

# Tensor Approach to Optimal Control problems with Fractional Elliptic Operator



ALGORITHMIC  
OPTIMIZATION

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## Application fields of fractional operators:

- viscoelastics
- biophysics
- nonlocal electrostatics
- anomalous diffusion
- heat equation in plasmonic nanostructure networks/composite materials
- ...

Given a function  $y_\Omega \in L^2(\Omega)$  on  $\Omega := (0, 1)^d$ , we consider the optimization problem

$$\begin{aligned} \min_{y, u} J(y, u) &:= \int_{\Omega} (y(x) - y_\Omega(x))^2 dx + \frac{\gamma}{2} \int_{\Omega} u^2(x) dx \\ \text{s. t. } &-\Delta y = \beta u \\ &y, u \in H_0^1(\Omega) \end{aligned}$$

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where  $\mathcal{A}^\alpha$  is the *spectral* fractional Laplacian operator for some  $\alpha \in (0, 1)$ .

$$\begin{bmatrix} id & 0 & \mathcal{A}^\alpha \\ 0 & \gamma id & -\beta id \\ \mathcal{A}^\alpha & -\beta id & 0 \end{bmatrix} \begin{pmatrix} y \\ u \\ p \end{pmatrix} = \begin{pmatrix} y_\Omega \\ 0 \\ 0 \end{pmatrix}$$

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$$\Rightarrow p = \frac{\gamma}{\beta} u$$
$$\Rightarrow y = \beta \mathcal{A}^{-\alpha} u$$

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Thus, we find the following necessary optimality conditions:

$$u = (\beta \mathcal{A}^{-\alpha} + \frac{\gamma}{\beta} \mathcal{A}^\alpha)^{-1} y_\Omega$$

for the control  $u$ , and

$$y = \beta \mathcal{A}^{-\alpha} u = (\mathcal{I} + \frac{\gamma}{\beta^2} \mathcal{A}^{2\alpha})^{-1} y_\Omega$$

for the state  $y$ .

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Thus, we find the following necessary optimality conditions:

$$u = \underbrace{(\beta \mathcal{A}^{-\alpha} + \frac{\gamma}{\beta} \mathcal{A}^\alpha)^{-1}}_{G_1} y_\Omega$$

for the control  $u$ , and

$$y = \beta \underbrace{\mathcal{A}^{-\alpha}}_{G_3} u = \underbrace{(\mathcal{I} + \frac{\gamma}{\beta^2} \mathcal{A}^{2\alpha})^{-1}}_{G_2} y_\Omega$$

for the state  $y$ .



Let  $\Omega \in \mathbb{R}^d$  be a bounded Lipschitz domain, and let  $\lambda_k$  and  $e_k$  be the eigenvalues and the corresponding eigenfunctions of the Laplacian, i. e.

$$\begin{aligned} -\Delta e_k &= \lambda_k e_k && \text{in } \Omega, \\ e_k &= 0 && \text{on } \partial\Omega, \end{aligned}$$

and the functions  $e_k$  are an orthonormal basis of  $L^2(\Omega)$ . Then, for  $\alpha \in [0, 1]$  and a function  $g \in H_0^1(\Omega)$

$$g = \sum_{k=1}^{\infty} a_k e_k,$$

we consider the operator

$$\mathcal{A}^\alpha g = \sum_{k=1}^{\infty} a_k \lambda_k^\alpha e_k.$$

For  $\alpha \in (0, 1)$ , the fractional Laplacian  $(-\Delta)^\alpha$  of a function  $g : \mathbb{R}^d \rightarrow \mathbb{R}$  at a point  $x \in \mathbb{R}^d$  is defined by

$$(-\Delta)^\alpha g(x) := C_{d,\alpha} \int_{\mathbb{R}^d} \frac{g(x) - g(y)}{\|x - y\|^{d+2\alpha}} dy.$$

