Near-optimal hierarchical matrix approximation from matrix-vector products

Tyler Chen

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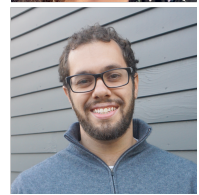
chen.pw/slides

Collaborators

Noah Amsel, Feyza Duman Keles, Diana Halikias,
David Persson, Chris Musco, Cameron Musco





Paper to appear at SODA 2025. Available at: `https://arxiv.org/abs/2407.04686`.

Matrix recovery and approximation

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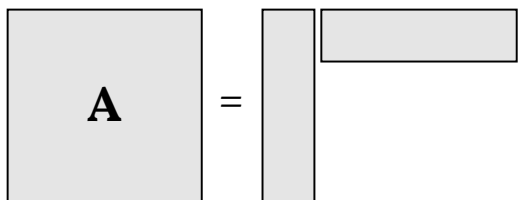

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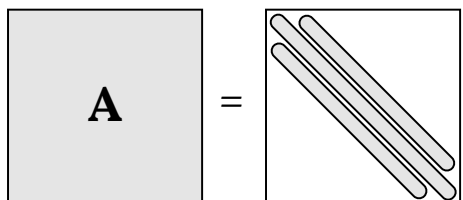

Matrix recovery and approximation

Let S be some family of matrices parameterized by a small number of parameters.

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

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

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

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

- 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

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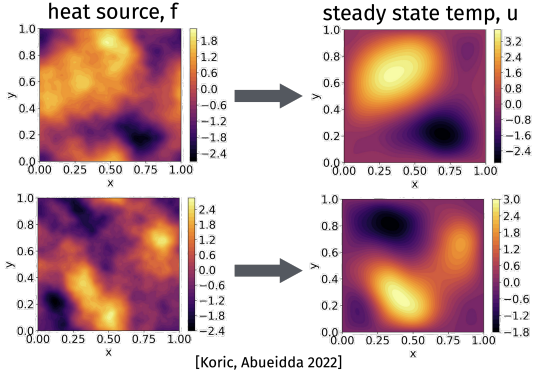
Operator Learning[1]

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



[Koric, Abueidda 2022]

[1]Boullé and Townsend 2024.

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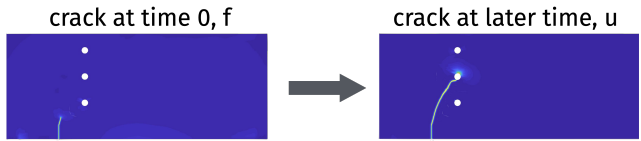

Goal: Learn mapping from input-output pairs: $(f_1, u_1), \ldots, (f_m, u_m)$.

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

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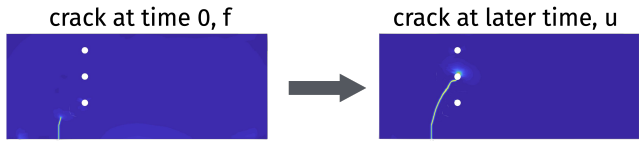

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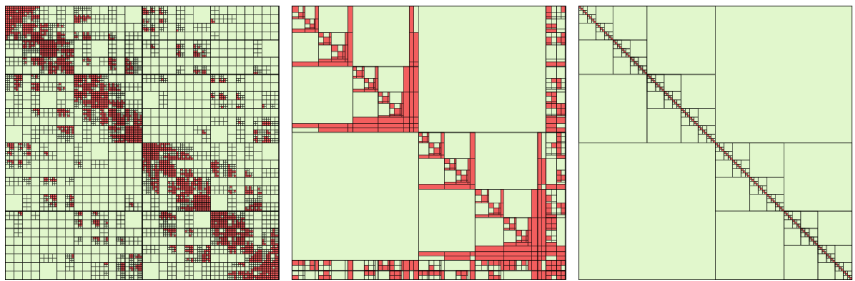
Hierarchical matrices

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.

