Variable-order approximation of integral operators

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Overview

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One-dimensional model problem

Integral equation: Find function u such that

$$\int_0^1 g(x,y)\,u(y)\,dy = f(x) \qquad \text{for all } x \in [0,1],$$

where the kernel function is given by $g(x,y) = -\log|x-y|$.

Galerkin discretization with basis functions $(\varphi_i)_{i=1}^n$ yields matrix $G \in \mathbb{R}^{n\times n}$ with

$$g_{ij} = \int_0^1 \varphi_i(x) \int_0^1 g(x,y)\varphi_j(y)\,dy\,dx \qquad \text{for all } i,j \in [1:n].$$

Challenge: Matrix G dense, storage $\sim n^2$.

Multi-dimensional model problem

Boundary integral equation: Find function u such that

$$\int_{\partial\Omega} g(x,y)\,u(y)\,dy = f(x) + \frac{1}{2}\int_{\partial\Omega} \frac{\partial g}{\partial n(y)}(x,y) f(y)\,dy \quad \text{for all } x \in \partial\Omega,$$

where g is the fundamental solution of an elliptic partial differential operator.

Examples of fundamental solutions:

$$g(x,y) = \frac{1}{4\pi\|x-y\|}, \qquad g(x,y) = \frac{\exp(i\kappa\|x-y\|)}{4\pi\|x-y\|}.$$

Challenge: Galerkin discretization again leads to dense matrices.

Compression methods

Toeplitz matrices:

- Only for very simple geometries.
- Only for translation-invariant kernel functions.
- Fast evaluation via FFT.

Wavelet compression:

- Very efficient compression.
- Wavelet bases for general geometries hard to find.
- Efficient implementation challenging.

Multipole and panel clustering:

- Good or excellent compression.
- Relatively simple and flexible.

Overview

Interpolation

Choose interpolation points $(\xi_\nu)_{\nu=0}^m$ and corresponding Lagrange polynomials $(\mathcal{L}_\nu)_{\nu=0}^m$.

Kernel function approximated by interpolating polynomial

$$g(x,y) \approx \sum_{\nu=0}^m \mathcal{L}_\nu(x) g(\xi_\nu, y).$$

Matrix approximated by low-rank factorization

$$g_{ij} \approx \sum_{\nu=0}^m \underbrace{\int_0^1 \varphi_i(x)\, \mathcal{L}_\nu(x)\, dx}_{=: V_{i\nu}} \underbrace{\int_0^1 \varphi_j(y)\, g(\xi_\nu, y)\, dy}_{=: B_{j\nu}} = (VB^*)_{ij}.$$

Advantage: Efficient matrix-vector multiplication $y = Gx \approx V(B^* x)$ requires only $\mathcal{O}(nm)$ operations instead of $\mathcal{O}(n^2)$.

Local interpolation

Problem: Kernel function g only locally smooth.

Approach: Use local interpolation in $\tau \times \sigma \subseteq [0,1] \times [0,1]$,

$$\tilde{g}_{\tau\sigma}(x,y) = \sum_{\nu=0}^{m} \sum_{\mu=0}^{m} \mathcal{L}_{\tau,\nu}(x) g(\xi_{\tau,\nu}, \xi_{\sigma,\mu}) \mathcal{L}_{\sigma,\mu}(y) \quad \text{for all } x \in \tau,\ y \in \sigma.$$

Matrix approximation results from discretization:

$$G|_{\hat{\tau}\times\hat{\sigma}} \approx V_\tau S_{\tau\sigma} V_\sigma^*$$

with index sets

$$\hat{\tau} := \{i \in [1:n] \ :\ \operatorname{supp} \varphi_i \subseteq \tau\}, \quad \hat{\sigma} := \{j \in [1:n] \ :\ \operatorname{supp} \varphi_j \subseteq \sigma\}.$$

Interpolation error

Assumption: $\tau \times \sigma$ is admissible, i.e., we have

$$\max\{\text{diam}(\tau), \text{diam}(\sigma)\} \leq \text{dist}(\tau, \sigma).$$

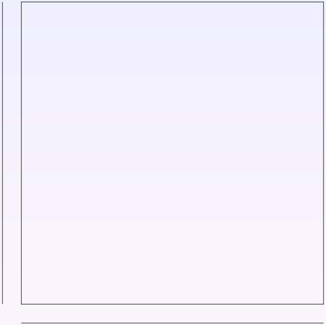
Analysis: For any $\varrho < 3 + 2\sqrt{2} \approx 5,83$ we find C such that

$$\|g - \tilde{g}\|_{\infty,\tau\times\sigma} \leq C\varrho^{-m} \qquad \text{for all } m \in \mathbb{N}.$$

(proof discussed lated)

Block tree

Idea: Recursively split matrix into submatrices corresponding to admissible subdomains $\tau \times \sigma$.



