# Near-optimal hierarchical matrix approximation from matrix-vector products

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January 11, 2025

chen.pw/slides

# Collaborators

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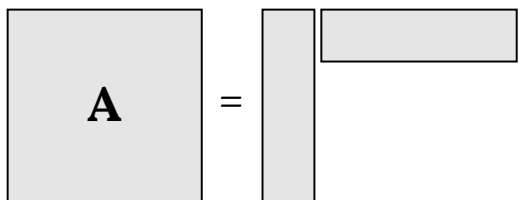

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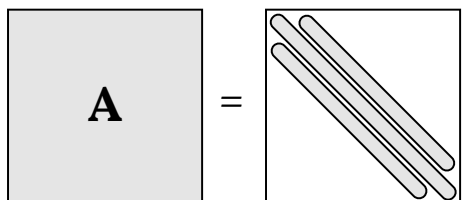

## Matrix recovery and approximation

**Recovery:** Promised $\mathbf{A} \in S$, learn parameterization of $\mathbf{A}$.

- past work for many classes: low-rank, sparse, circulant, hierarchical (HODLR, HSS, etc.), butterfly, etc.[1]

**Approximation:** Arbitrary $\mathbf{A}$, learn (parameterization of) $\widetilde{\mathbf{A}} \in S$ such that

$$\|\mathbf{A} - \widetilde{\mathbf{A}}\| \leq (1 + \varepsilon) \min_{\mathbf{X} \in S} \|\mathbf{A} - \mathbf{X}\|.$$

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# Access model

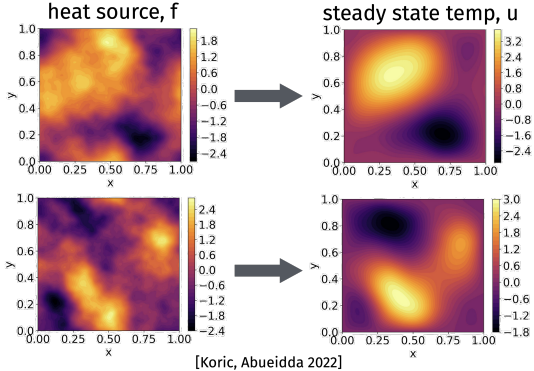
Assume we can only access $\mathbf{A}$ using matrix-vector (matvec) queries $\mathbf{x} \mapsto \mathbf{A}\mathbf{x}$ or $\mathbf{y} \mapsto \mathbf{A}^T\mathbf{y}$.

Why might this access model arise?

- if $\mathbf{A} = \mathbf{B}^{-1}$, we can compute $\mathbf{A}\mathbf{x}$ using a fast solver
- the action of $\mathbf{A}$ could also correspond to some physical process

# Operator Learning[2]

Physical processes often map a function $f$ to a function $u$. I.e., implement some operator $\Phi(f) = u$.




[Koric, Abueidda 2022]

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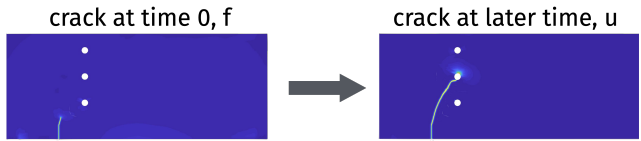


**Goal:** Learn mapping from input-output pairs: $(f_1, u_1), \ldots, (f_m, u_m)$.

**Scientific ML:** Assume $S$ is some parameterized family (e.g. neural net as in DeepONet, DeepGreen, etc.)

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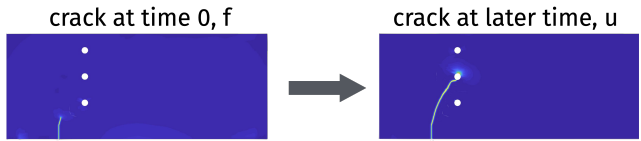


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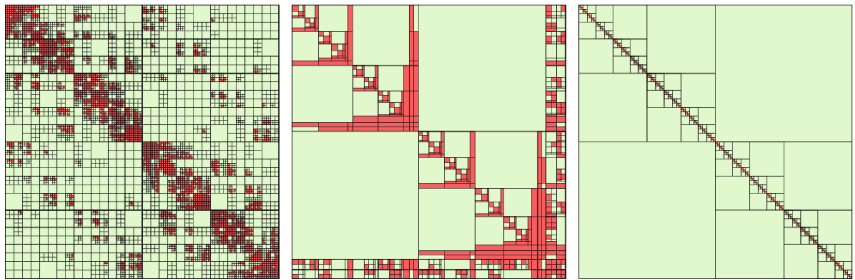
# Hierarchical matrices

Today, $S$ will be some family of hierarchical matrices.



**example classes:** hierarchical off-diagonal low-rank (HODLR), hierarchical semi-seperable (HSS), $\mathcal{H}^1$, $\mathcal{H}^2$, hierarchical off-diagonal butterfly, etc.

# Why hierarchical matrices?

Hierarchical matrices are useful for applications involving physical applications due to the presence of multiscale phenomena.

