Fast iterative or fast direct solution of boundary element systems

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Outline

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1. Review of $\mathcal{H}$-matrices
   - $\mathcal{H}$-matrix arithmetic
   - ACA
2. $\mathcal{H}$-matrix preconditioners
   - $\mathcal{H}$-LU decomposition
3. Computational Experiments

Outline

Fredholm integral equation

$$\lambda u + \mathcal{K} u = f, \quad \lambda \in \mathbb{R},$$

where

$$(\mathcal{K}u)(x) = \int_\Gamma \kappa(x,y) u(y)\, \mathrm{d}s_y, \quad x \in \mathbb{R}^3,$$

is an elliptic pseudo-differential operator, $\Gamma \subset \mathbb{R}^3$.

Finite dimensional ansatz space $V_h := \mathrm{span}\{\varphi_i\}$.
Stiffness matrix $K \in \mathbb{R}^{n\times n}$ with entries

$$K_{ij} := \int_\Gamma \int_\Gamma \varphi_i(x) \kappa(x,y) \varphi_j(y)\, \mathrm{d}s_x\, \mathrm{d}s_y, \quad i,j = 1,\ldots,n.$$

Critical properties of K

- κ usually non-local $\implies$ K is dense
- $\lambda M + K$ may be ill-conditioned

For simplicity let $\lambda = 0$.

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Asymptotic smoothness

$\mathcal{K}$ elliptic operator $\Longrightarrow$ κ has Calderón-Zygmund property

Asymptotic smoothness

There are $c_1, c_2 > 0$ and $g \in \mathbb{R}$ s.t. for all $\alpha \in \mathbb{N}_0^3$ it holds that

$$|\partial_y^\alpha \kappa(x,y)| \le c_1 |\alpha|! \, (c_2|x-y|)^{g-|\alpha|}, \quad x \neq y.$$

Want *degenerate approximation* on $D_1 \times D_2$

$$\kappa(x,y) \approx \tilde{\kappa}(x,y) = \sum_{\ell=1}^{k} u_\ell(x) v_\ell(y).$$

Far field condition ($0 < \eta < 1$ given)

$$\min\{\operatorname{diam} D_1, \operatorname{diam} D_2\} \le \eta \operatorname{dist}(D_1, D_2).$$

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Fast summation methods

E.g. by Taylor expansion: $\|\kappa - \tilde{\kappa}\|_{\infty,D_1\times D_2} \sim \eta^p \|\kappa\|_{\infty,D_1\times D_2}$.

Analytic expansions:
Fast multipole [Rokhlin '85] and panel clustering [Hackbusch/Nowak '89]

Analysis $\leftrightarrow$ algebra

	$\kappa(x,y)$	$\approx$	$\sum_{\ell=1}^{k} u_\ell(x)v_\ell(y)$	*degenerate approximation*
$\longleftrightarrow$	$K\|_b$	$\approx$	UV^T	low-rank approximation.

Algebraic methods: (hierarchical matrices)
Pseudo-skeletons [Tyrtyshnikov '97]

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Admissibility condition

Stiffness matrix $K \in \mathbb{R}^{n\times n}$

Basis functions φ_i, $i = 1,\ldots,n$, with supports $X_i := \operatorname{supp}\varphi_i$,

$$K_{ij} = a(\varphi_j, \varphi_i), \quad i,j = 1,\ldots,n.$$

For entry K_{ij} $\longleftrightarrow$ κ evaluated on $X_i \times X_j$
block $b = s \times t$ $\longleftrightarrow$ pair $X_s \times X_t$, where $X_t := \bigcup_{i\in t} X_i$.

Admissibility condition on block $b = s \times t$

$$\min\{\operatorname{diam} X_s, \operatorname{diam} X_t\} \le \eta \operatorname{dist}(X_s, X_t) \quad \text{or} \quad \min\{\#s, \#t\} \le n_{\min}.$$

Number of generated blocks is $\mathcal{O}(\eta^{-4} n \log n)$.
Note: arbitrary grids (no grid hierarchy required!)