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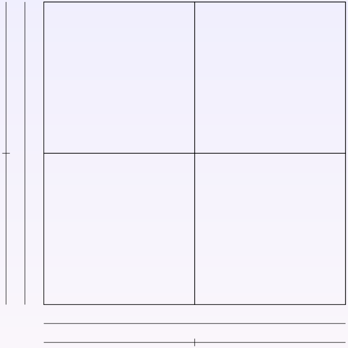

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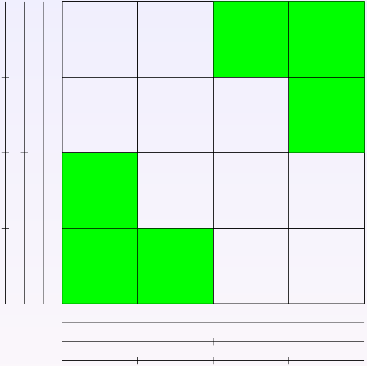

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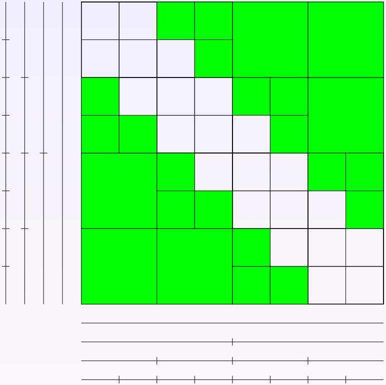

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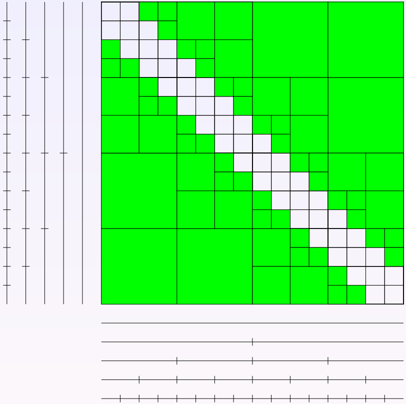

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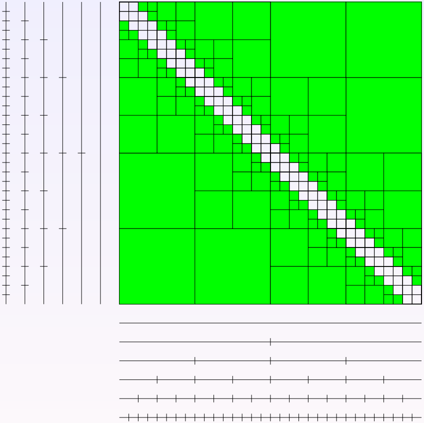

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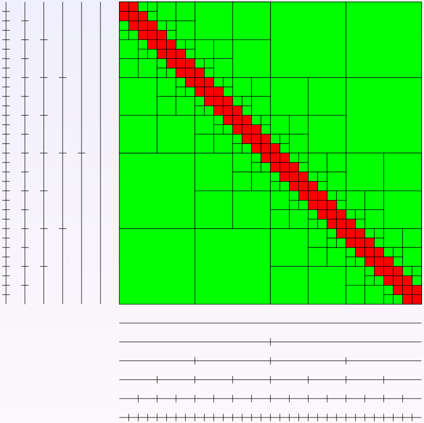

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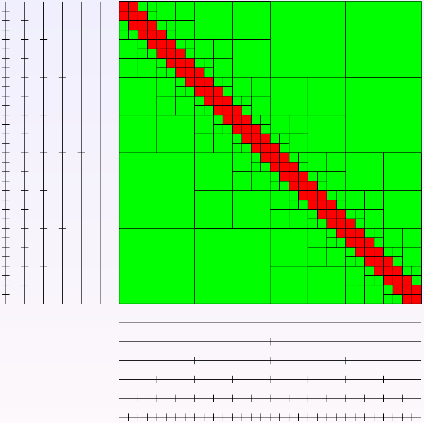

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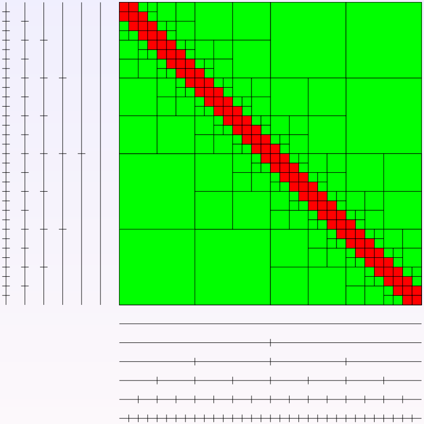
Result:

- Domain split in cluster tree.
- Matrix split in block tree.