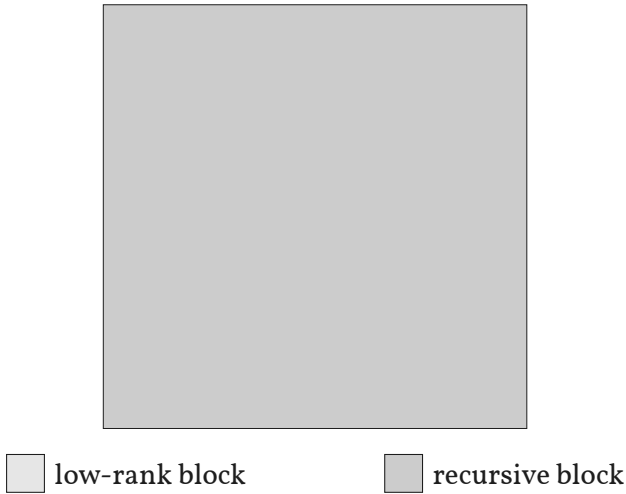
Argonne NATIONAL LABORATORY

BERKELEY LAB
Lawrence Berkeley National Laboratory

ButterflyPACK
Fast PDE solvers and transforms


HODLRlib

# HODLR matrices



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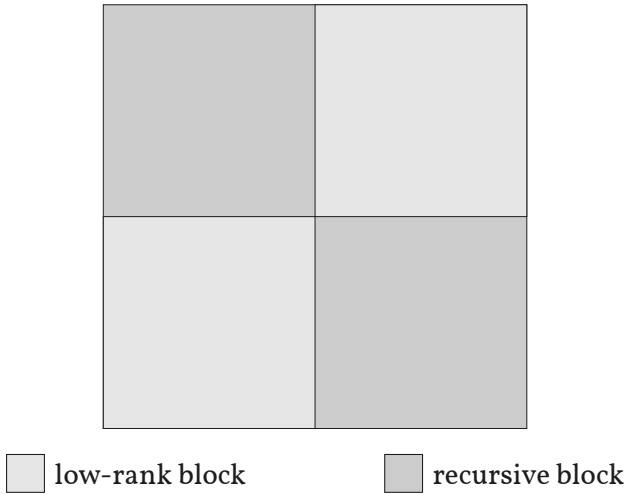

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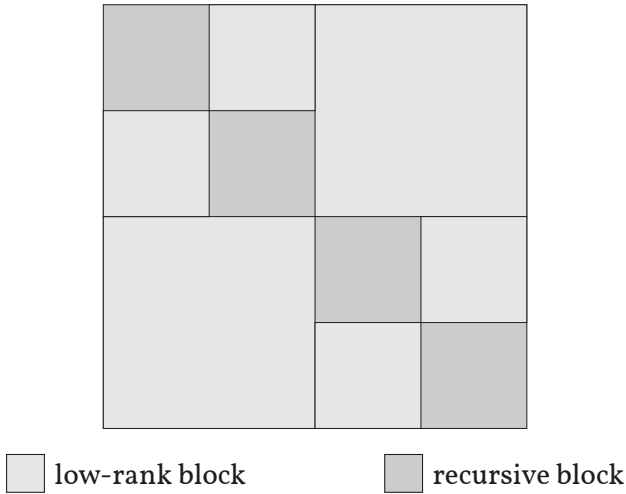

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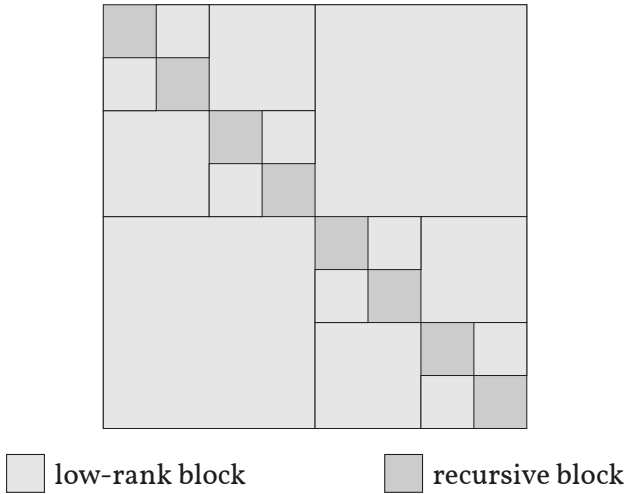


## HODLR Matrices

**Definition.** Fix a rank parameter $k$. We say a $n \times n$ matrix $\mathbf{A}$ is HODLR($k$) if $n \leq k$ or $\mathbf{A}$ can be partitioned into $(n/2) \times (n/2)$ blocks

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{1,1} & \mathbf{A}_{1,2} \\ \mathbf{A}_{2,1} & \mathbf{A}_{2,2} \end{bmatrix}$$

such that $\mathbf{A}_{1,2}$ and $\mathbf{A}_{2,1}$ are of rank at most $k$ and $\mathbf{A}_{1,1}$ and $\mathbf{A}_{2,2}$ are each HODLR($k$).

HODLR matries have $O(kn \log(n))$ parameters.

There are several matvec algorithms for the recovery problem.[3]

[3] Lin, Lu, and Ying 2011; Martinsson 2016; Levitt and Martinsson 2022; Halikias and Townsend 2023.

## Low-rank approximation from matrix-vector products

The Randomized SVD (RSVD) is a well-known algorithm for obtaining a low-rank approximation to a matrix $\mathbf{B}$:

1. Sample Gaussian matrix $\mathbf{\Omega}$
2. Form $\mathbf{Q} = \text{orth}(\mathbf{B\Omega})$
3. Compute $\mathbf{X} = \mathbf{Q}^\mathsf{T}\mathbf{B}$ (minimize: $\|\mathbf{B} - \mathbf{QX}\|_\mathsf{F}$)
4. Output $\mathbf{Q}[\![\mathbf{X}]\!]_k$

> **Theorem.** If $\mathbf{B}$ is rank-$k$, and $\mathbf{\Omega}$ has $O(k)$ columns, then $\mathbf{Q}[\![\mathbf{X}]\!]_k = \mathbf{B}$ (a.s.).