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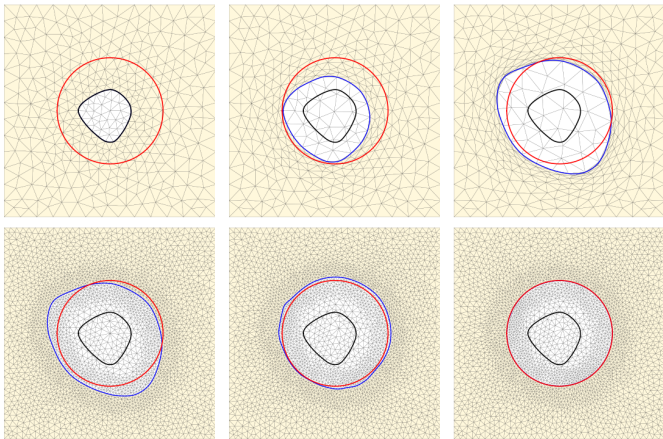
- coincides with  $\mathcal{A}^\alpha$  on  $\mathbb{R}^d$ , cf. details in: Lischke et al. (2018, arXiv:1801.09767)
- leads to multilevel Toeplitz structures on tensor grids (Ch. Vollmann, V. Schulz, CVS 2019)

$$L_{\phi}g(x) = \int_{\Omega} g(x)\phi(x, y) - g(y)\phi(y, x)dy$$

- nonlocal calculus developed by Max Gunzburger et. al.
- unstructured discretization and shape optimization discussed in
  - Ch. Vollmann: *Nonlocal Models with Truncated Interaction Kernels– Analysis, Finite Element Methods and Shape Optimization*, PhD dissertation Trier University, 2019
  - V. Schulz, Ch. Vollmann: *Shape optimization for interface identification in nonlocal models*, arXiv:1909.08884, 2019

→ more details in 2nd RICAM workshop in two weeks...

# Example of nonlocal shape numerics



On a bounded domain, the operators are different.

## Theorem, Servadei/Valdinoci (2014)

The operators  $\mathcal{A}^\alpha$  and  $(-\Delta)^\alpha$  are not the same, since they have different eigenvalues and eigenfunctions (with respect to Dirichlet boundary conditions). In particular,

- the first eigenvalues of  $(-\Delta)^\alpha$  is strictly less than that of  $\mathcal{A}^\alpha$
- the eigenfunctions of  $(-\Delta)^\alpha$  are only Hölder continuous up to the boundary, in contrast with those of  $\mathcal{A}^\alpha$ , which are as smooth up to the boundary as the boundary allows.

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Lischke et al. (2018, arXiv:1801.09767): Numerical tests for the error between  $\mathcal{A}^\alpha$  and  $(-\Delta)^\alpha$ .

$${}^R L^\beta := - {}^R D_{x_1}^{\beta_1} - {}^R D_{x_2}^{\beta_2}, \quad \beta_1, \beta_2 \in (1, 2)$$

${}^R D_{x_i}^{\beta_i}$  : 1D Riemann-Liouville derivative



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$${}^R D_{x_i}^{\beta_i} : \text{1D Riemann-Liouville derivative}$$

This operator is considered in the related publications:

- S. Dolgov, J. W. Pearson, D. V. Savostyanov, M. Stoll: *Fast tensor product solvers for optimization problems with fractional differential equations as constraints*, Applied Mathematics and Computation, 2016
- T. Breiten, V. Simoncini, M. Stoll: *Low-rank solvers for fractional differential equations*, ETNA 2016
- S. Pougkakiotis, J. W. Pearson, S. Leveque, J. Gondzio: *Fast Solution Methods for Convex Fractional Differential Equation Optimization*, arXiv:1907.13428, 2019

Note:

$$(-\Delta)^\alpha \neq \mathcal{A}^\alpha \neq {}^R L^{(2\alpha, 2\alpha)}$$



For a function with separated variables, the Laplacian can be applied in one dimension: Let

$$g : (0, 1)^2 \rightarrow \mathbb{R}, \quad g(x_1, x_2) = g_1(x_1)g_2(x_2).$$

Then

$$-\Delta g(x_1, x_2) = -g_1''(x_1)g_2(x_2) - g_1(x_1)g_2''(x_2).$$



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The case

$$g(x_1, x_2) = \sum_{j=1}^S g_1^{(j)}(x_1)g_2^{(j)}(x_2)$$

follows immediately.