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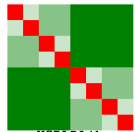
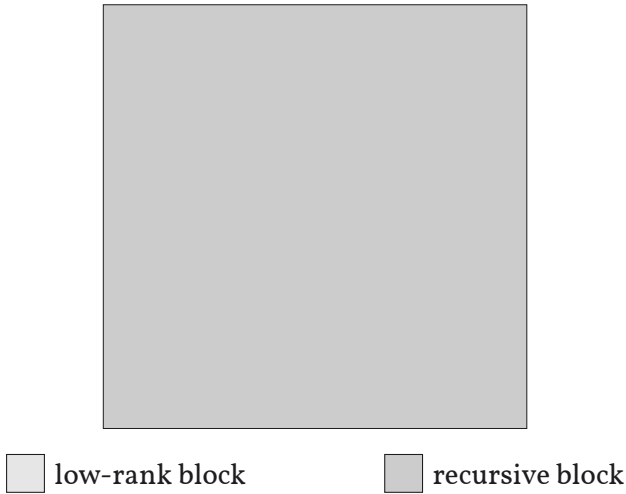
ButterflyPACK
Fast PDE solvers and transforms


HODLRlib

HODLR matrices



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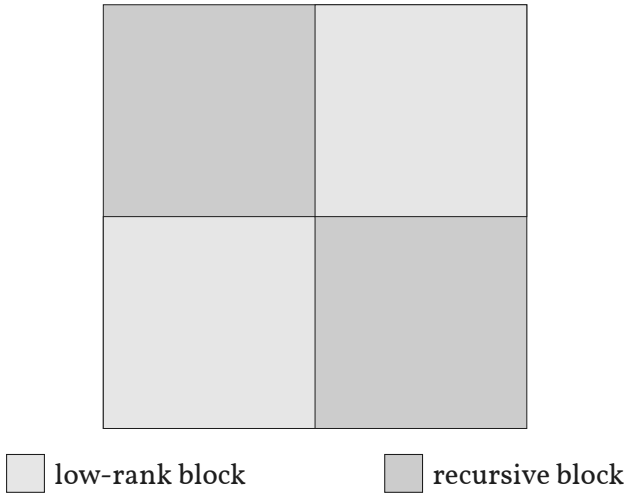

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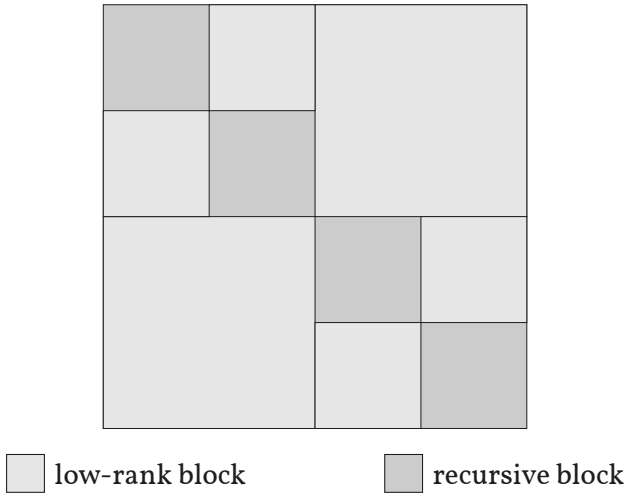