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What are $\mathcal{H}$-matrices ?

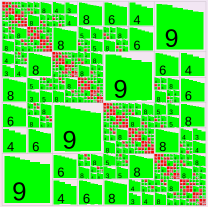
Basic principles

1. Hierarchical partition of the matrix into blocks
2. Restriction to low-rank matrices on each block

$$P = \{b = s \times t,\ s,t \subset I\}, \quad I := \{1,\dots,N\}$$

with pairwise disjoint P and

$$I \times I = \bigcup_{b \in P} b.$$



Blockwise low-rank matrices (M has full rank !)

Definition

$$\mathcal{H}(P,k) := \{M \in \mathbb{R}^{N \times N} : \operatorname{rank} M|_b \le k \text{ for all } b \in P\}$$

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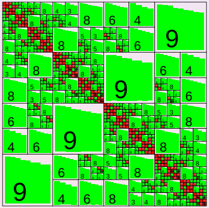

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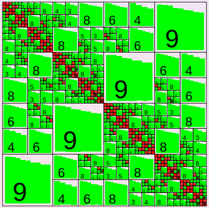

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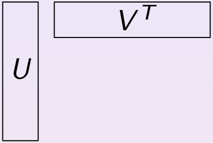
Low-rank matrices

Outer product representation

$A \in \mathbb{R}^{m\times n}$: rank $A \leq k$

$\iff \exists U \in \mathbb{R}^{m\times k},\ V \in \mathbb{R}^{n\times k}$ s.t. $A = UV^T$.



Storage

Instead of $m \cdot n$ for A

$k(m+n)$ units of memory for U, V.

Cost of MV-multiply

Instead of $\mathcal{O}(m \cdot n)$ for Ax

$\mathcal{O}(k(m+n))$ operations for $UV^Tx = U(V^Tx)$.

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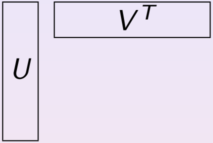

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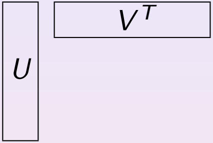

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$\mathcal{H}$-matrix arithmetic

$\mathcal{H}$-MV multiply

can be done without approximation.

Sum of two rank-k matrices exceeds rank k
$\Longrightarrow \mathcal{H}(P,k)$ is *not* a linear space.

SVD of AB^T, $A \in \mathbb{R}^{m\times k}$, $B \in \mathbb{R}^{n\times k}$

(i)	QR decompositions: $A = Q_A R_A$, $B = Q_B R_B$	$k^2(m+n)$
(ii)	SVD of $M := R_A R_B^T \in \mathbb{R}^{k\times k}$: $M = U\Sigma V^T$	k^3

then $(Q_A U)\Sigma(Q_B V)^T$ is SVD of AB^T.

$\mathcal{H}$-Addition

Blockwise truncated addition with precision ε

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$\mathcal{H}$-MM-Multiplication

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{bmatrix}$$

$\mathcal{H}$-Inversion

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} = \begin{bmatrix} A_{11}^{-1} + A_{11}^{-1}A_{12}S^{-1}A_{21}A_{11}^{-1} & -A_{11}^{-1}A_{12}S^{-1} \\ -S^{-1}A_{21}A_{11}^{-1} & S^{-1} \end{bmatrix},$$

where $S := A_{22} - A_{21}A_{11}^{-1}A_{12}$ is the Schur complement.

$\mathcal{H}$-operations: $\mathcal{O}(N \log^* N)$ [Grasedyck/Hackbusch '03].

Adaptive Cross Approximation (ACA)

Let $k = 1$; $Z = \varnothing$

repeat

if $k > 1$ **then** $i_k := \operatorname{argmax}_{i \notin Z} |(u_{k-1})_i|$

else $i_k := \min\{1, \dots, m\} \setminus Z$

$\tilde{v}_k := a_{i_k,1:n} - \sum_{\ell=1}^{k-1} (u_\ell)_{i_k} v_\ell$

$Z := Z \cup \{i_k\}$

if $\tilde{v}_k$ does not vanish **then**

$j_k := \operatorname{argmax}_{j=1,\dots,n} |(\tilde{v}_k)_j|$; $\quad v_k := (\tilde{v}_k)_{j_k}^{-1} \tilde{v}_k$

$u_k := a_{1:m,j_k} - \sum_{\ell=1}^{k-1} (v_\ell)_{j_k} u_\ell$.

