

Adaptive Near-Minimal Rank Approximation for High Dimensional Operator Equations

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Contents

- 1 Motivation, Background
- 2 Tractability
- 3 Tensor Formats
- 4 High-Dimensional Diffusion Equations
 - Where do we Stand?
 - Basic Strategy
 - Main Result
- 5 First Experiments

High Dimensional PDEs

Examples:

- (i) Electronic Schrödinger equation: $d = 3n$, $n = \#$ of particles
- (ii) Fokker-Planck equations: $d = 3K$, $K =$ length of bead string for polymer model
- (iii) Parameter dependent (stochastic) PDEs: $d = \infty$

Core task for (i), (ii): solution of high dimensional elliptic PDEs

Curse of Dimensionality, Tractability - Novak, Woźniakowski

$u(x_1, \dots, x_d)$, $N(\varepsilon, d) := \#\text{lin information for accuracy } \varepsilon$

- Intractable:

$$\liminf_{\varepsilon \rightarrow 0, d \rightarrow \infty} \frac{\log N(\varepsilon, d)}{\varepsilon^{-1} + d} > 0$$

- Weakly tractable:

$$\lim_{\varepsilon \rightarrow 0, d \rightarrow \infty} \frac{\log N(\varepsilon, d)}{\varepsilon^{-1} + d} = 0$$

- Polynomially intractable:

$$\nexists C, s, q \text{ s.t. } N(\varepsilon, d) \leq C\varepsilon^{-s}d^q, \quad \forall \varepsilon \in (0, 1)$$

$u \in C^\infty$, $\|u\|_{C^k} \leq M$, $k \in \mathbb{N}$: \rightsquigarrow polynomially intractable

Remedies?...

- “Excessive” regularity (Korobov spaces)
- “Hidden sparsity” with respect to a
“problem dependent dictionary”

Separation of variables, tensors...

$$u(x) = u(x_1, \dots, x_d) \in C^s$$

$$\varepsilon \sim n^{-s} \rightsquigarrow N \sim n^d$$

$$N(\varepsilon, d) \sim \varepsilon^{-d/s} \text{ or } C^{\alpha d} \varepsilon^{-1/s}$$

$$u(x) \approx \sum_{k=1}^{r(\varepsilon)} u_{k,1}(x_1) \cdots u_{k,d}(x_d)$$

$$\varepsilon \sim r(\varepsilon) d n^{-s} \rightsquigarrow N \sim r(\varepsilon) d n$$

$$N(\varepsilon, d) \sim r(\varepsilon)^{\frac{1}{s}} d^{1+\frac{1}{s}} \varepsilon^{-1/s}$$

Tractability of High-Dimensional PDEs

- $Au = f?$
- u cannot be queried directly
- “Inversion Complexity” – “Representation Complexity”

THEOREM: [D./DeVore/Grasedyck/Süli]

The inversion complexity of the high-dimensional Poisson problem is computationally polynomially tractable

- Important tools: exponential sums of operators, canonical format
- What about more general diffusion coefficients

$$\operatorname{div}(a \nabla u) = f, \quad a \in \mathbb{R}^{d \times d}?$$

A Nasty Pitfall [de Silva...]

$$\begin{aligned}
 & \underbrace{u_{n,1} \otimes u_{n,2} \otimes u_{n,3}}_{n(a + \frac{1}{n}e) \otimes b \otimes c} + \underbrace{v_{n,1} \otimes v_{n,2} \otimes v_{n,3}}_{-na \otimes (b - \frac{1}{n}e) \otimes (c + \frac{1}{n}f)} \\
 = & \quad \color{blue}{na \otimes b \otimes c + e \otimes b \otimes c} - \color{blue}{na \otimes b \otimes c} + a \otimes e \otimes c \\
 & \quad - a \otimes b \otimes f + \frac{1}{n}a \otimes e \otimes f \\
 \rightarrow & \quad \color{blue}{e \otimes b \otimes c + a \otimes e \otimes c} - a \otimes b \otimes f
 \end{aligned}$$

... The limit of rank-2 tensors can have rank 3 ... best approximations don't exist ...

Stable Tensor-Formats

de Silva, Lathauwer, Hackbusch, Falco, Grasedyck, Oseledets, Schneider...