Uniform hierarchical matrix

Approach: Interpolation in admissible subdomains $\tau \times \sigma$ leads to low-rank factorization $V_\tau S_{\tau\sigma} V_\sigma^*$.



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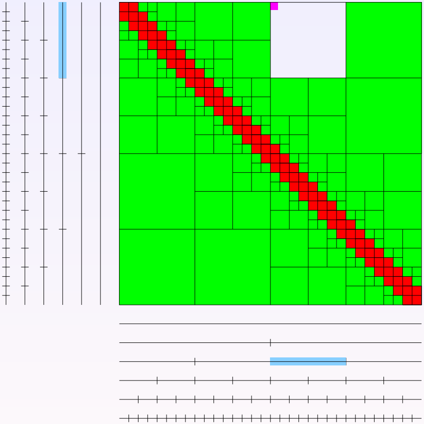

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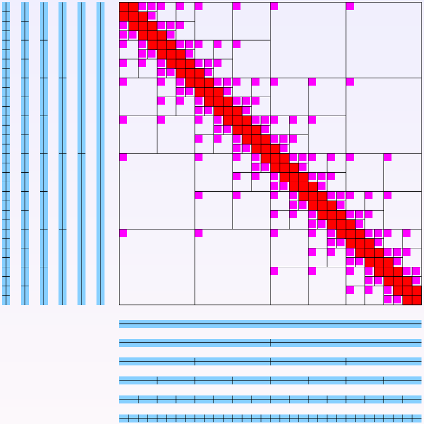

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Result:

- Storage $\mathcal{O}(nm\log(n))$,
- Accuracy $\mathcal{O}(\varrho^{-m})$.

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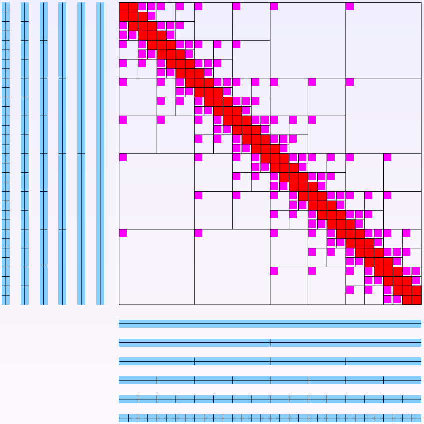

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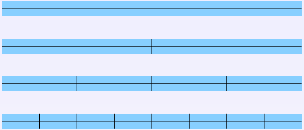
Goal: Linear complexity $\mathcal{O}(nm)$.

Nested basis

Challenge: Cluster basis (V_τ) requires $\sim nm\log(n)$ units of storage.



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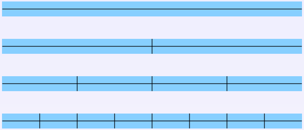

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$$\mathcal{L}_{\tau,\nu} = \sum_{\nu'=0}^{m} \underbrace{\mathcal{L}_{\tau,\nu}(\xi_{\tau',\nu'})}_{=e_{\tau',\nu'\nu}} \mathcal{L}_{\tau',\nu'}$$

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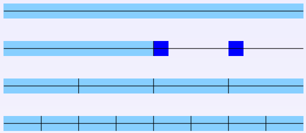

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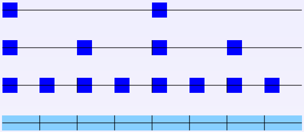

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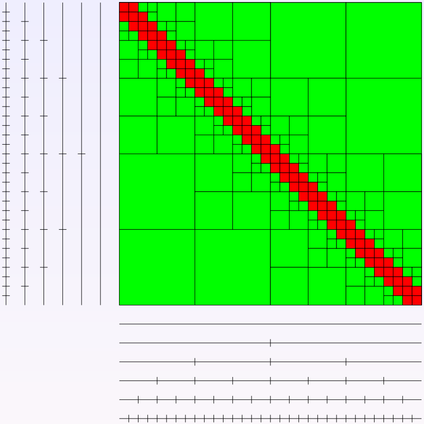
Approach: Store V_τ only for leaf clusters and use transfer matrices E_τ $\rightarrow$ storage $\mathcal{O}(nm)$ for the entire cluster basis.

$\mathcal{H}^2$-matrix



Matrix split into blocks.

