

The uniform sparse FFT

with application to PDEs with random coefficients

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joint work with Lutz Kämmerer and Daniel Potts

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1. Introduction

Setting The sparse FFT

2. The uniform sparse FFT The key idea

Main result

3. Numerical examples

Affine random coefficient Lognormal random coefficient



We consider the PDE problem

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

- ▶ spatial variable $x \in D \subset \mathbb{R}^{d_x}$, typically with $d_x = 1, 2, 3$
- ▶ random variable $y = (y_j)_{j=1}^d \in D_y$, typically very high-dimensional or even infinite-dimensional

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 affine random coefficient [Cohen, DeVore, Schwab '10], [Dick, Kuo, Le Gia, Schwab '16], [Bachmayr, Cohen, Dahmen '18],[Gantner, Herrmann, Schwab '18], [Nguyen, Nuyens '21], ...

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

periodic random coefficient

[Kaarnioja, Kuo, Sloan '20], [Kaarnioja, Kazashi, Kuo, Nobile, Sloan '20]

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

with Θ_j periodic, e.g., $\Theta_j(\boldsymbol{y}) \coloneqq \frac{1}{\sqrt{6}} \sin(2\pi y_j)$

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

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

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- Common aim: Approximation of the solution $u(\boldsymbol{x}, \boldsymbol{y})$ or some quantity of interest, e.g., the expectation value $\mathbb{E}[F(\boldsymbol{y})]$ of some functional $F(\boldsymbol{y}) \coloneqq F[u(\cdot, \boldsymbol{y})]$, using samples of the function.
- Main problem: high-dimensional approximation!



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- Main problem: high-dimensional approximation!
- 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], ...



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- 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!



• We aim for an approximation of $u(x_0, \cdot)$ for fixed $x_0 \in D$ using the sparse FFT (sFFT) based on rank-1 lattice sampling.

[Potts, Volkmer '16], [Kämmerer, Krahmer, Volkmer '20], [Kämmerer, Potts, Volkmer '21]



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The goal of the sFFT is the computation of the index set I = supp p̂ ⊂ Z^d in the given search space Γ ⊃ I and the coefficients p̂_k, k ∈ I, of the multivariate trigonometric polynomial

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

from sampling values.



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Function approximation of u(x₀, ·) can be realized using the sFFT by assuming it to be a trigonometric polynomial p with some noise η, i.e.,

$$u(\boldsymbol{x}_0, \boldsymbol{y}) = p(\boldsymbol{y}) + \eta(\boldsymbol{y}).$$



























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

 $\begin{array}{c} 1-dim.\\ -8 \\ 0 \\ 0 \\ 0 \\ k1 \\ 8 \\ \text{detected frequencies I}^{(1)} \end{array}$





















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- ▶ Back to our original problem: Approximating $u_{x_0}(y) \coloneqq u(x_0, y)$ for a given $x_0 \in D$.
- ► Up to now:

$$u_{\boldsymbol{x}_0}(\boldsymbol{y}) pprox u_{\boldsymbol{x}_0}^{\mathrm{sFFT}}(\boldsymbol{y}) \coloneqq \sum_{\boldsymbol{k} \in \mathrm{I}_{\boldsymbol{x}_0}} c_{\boldsymbol{k}}^{\mathrm{sFFT}}(u_{\boldsymbol{x}_0}) \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{y}}$$



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Up to now:

$$u_{\boldsymbol{x}_0}(\boldsymbol{y}) \approx u_{\boldsymbol{x}_0}^{\mathrm{sFFT}}(\boldsymbol{y}) \coloneqq \sum_{\boldsymbol{k} \in \mathrm{I}_{\boldsymbol{x}_0}} c_{\boldsymbol{k}}^{\mathrm{sFFT}}(u_{\boldsymbol{x}_0}) \, \mathrm{e}^{2 \pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{y}}$$

- ▶ In practice: Consider $\{x_g \in D, g = 1, ..., G\}$ instead of $\{x_0 \in D\}$.
- ▶ Need G calls of the sFFT to compute $I_{\boldsymbol{x}_g}$ and $c_{\boldsymbol{k}}^{\text{sFFT}}(u_{\boldsymbol{x}_g}), g = 1, \dots, G$.



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- Problem: Sampling is very expensive!
 One sample u_{x_g}(y) = one call of the PDE solver for fixed y
- \blacktriangleright Sampling nodes y differ for each $x_g \longrightarrow$ we can't reuse the PDE solutions.



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Solution: the uniform sFFT!

















