large

Affine random coefficient

$\boldsymbol{y}$ typically uniformly distributed in $D_{\boldsymbol{y}}$, e.g. $\boldsymbol{y} \sim \mathcal{U}\left([-1,1]^d\right)$

$$a(\boldsymbol{x},\boldsymbol{y}) = a_0(\boldsymbol{x}) + \sum_{j=1}^{d} y_j\,\psi_j(\boldsymbol{x})$$

[Cohen, DeVore, Schwab '10], [Dick, Kuo, Le Gia, Schwab '16], [Bachmayr, Cohen, Dahmen '18], [Gantner, Herrmann, Schwab '18], ...

Lognormal random coefficient

$\boldsymbol{y}$ typically normally distributed in $D_{\boldsymbol{y}} = \mathbb{R}^d$, i.e. $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{0},\boldsymbol{I})$

$$a(\boldsymbol{x},\boldsymbol{y}) = a_0(\boldsymbol{x}) + \exp(b(\boldsymbol{x},\boldsymbol{y})), \qquad b(\boldsymbol{x},\boldsymbol{y}) = b_0(\boldsymbol{x}) + \sum_{j=1}^{d} y_j\,\psi_j(\boldsymbol{x})$$

[Graham, Kuo, Nichols, Scheichl, Schwab, Sloan '13],[Cheng, Hou, Yan, Zhang '13], [Bachmayr, Cohen, DeVore, Migliorati '17], [Nguyen, Nuyens '21], ...

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Approximation of the solution $u(\boldsymbol{x}, \boldsymbol{y})$

Main problem

d typically very large
$\Longrightarrow$ Curse of Dimensionality

Examples of other approaches:

- Quasi-Monte Carlo methods [Kuo, Schwab, Sloan '15], [Dick, Le Gia, Schwab '16], [Nguyen, Nuyens '21], ...
- collocation methods [Cheng, Hou, Yan, Zhang '13], [Ernst, Sprungk '14], [Zhang, Hu, Hou, Lin, Yan '14], ...
- methods based on certain (tensorized) functions (e.g., Legendre polynomials) [Cohen, DeVore, Schwab '10], [Bachmayr, Cohen, Migliorati '17], ...

These approaches are often heavily influenced by the choice (or computation) of some weights, functions or kernels in advance!
Also, they often just approximate some quantity of interest (e.g. $\mathbb{E}[F(u(\cdot, \boldsymbol{y}))]$).

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Main Tool

a sparse FFT (sFFT) approach [Indyk, Kapralov '12], [Potts, Volkmer '16]

The sFFT was originally designed to recover sparse trigonometric polynomials

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

with unknown frequency set $\mathrm{I} \subset \mathbb{Z}^d$.

Input

- search space $\Gamma \subset \mathbb{Z}^d$
- sparsity $s \geq |\mathrm{I}|$
- black box sampling $(\boldsymbol{y} \mapsto p(\boldsymbol{y}))$

Output

- frequency set $\mathrm{I} = \operatorname{supp} \hat{p} \subset \Gamma \subset \mathbb{Z}^d$
- coefficients $\hat{p}_{\boldsymbol{k}}, \boldsymbol{k} \in \mathrm{I}$

Function approximation using the sFFT is realized via thresholding.

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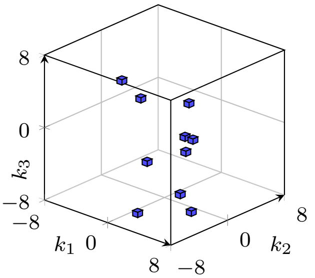

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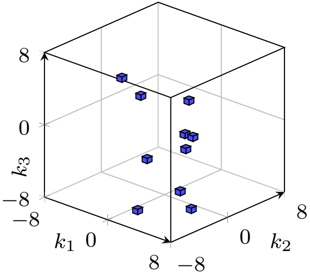
$$\hat{p}_{k_1} := \frac{1}{17} \sum_{\ell=0}^{16} p\left(\begin{pmatrix} \ell/17 \\ x_2' \\ x_3' \end{pmatrix}\right) \mathrm{e}^{-2\pi\mathrm{i}\frac{\ell k_1}{17}}$$

$k_1 = -8, \ldots, 8$

frequency candidates

sampling nodes $\{(\frac{\ell}{17}, x_2', x_3')\}_{\ell=0}^{16}$



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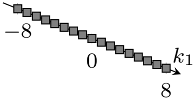