- Subspace based methods (Grassmann manifolds)
- Orthogonal projections, SVD, existence of best approximations...
- But, only in \mathbb{R}^d , $f(\nu_1, \dots, \nu_d)$, $\nu \in \mathcal{J} = \mathcal{J}_1 \times \dots \times \mathcal{J}_d$, $\#(\mathcal{J}_j) < \infty$
- Extension to $\ell_2(\mathcal{J}^d)$, $\#(\mathcal{J}) = \infty$, by Hilbert-Schmidt

“background basis” \rightsquigarrow function spaces... But: scaling problem!

Tucker/Hierarchical Tucker Format

View $\mathbf{u} = (u_{\nu_1, \dots, \nu_d})_{(\nu_1, \dots, \nu_d) \in \mathcal{J}^d}$ as **order- d -tensor**

Mode frames: $\mathbf{U}_k^{(j)} \in \ell_2(\mathcal{J}), j = 1, \dots, d, \langle \mathbf{U}_k^{(i)}, \mathbf{U}_l^{(i)} \rangle = \delta_{kl}, k, l \in \mathbb{N}$

$$\mathbf{u} = \sum_{k_1=1}^{\infty} \cdots \sum_{k_d=1}^{\infty} \langle \mathbf{u}, \mathbf{U}_{k_1}^{(1)} \otimes \cdots \otimes \mathbf{U}_{k_d}^{(d)} \rangle \mathbf{U}_{k_1}^{(1)} \otimes \cdots \otimes \mathbf{U}_{k_d}^{(d)} =: \sum_{\mathbf{k} \in \mathbb{N}^d} \mathbf{a}_{\mathbf{k}} \mathbb{U}_{\mathbf{k}}$$

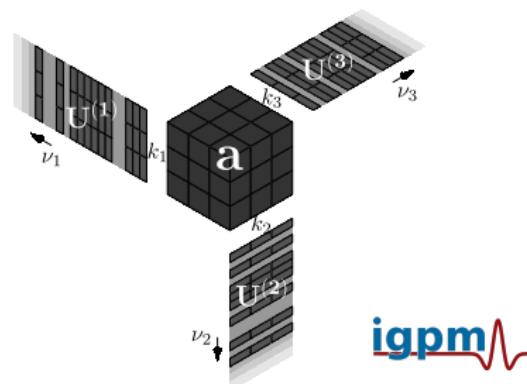
$$\mathbf{U}_k^{(j)} = (\delta_{k,n})_{n \in N} \rightsquigarrow \mathbf{a} = \mathbf{u}$$

Hierarchical Tucker (H-T)-format:

hierarchical factorization of $(\mathbf{a}_{\mathbf{k}})_{\mathbf{k} \in \mathbb{N}^d}$

rank $r \rightsquigarrow$ rank-vector $\mathbf{r} \in \mathbb{N}^d$

How to find good mode frames?



Workhorse SVD... [DeLathauwer, Hackbusch, Khoromskij...]

- Matricization: $\mathbf{v} = (\nu_\nu)_{\nu \in \mathcal{J}^d} \rightsquigarrow M_{\mathbf{v}}^{(i)} = (\nu_{\nu_1, \dots, \nu_{i-1}, \nu_i, \nu_{i+1}, \dots, \nu_d})_{\nu_i \in \mathcal{J}, \nu_j \in \mathcal{J}^{d-1}}$

Tucker ranks: $\text{rank}_i(\mathbf{u}) := \dim \text{range}(M_{\mathbf{u}}^{(i)})$, $i = 1, \dots, d$

- Tucker Format: SVD for $M_{\mathbf{u}}^{(i)} \rightsquigarrow$ left singular vectors $U_k^{(i)}$: \rightsquigarrow HOSVD

$$\lesssim d |\tilde{\mathbf{r}}|_{\infty}^{d+1} + C |\tilde{\mathbf{r}}|_{\infty}^2 \sum_{i=1}^d \#\text{supp}_i(\mathbf{u}), \quad \text{supp}_i(\mathbf{u}) := \bigcup_{z \in \text{range } M_{\mathbf{u}}^{(i)}} \text{supp } z$$

- Hierarchical Tucker Format: \mathcal{H} SVD

[Espig, Grasedyck, Hackbusch, Kolda, Khoromskij, Oseledets,...]