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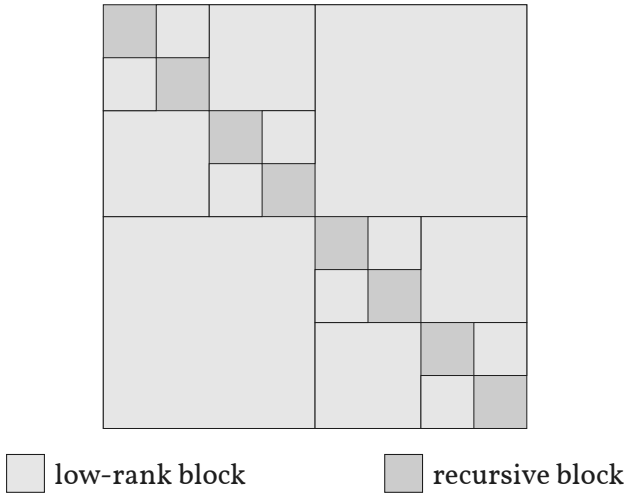


HODLR Matrices

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.[2]

[2] 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[3]

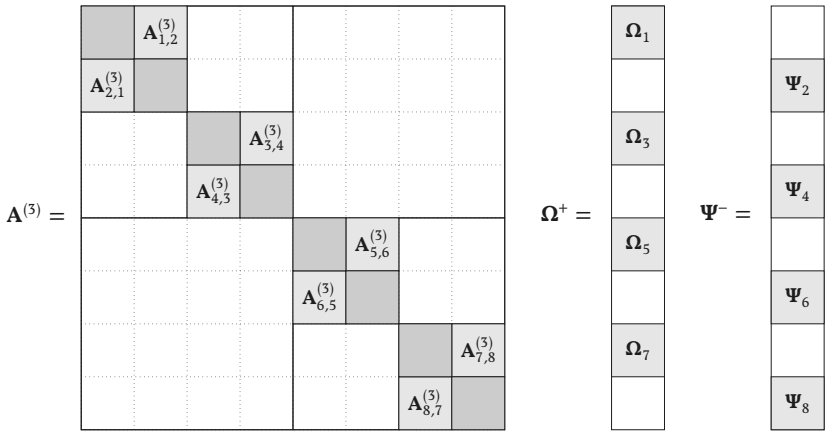
The algorithm works from the top layer down.

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

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

Peeling: an algorithm for the recovery problem



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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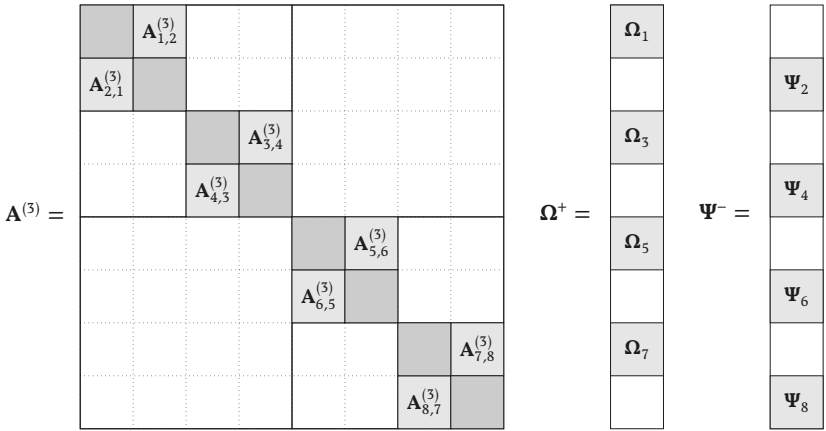

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Peeling: an algorithm for the recovery problem

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.

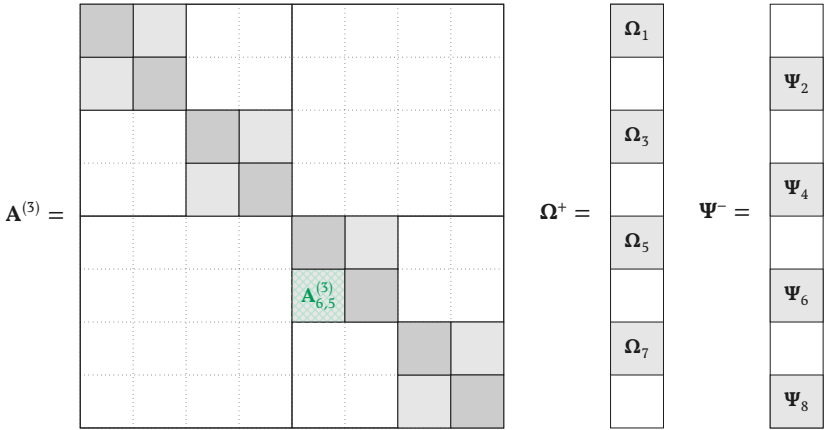
Peeling with error?