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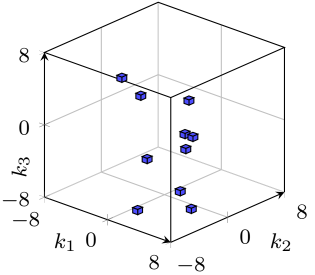

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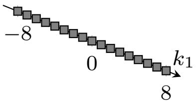
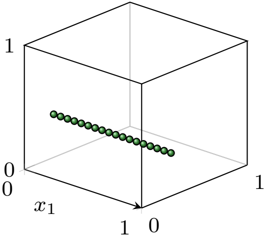


frequency candidates

construct $\longrightarrow$ sampling set



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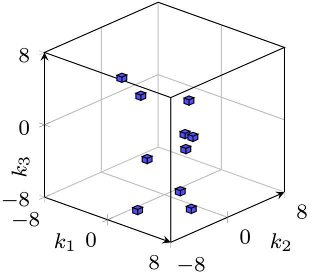

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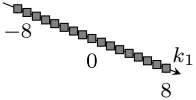
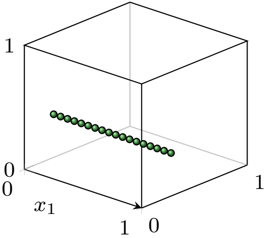


frequency candidates

1-dim. ⟵ FFT



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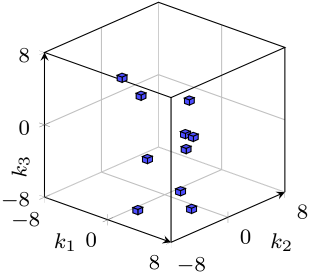

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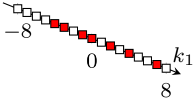
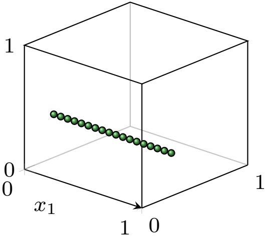
$$= \sum_{\substack{(h_2,h_3)\in\{-8,\ldots,8\}^2 \\ (k_1,h_2,h_3)^\top \in \operatorname{supp}\hat{p}}} \hat{p}_{\begin{pmatrix} k_1 \\ h_2 \\ h_3 \end{pmatrix}} \mathrm{e}^{2\pi\mathrm{i}(h_2 x_2' + h_3 x_3')},$$