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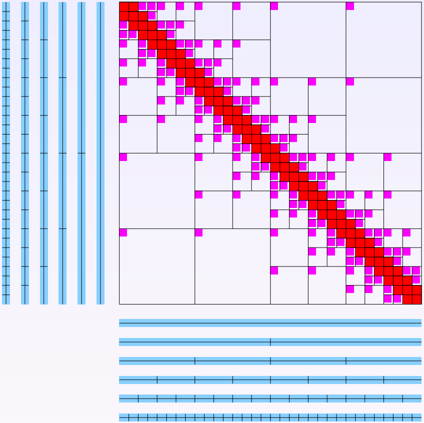

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Low-rank factorization $V_\tau S_{\tau\sigma} V_\sigma^*$ of admissible blocks $\tau \times \sigma$.

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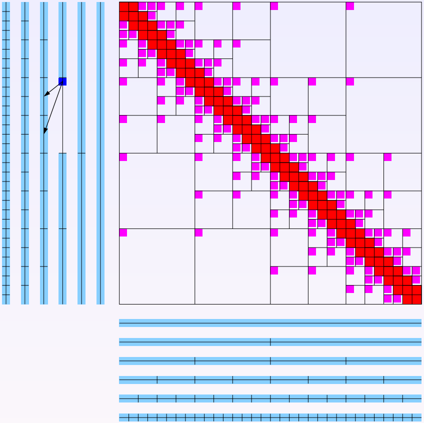

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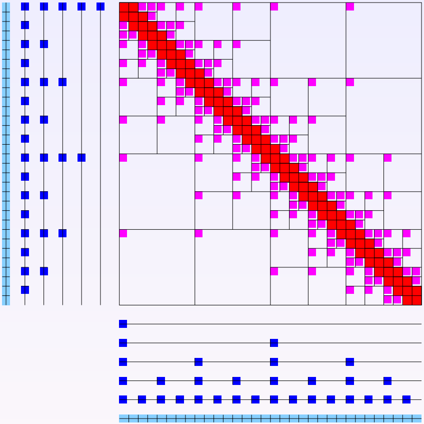

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Result: $\mathcal{H}^2$-matrix with complexity $\mathcal{O}(nm)$ and accuracy $\mathcal{O}(\varrho^{-m})$.

Overview

Projection and stability

Interpolation operator for $[-1, 1]$ given by

$$\mathfrak{I}_m \colon C[-1,1] \to \Pi_m, \qquad f \mapsto \sum_{\nu=0}^{m} f(\xi_\nu)\mathcal{L}_\nu.$$

Projection: Polynomials are fixed points.

$$\mathfrak{I}_m[p] = p \qquad \text{for all } p \in \Pi_m.$$

Stability: Maximum norm bounded.

$$\|\mathfrak{I}_m[f]\|_{\infty,[-1,1]} \leq \Lambda_m \|f\|_{\infty,[-1,1]} \qquad \text{for all } f \in C[-1,1].$$

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Result: Best-approximation property for all $f \in C[-1, 1]$:

$$\|f - \mathfrak{I}_m[f]\|_{\infty,[-1,1]} \leq (\Lambda_m + 1)\|f - p\|_{\infty,[-1,1]} \qquad \text{for all } p \in \Pi_m.$$

Bernstein ellipses

If f is holomorphic in the Bernstein ellipse

$$\mathcal{B}_\varrho := \left\{ x + iy \ : \ \left(\frac{2x}{\varrho + 1/\varrho} \right)^2 + \left(\frac{2y}{\varrho - 1/\varrho} \right)^2 \leq 1 \right\},$$

there is a $C \in \mathbb{R}_{>0}$ such that

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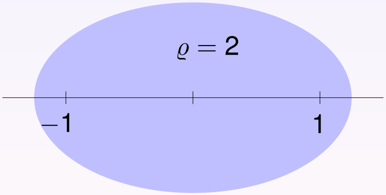

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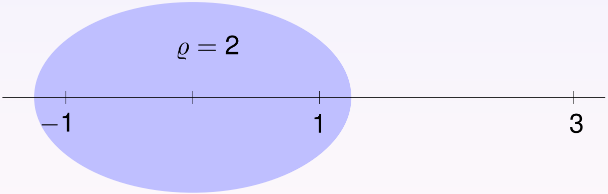

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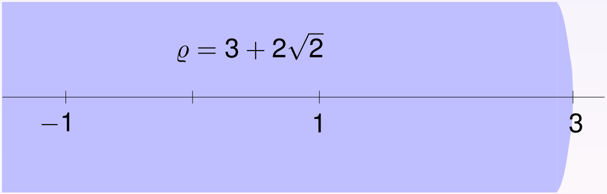