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).[4]

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

[4] Boullé and Townsend 2022.

Does peeling work on non-HODLR matrices?



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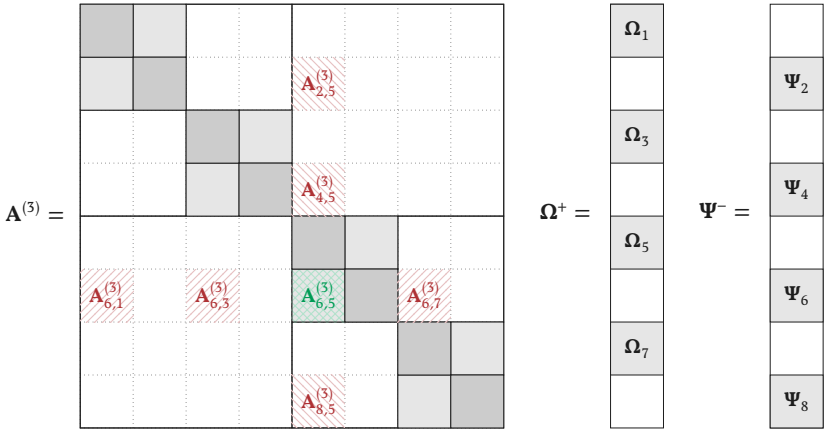

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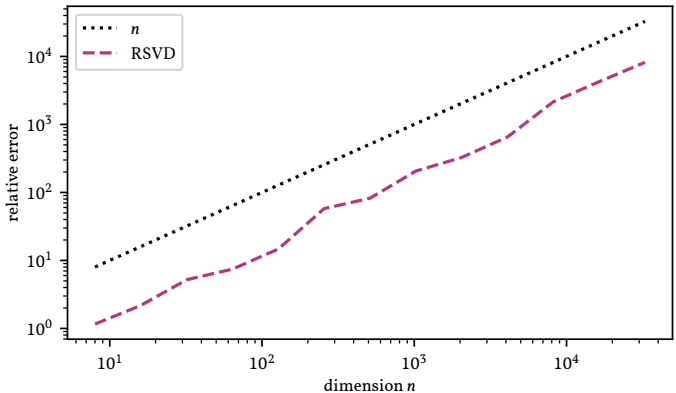
Does peeling work on non-HODLR matrices?

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[5]

Problem. Given an $n \times n$ matrix $\mathbf{A}$, accessible only by matrix-vector products, a rank parameter k, and an accuracy parameter ε, 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[6]

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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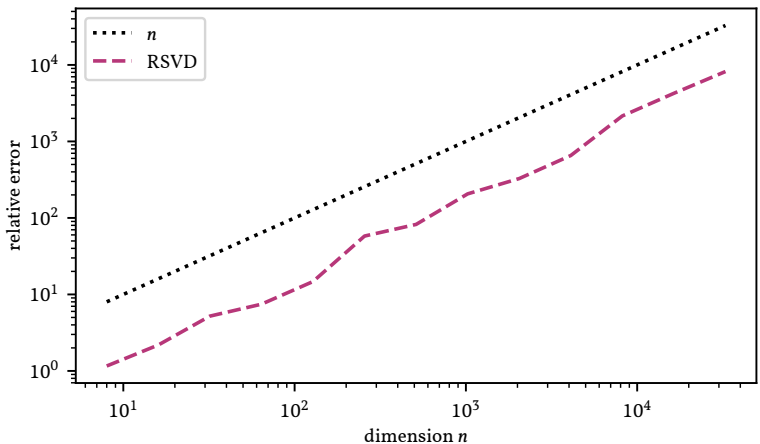