## Peeling: an algorithm for the recovery problem[4]

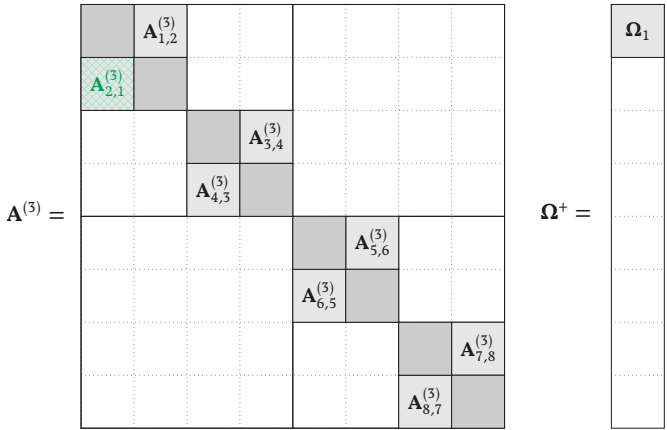
The algorithm works from the top layer down.

At each level, we simultaneosly apply the RSVD to the low-rank off-diagonal blocks.

We then "peel" off these blocks before proceeding to the next level

[4] Lin, Lu, and Ying 2011; Martinsson 2016.

# Peeling: an algorithm for the recovery problem



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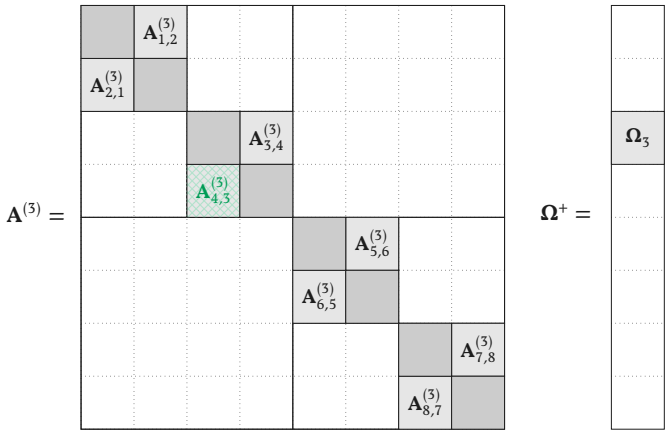

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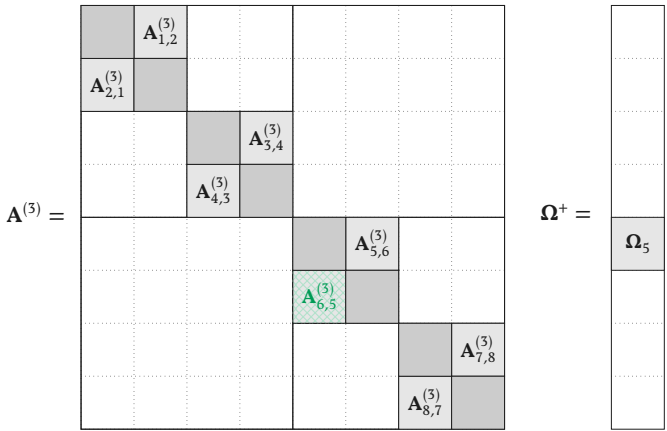

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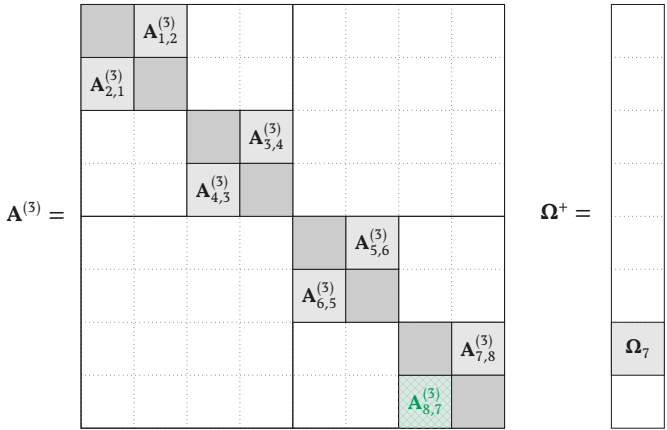

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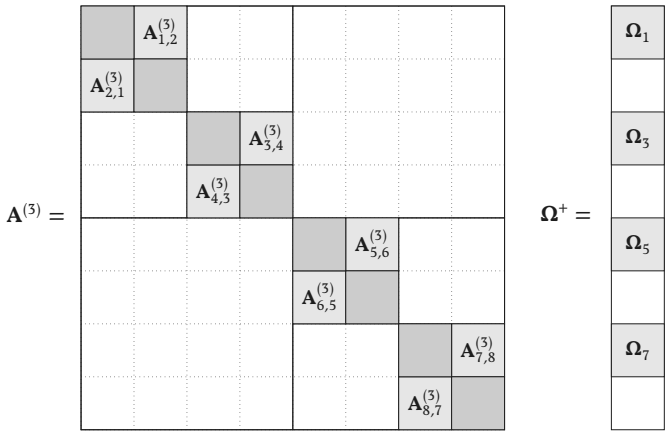


From $\mathbf{A}^{(3)}\boldsymbol{\Omega}^{+}$ we get sketches: $\mathbf{A}^{(3)}_{2,1}\boldsymbol{\Omega}_1$, $\mathbf{A}^{(3)}_{4,3}\boldsymbol{\Omega}_3$, $\mathbf{A}^{(3)}_{6,5}\boldsymbol{\Omega}_5$, $\mathbf{A}^{(3)}_{8,7}\boldsymbol{\Omega}_7$.