$k_1 = -8, \ldots, 8$

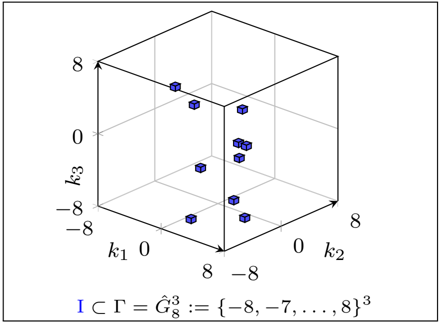


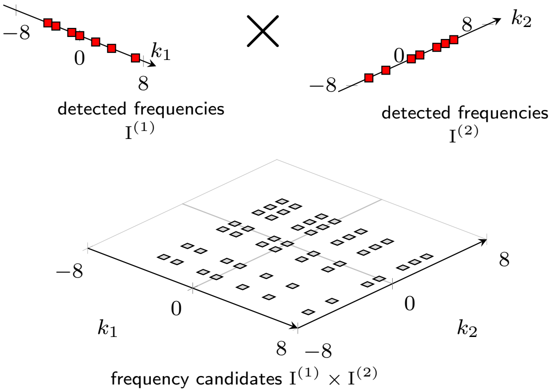
detected frequencies $\mathrm{I}^{(1)}$

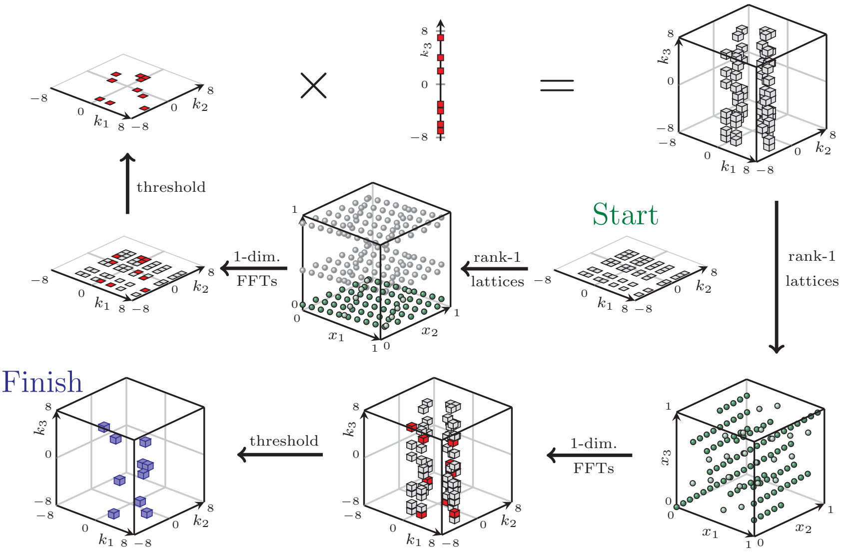
1-dim.
$\longleftarrow$
FFT



sampling nodes $\left\{\left(\frac{\ell}{17}, x_2', x_3'\right)\right\}_{\ell=0}^{16}$


8
0
k_3
−8
−8
k_1 0
8 −8
0 k_2
8
$\mathrm{I} \subset \Gamma = \hat{G}_8^3 := \{-8, -7, \ldots, 8\}^3$


−8
0
k_1
8
detected frequencies
$\mathrm{I}^{(1)}$
k_2
8
0
−8
detected frequencies
$\mathrm{I}^{(2)}$
−8
0
k_1
8 −8
0
k_2
8
frequency candidates $\mathrm{I}^{(1)} \times \mathrm{I}^{(2)}$


Start
rank-1 lattices
1-dim. FFTs
threshold
×
=
rank-1 lattices
1-dim. FFTs
threshold
Finish

Aim

Find an approximation of $u(\boldsymbol{x}, \boldsymbol{y})$.

Spatial discretization

Fix $\boldsymbol{x}_g \in \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_G\}$ and consider the d-variate function $u(\boldsymbol{x}_g, \cdot)$.

Adaptive approximation at each $\boldsymbol{x}_g$

$$u^{\mathrm{sFFT}}(\boldsymbol{x}_g, \boldsymbol{y}) := \sum_{\boldsymbol{k} \in \mathrm{I}_{\boldsymbol{x}_g}} c^{\mathrm{sFFT}}_{\boldsymbol{k}, \boldsymbol{x}_g} \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{y}}$$

Problem: Amount of samples

$G \cdot \mathcal{O}\left(d\, s \, \max(s, N_\Gamma) \log^2 \frac{d\, s\, N_\Gamma}{\delta}\right)$

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$u(\boldsymbol{x}_1, \cdot)$	different functions	$u(\boldsymbol{x}_2, \cdot)$
$\downarrow$		$\downarrow$
$\mathrm{I}_{\boldsymbol{x}_1}$	different index sets	$\mathrm{I}_{\boldsymbol{x}_2}$
$\downarrow$		$\downarrow$
$K_{\boldsymbol{x}_1}$	different candidate sets	$K_{\boldsymbol{x}_2}$
$\downarrow$		$\downarrow$
$S_{\boldsymbol{x}_1}$	different sampling nodes	$S_{\boldsymbol{x}_2}$

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$$G \cdot \mathcal{O}\left(d\, s\, \max(s, N_\Gamma) \log^2 \frac{d\, s\, N_\Gamma}{\delta}\right)$$

$u(\boldsymbol{x}_1, \cdot)$	slightly different functions	$u(\boldsymbol{x}_2, \cdot)$
↓ $\mathrm{I}_{\boldsymbol{x}_1}$	slightly different index sets	↓ $\mathrm{I}_{\boldsymbol{x}_2}$
↓ $K_{\boldsymbol{x}_1}$	slightly different candidate sets	↓ $K_{\boldsymbol{x}_2}$
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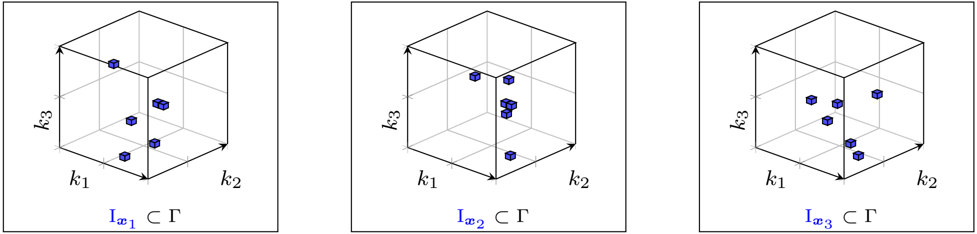
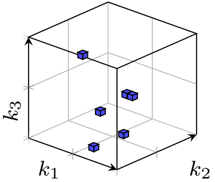
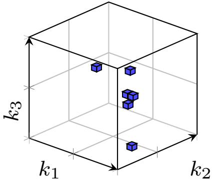
$\downarrow$		$\downarrow$
$K_{\boldsymbol{x}_1}$	slightly different candidate sets	$K_{\boldsymbol{x}_2}$
$\downarrow$		$\downarrow$
$S_{\boldsymbol{x}_1}$	different sampling nodes	$S_{\boldsymbol{x}_2}$