$k := k + 1$

endif

until $\|u_k\|_2 \, \|v_k\|_2 < \varepsilon \, \| \sum_{\ell=1}^{k-1} u_\ell v_\ell^T \|_F$.

Theorem

Let (X_s, X_t) satisfy the far field condition and κ be asymptotically smooth. Then for $|Z| \geq n_p$ it holds that

$$|(A - \sum_{\ell=1}^{k} u_\ell v_\ell^T)_{ij}| \leq c \operatorname{dist}^g(X_s, X_t) \, \|\varphi_i\|_{L^1} \, \|\varphi_j\|_{L^1} \, \eta^p, \quad 0 < \eta < \frac{1}{3}.$$

[B. '99, B. & Rjasanow '03]

Parallelization of ACA and $\mathcal{H}$-MV-multiplication [B. & Kriemann '04]

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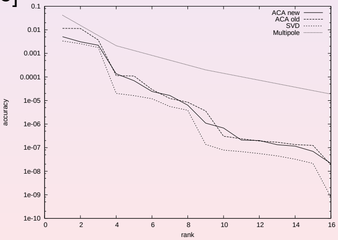

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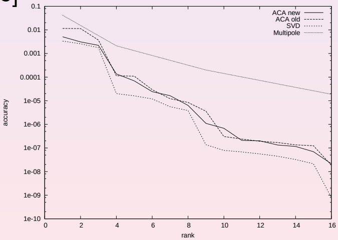

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$\mathcal{H}$-matrix preconditioners

Iterative solution using $\mathcal{H}$-MV multiplication
Problem: stiffness matrix K may be ill-conditioned
If $\mathcal{K}$ is operator of order m, $\operatorname{cond}_2(K) \sim h^{-|m|}$.

Idea [Steinbach/Wendland '98] based on mapping properties only.
Let $\mathcal{A} : V \to V'$ and $\mathcal{B} : V' \to V$ be V-coercive and V'-coercive.
Then for all $v \in V$

$$\alpha_1 \|v\|_V^2 \leq (\mathcal{A}v, v)_{L^2} \leq \alpha_2 \|v\|_V^2$$
$$\beta_1 \|v\|_V^2 \leq (\mathcal{B}^{-1}v, v)_{L^2} \leq \beta_2 \|v\|_V^2.$$

$\mathcal{A}$ and $\mathcal{B}^{-1}$ are spectrally equivalent

$$\frac{\alpha_1}{\beta_2}(\mathcal{B}^{-1}v, v) \leq (\mathcal{A}v, v) \leq \frac{\alpha_2}{\beta_1}(\mathcal{B}^{-1}v, v) \quad \text{for all } v \in V.$$

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Use hypersingular operator to precondition single layer operator. ($\rightarrow$ ACA).
Even for small n: $\mathrm{cond}_2(K)$ large due to geometry/discretisation.

Aim: compute preconditioner $C_{\mathcal{H}} \in \mathcal{H}(P, k)$ such that

$$\|K - C_{\mathcal{H}}\|_2 \leq \delta \|K\|_2, \quad \delta \mathrm{cond}_2(K) \leq \delta' < 1$$

then

$$\mathrm{cond}_2(C_{\mathcal{H}}^{-1} K) \leq \frac{1+\delta'}{1-\delta'}.$$

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Another idea:

- Inverse $\mathcal{K}^{-1}$ of elliptic ΨDO $\mathcal{K}$ also ΨDO with order $-m$.
- kernel function of $\mathcal{K}^{-1}$ has Calderón-Zygmund property
- Could use low-precision $\mathcal{H}$-inverse.