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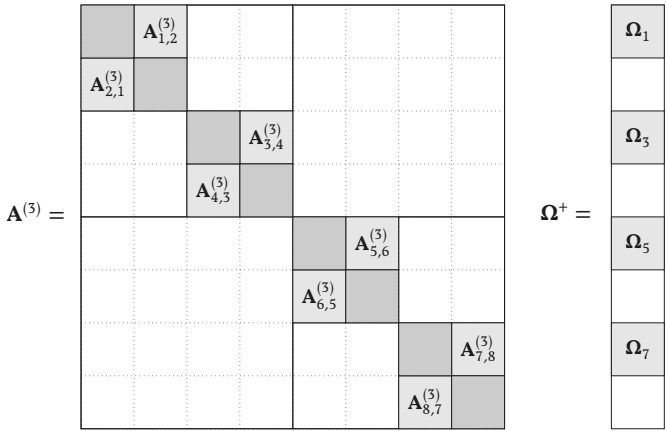


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## Peeling: an algorithm for the recovery problem

At each level we use $O(k)$ matrix-vector products with $\mathbf{A}$ and $\mathbf{A}^\mathsf{T}$.

There are $\log_2(n/k) \leq \log_2(n)$ levels until the blocks are of size $k$

- then we can directly recover them at once with $k$ products

> **Theorem.** We can recover a HODLR matrix using $O\big(k \log_2(n)\big)$ matvecs.

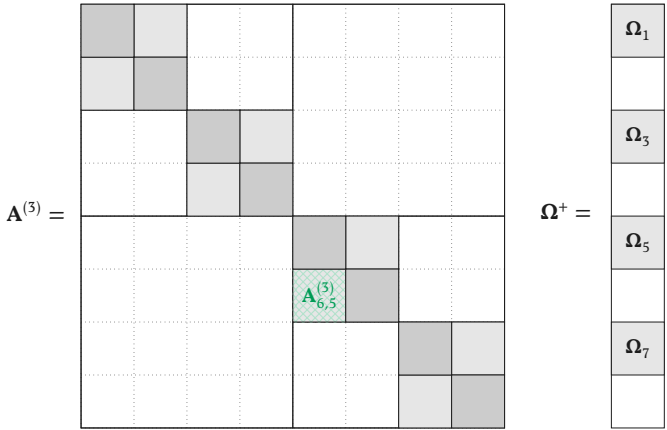
## Peeling with error?

A variant of the peeling algorithm can be used to approximate the solution operator of elliptic PDEs (2024 SIAM Linear Algebra Best Paper Prize winner).[5]

> **Boullé and Townsend 2022:** Is there a peeling-type algorithm that works for nearly-HODLR matrices?

[5] Boullé and Townsend 2022.

# Does peeling work on non-HODLR matrices?



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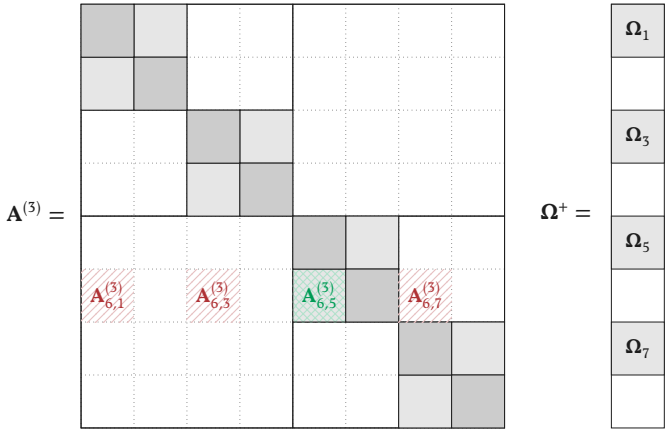


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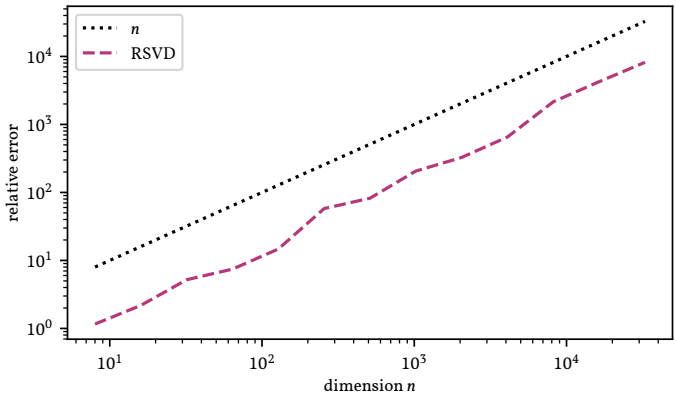
## Does peeling work on non-HODLR matrices?

If all the error at a level can propagate to the next level, then the total error doubles at each level. Exponential blow-up in the number of levels (linear in $n$)!



## The HODLR approximation problem[6]

**Problem.** Given an $n \times n$ matrix $\mathbf{A}$, accessible only by matrix-vector products, a rank parameter $k$, and an accuracy parameter $\varepsilon$, find a HODLR($k$) matrix $\widetilde{\mathbf{A}}$ such that

$$\|\mathbf{A} - \widetilde{\mathbf{A}}\|_{\mathsf{F}} \leq (1+\varepsilon) \min_{\mathbf{H} \in \mathrm{HODLR}(k)} \|\mathbf{A} - \mathbf{H}\|_{\mathsf{F}}.$$

**Theorem.** There is an efficient matvec algorithm for HODLR approximation.

**Note:** The best HODLR approximation to $\mathbf{A}$ is obtained by applying a rank-$k$ SVD to each low-rank block of $\mathbf{A}$.

- This is too expensive in the matrix-vector product model ($n$ products)

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## A perturbation bound for the RSVD

We prove a perturbation bound for the RSVD. This is likely of independent interest.