Now consider (FEM/FDM) discretizations  $A_{(1)}$ ,  $A_{(2)}$  of the one-dimensional Laplacian in the first and variables, respectively. The a discretization of  $\mathcal{A} = -\Delta$  on  $(0, 1)^2$  is given by

$$A = A_{(1)} \otimes I_2 + I_1 \otimes A_{(2)}.$$

Let  $\mathbf{g} = \mathbf{g}_1 \otimes \mathbf{g}_2$  be the function  $g$  evaluated on the grid. It follows that

$$A\mathbf{g} = A_{(1)}\mathbf{g}_1 \otimes \mathbf{g}_2 + \mathbf{g}_1 \otimes A_{(2)}\mathbf{g}_2.$$

$\Rightarrow$  The Laplacian  $\mathcal{A}$  admits a tensor product representation with *Kronecker rank 2*.



Therefore, the discrete Laplacian  $A$  can be applied efficiently to function  $g$ , given by

$$g(x_1, x_2) = \sum_{j=1}^S g_1^{(j)}(x_1) g_2^{(j)}(x_2).$$

We get

$$A\mathbf{g} = \sum_{j=1}^S \left( A_{(1)}\mathbf{g}_1^{(j)} \otimes \mathbf{g}_2^{(j)} + \mathbf{g}_1^{(j)} \otimes A_{(2)}\mathbf{g}_2^{(j)} \right),$$

for discretizations  $\mathbf{g}_i^{(j)}$  of  $g_i^{(j)}$ .

**From now on:** Let  $A^\alpha$  be the discretization of  $\mathcal{A}^\alpha$ .

Gavrilyuk/Hackbusch/Khoromskij (2005): using the integral representation

$$\mathcal{A}^{-\alpha} = \frac{1}{\Gamma(\alpha)} \int_0^{\infty} t^{\alpha-1} e^{-tA} dt$$

(based on the Laplace transform), it can be shown that (discretized)  $A^{-\alpha}$  has exponentially decaying singular values, and thus admits a low Kronecker rank approximation.

**Proof:** Sinc quadrature  $\rightarrow$  exponentially decaying coefficients.

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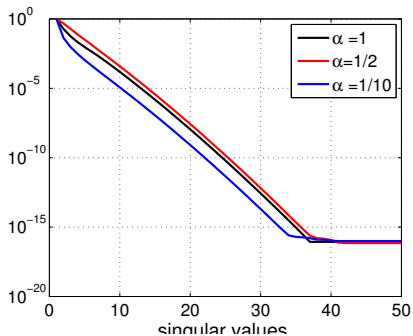
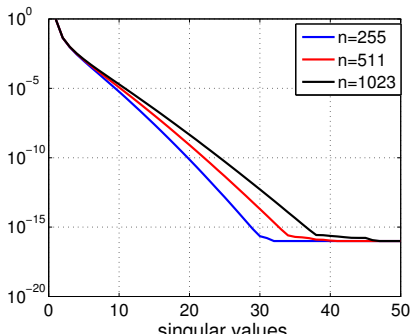
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**Open question:** Similar results for

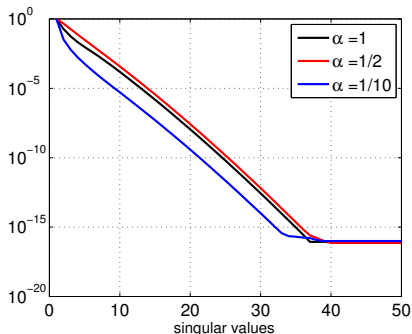
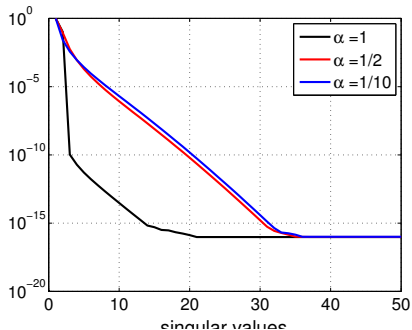
$$G_1 := (\beta A^{-\alpha} + \frac{\gamma}{\beta} A^{\alpha})^{-1}, \quad G_2 := (I + \frac{\gamma}{\beta^2} A^{2\alpha})^{-1}.$$

**But:** Numerical experiments (later) show similar behaviour for all three operators.



Decay of singular values with  $\alpha = 1$  in vs.  $n$  (left);  
singular values vs.  $\alpha > 0$  with fixed  $n = 511$  (right).