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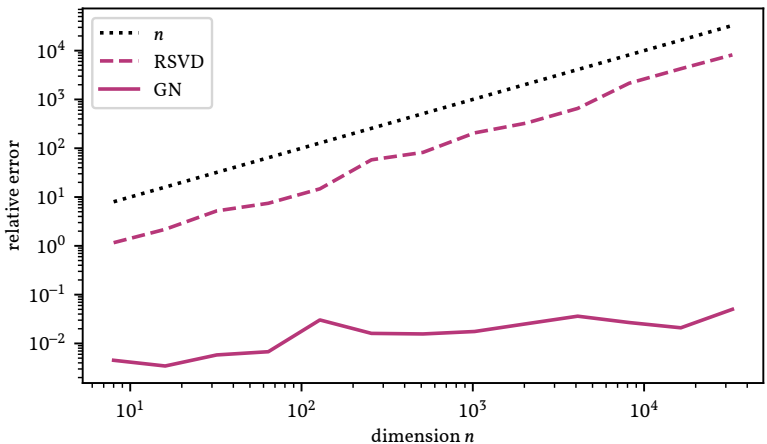
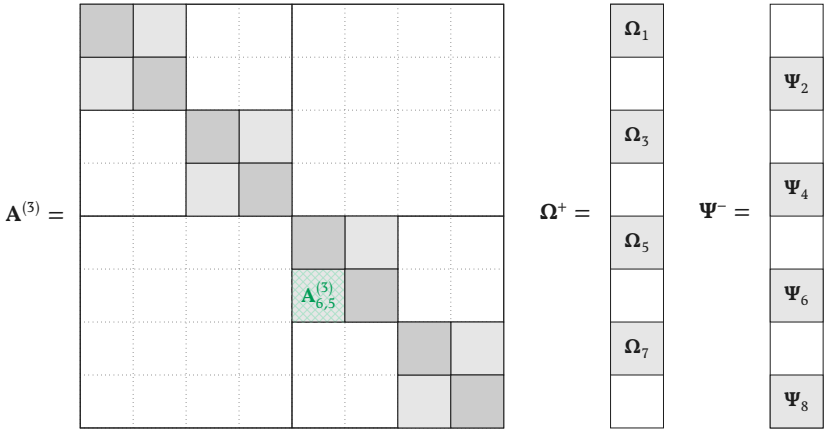


Another approach: perforated sketches

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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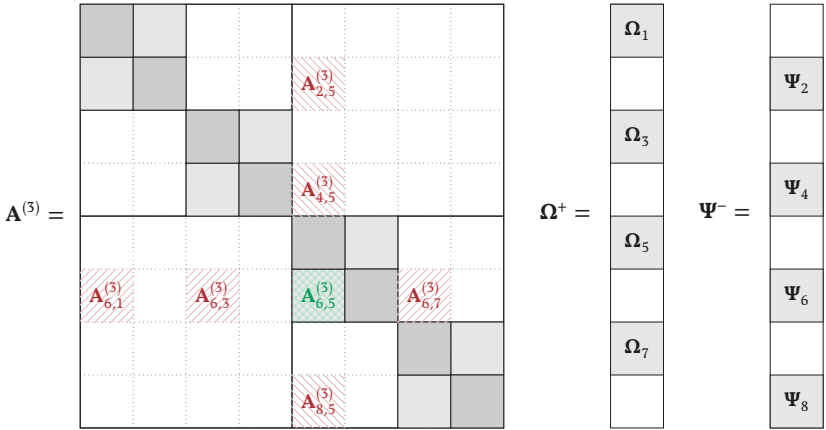