**Theorem.** Let $\mathbf{Q} = \operatorname{orth}(\mathbf{B}\boldsymbol{\Omega} + \mathbf{E}_1)$ and $\mathbf{X} = \mathbf{Q}^\mathsf{T}\mathbf{B} + \mathbf{E}_2$. Then

$$\|\mathbf{B} - \mathbf{Q}[\![\mathbf{X}]\!]_k\|_\mathsf{F} \leq \underbrace{\|\mathbf{E}_1\boldsymbol{\Omega}_{\text{top}}^\dagger\|_\mathsf{F} + 2\|\mathbf{E}_2\|_\mathsf{F}}_{\text{perturbations}} + \underbrace{\left(\|\boldsymbol{\Sigma}_{\text{bot}}\|_\mathsf{F}^2 + \|\boldsymbol{\Sigma}_{\text{bot}}\boldsymbol{\Omega}_{\text{bot}}\boldsymbol{\Omega}_{\text{top}}^\dagger\|_\mathsf{F}^2\right)^{1/2}}_{\text{classical RSVD bound}}.$$

When $\boldsymbol{\Omega}$ has $O(k/\varepsilon)$ columns, $\boldsymbol{\Omega}_{\text{top}}$ is a $k \times O(k/\varepsilon)$ Gaussian matrix which has a small pseudoinverse:

$$\mathbb{E}\left[(\boldsymbol{\Omega}_{\text{top}}^\dagger)^\mathsf{T}\boldsymbol{\Omega}_{\text{top}}^\dagger\right] = \mathbb{E}\left[(\boldsymbol{\Omega}_{\text{top}}\boldsymbol{\Omega}_{\text{top}}^\mathsf{T})^{-1}\right] = \varepsilon\mathbf{I}.$$

**Takeaway:** The pseudoinverse will help damp the perturbation $\mathbf{E}_1$, but (unsurprisingly) all of the perturbation $\mathbf{E}_2$ can propagate.

## Generalized Nyström[7]

The RSVD tries to compute $\mathbf{Q}^\mathsf{T}\mathbf{B}$ directly; this is the solution to:

$$\min_{\mathbf{X}} \|\mathbf{A} - \mathbf{Q}\mathbf{X}\|_\mathsf{F}.$$

Instead, we can solve a sketched problem:

$$\min_{\mathbf{X}} \|\mathbf{\Psi}^\mathsf{T}\mathbf{A} - \mathbf{\Psi}^\mathsf{T}\mathbf{Q}\mathbf{X}\|_\mathsf{F}.$$

This means $\mathbf{X} = (\mathbf{\Psi}^\mathsf{T}\mathbf{Q})^\dagger \mathbf{\Psi}^\mathsf{T}\mathbf{A}$.

**Observation.** By adding columns to $\mathbf{\Psi}$, we can damp errors in the product $\mathbf{\Psi}^\mathsf{T}\mathbf{A}$.

The algorithm is also non-adaptive (we can do products with $\mathbf{\Psi}$ in advance)

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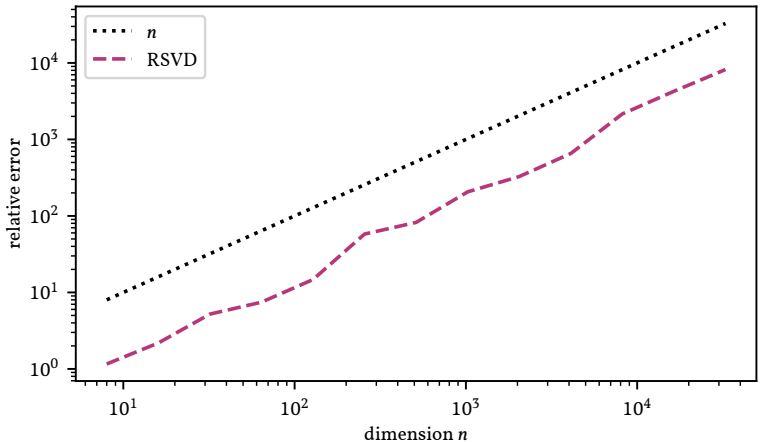

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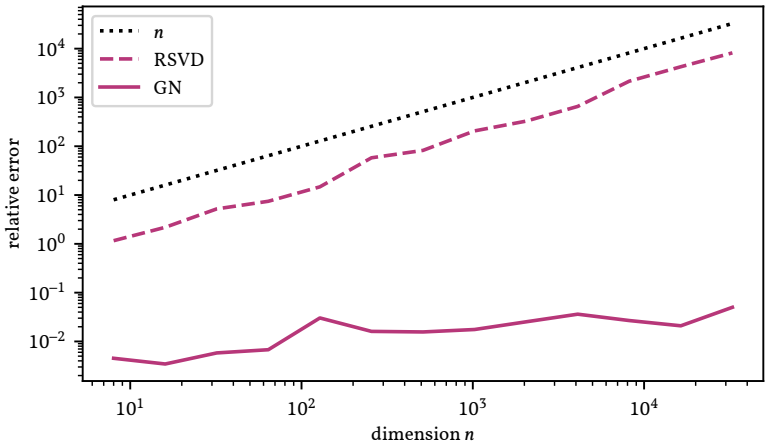
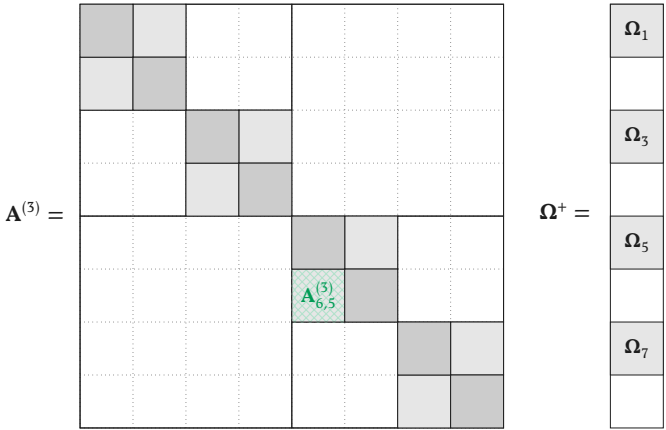


# Another approach: perforated sketches

Because of the structure of peeling, the error happens when blocks of our sketch hit the error from our approximation of low-rank blocks at previous levels.

