Integral Equation Methods for Numerical Solutions of Partial Differential Equations

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Learning Objectives

By the end of this talk, participants should be able to:

1. Be more familiar with the development of numerical methods for PDEs.
2. Understand the workflow of integral equation methods.
3. Know the advantages and disadvantages of integral equation methods, and use it appropriately in future research.
4. Know a subset of active problems arising from this field.

Introduction

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These requirements don't hold universally.

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What's the advantage of the formulations?

Example: Laplace's equation

Definition

Laplace's equation with Dirichlet boundary condition

$$-\nabla^2 u(x) = 0 \quad \text{for } x \in \Omega \tag{1}$$

$$u(x) = f(x) \quad \text{for } x \in \partial\Omega \tag{2}$$

We want to find a solution to it that takes the form

$$u(x) = \int_{\partial\Omega} d(x,y)\sigma(y)ds(y), \quad x \in \Omega,$$

where $d(x,y)$ is the normal derivative to the Green's function of Laplace's equation at the boundary point y
($d(x,y) = n(y) \cdot \nabla_y \phi(x-y) = \frac{n(y)\cdot(x-y)}{2\pi|x-y|^2}$ and $n(y)$ is the unit length inwards pointing normal to $\partial\Omega$ at $y \in \partial\Omega$).

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Questions

- Q: Why can we assume that the solution is written in this weird integral form?
- Q: Why do we pick this specific kernel function $d(x,y)$ instead of others?

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Remarks

Our kernel function $d(x, y)$ has a singularity as $x \to y$, which leads to an extra term as we take the limit

$$\lim_{x' \to x, x' \in \Omega} u(x') = -\frac{1}{2}\sigma(x) + \int_{\partial\Omega} d(x, y)\sigma(y)ds(y).$$

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$$\lim_{x' \to x, x' \in \Omega} u(x') = -\frac{1}{2}\sigma(x) + \int_{\partial\Omega} d(x, y)\sigma(y) ds(y).$$

Therefore, we got the integral equation that $\sigma(x)$ satisfies:

$$-\frac{1}{2}\sigma(x) + \int_{\partial\Omega} d(x, y)\sigma(y) ds(y) = f(x), \quad x \in \partial\Omega.$$

Integral equation formulations of Laplace's equation

References

- J. Levandosky, Notes on potential theory, Stanford University, 2003.
- P.G. Martinsson, Direct Solvers for Integral Equations, CBMS/NSF Conference on Fast Direct Solvers, 2014.
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Discretization of the integral equation

The density function $\sigma(x)$ satisfies a Fredholm integral equation of second kind:

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We discretize the integral equation by replacing the integral with a representative weighted sum, i.e., a selected quadrature rule:

$$\int_{\partial\Omega} \phi(y)ds(y) = \sum_{j=1}^{N} w_j \phi(x_j), \quad \text{for a certain class of } \phi.$$

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Then the discretized integral equation becomes a $N \times N$ linear system

$$-\frac{1}{2}\sigma(x_i) + \sum_{j=1}^{N} w_j d(x_i,x_j)\sigma(x_j) = f(x_i), \quad i = 1,2,\ldots,N.$$

Discretization of the integral equation

Examples of common quadrature rules

- Trapezoidal rule: Converge super-algebraically when the boundary condition f is C^∞ and periodic, plus the boundary of the domain is smooth. Easy to code.
- Composite Gaussian quadrature: Customized convergence rate depending on the selected order of quadrature. Allows for local refinement, which is good for domains with corners and edges.
- Singular integral quadrature: Necessary when we need to evaluate the integral of a singular kernel. We don't need it in our example, but it's required for more sophisticated problems, e.g., Helmholtz equation.

Discretization of the integral equation

To write the discretized integral equation

$$-\frac{1}{2}\sigma(x_i) + \sum_{j=1}^{N} w_j d(x_i, x_j)\sigma(x_j) = f(x_i)$$

as a $N \times N$ linear system, we define vectors $\sigma, f \in R^n$ via

$$f(i) = \sqrt{w_i} f(x_i), \quad \sigma(i) = \sqrt{w_i}\sigma(x_i),$$

and define matrix $A \in R^{N \times N}$ via

$$A(i,j) = \sqrt{w_i} d(x_i, x_j)\sqrt{w_j} - \frac{1}{2}\delta_{i,j}. \tag{3}$$

Finally, we get a linear system $A\sigma = f$ to solve.