- How to utilize this?
- Solution: the uniform sFFT (usFFT)

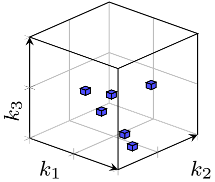

k_3
k_1
k_2
$\mathrm{I}_{\boldsymbol{x}_1} \subset \Gamma$
k_3
k_1
k_2
$\mathrm{I}_{\boldsymbol{x}_2} \subset \Gamma$
k_3
k_1
k_2
$\mathrm{I}_{\boldsymbol{x}_3} \subset \Gamma$



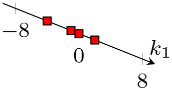
$\mathrm{I}_{\boldsymbol{x}_1} \subset \Gamma$



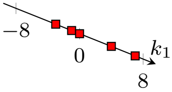
$\mathrm{I}_{\boldsymbol{x}_2} \subset \Gamma$



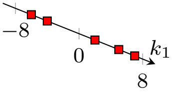
$\mathrm{I}_{\boldsymbol{x}_3} \subset \Gamma$



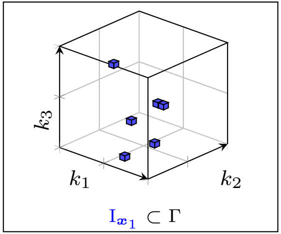
detected frequencies $\mathrm{I}_{\boldsymbol{x}_1}^{(1)}$

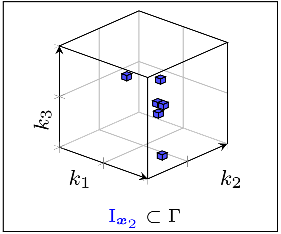


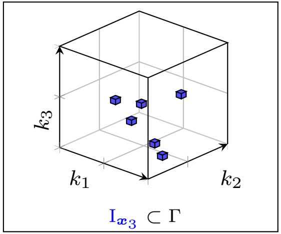
detected frequencies $\mathrm{I}_{\boldsymbol{x}_2}^{(1)}$

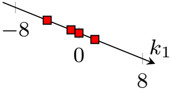


detected frequencies $\mathrm{I}_{\boldsymbol{x}_3}^{(1)}$



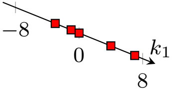






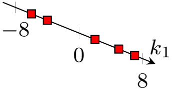
detected frequencies
$I^{(1)}_{\boldsymbol{x}_1}$