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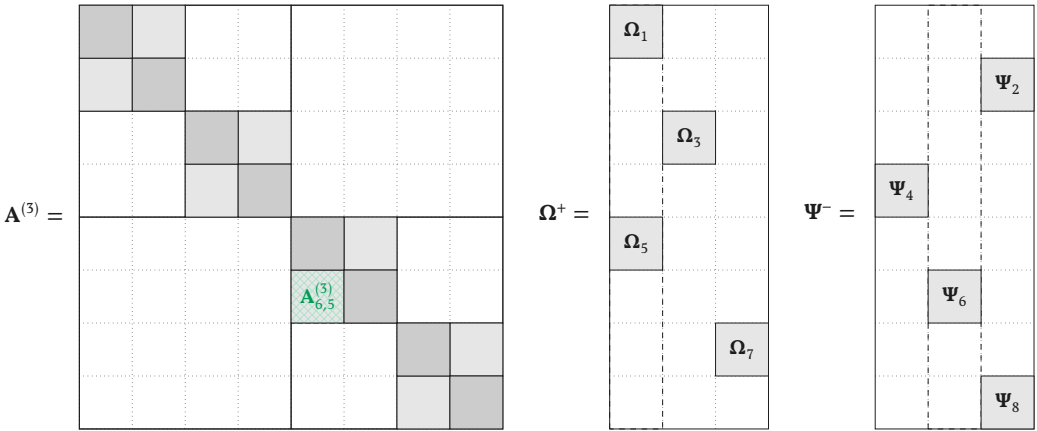

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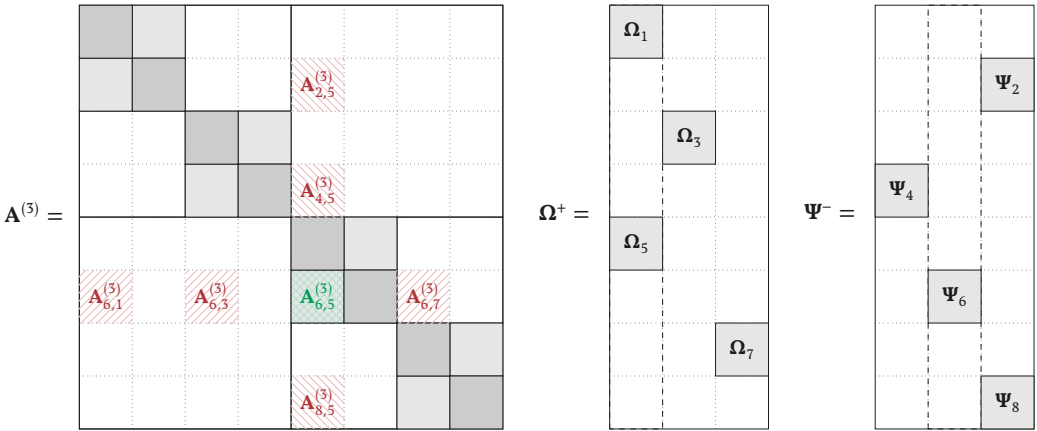