Why do we need the $\sqrt{w}$ weighting scheme?

Such weighting scheme allows the matrix to capture the L^2 behaviour of an integral operator rather than its pointwise behavior, which leads to a better-conditioned linear system due to some intrinsic property of our integral equation.

Discretization of the integral equation

References

- J Bremer, Z Gimbutas, V Rokhlin, A nonlinear optimization procedure for generalized Gaussian quadratures, SIAM Journal on Scientific Computing, 2010
- S Hao, AH Barnett, PG Martinsson, P Young, High-order accurate methods for Nyström discretization of integral equations on smooth curves in the plane, Advances in Computational Mathematics, 2014
- J. Bremer, A fast direct solver for the integral equations of scattering theory on planar curves with corners, Journal of Computational Physics, 2012
- J. Bremer, A Nyström method for weakly singular integral operators on surfaces, Journal of Computational Physics, 2012

Fast algorithms for rank-structured matrices

Let's take a close look at the matrix A where

$$A(i,j) = \sqrt{w_i}\, d(x_i, x_j) \sqrt{w_j} - \frac{1}{2}\delta_{i,j}. \tag{4}$$

Unlike the usual sparse matrices arising from the common numerical PDE methods, our matrix is dense and rank-structured! This tells us...

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- Conventional matrix solvers will be slow.
- The matrix requires more storage as its columns can't be stored sparsely.

Rank-structured matrix

What's special about our matrix

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Definition: Given an error tolerance ϵ, if A is a $m \times n$ low-rank matrix with numerical rank k, then we have $U \in R^{m \times k}$ and $V \in R^{k \times n}$

$$A \approx UV,$$

and the numerical rank k is the smallest integer such that $|A - UV|_2 < \epsilon$:

$$\text{numrank}(A, \epsilon) = \min\{k : \exists U \in R^{m \times k}, V \in R^{k \times n}, s.t., |A - UV|_2 < \epsilon\}.$$

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Remarks

The numerical rank of a low rank matrix is usually far lower than the actual rank, i.e., $k << \min(m, n)$.
What happens to the storage?

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Low-rank approximation

How do we compute a low-rank approximation of the matrix?

Examples

- SVD: Optimal! (by Eckart-Young-Mirsky Theorem) But...
- Randomized range finder: Fast. Receiving more and more attentions nowadays. However, its advantage is not obvious compared to the next example in our application...
- Interpolatory decomposition: Widely used by the integral equation method researchers! Nearly optimal, reasonably fast, no need to construct the whole matrix A when integrated into our algorithm (by exploiting the analytical property of our kernel...)

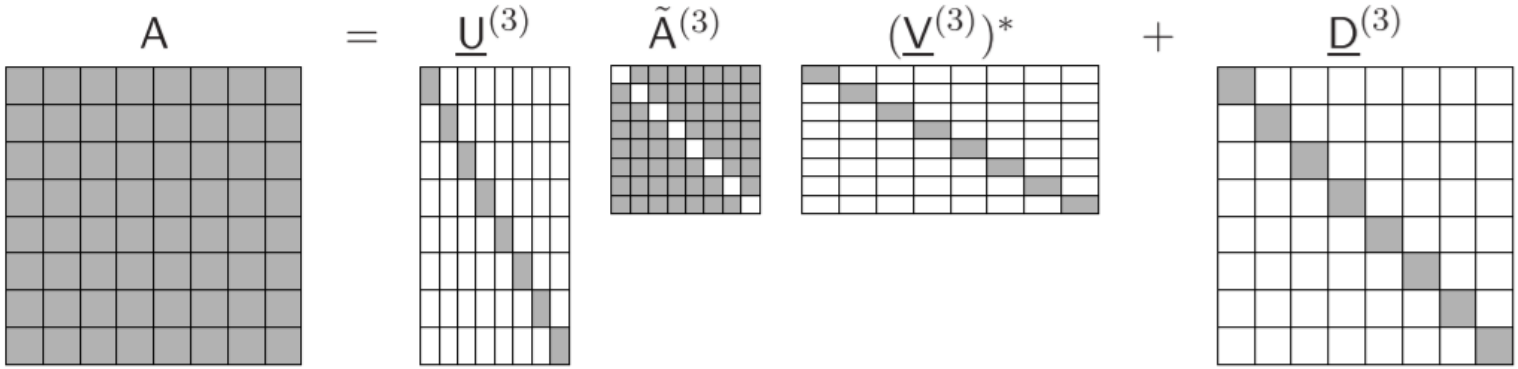
Rank-structured matrix and low-rank approximation