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

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



detected frequencies $I_{{m x}_3}^{(1,2)}$













detected frequencies $I_{\boldsymbol{x}_1}^{(1,2)}$

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

detected frequencies $I_{\mathbf{z}_3}^{(1,2)}$



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<u>i</u>







Result:

$$u_{\boldsymbol{x}_g}(\boldsymbol{y}) \approx u_{\boldsymbol{x}_g}^{\text{usFFT}}(\boldsymbol{y}) \coloneqq \sum_{\boldsymbol{k} \in \mathbf{I}} c_{\boldsymbol{k}}^{\text{usFFT}}(u_{\boldsymbol{x}_g}) e^{2\pi i \boldsymbol{k} \cdot \boldsymbol{y}} \qquad g = 1, \dots, G$$

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- index set $I \in \Gamma$ with $I_{\boldsymbol{x}_g} \subset I$ for all g = 1, ..., G
- approximations $c_{k}^{\text{usFFT}}(u_{x_{g}}), k \in I$, for all g = 1, ..., G



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▶ samples $\hat{=}$ amount of PDE solutions needed:

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



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computational complexity of the usFFT:

$$\mathcal{O}\left(d^2 s^2 G^2 N_{\Gamma} \log^3 \frac{d s G N_{\Gamma}}{\delta}\right)$$
 with high probability $1 - \delta$
$$\mathcal{O}\left(d^2 s^3 G^2 N_{\Gamma} \log^3 \frac{d s G N_{\Gamma}}{\delta}\right)$$
 worst case



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- ▶ approximations $c_{k}^{\text{usFFT}}(\tilde{u_{x_{g}}}), k \in I$, for all g = 1, ..., G
- ▶ samples $\hat{=}$ amount of PDE solutions needed: $G \lesssim ds$

$$\mathcal{O}\left(d\,s\,\max(s,N_{\Gamma})\,\log^2rac{d\,s\,G\,N_{\Gamma}}{\delta}\!+\!\max(sG,N_{\Gamma})\,\lograc{d\,s\,G}{\delta}
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$$\mathcal{O}\left(d^2 s^3 \frac{G^2}{\delta} N_{\Gamma} \log^3 \frac{d s \frac{G}{\delta} N_{\Gamma}}{\delta}\right)$$
 worst case

Numerical examples Affine random coefficient

Consider the problem

$$\begin{aligned} -\nabla_{\boldsymbol{x}} \cdot (a(\boldsymbol{x},\boldsymbol{y}) \nabla_{\boldsymbol{x}} u(\boldsymbol{x},\boldsymbol{y})) &= 1 & \boldsymbol{x} \in D, \, \boldsymbol{y} \in D_{\boldsymbol{y}} \\ u(\boldsymbol{x},\boldsymbol{y}) &= 0 & \forall \boldsymbol{x} \in \partial D, \, \boldsymbol{y} \in D_{\boldsymbol{y}} \end{aligned}$$

with $D=(0,1)^2$, $D_{\bm{y}}=[-1,1]^{20}$, $\bm{y}\sim\mathcal{U}\left([-1,1]^{20}\right)$ and the random coefficient

$$a(\boldsymbol{x}, \boldsymbol{y}) = 1 + \sum_{j=1}^{20} y_j \psi_j(\boldsymbol{x})$$

with

$$\psi_j(\boldsymbol{x}) \coloneqq \frac{0.9}{\zeta(2)} j^{-2} \cos(2\pi m_1(j)x_1) \cos(2\pi m_2(j)x_2), \quad \boldsymbol{x} \in D, \ j \ge 1.$$

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	

Example taken from

M. Eigel, C. J. Gittelson, C. Schwab and E. Zander.

Adaptive stochastic Galerkin FEM.

Comput. Methods Appl. Mech. Engrg., 270: 247-269, 2014.

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Numerical examples Affine random coefficient



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

$$\mathsf{err}_{2}^{\eta}(\pmb{x}_{g}) \coloneqq \sqrt{\frac{1}{n_{\mathsf{test}}}\sum_{j=1}^{n_{\mathsf{test}}} \left|\check{u}\left(\pmb{x}_{g},\pmb{y}^{(j)}\right) - u^{\mathsf{usFFT}}\left(\pmb{x}_{g},\pmb{y}^{(j)}\right)\right|^{2}}$$

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number ℓ of non-zero frequency components

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

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

Consider the problem

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

with $f(\boldsymbol{x}) = \sin(1.3\pi x_1 + 3.4\pi x_2)\cos(4.3\pi x_1 - 3.1\pi x_2)$, $D = (0, 1)^2$, $D_{\boldsymbol{y}} = \mathbb{R}^{10}$, $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$ and the random coefficient

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

Example taken and modified from M. Cheng, T. Y. Hou, M. Yan and Z. Zhang. A data-driven stochastic method for elliptic PDEs with random coefficients. SIAM/ASA J. Uncertain. Quantif., 1: 452-493, 2013.





Figure: Largest error err_2^η w.r.t. the nodes x_g for different parameter settings, i.e., s = 100, 250, 500, 1000, 2000, for the lognormal example.

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





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

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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
- adapts easily to other domains, boundary conditions, ...
- non-intrusive and parallelizable



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- Lutz K\u00e4mmerer, 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!