Decay of singular values of  $G_1$  (left) and  $G_2$  (right) vs.  
 $\alpha = 1, 1/2, 1/10$  for  $n = 511$ .

Let  $A_{(i)}$  be the discretized one-dimensional Laplacian on a uniform grid. Then  $A_{(i)}$  is diagonalized in the sine basis, i. e.

$$A_{(i)} = F_i^* \Lambda_{(i)} F_i,$$

where  $\Lambda_{(i)} = \text{diag}\{\lambda_1, \dots, \lambda_n\}$ , and the action of  $F_i$  ( $F_i^*$ ) is given by the (inverse) sine transform.

Thus, we can write

$$\begin{aligned} A &= (F_1^* \otimes F_2^*)(\Lambda_1 \otimes I_2)(F_1 \otimes F_2) + (F_1^* \otimes F_2^*)(I_1 \otimes \Lambda_2)(F_1 \otimes F_2) \\ &= (F_1^* \otimes F_2^*) \underbrace{((\Lambda_1 \otimes I_2) + (I_1 \otimes \Lambda_2))}_{=: \Lambda} (F_1 \otimes F_2), \end{aligned}$$

and, for a function  $f$  applied to  $A$ , we get

$$f(A) = (F_1^* \otimes F_2^*) f(\Lambda) (F_1 \otimes F_2).$$

Now assume that  $f(A)$  may be approximated by a linear combination of Kronecker rank 1 matrices. Then, to approximate  $f(A)$ , it is sufficient to approximate  $f(\Lambda)$  (e. g. by a truncated SVD).

Assume we have a decomposition

$$f(\Lambda) = \sum_{k=1}^R \text{diag}(\mathbf{u}_1^{(k)} \otimes \mathbf{u}_2^{(k)}),$$

and let

$$\mathbf{x} = \sum_{j=1}^S \mathbf{x}_1^{(j)} \otimes \mathbf{x}_2^{(j)}.$$

Now we can compute a matrix-vector product

$$\begin{aligned} f(A)\mathbf{x} &= (F_1^* \otimes F_2^*) \left( \sum_{k=1}^R \text{diag}(\mathbf{u}_1^{(k)} \otimes \mathbf{u}_2^{(k)}) \right) (F_1 \otimes F_2) \left( \sum_{j=1}^S \mathbf{x}_1^{(j)} \otimes \mathbf{x}_2^{(j)} \right) \\ &= \sum_{k=1}^R \sum_{j=1}^S F_1^*(\mathbf{u}_1^{(k)} \odot F_1 \mathbf{x}_1^{(j)}) \otimes F_2^*(\mathbf{u}_2^{(k)} \odot F_2 \mathbf{x}_2^{(j)}), \end{aligned}$$

where  $\odot$  denotes the componentwise (Hadamard) product.

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$\Rightarrow$  Can be computed in  $\mathcal{O}(RSn \log n)$  flops

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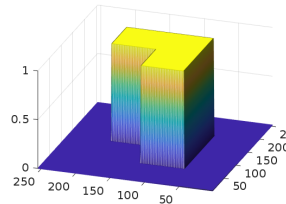
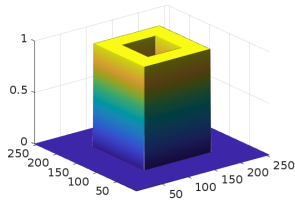
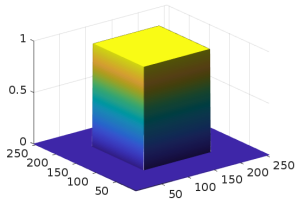
$$\begin{aligned}
 f(A)\mathbf{x} &= (F_1^* \otimes F_2^*) \left( \sum_{k=1}^R \text{diag}(\mathbf{u}_1^{(k)} \otimes \mathbf{u}_2^{(k)}) \right) (F_1 \otimes F_2) \left( \sum_{j=1}^S \mathbf{x}_1^{(j)} \otimes \mathbf{x}_2^{(j)} \right) \\
 &= \sum_{k=1}^R \sum_{j=1}^S F_1^*(\mathbf{u}_1^{(k)} \odot F_1 \mathbf{x}_1^{(j)}) \otimes F_2^*(\mathbf{u}_2^{(k)} \odot F_2 \mathbf{x}_2^{(j)}),
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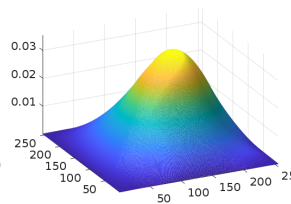
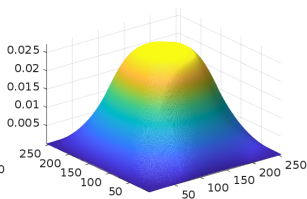
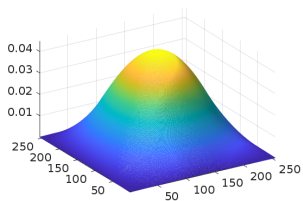
Computational time on a  $2^{15}$ -by- $2^{15}$  grid ( $> 10^9$ ): under 1 s