Successive SVD for $M_{\mathbf{u}}^{(\alpha)} = (u_{\nu_\alpha, \nu_\beta})_{\nu_\alpha \in \mathcal{J}^{|\alpha|}, \nu_\beta \in \mathcal{J}^{|\beta|}}$, $\alpha \subset \{1, \dots, d\}$

$$\lesssim d |\tilde{\mathbf{r}}|_{\infty}^4 + C \left(\max_i \tilde{r}_i \right)^2 \sum_{i=1}^d \#\text{supp}_i(\mathbf{u})$$

- Projections: $\|\mathbf{u} - P_{\mathbb{U}(\mathbf{u}), \tilde{\mathbf{r}}} \mathbf{u}\| \leq \sqrt{2d-3} \inf \{ \|\mathbf{u} - \mathbf{v}\| : \mathbf{v} \in \mathcal{H}(\tilde{\mathbf{r}}) \}$

PDEs on $\Omega := \Omega_1 \times \cdots \times \Omega_d$

Model problem:

$$Au = - \sum_{i,j=1}^d \partial_{x_i} (a_{i,j} \partial_{x_j} u) + cu, \quad a(u, v) := \langle v, Au \rangle : \tilde{H}^1(\Omega) \times \tilde{H}^1(\Omega) \rightarrow \mathbb{R}$$

For $f \in (\tilde{H}^1(\Omega))'$ find $u \in H := \tilde{H}^1(\Omega)$ such that

$$a(u, v) = \langle f, v \rangle, \quad v \in H$$

- A has finite (Tucker-) rank
- When $A = -(\partial_{x_1}^2 \otimes I \otimes \cdots \otimes I + \cdots + I \otimes \cdots \otimes I \otimes \partial_{x_d}^2)$
 f “tensor-sparse” $\Rightarrow u = A^{-1}f$ “tensor-sparse”

[D/DeVore/Grasedyck/Süli]



Some Obstructions

- Stable tensor formats not defined for functions (except perhaps $L_2(D^d)$)
- $A : H \rightarrow H'$ isomorphism, i.e., $\|u - v\|_H \sim \|f - Av\|_{H'}$

$$H = \bigcap_{j=1}^d L_2(\Omega_1) \otimes \cdots \otimes L_2(\Omega_{j-1}) \otimes H^1(\Omega_j) \otimes L_2(\Omega_{j+1}) \otimes \cdots \otimes L_2(\Omega_d)$$

does **not** have a “cross-norm”

- $A^{-1} : H' \rightarrow H$ has **infinite rank** because eigenvalues have the form

$$\lambda_\nu = \lambda_{1,\nu_1} + \cdots + \lambda_{d,\nu_d}, \quad \nu \in \mathbb{N}^d$$

\rightsquigarrow a “scaling trap”

Tensor methods for Operator equations

So far...

[Ehrlacher, Falcó, Hackbusch, Khoromskij, Kressner, Mohlenkamp/Beylkin, Nouy, Oseledets, Schneider,...]

- initial reduction to a **fixed discrete** system
- accuracy considerations **detached from continuous** solution
- approximation error and residuals are measured in the **same** (Euclidean) norm - **"scaling trap"**
- accuracy and rank growth **cannot** be controlled simultaneously
- PGD...convergence, ranks?... [Falcó, Chinesta, Ladevez, Nouy,...]

What is different here... (building on existing tools +...)

- Transformation into an **equivalent ∞ -dimensional** problem on $\ell_2(\mathcal{J}^d)$
- Use stable tensor formats on $\ell_2(\mathcal{J}^d)$
- Establish correct mapping properties by diagonal scaling \rightsquigarrow infinite ranks
- Control ranks by adaptive separable scaling approximations - **exponential sums**

Reduction to Problem in $\ell_2(\mathcal{J}^d)$

“Universal background” basis: $\Omega := \Omega_1 \times \cdots \times \Omega_d$

$$\{\psi_\nu = \psi_{\nu_1} \otimes \cdots \otimes \psi_{\nu_d} : \nu \in \mathcal{J}^d\} \text{ O.N.B. for } L_2(\Omega) \rightsquigarrow$$

$$\Psi = \left\{ \left(\sum_{i=1}^d 2^{2|\nu_i|} \right)^{-\frac{1}{2}} \psi_\nu =: s_\nu^{-1} \psi_\nu \right\}_{\nu \in \mathcal{J}^d} \text{ Riesz-basis for } H \subset L_2(\Omega)$$

$$Au = f \Leftrightarrow A\mathbf{u} = \mathbf{f}, \quad \mathbf{A} = \underbrace{\left(s_\nu^{-1} a(\psi_\nu, \psi_\mu) s_\mu^{-1} \right)_{\nu, \mu \in \mathcal{J}}}_{\mathbf{S}^{-1} \mathbf{T} \mathbf{S}^{-1}}, \quad \mathbf{f} = \underbrace{\left(\langle f, s_\nu^{-1} \psi_\nu \rangle \right)_{\nu \in \mathcal{J}}}_{\mathbf{S}^{-1} \mathbf{g}}$$