$\bigcup$

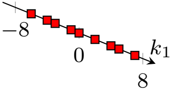


detected frequencies
$I^{(1)}_{\boldsymbol{x}_2}$

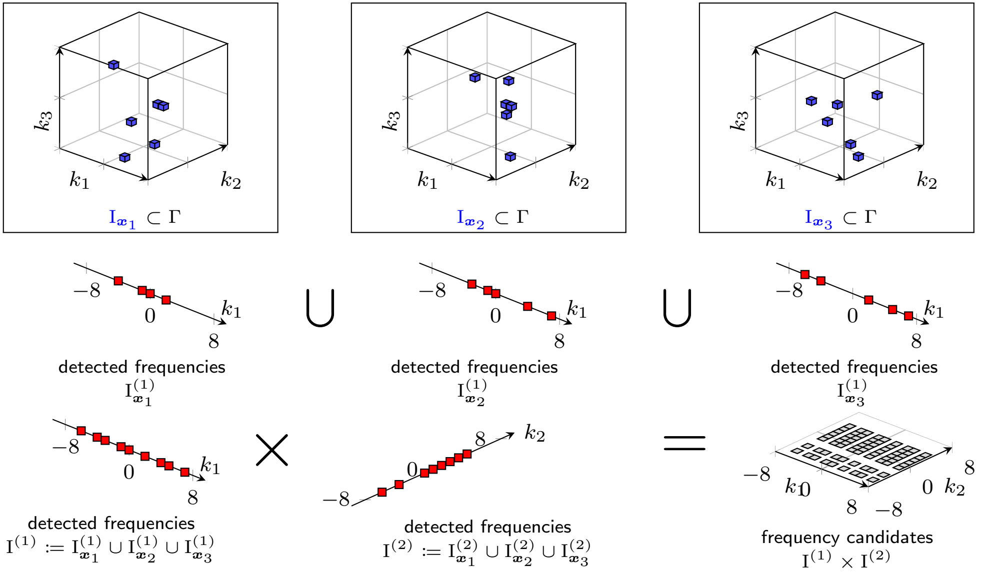
$\bigcup$

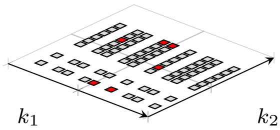


detected frequencies
$I^{(1)}_{\boldsymbol{x}_3}$

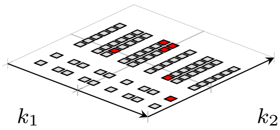


detected frequencies
$I^{(1)} := I^{(1)}_{\boldsymbol{x}_1} \cup I^{(1)}_{\boldsymbol{x}_2} \cup I^{(1)}_{\boldsymbol{x}_3}$

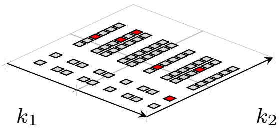

k_3
k_1
k_2
$I_{x_1} \subset \Gamma$
$I_{x_2} \subset \Gamma$
$I_{x_3} \subset \Gamma$
−8
0
8
$\cup$
detected frequencies
$I^{(1)}_{x_1}$
$I^{(1)}_{x_2}$
$I^{(1)}_{x_3}$
$\times$
=
detected frequencies
$I^{(1)} := I^{(1)}_{x_1} \cup I^{(1)}_{x_2} \cup I^{(1)}_{x_3}$
detected frequencies
$I^{(2)} := I^{(2)}_{x_1} \cup I^{(2)}_{x_2} \cup I^{(2)}_{x_3}$
frequency candidates
$I^{(1)} \times I^{(2)}$



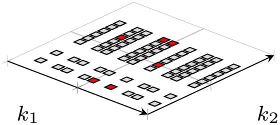
detected frequencies
$\mathrm{I}_{\boldsymbol{x}_1}^{(1,2)}$



detected frequencies
$\mathrm{I}_{\boldsymbol{x}_2}^{(1,2)}$

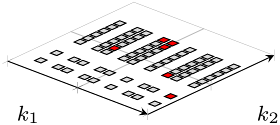


detected frequencies
$\mathrm{I}_{\boldsymbol{x}_3}^{(1,2)}$



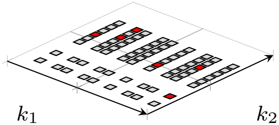
detected frequencies
$\mathrm{I}_{\boldsymbol{x}_1}^{(1,2)}$

$\cup$

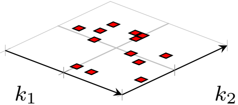


detected frequencies
$\mathrm{I}_{\boldsymbol{x}_2}^{(1,2)}$

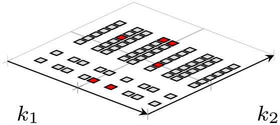
$\cup$



detected frequencies
$\mathrm{I}_{\boldsymbol{x}_3}^{(1,2)}$

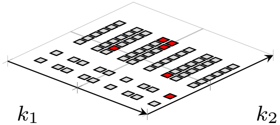


detected frequencies
$\mathrm{I}^{(1,2)} := \mathrm{I}_{\boldsymbol{x}_1}^{(1,2)} \cup \mathrm{I}_{\boldsymbol{x}_2}^{(1,2)} \cup \mathrm{I}_{\boldsymbol{x}_3}^{(1,2)}$



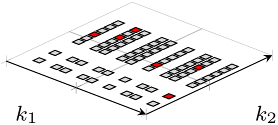
detected frequencies
$\mathrm{I}_{\boldsymbol{x}_1}^{(1,2)}$