Preprocessing time: 300 s



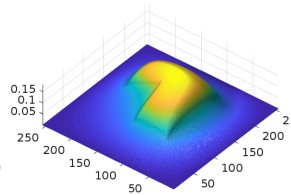
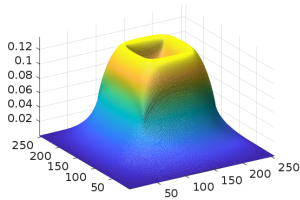
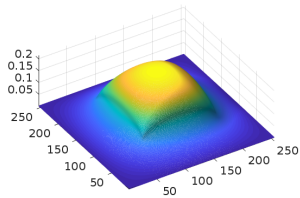
Shapes of the right-hand side  $y_\Omega$  computed with  $n=255$ .

# Computed $u$ with $\alpha = 1$

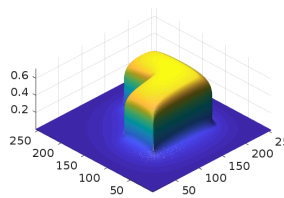
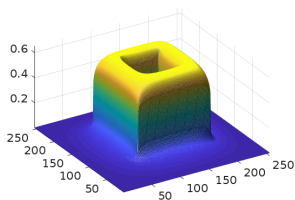
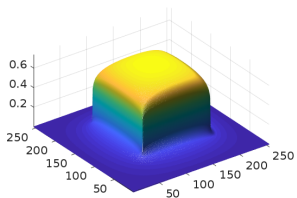


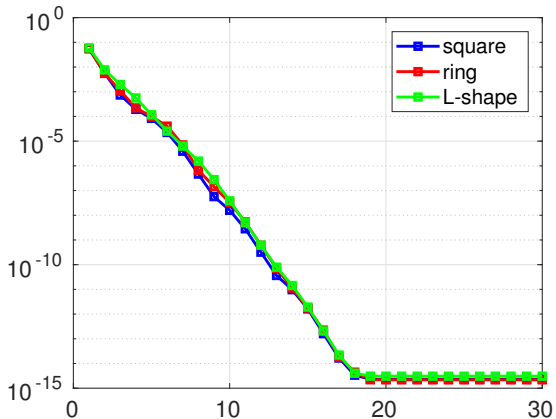


# Computed $u$ with $\alpha = 1/2$



# Computed $u$ with $\alpha = 1/10$



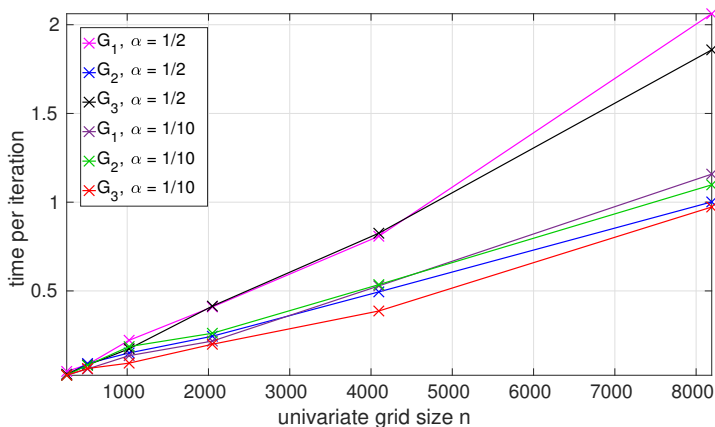


Error norm of optimal solution in full rank vs low rank format with  $n = 255$  and  $\alpha = 1/2$ .