What if we just reduce how often this happens?

# Perforated Block CountSketch



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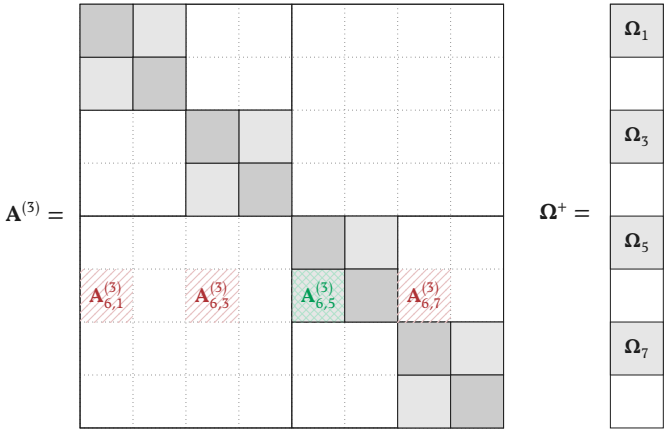


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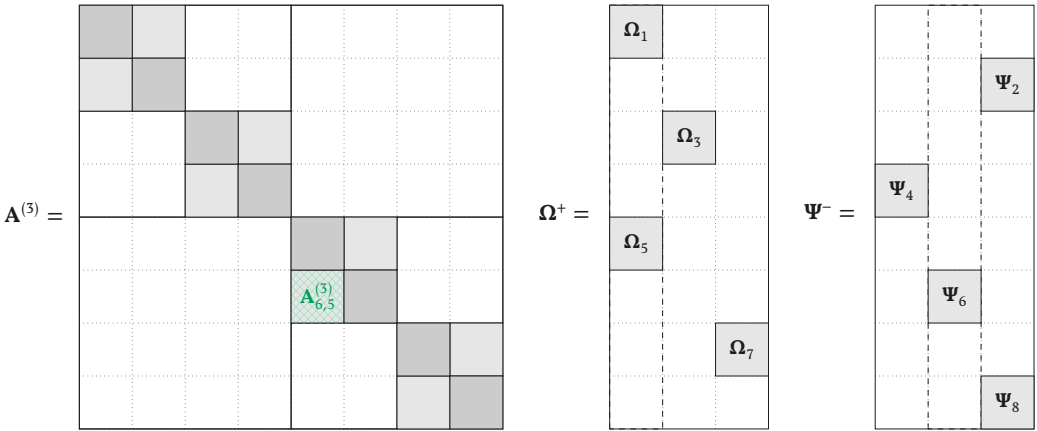


$$\mathbf{A}^{(3)}_{6,5}\mathbf{\Omega}_5$$

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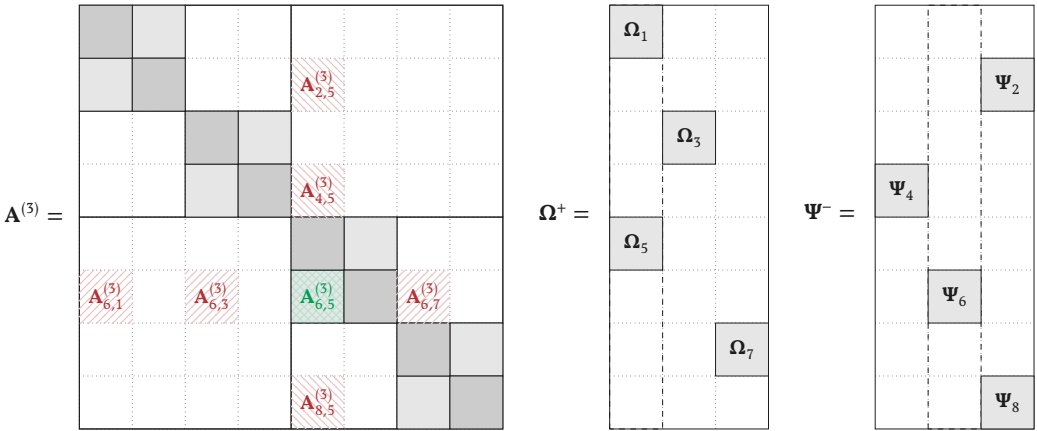


$$\mathbf{A}^{(3)}_{6,5}\mathbf{\Omega}_5 + \mathbf{A}^{(3)}_{6,1}\mathbf{\Omega}_1$$

## Our main result

**Theorem.** There exist matvec algorithms which use $O\big(k\log(n)/\beta^3\big)$ products with $\mathbf{A}$ to obtain a HODLR$(k)$ matrix $\widetilde{\mathbf{A}}$ satisfying

$$\|\mathbf{A}-\widetilde{\mathbf{A}}\|_{\mathsf{F}} \le (1+\beta)^{\log_2(n)} \min_{\mathbf{H}\in\mathrm{HODLR}(k)} \|\mathbf{A}-\mathbf{H}\|_{\mathsf{F}}.$$

**Corollary.** $(1+\varepsilon)$-optimal approximation with $O\big(k\log(n)^4/\varepsilon^3\big)$ matvecs

**Corollary.** $n^{0.01}$-optimal approximation with $O\big(k\log(n)\big)$ matvecs

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**Theorem.** There exist matvec algorithms which use $O\big(k\log(n)/\beta^3\big)$ products with $\mathbf{A}$ to obtain a HODLR$(k)$ matrix $\widetilde{\mathbf{A}}$ satisfying