$\cup$

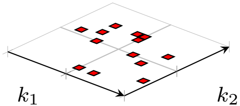


detected frequencies
$\mathrm{I}_{\boldsymbol{x}_2}^{(1,2)}$

$\cup$

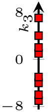


detected frequencies
$\mathrm{I}_{\boldsymbol{x}_3}^{(1,2)}$



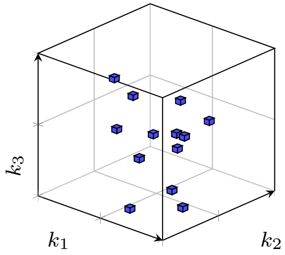
detected frequencies
$\mathrm{I}^{(1,2)} := \mathrm{I}_{\boldsymbol{x}_1}^{(1,2)} \cup \mathrm{I}_{\boldsymbol{x}_2}^{(1,2)} \cup \mathrm{I}_{\boldsymbol{x}_3}^{(1,2)}$

$\times$



detected frequencies
$\mathrm{I}^{(3)} := \mathrm{I}_{\boldsymbol{x}_1}^{(3)} \cup \mathrm{I}_{\boldsymbol{x}_2}^{(3)} \cup \mathrm{I}_{\boldsymbol{x}_3}^{(3)}$

$=$ $\ldots$



$\mathrm{I} := \mathrm{I}_{\boldsymbol{x}_1} \cup \mathrm{I}_{\boldsymbol{x}_2} \cup \mathrm{I}_{\boldsymbol{x}_3}$

- Result:

$$u(\boldsymbol{x}_g, \boldsymbol{y}) \approx u^{\texttt{usFFT}}(\boldsymbol{x}_g, \boldsymbol{y}) := \sum_{\boldsymbol{k} \in \mathrm{I}} c_{\boldsymbol{k}, \boldsymbol{x}_g}^{\texttt{usFFT}} \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{y}} \qquad g = 1, \ldots, G$$

Output of the usFFT

- index set $\mathrm{I} \subset \Gamma \subset \mathbb{Z}^d$ with $\mathrm{I}_{\boldsymbol{x}_g} \subset \mathrm{I}$ for all $g = 1, \ldots, G$
- approximations $c^{\mathtt{usFFT}}_{\boldsymbol{k},\boldsymbol{x}_g}, \boldsymbol{k} \in \mathrm{I}$, for all $g = 1, \ldots, G$

Sample Complexity (= how often do we have to solve the PDE)

$$\mathcal{O}\left(d\, s\, \max(s, N_\Gamma)\, \log^2 \frac{d\, s\, G\, N_\Gamma}{\delta} + \max(sG, N_\Gamma)\, \log \frac{d\, s\, G}{\delta}\right)$$

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PDE (Example from [Eigel, Gittelson, Schwab, Zander 14'])

$$-\nabla_{\boldsymbol{x}} \cdot (a(\boldsymbol{x},\boldsymbol{y})\nabla_{\boldsymbol{x}} u(\boldsymbol{x},\boldsymbol{y})) = 1 \qquad \boldsymbol{x} \in D,\ \boldsymbol{y} \in D_{\boldsymbol{y}}$$

$$u(\boldsymbol{x},\boldsymbol{y}) = 0 \qquad \forall \boldsymbol{x} \in \partial D,\ \boldsymbol{y} \in D_{\boldsymbol{y}}$$

Spatial domain

$$D = (0,1)^2$$

Random domain

$$D_{\boldsymbol{y}} = [-1,1]^{20}$$

Distribution

$$\boldsymbol{y} \sim \mathcal{U}\left([-1,1]^{20}\right)$$

Affine random coefficient

$$a(\boldsymbol{x},\boldsymbol{y}) = 1 + \sum_{j=1}^{20} y_j \psi_j(\boldsymbol{x}) \quad \text{with} \quad \psi_j(\boldsymbol{x}) := \frac{0.9}{\zeta(2)} j^{-2} \cos(2\pi m_1(j) x_1) \cos(2\pi m_2(j) x_2)$$

and

j	1	2	3	4	5	6	7	8	9	10	11	12	13	14	...
$m_1(j)$	0	1	0	1	2	0	1	2	3	0	1	2	3	4	...
$m_2(j)$	1	0	2	1	0	3	2	1	0	4	3	2	1	0	...