		$G_1$				$G_2$				$G_3$			
$r \backslash n$	$n$	256	512	1024	2048	256	512	1024	2048	256	512	1024	2048
4	4	4	4	4	5	4	4	4	5	3	4	4	4
5	3	3	3	4	4	3	4	4	4	3	3	3	4
6	3	3	3	3	4	3	3	3	4	2	3	3	3
7	2	3	3	3	3	2	3	3	3	2	2	3	3
8	2	2	2	2	3	2	2	2	3	2	2	2	3
9	2	2	2	2	2	2	2	2	2	2	2	2	3
10	2	2	2	2	2	2	2	2	2	2	2	2	2

- univariate grid size  $n$
- preconditioner rank  $r$
- convergence to relative residual of  $10^{-6}$



CPU times (sec) vs. univariate grid size  $n$  for a single PCG iteration for a 2D problem, for different fractional operators and fixed preconditioner

rank  $r = 5$

Low-rank  $m \times n$  matrix given by the *singular value decomposition*:

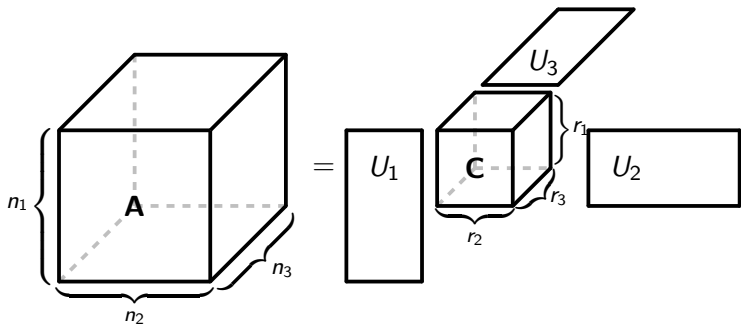
$$\begin{aligned}
 \begin{matrix} m \\ \left\{ \begin{array}{c} \square \\ A \\ \square \end{array} \right. \\ \underbrace{\hspace{2cm}} \\ n \end{matrix} &= \begin{matrix} \square \\ U \\ \square \end{matrix} \underbrace{\begin{matrix} \square \\ \Sigma \\ \square \end{matrix}}_r \begin{matrix} \square \\ V^T \\ \square \end{matrix} \\
 &= \sigma_1 \begin{matrix} \overline{\mathbf{v}_1^T} \\ \left| \begin{array}{c} \\ \mathbf{u}_1 \end{array} \right. \end{matrix} + \cdots + \sigma_r \begin{matrix} \overline{\mathbf{v}_r^T} \\ \left| \begin{array}{c} \\ \mathbf{u}_r \end{array} \right. \end{matrix}
 \end{aligned}$$

Low-rank  $m \times n$  matrix given by the *singular value decomposition*:

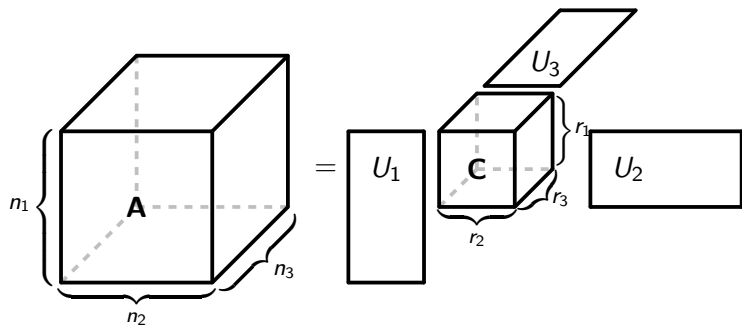
$$\begin{array}{c}
 \left. \begin{array}{|c|} \hline m \\ \hline \end{array} \right\} \begin{array}{|c|} \hline A \\ \hline \end{array} \underbrace{\hspace{10em}}_n = \begin{array}{|c|} \hline U \\ \hline \end{array} \underbrace{\begin{array}{|c|} \hline \Sigma \\ \hline \end{array}}_r \begin{array}{|c|} \hline V^T \\ \hline \end{array} \\
 \\
 = \sigma_1 \begin{array}{|c|} \hline \mathbf{v}_1^T \\ \hline \end{array} + \dots + \sigma_r \begin{array}{|c|} \hline \mathbf{v}_r^T \\ \hline \end{array} \\
 \begin{array}{|c|} \hline \mathbf{u}_1 \\ \hline \end{array} \begin{array}{|c|} \hline \mathbf{u}_r \\ \hline \end{array}
 \end{array}$$