References

- A. Kloeckner, Tools for Low-Rank Linear Algebra, Fast Algorithms and Integral Equation Methods, Fall 2019
- P.G. Martinsson, Fast Direct Solvers for Elliptic PDEs, SIAM, 2019

Low-rank approximation of our matrix

Low-rank approximation of the first level (cited from [Gillman, et al])



Final Low-rank approximation (cited from [Gillman, Young, Martinsson])

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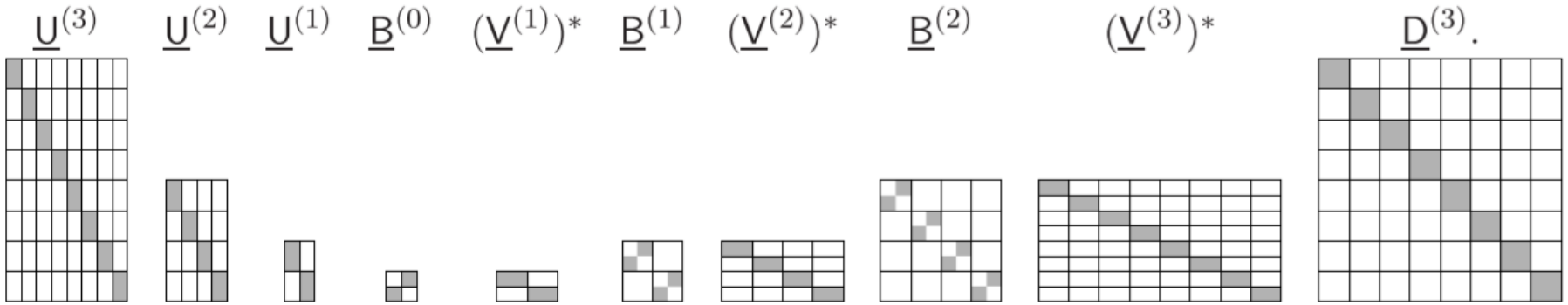
The block structure of the right hand side of (4.4) is:



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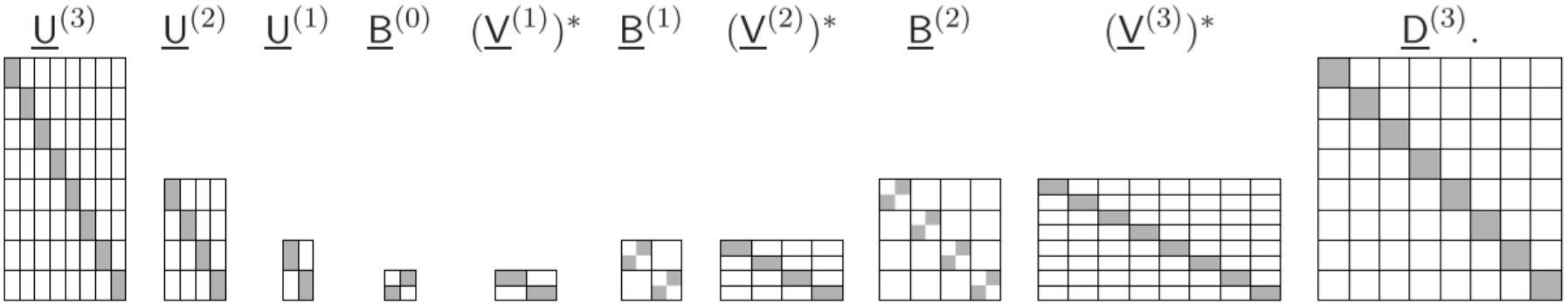