More efficient: $\mathcal{H}$-LU decomposition $C_{\mathcal{H}} = LU$.
Apply $C_{\mathcal{H}}^{-1}$ to b using forward/backward substitution: $Ly = b$, $Ux = y$, where

$$\begin{bmatrix} L_{11} & \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

is solved by

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$\mathcal{H}$-LU Decomposition

Idea: Block-LU decomposition

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ & U_{22} \end{bmatrix}$$

is recursively computed by:

$$\begin{aligned} L_{11}U_{11} &= A_{11} \\ L_{11}U_{12} &= A_{12} \\ L_{21}U_{11} &= A_{21} \\ L_{22}U_{22} &= A_{22} - L_{21}U_{12} \end{aligned}$$

First and last: LU decompositions of half the size.

Second: solve $LB = A$ for B.

$$\begin{bmatrix} L_{11} & \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

B can be found from

$$\begin{aligned} L_{11}B_{11} &= A_{11} \\ L_{11}B_{12} &= A_{12} \\ L_{22}B_{21} &= A_{21} - L_{21}B_{11} \\ L_{22}B_{22} &= A_{22} - L_{21}B_{12}, \end{aligned}$$

- replace usual operations $+, *$ by $\mathcal{H}$-versions with accuracy δ
- on the leaves of the tree use usual matrix operations
- Cholesky decomposition

Accuracy of *storing* and of each *arithmetical operation* is δ.
Product LU is backward stable, i.e.,

$$\|A - LU\|_2 < c\rho\delta\|A\|_2,$$

where the *growth factor*

$$\rho := \frac{\max_{ij} |u_{ij}|}{\max_{ij} |a_{ij}|}$$

is bounded in practice.

Complexity of $\mathcal{H}$-LU: $n|\log\delta|^4 \log^2 n$.
Preconditioner $C_{\mathcal{H}}$, $\operatorname{cond}_2(C_{\mathcal{H}}^{-1}K) \leq 10$, with complexity $\mathcal{O}(n\log^6 n)$.

Inner Dirichlet Problem Laplace

Boundary integral equation

$$\mathcal{V}v = (\frac{1}{2}\mathcal{I} + \mathcal{K})g.$$

Building the $\mathcal{H}$-matrix approximants
single layer 28288×28288 and 113152×113152
double layer 28288×14146 and 113152×56578

	$n = 28288$				$n = 113152$			
	single layer		double layer		single layer		double layer	
η	MB	time	MB	time	MB	time	MB	time
0.6	76	132 s	154	772 s	378	698 s	756	3972 s
0.8	78	99 s	156	596 s	391	497 s	765	2971 s
1.0	83	79 s	164	491 s	422	397 s	807	2408 s
1.2	88	71 s	172	448 s	458	353 s	860	2195 s

Computing $\mathcal{H}$-LU decomposition and solving

Recompress a copy to prescribed accuracy δ and compute hierarchical Cholesky decomposition with precision δ.

	$n = 28288$			$n = 113152$		
δ	recompr.	MB	decomp.	recompr.	MB	decomp.
$1e-1$	3.6 s	11	3.4 s	20.4 s	54	13.7 s
$1e-2$	8.1 s	40	5.7 s	40.1 s	224	53.0 s
$1e-3$	6.0 s	73	21.4 s	11.3 s	366	135.1 s

Solve $A_{\mathcal{H}}x = b$, $b = (\frac{1}{2}M + B_{\mathcal{H}})g$.

	$n = 28288$		$n = 113152$	
δ	steps	time	steps	time
$1e-1$	39	3.6 s	40	20.1 s
$1e-2$	21	2.6 s	21	14.1 s
$1e-3$	6	1.0 s	6	5.2 s

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Summary

We have presented a preconditioning technique that is

- building matrix using original matrix entries
- spectrally equivalent preconditioning (also for small n)
- *fast*: $\mathcal{O}(n \log^* n)$ complexity
- expensive parts parallelized
- *black-box*: can equally be applied to any elliptic operator

Software library for $\mathcal{H}$-matrices:
http://www.math.uni-leipzig.de/~bebendorf/AHMED.html