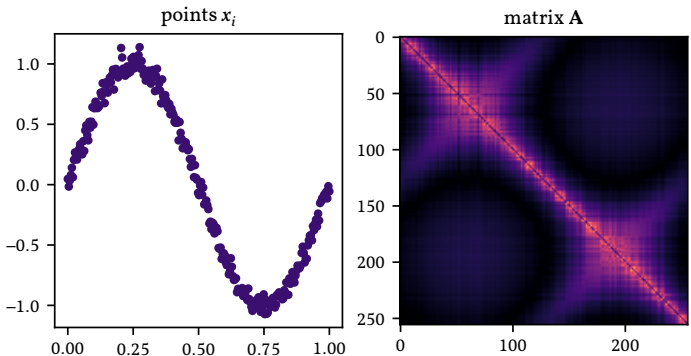
$$\|\mathbf{A}-\widetilde{\mathbf{A}}\|_{\mathsf{F}} \le (1+\beta)^{\log_2(n)} \min_{\mathbf{H}\in\mathrm{HODLR}(k)} \|\mathbf{A}-\mathbf{H}\|_{\mathsf{F}}.$$

**Corollary.** $(1+\varepsilon)$-optimal approximation with $O\big(k\log(n)^4/\varepsilon^3\big)$ matvecs

**Corollary.** $n^{0.01}$-optimal approximation with $O\big(k\log(n)\big)$ matvecs

# Another experiment

Given points $x_i \in \mathbb{R}^2$, define $[\mathbf{A}]_{i,j} = -\log(\|x_i - x_j\|)$



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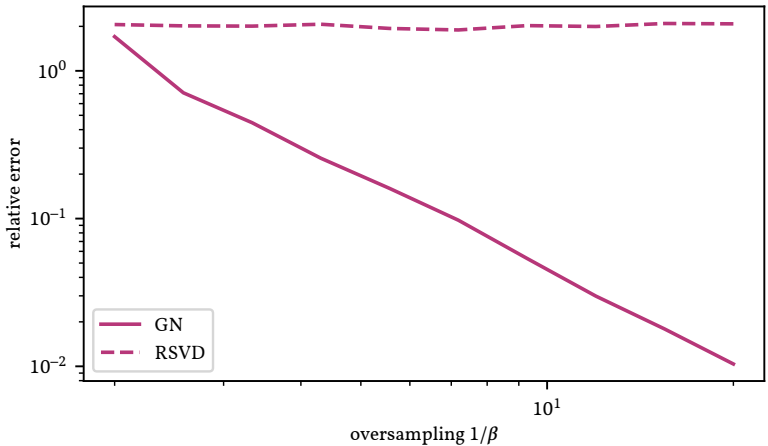


## Lower bounds?

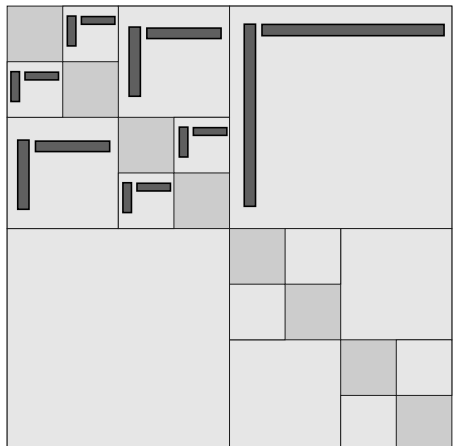
The matrix-vector query model often lets us prove lower-bounds against any matvec algorithm for a given task; i.e. study the complexity of a task.

This provides a very different approach for understanding how good algorithms are (compared to classical numerical analysis).

> **Theorem.** There is a constant $C > 0$ such that for any $k, n, \varepsilon$, there exists a matrix $\mathbf{A}$ such that getting a $(1+\varepsilon)$-optimal HODLR approximation requires at least $C\big(k \log_2(n/k) + k/\varepsilon\big)$ matvecs.

# HSS matrices

The low-rank blocks of HSS matrices are related: $O(nk)$ parameters.



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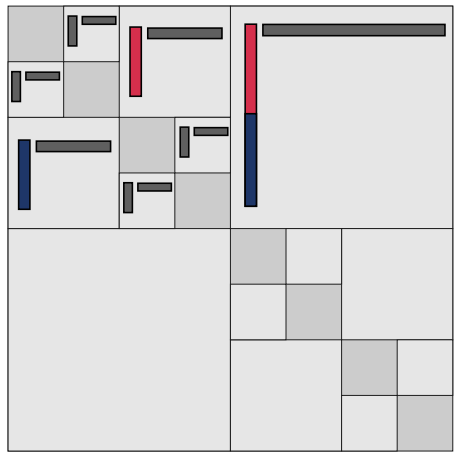

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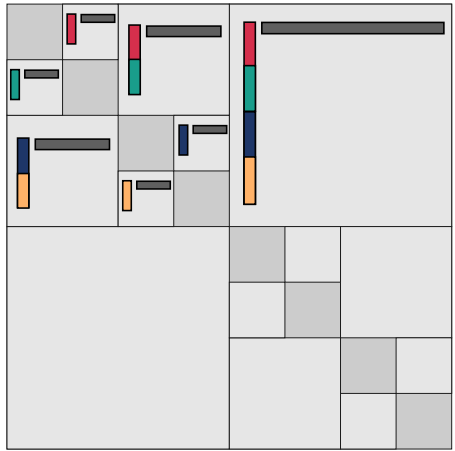

## HSS is tricky!

Many papers study HSS recovery.[8]

The nestedness of column-spaces across levels adds lots of relations which make the approximation problem much harder.

- No known polynomial algorithm known for constant factor HSS approximation?!
- In fact, not even clear what to do in exponential time.

We prove:

> **Theorem.** Can get $O(\log(n))$-optimal HSS approximation in $O(kn^2)$ time.

[8] Xia, Chandrasekaran, Gu, and Li 2010; Levitt and Martinsson 2022; Halikias and Townsend 2023.