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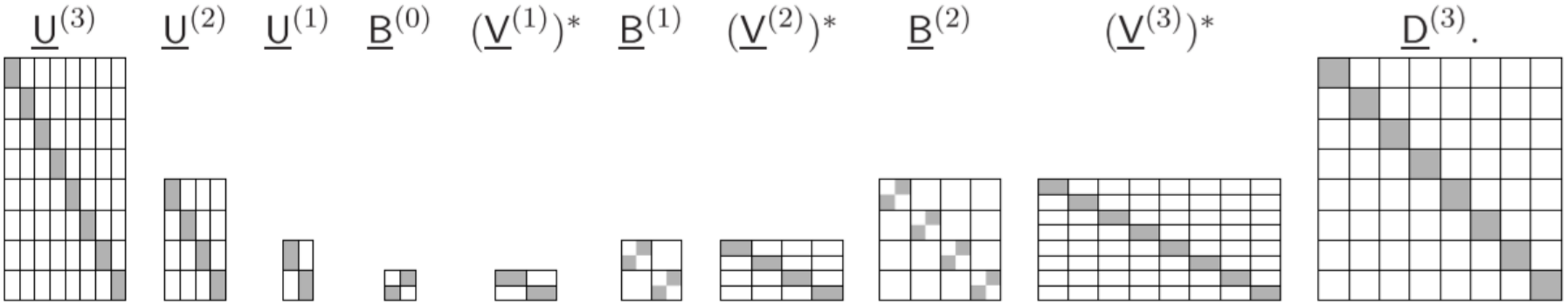

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- Time complexity of matvec: $O(kN)$.

Iterative methods for rank-structured matrices

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- Analytical expansion vs matrix factorization.
- Strong admissibility vs weak admissibility.

Iterative methods for rank-structured matrices

References

- A. Gillman, P. Young, P.G. Martinsson, A direct solver with O(N) complexity for integral equations on one-dimensional domains, Front. Math. China, 7 (2012), pp. 217–247.
- R. Beatson, L. Greengard, A short course on fast multipole methods
- L. Greengard, V. Rokhlin, A fast algorithm for particle simulations, Journal of Computational Physics, 1987

Direct solver for rank-structured matrices

Why do we need a direct solver?

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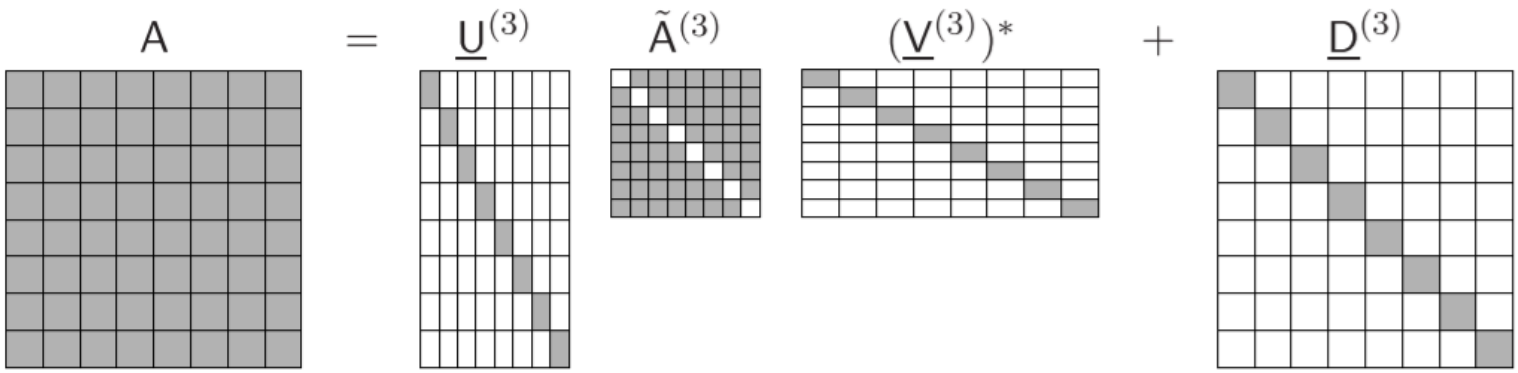
Next question: How to compute the inverse of our factorized matrix?



There's a name for such factorization...