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Our main result

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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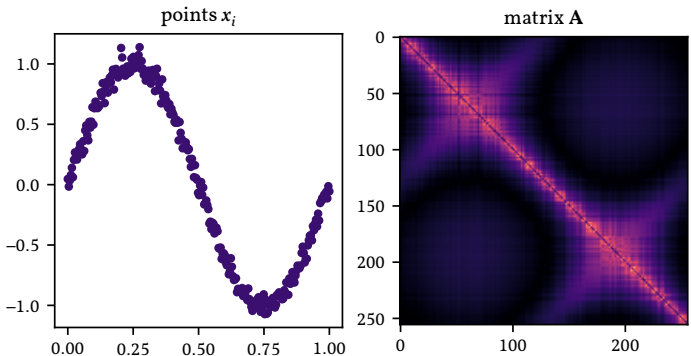
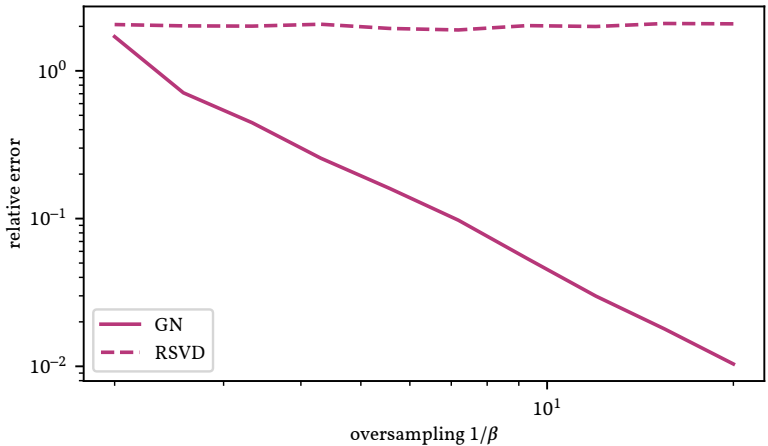
Another experiment

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



Another experiment



Lower bounds?

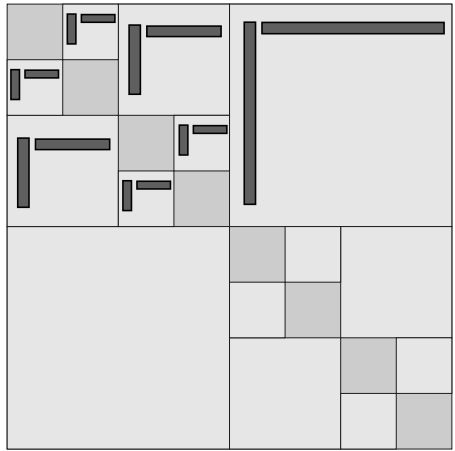
The matrix-vector query model often lets us prove lower-bounds against any matvec algorithm for a given task; i.e. study the complexity of a task.

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, ε, 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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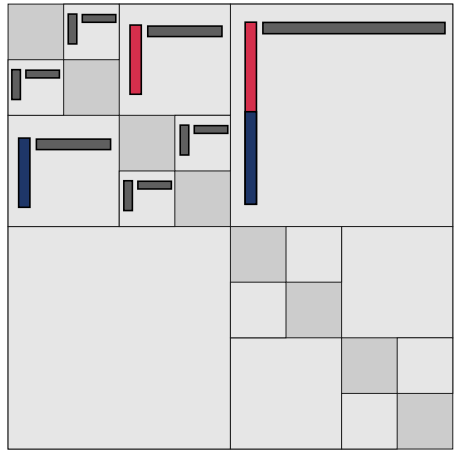

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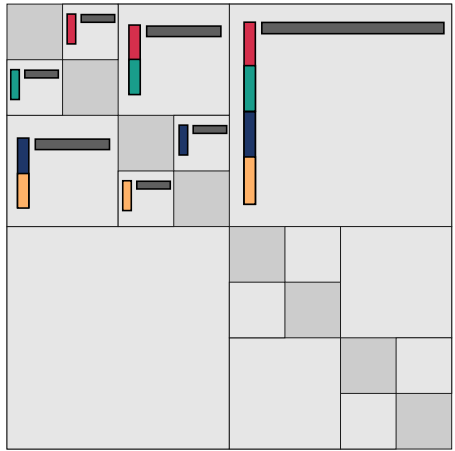

HSS is tricky!

Many papers study HSS recovery.[7]

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 $O(\log(n))$ HSS approximation in $O(kn^2)$ time.

[7] 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 ε 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

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:

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

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.

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