Theorem:

$$\kappa(\mathbf{A}) := \|\mathbf{A}\| \|\mathbf{A}^{-1}\| \lesssim 1$$

$$u \in H \Leftrightarrow \mathbf{u} = (u_\nu)_{\nu \in \mathcal{J}^d} \in \ell_2(\mathcal{J}^d)$$

Scheme: Perturbed “Ideal Iteration”

Strategy:

$$\mathbf{u}^{k+1} = \mathbf{C}_{\varepsilon_3(k)} \left(\mathbf{P}_{\varepsilon_2(k)} (\mathbf{u}^k + \omega(\mathbf{f} - \mathbf{A}\mathbf{u}^k)) \right) \rightsquigarrow \|\mathbf{u} - \mathbf{u}^{k+1}\| \leq \rho \|\mathbf{u} - \mathbf{u}^k\|, \quad \rho < 1$$

- keep the \mathbf{u}^k in hierarchical Tucker format
- $\mathbf{C}_{\varepsilon_3(k)}$ coarsening of mode frames
- $\mathbf{P}_{\varepsilon_2(k)}$ \mathcal{H} SVD projection to near-optimal subspaces
 - rightsquigarrow simultaneous control of ranks and mode frame sparsity
- control tolerances so as to ensure convergence

Some New Conceptual Ingredients...

- Tensor-Compression-Coarsening Lemma: $a > 1, b < 1$

$$\|\mathbf{u} - \mathbf{v}\| \leq \eta \quad \rightsquigarrow \quad \|\mathbf{P}_{\mathbb{U}(\mathbf{v}), r(a\eta)} \mathbf{v} - \mathbf{u}\| \leq C \inf_{\mathbf{w} \in \mathcal{H}(br(a\eta))} \|\mathbf{u} - \mathbf{w}\|$$

- Contractions:

$$\pi^{(i)}(\mathbf{u}) = (\pi_{\nu_i}^{(i)}(\mathbf{u}))_{\nu_i \in \mathcal{J}} := \left(\left(\sum_{\nu_1, \dots, \nu_{i-1}, \nu_{i+1}, \dots, \nu_d} |u_\nu|^2 \right)^{\frac{1}{2}} \right)_{\nu_i \in \mathcal{J}} \rightsquigarrow$$

$$\pi_{\nu}^{(i)}(\mathbf{u}) = \left(\sum_k |\mathbf{U}_{\nu, k}^{(i)}|^2 |\sigma_k^{(i)}|^2 \right)^{\frac{1}{2}}, \quad \pi_{\nu}^{(i)}(\mathbf{P}_{\mathbb{U}(\mathbf{u}), r} \mathbf{u}) \leq \pi_{\nu}^{(i)}(\mathbf{u}), \quad \nu \in \mathcal{J}$$

\rightsquigarrow sparsity of $\pi^{(i)}(\mathbf{u}) \leftrightarrow$ joint sparsity of i th mode-frames

- Exponential sum approximation to (non-separable) scaling matrices

$$\mathbf{S} = (s_{\nu} \delta_{\nu, \mu})_{\nu, \mu \in \mathcal{J}^d} \text{ in } \mathbf{A} = \mathbf{S}^{-1} \mathbf{T} \mathbf{S}^{-1}$$

$$s_{\nu}^{-1} = (s_{1, \nu_1} + \dots + s_{d, \nu_d})^{-1/2} \approx \sum_{k=1}^r \omega_k e^{-\alpha_k s_{\nu}^2} = \sum_{k=1}^r \omega_k \prod_{j=1}^d e^{-\alpha_k s_{j, \nu_j}}$$


Controlling Rank Growth

Lemma:

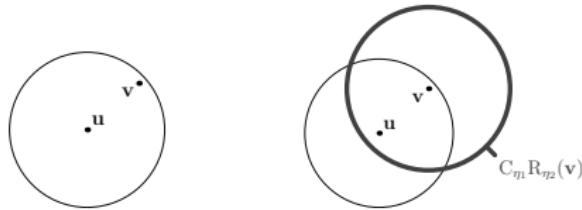
Fix $\alpha > 0$. Let $\|\mathbf{u} - \mathbf{v}\| \leq \eta$, set $\mathbf{w}_\eta := R_{q_d(1+\alpha)\eta} \mathbf{v} = P_{\mathbb{U}(\mathbf{v}), q_d(1+\alpha)\eta} \mathbf{v}$. Then

$$\|\mathbf{u} - \mathbf{w}_\eta\| \leq (1 + q_d(1 + \alpha))\eta$$

and

$$|\text{rank}(\mathbf{w}_\eta)|_\infty \leq \min\{|r|_\infty : r \text{ such that } \exists \tilde{\mathbf{w}}, \text{rank}(\tilde{\mathbf{w}}) \leq r: \|\mathbf{u} - \tilde{\mathbf{w}}\| \leq \alpha\eta\}.$$

- Combine with coarsening: similar result for $C_{\eta_1} R_{\eta_2}$



Exponential Sums Braess/Hackbusch

THEOREM:

Let $\alpha(x) := \ln^2(1 + e^x)$, $w(x) := 2\pi^{-1/2}(1 + e^{-x})^{-1}$, and for given $h > 0$, $n^+, n^- \in \mathbb{N}$, let

$$\varphi_{h,n^+,n^-}(t) := \sum_{k=-n^-}^{n^+} h w(kh) e^{-\alpha(kh)t}. \quad (1)$$

Let $\delta_0 \in (0, 1)$, fix $h \in \left(0, \frac{\pi^2}{5(|\ln \delta_0| + 4)}\right]$, $n^+ \geq N_0^+(\delta_0) := \lceil h^{-1} \max\{2, \sqrt{|\ln \delta_0|}\} \rceil$, then

$$\left| \frac{1}{\sqrt{t}} - \varphi_{h,n^+,\infty}(t) \right| \leq \frac{\delta_0}{\sqrt{t}} \quad \text{for all } t \in [1, \infty). \quad (2)$$

Furthermore, for any $\varepsilon > 0$ and for all $n^- \geq \lceil h^{-1}(\ln 2\pi^{-\frac{1}{2}} + |\ln \varepsilon|) \rceil$, we have

$$|\varphi_{h,n^+,\infty}(t) - \varphi_{h,n^+,n^-}(t)| \leq \varepsilon \quad \text{for all } t \in [1, \infty). \quad (3)$$

The Algorithm

Ideal Iteration:

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \omega(\mathbf{f} - \mathbf{A}\mathbf{u}^n), \quad n = 0, 1, 2, \dots, \quad \mathbf{A} = \mathbf{S}^{-1}\mathbf{T}\mathbf{S}^{-1}, \quad \mathbf{f} = \mathbf{S}^{-1}\mathbf{g}$$

Approximate separable scaling:

$$\tilde{\mathbf{S}}_m^{-1} = \sum_{k=-m}^{N^+} \omega_{m,k} \mathbf{e}_{k,1} \otimes \cdots \otimes \mathbf{e}_{k,d}, \quad (\mathbf{e}_{k,j})_{\nu_j, \mu} = e^{-\alpha_{m,k} 2^{2|\nu_j|}} \delta_{\nu_j, \mu}, \quad \tilde{\mathbf{S}} := \tilde{\mathbf{S}}_\infty$$

$$\|\mathbf{S}\tilde{\mathbf{S}}^{-1}\| \sim 1, \quad \|\mathbf{S}(\tilde{\mathbf{S}}^{-1} - \tilde{\mathbf{S}}_m^{-1})\mathbf{v}\| \leq \textcolor{red}{\eta} \|\mathbf{v}\| \quad \text{if } m \gtrsim |\ln \textcolor{red}{\eta}|, C \max_{\nu \in \text{supp } \mathbf{v}} |\nu|$$

Perturbed Iteration:

$$\bar{\mathbf{u}}^{n+1} = C_{\eta_1(n)} R_{\eta_2(n)} \left(\bar{\mathbf{u}}^n + \omega \underbrace{(\tilde{\mathbf{S}}_{m_{\eta_4(n)}} \mathbf{g}_{\eta_3(n)})}_{\approx \mathbf{f}} - \underbrace{(\tilde{\mathbf{S}}_{m_{\eta_4(n)}} \mathbf{T}_{\eta_3(n)} \tilde{\mathbf{S}}_{m_{\eta_4(n)}}) \bar{\mathbf{u}}^n}_{\approx \mathbf{A}} \right)$$



What is to be shown?...Sparsity Notions...