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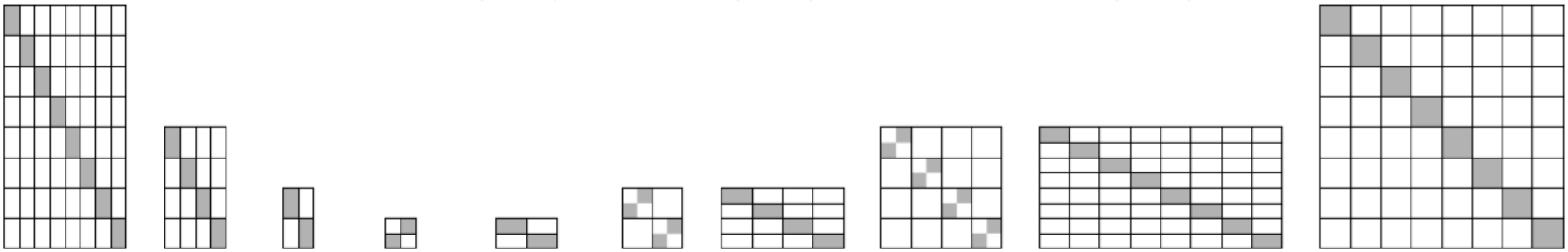

- Sherman–Morrison-Woodbury formula

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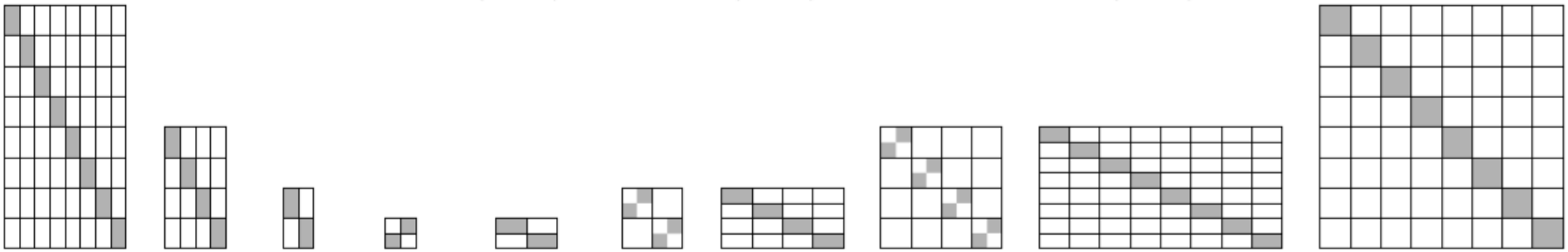

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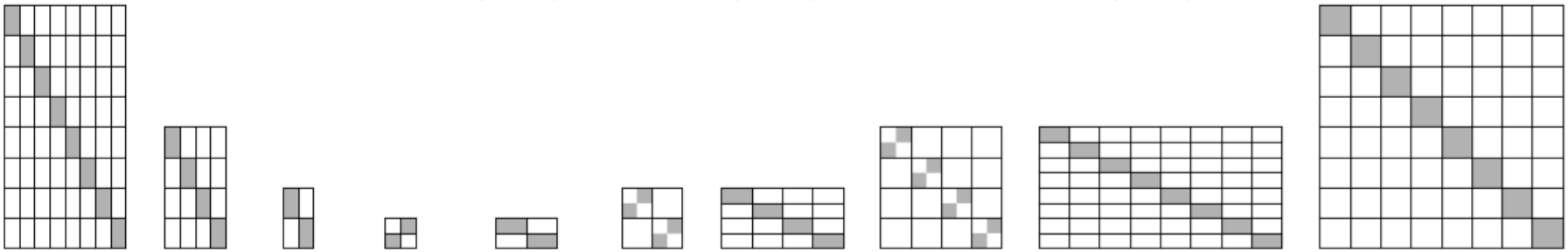

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- Time complexity of applying the inverse: $O(Nk)$

Direct solver for rank-structured matrices

References

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- A. Gillman, P. Young, P.G. Martinsson, A direct solver with O(N) complexity for integral equations on one-dimensional domains, Front. Math. China, 7 (2012), pp. 217–247.
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- Z. Shen, lap2d: A Fast Direct Dense Solver for 2-D Laplace's Equation, 2020

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- Be able to achieve machine precision accuracy.
- Works well for exterior problems (acoustics, electromagnetic scattering).
- Capability of exploiting all kinds of analytical properties of PDEs. Nice combination between analysis and numerical linear algebra!

Summary

Disadvantages

- Harder to code.

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- Harder to code.
- Special considerations need to be done when the problem has body load, singular kernels, a domain with corners, mixed boundary condition, etc.

Questions?

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Thanks to prof. Kirill Serkh and Xinyue Lu for providing suggestions to the talk.