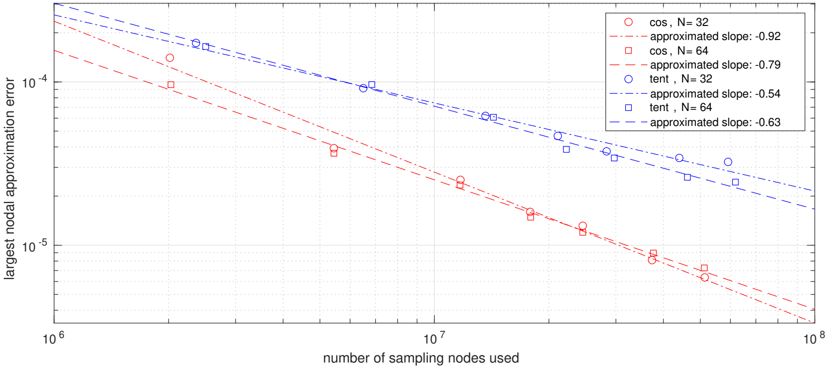

Figure: Largest error err_2^η w.r.t. the nodes $\boldsymbol{x}_g$ for different parameter settings, i.e., $s \in \{100, 250, 500, 750, 1000, 1500, 2000\}$, for the affine example.

$$\text{err}_2^\eta(\boldsymbol{x}_g) := \sqrt{\frac{1}{n_{\text{test}}} \sum_{j=1}^{n_{\text{test}}} \left|\check{u}\left(\boldsymbol{x}_g, \boldsymbol{y}^{(j)}\right) - u^{\text{usFFT}}\left(\boldsymbol{x}_g, \boldsymbol{y}^{(j)}\right)\right|^2}$$

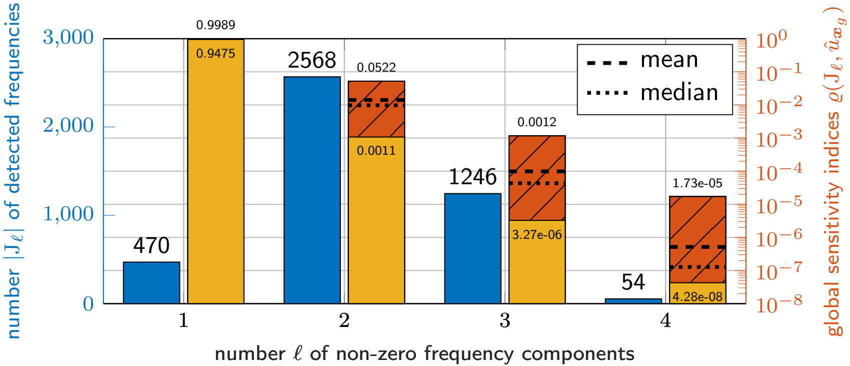

Figure: Analysis of the approximation for the affine example with $s = 2000,\ N = 32$.

$$\varrho(\mathrm{J}, \tilde{u}^{\mathrm{usFFT}}_{\boldsymbol{x}_g}) := \frac{\sigma^2(\tilde{u}^{\mathrm{usFFT}}_{\boldsymbol{x}_g,\mathrm{J}})}{\sigma^2(\tilde{u}^{\mathrm{usFFT}}_{\boldsymbol{x}_g})} = \frac{\sum_{\boldsymbol{k}\in\mathrm{J}\setminus\{\mathbf{0}\}} |c^{\mathrm{usFFT}}_{\boldsymbol{k}}(\tilde{u}_{\boldsymbol{x}_g})|^2}{\sum_{\boldsymbol{k}\in\mathrm{I}\setminus\{\mathbf{0}\}} |c^{\mathrm{usFFT}}_{\boldsymbol{k}}(\tilde{u}_{\boldsymbol{x}_g})|^2} \in [0,1],$$

PDE (Example from [Cheng, Hou, Yan, Zhang 13'], modified)

$$-\nabla_{\boldsymbol{x}} \cdot (a(\boldsymbol{x},\boldsymbol{y})\nabla_{\boldsymbol{x}} u(\boldsymbol{x},\boldsymbol{y})) = f(\boldsymbol{x}) \qquad \boldsymbol{x} \in D,\ \boldsymbol{y} \in D_{\boldsymbol{y}}$$

$$u(\boldsymbol{x},\boldsymbol{y}) = 0 \qquad \forall \boldsymbol{x} \in \partial D,\ \boldsymbol{y} \in D_{\boldsymbol{y}}$$

with $f(\boldsymbol{x}) = \sin(1.3\pi x_1 + 3.4\pi x_2)\cos(4.3\pi x_1 - 3.1\pi x_2)$

Spatial domain

$$D = (0,1)^2$$

Random domain

$$D_{\boldsymbol{y}} = \mathbb{R}^{10}$$

Distribution

$$\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

Lognormal random coefficient

$$\log a(\boldsymbol{x},\boldsymbol{y}) = \sum_{j=1}^{10} \frac{y_j}{j} \sin(2\pi j x_1)\cos(2\pi(11-j)x_2)$$