Formally:  $A = U\Sigma V^T = \sum_{k=1}^r \sigma_k \mathbf{u}_k \mathbf{v}_k^T =: \sum_{k=1}^r \sigma_k \mathbf{u}_k \circ \mathbf{v}_k$

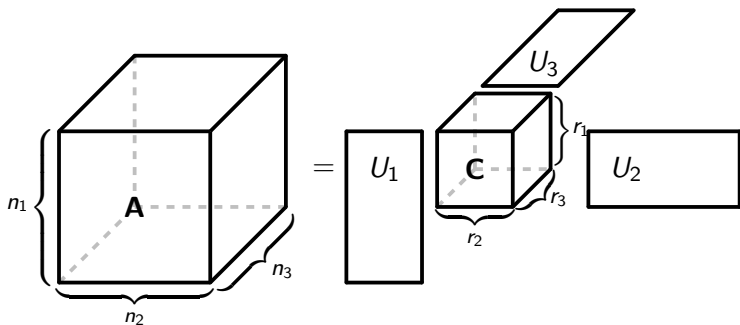
# ...over the Tucker format...







$$\text{Formally: } A = \mathbf{C} \times_1 U_1 \cdots \times_d U_d = \mathbf{C} \times_{i=1}^d U_i$$



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Storage cost:  $\mathcal{O}(r^d + dnr)$

## ... to the truncated HOSVD



A Tucker decomposition of a rank- $\mathbf{r}$  tensor can be computed by computing an SVD for each tensor mode.



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**Remark:**

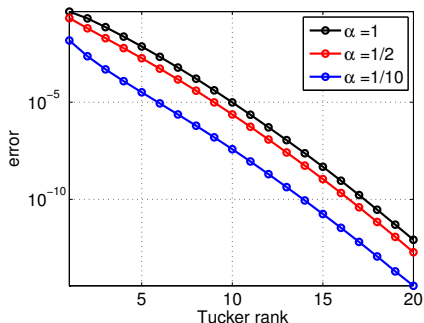
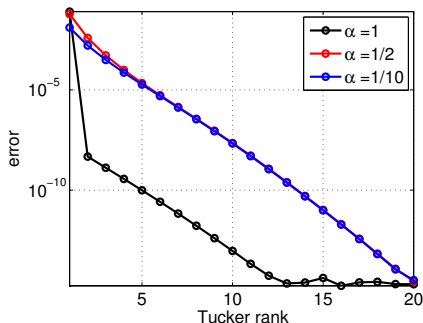
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## Remark:

- $P_{\mathbf{r}}^{\text{HO}}$  only gives a *quasi-best* rank- $\mathbf{r}$  approximation



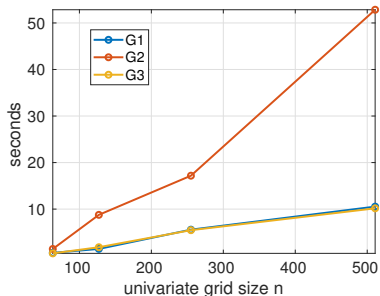
Tucker-ALS approximation error of  $G_1$  (left) and  $G_2$  (right) vs.  $\alpha = 1, 1/2, 1/10$  for  $d = 3$ .