Benchmarks/Assumptions:

- \mathbf{u} is tensor sparse: $\mathbf{u} \in \mathcal{R}^\gamma(\ell_2(\mathcal{J}^d)) =: \mathcal{R}^\gamma$, i.e. for $\gamma(r) \nearrow \infty$ (e.g. $\gamma(r) = e^{\alpha r}$)

$$\sup_{r \in \mathbb{N}} \left\{ \gamma(r) \inf_{\mathbf{w} \in \mathcal{H}(r)} \|\mathbf{u} - \mathbf{w}\| \right\} := \|\mathbf{u}\|_{\mathcal{R}^\gamma} < \infty$$

i.e. optimal ranks for target accuracy ε satisfy $r(\varepsilon) \lesssim \gamma^{-1}(\|\mathbf{u}\|_{\mathcal{R}^\gamma}/\varepsilon)$

- $\pi^{(i)}(\mathbf{u}) \in \mathcal{A}^s = \mathcal{A}^s(\ell_2(\mathcal{J}))$, $1 \leq i \leq d$, i.e.

$$\mathbf{v} \in \mathcal{A}^s \Leftrightarrow \sup_n n^s \left\{ \inf_{\text{supp } \mathbf{z} \leq n} \|\mathbf{v} - \mathbf{z}\| \right\} =: |\mathbf{v}|_{\mathcal{A}^s} < \infty \}$$

- The low-dimensional components of \mathbf{A} are s^* -compressible with $s^* > s$

$\gamma(r) = e^{\alpha r}$, ε -accuracy: $\sim d^b |\log \varepsilon|^{1/\alpha} \varepsilon^{-1/s}$

Show that the approximate solution \mathbf{u}_ε produced by the iteration has this sparsity



Convergence and Complexity

THEOREM:

Assume that problem has some excess regularity:

for $\varepsilon > 0$ the **Algorithm** produces a \mathbf{u}_ε with $\|\mathbf{u} - \mathbf{u}_\varepsilon\| \leq \varepsilon$ s.t.:

$$|\text{rank } \mathbf{u}_\varepsilon|_\infty \leq C(d) |\log \varepsilon|^b \gamma^{-1} (\|\mathbf{u}\|_{\mathcal{R}^\gamma} / \varepsilon)$$

$$\sum_{i=1}^d \#(\text{supp}(\pi^{(i)}(\mathbf{u}_\varepsilon))) \leq C(d) \left(\sum_{i=1}^d \|\pi^{(i)}(\mathbf{u})\|_{\mathcal{A}^s} / \varepsilon \right)^{\frac{1}{s}}$$

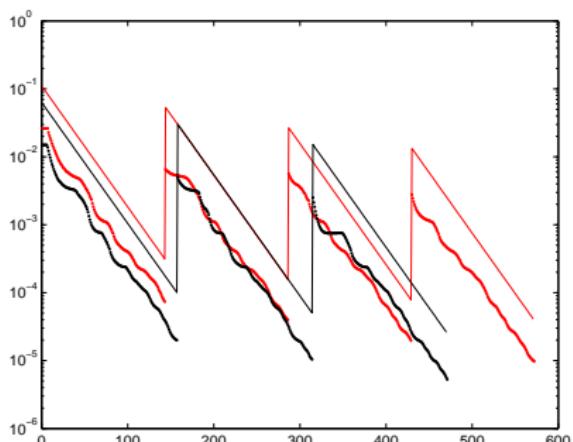
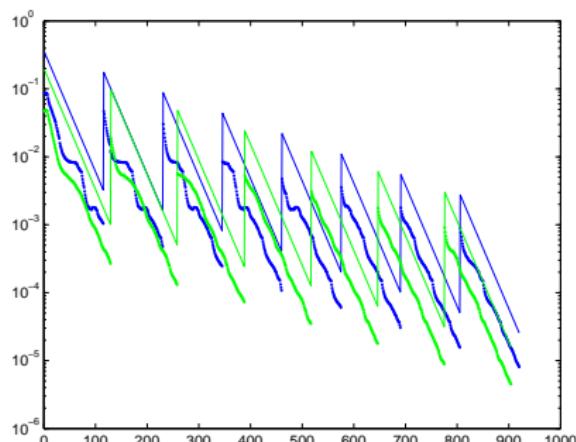
$$\|\mathbf{u}_\varepsilon\|_{\mathcal{R}^\gamma} \leq C(d) \|\mathbf{u}\|_{\mathcal{R}^\gamma}, \quad \sum_{i=1}^d \|\pi^{(i)}(\mathbf{u}_\varepsilon)\|_{\mathcal{A}^s} \leq C(d) \sum_{i=1}^d \|\pi^{(i)}(\mathbf{u})\|_{\mathcal{A}^s}$$