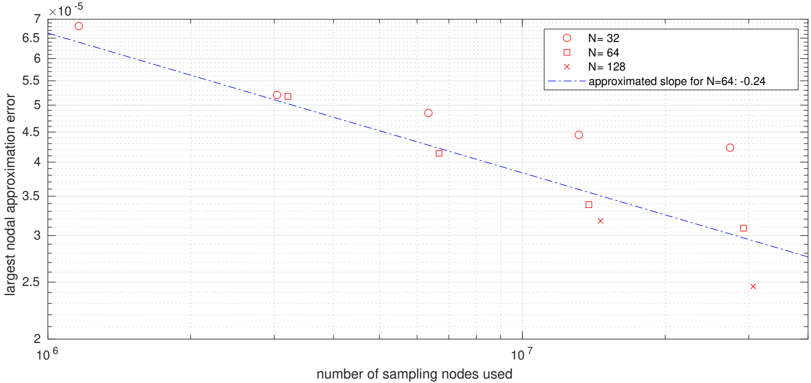

Figure: Largest error err_2^η w.r.t. the nodes $\boldsymbol{x}_g$ for different parameter settings, i.e., $s \in \{100, 250, 500, 1000, 2000\}$, for the lognormal example.

$$\mathrm{err}_2^\eta(\boldsymbol{x}_g) := \sqrt{\frac{1}{n_{\text{test}}} \sum_{j=1}^{n_{\text{test}}} \left|\breve{u}\left(\boldsymbol{x}_g, \boldsymbol{y}^{(j)}\right) - u^{\text{usFFT}}\left(\boldsymbol{x}_g, \boldsymbol{y}^{(j)}\right)\right|^2}$$

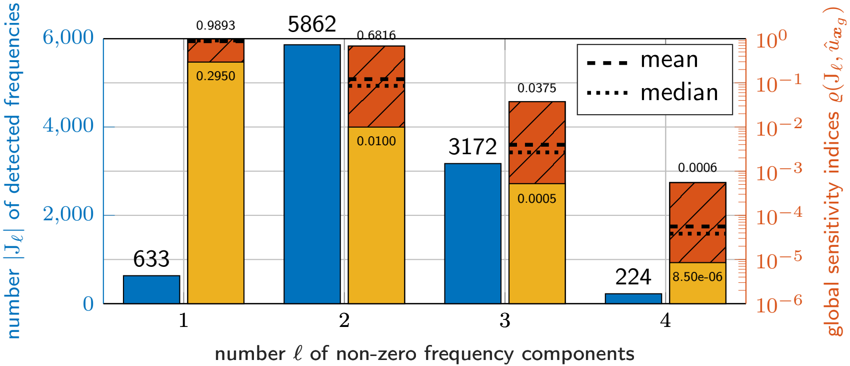

Figure: Analysis of the approximation for the lognormal example with $s = 2000,\ N = 32$.

$$\varrho(\mathrm{J}, \tilde{u}^{\mathrm{usFFT}}_{\boldsymbol{x}_g}) := \frac{\sigma^2(\tilde{u}^{\mathrm{usFFT}}_{\boldsymbol{x}_g,\mathrm{J}})}{\sigma^2(\tilde{u}^{\mathrm{usFFT}}_{\boldsymbol{x}_g})} = \frac{\sum_{\boldsymbol{k}\in\mathrm{J}\setminus\{\boldsymbol{0}\}} |c^{\mathrm{usFFT}}_{\boldsymbol{k}}(\tilde{u}_{\boldsymbol{x}_g})|^2}{\sum_{\boldsymbol{k}\in\mathrm{I}\setminus\{\boldsymbol{0}\}} |c^{\mathrm{usFFT}}_{\boldsymbol{k}}(\tilde{u}_{\boldsymbol{x}_g})|^2} \in [0,1],$$

- Main advantages of the usFFT:
  - fully adaptive, no critical a priori choice needed
  - sample efficient (in terms of sampling locations)
  - approximation gives insight on the influence and interactions of the y_j
  - non-intrusive (does not affect the PDE solver) and parallelizable
  - adapts easily to other domains, boundary conditions, ...

- Lutz Kämmerer, Daniel Potts, Fabian Taubert
  The uniform sparse FFT with application to PDEs with random coefficients
  ArXiv e-prints, 2021. arXiv:2109.04131 [math.NA]

- Thank you for your attention!

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