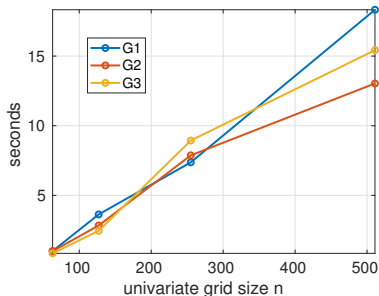


		$G_1$				$G_2$				$G_3$			
$r \backslash n$		64	128	256	512	64	128	256	512	64	128	256	512
4		1	2	1	1	1	6	1	2	1	2	1	1
5		1	1	1	2	1	1	8	4	1	1	1	2
6		1	1	1	1	2	2	1	1	1	1	1	1
7		1	3	1	2	1	1	5	4	1	2	1	2
8		1	1	1	1	1	1	1	1	1	1	1	1
9		1	1	1	2	1	6	5	4	1	1	1	2
10		1	1	1	1	1	6	1	1	1	1	1	1

- univariate grid size  $n$
- preconditioner rank  $r$
- convergence to relative residual of  $10^{-6}$



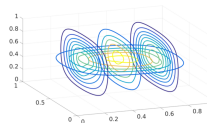
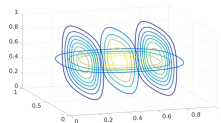
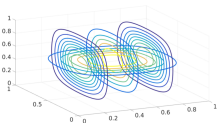
$$\alpha = 1/2, r = 4$$



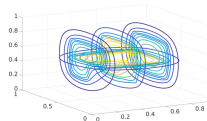
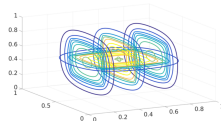
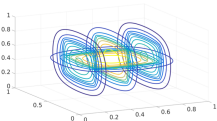
$$\alpha = 1/10, r = 7$$

CPU times (in seconds) vs. grid size  $n$  of a single PCG iteration for a 3D problem, for different fractional operators and fixed preconditioner rank  $r$ .

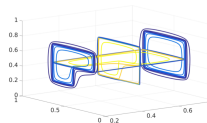
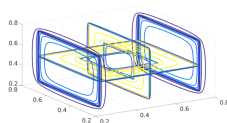
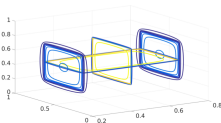
$\alpha = 1$ :



$\alpha = \frac{1}{2}$ :



$\alpha = \frac{1}{10}$ :



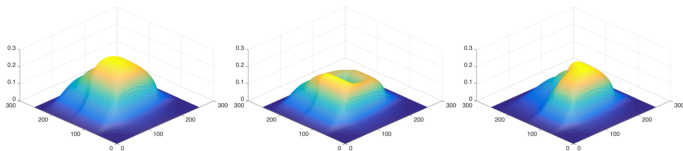
Solutions  $u$  for analogous right-hand sides ( $n = 255$ ).

Generalization to different elliptic equation [Schmitt 2019]:

$$(-\operatorname{div}(\mathbb{A}\operatorname{grad}))^\alpha y = \beta u, \quad \mathbb{A}(x_1, x_2) = \begin{bmatrix} a_1(x_1) & 0 \\ 0 & a_2(x_2) \end{bmatrix}$$

- needs affordable preparation step for 1D eigenvalues/vectors
- similarly good numerical complexity
- more general  $\mathbb{A}$  in preparation

$$\alpha = \frac{1}{2}:$$



- Gennadij Heidel: *Optimization in Tensor Spaces for Data Science and Scientific Computing*, PhD Dissertation, Trier University 2019
- Gennadij Heidel, Venera Khoromskaia, Boris N. Khoromskij, Volker Schulz: *Tensor approach to optimal control problems with fractional  $d$ -dimensional elliptic operator in constraints*, 2018, arXiv:1809.01971 (revised version submitted to SICON)
- Britta Schmitt: *Niedrigrang-Tensorapproximation bei heterogen verteilten Optimalsteuerungsproblemen*, Masters's Thesis, Trier University, 2019
- Britta Schmitt, Venera Khoromskaia, Boris N. Khoromskij, Volker Schulz: *Low-Rank Tensor Approximation of Heterogenously Distributed Optimal Control Problems* (in preparation)

- Solution of a nonlocal PDE on a tensor grid in  $\mathcal{O}(RSn \log n) \ll \mathcal{O}(n^d)$
- Numerical complexity independent of  $d$
- Even for  $\alpha = 1$  the methodology is significantly faster than multigrid
- Numerical results convincing; theoretical justification w.r.t. low rank still open