# What's next?

**Big goal:** general theory for structured matrix approximation problem

- Correct $\log(n)$ and $\varepsilon$ rates for the algorithms we study?
  - Limited by the best known bounds for Generalized Nyström: $O(k/\varepsilon^3)$
- True stability analysis (e.g. for floating point arithmetic)
  - Working on with students at NYU
- Adaptive algorithms
- Other hierarchical classes?
- Better understanding of (non-adaptive) low-rank approximation

## Generalized Nyström (perturbation) analysis

Extend $\mathbf{Q}$ to an orthogonal matrix $[\mathbf{Q}\ \widehat{\mathbf{Q}}]$, and write $\mathbf{\Psi}_1 = \mathbf{\Psi}^\mathsf{T}\mathbf{Q}$ and $\mathbf{\Psi}_2 = \mathbf{\Psi}^\mathsf{T}\widehat{\mathbf{Q}}$.

By orthogonal invariance, $\mathbf{\Psi}_1$ and $\mathbf{\Psi}_2$ are independent Gaussian matrices!

First observe:

$$\mathbf{\Psi}^\mathsf{T}\mathbf{B} = \mathbf{\Psi}^\mathsf{T}(\mathbf{Q}\mathbf{Q}^\mathsf{T} + \widehat{\mathbf{Q}}\widehat{\mathbf{Q}}^\mathsf{T})\mathbf{B} = \mathbf{\Psi}_1\mathbf{Q}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_2\widehat{\mathbf{Q}}^\mathsf{T}\mathbf{B}.$$

Therefore:

$$\mathbf{X} = (\mathbf{\Psi}^\mathsf{T}\mathbf{Q})^\dagger(\mathbf{\Psi}^\mathsf{T}\mathbf{B}) = \mathbf{\Psi}_1^\dagger\mathbf{\Psi}_1\mathbf{Q}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_1^\dagger\mathbf{\Psi}_2\widehat{\mathbf{Q}}^\mathsf{T}\mathbf{B} = \mathbf{Q}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_1^\dagger\mathbf{\Psi}_2\widehat{\mathbf{Q}}^\mathsf{T}\mathbf{B}.$$

Adding more columns to $\mathbf{\Psi}$ (and hence $\mathbf{\Psi}_1$) reduces the error in the second term.

## Generalized Nyström (perturbation) analysis

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By orthogonal invariance, $\mathbf{\Psi}_1$ and $\mathbf{\Psi}_2$ are independent Gaussian matrices!

First observe:

$$\mathbf{\Psi}^\mathsf{T}\mathbf{B} + \mathbf{E} = \mathbf{\Psi}^\mathsf{T}(\mathbf{Q}\mathbf{Q}^\mathsf{T} + \widehat{\mathbf{Q}}\widehat{\mathbf{Q}}^\mathsf{T})\mathbf{B} + \mathbf{E} = \mathbf{\Psi}_1\mathbf{Q}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_2\widehat{\mathbf{Q}}^\mathsf{T}\mathbf{B} + \mathbf{E}.$$

Therefore:

$$\mathbf{X} = (\mathbf{\Psi}^\mathsf{T}\mathbf{Q})^\dagger(\mathbf{\Psi}^\mathsf{T}\mathbf{B} + \mathbf{E}) = \mathbf{\Psi}_1^\dagger\mathbf{\Psi}_1\mathbf{Q}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_1^\dagger\mathbf{\Psi}_2\widehat{\mathbf{Q}}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_1^\dagger\mathbf{E} = \mathbf{Q}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_1^\dagger\mathbf{\Psi}_2\widehat{\mathbf{Q}}^\mathsf{T}\mathbf{B} + \mathbf{\Psi}_1^\dagger\mathbf{E}.$$

Adding more columns to $\mathbf{\Psi}$ (and hence $\mathbf{\Psi}_1$) reduces the error in the second term.

# References I


Boullé, Nicolas and Alex Townsend (Jan. 2022). "Learning Elliptic Partial Differential Equations with Randomized Linear Algebra". In: *Foundations of Computational Mathematics* 23.2, pp. 709–739.

— (2024). "A mathematical guide to operator learning". In: *Numerical Analysis Meets Machine Learning*. Elsevier, pp. 83–125.

Chen, Tyler et al. (2025). "Near-optimal hierarchical matrix approximation from matrix-vector products". In: *Symposium on Discrete Algorithms (SODA)*.

Clarkson, Kenneth L. and David P. Woodruff (May 2009). "Numerical linear algebra in the streaming model". In: *Proceedings of the forty-first annual ACM symposium on Theory of computing*. STOC '09. ACM.

Halikias, Diana and Alex Townsend (Sept. 2023). "Structured matrix recovery from matrix-vector products". In: *Numerical Linear Algebra with Applications* 31.1.

Levitt, James and Per-Gunnar Martinsson (2022). *Randomized Compression of Rank-Structured Matrices Accelerated with Graph Coloring*.

Lin, Lin, Jianfeng Lu, and Lexing Ying (May 2011). "Fast construction of hierarchical matrix representation from matrix–vector multiplication". In: *Journal of Computational Physics* 230.10, pp. 4071–4087.

Martinsson, Per-Gunnar (Jan. 2016). "Compressing Rank-Structured Matrices via Randomized Sampling". In: *SIAM Journal on Scientific Computing* 38.4, A1959–A1986.

Nakatsukasa, Yuji (2020). "Fast and stable randomized low-rank matrix approximation". In: *ArXiv* abs/2009.11392.

Tropp, Joel A. et al. (Jan. 2017). "Practical Sketching Algorithms for Low-Rank Matrix Approximation". In: *SIAM Journal on Matrix Analysis and Applications* 38.4, pp. 1454–1485.

# References II

Xia, Jianlin et al. (Nov. 2010). “Fast algorithms for hierarchically semiseparable matrices”. In: *Numerical Linear Algebra with Applications* 17.6, pp. 953–976.