$$\#(\text{ops}) \lesssim C(d) |\log \varepsilon|^b \varepsilon^{-\frac{1}{s}} \left(\sum_{i=1}^d \max\{\|\pi^{(i)}(\mathbf{u})\|_{\mathcal{A}^s}, \|\pi^{(i)}(\mathbf{f})\|_{\mathcal{A}^s}\} \right)^{\frac{1}{s}}$$

a) High-dim PDE: $C(d) \lesssim d^{\ln d}$, $b \lesssim \ln d$ b) Parametric PDE: $C(d) \leq d^{\bar{a}}$

Preliminary Numerical Tests

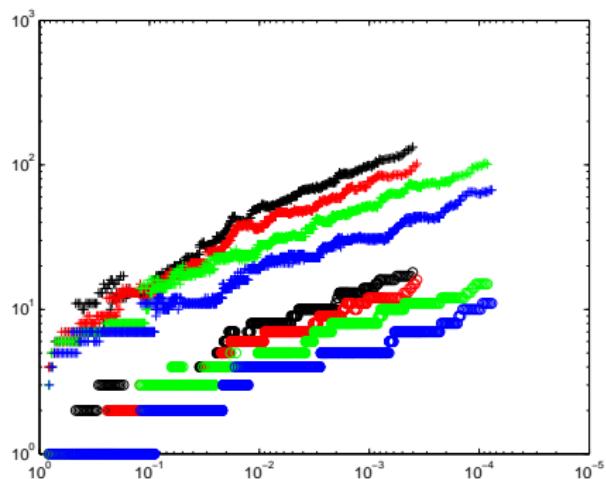
Test problem $-\Delta u = 1$, $u \in H_0^1((0, 1)^d)$, $d = 4, 8, 16, 32$.



x -axis: iteration number, y -axis: residual estimate $\|\tilde{\mathbf{f}}_\eta - \tilde{\mathbf{A}}_\eta(\mathbf{u}_j)\|$ (dots),
current error tolerance (lines)

Preliminary Numerical Tests

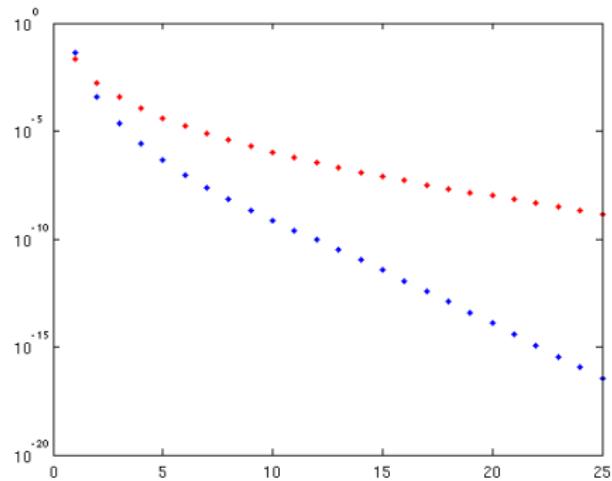
$$d = 4, 8, 16, 32$$



x-axis: estimate of relative residual $\| \mathbf{A} \mathbf{u} - \mathbf{f} \| / \| \mathbf{f} \|$,

y-axis: max. ranks of u_j (\circ) and of intermediate quantities (+)

Concluding Remarks



- wider applicability
- weak tractability
- Poisson: polynomial tractability [D./DeVore/Grasedyck/Süli]
- dependence of $\text{cond}_2(\mathbf{A})$ on d

References

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