Tensor interpolation

Transformed interpolation: Use $\Phi(x) = \frac{b+a}{2} + \frac{b-a}{2}x$, define

$$\mathfrak{I}_{[a,b],m}[f] = \mathfrak{I}_m[f \circ \Phi] \circ \Phi^{-1}.$$

Tensor interpolation for $\tau = [a_1, b_1] \times [a_2, b_2]$ given by

$$\mathfrak{I}_{\tau,m} = \mathfrak{I}_{[a_1,b_1],m} \otimes \mathfrak{I}_{[a_2,b_2],m}.$$

Error estimate obtained via stability property

$$\begin{aligned} \|f - \mathfrak{I}_{\tau,m}[f]\|_{\infty,\tau} \leq \quad & \|f - (\mathfrak{I}_{[a_1,b_1],m} \otimes I)[f]\|_{\infty,\tau} \\ & + \Lambda_m \|f - (I \otimes \mathfrak{I}_{[a_2,b_2],m})[f]\|_{\infty,\tau}. \end{aligned}$$

Interpolation error

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Laplace problem: $g(x, y) = \frac{1}{4\pi\|x-y\|}$ leads to

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Helmholtz problem: $g(x, y) = \frac{\exp(i\kappa\|x-y\|)}{4\pi\|x-y\|}$ significantly more challenging, since holomorphic extension grows exponentially.
$\rightarrow$ Use modified interpolation to construct $\mathcal{DH}^2$-matrices.

Variable order

Already established: Maximum-norm estimate

$$\|g - \tilde{g}_{\tau\sigma}\|_{\infty,\tau\times\sigma} \leq C\varrho^{-m}.$$

Integral equation requires estimate in L^2-norm,

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Idea of variable-order methods:

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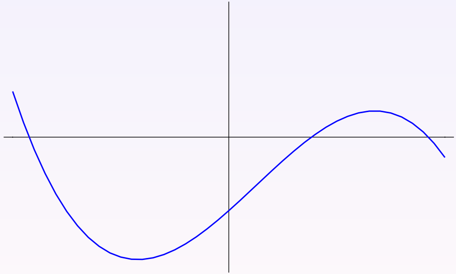
Result: Accuracy $\mathcal{O}(h)$ with complexity $\mathcal{O}(n)$.

Re-interpolation

Problem: Cluster basis for variable order no longer nested.

Approach: Approximate Lagrange polynomials by interpolation.

$$\widetilde{\mathcal{L}}_{\tau,\nu}(x) = \begin{cases} \mathcal{L}_{\tau,\nu}(x) & \text{if } \tau \text{ is a leaf,} \\ \sum_{\nu'=0}^{m'} \mathcal{L}_{\tau,\nu}(\xi_{\tau',\nu'})\widetilde{\mathcal{L}}_{\tau',\nu'}(x) & \text{if } x \in \tau',\ \tau' \in \operatorname{sons}(\tau). \end{cases}$$



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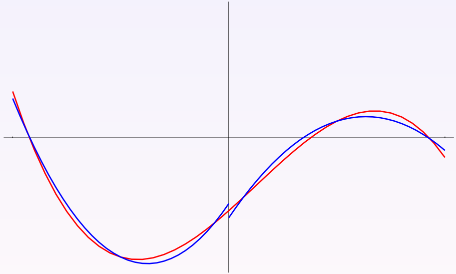

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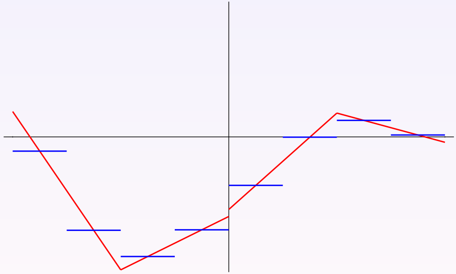

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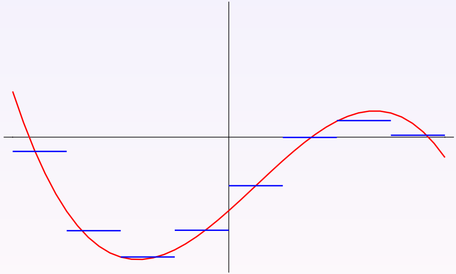
Approach: Approximate Lagrange polynomials by interpolation.

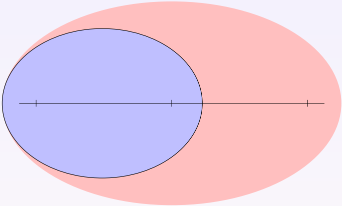
$$\widetilde{\mathcal{L}}_{\tau,\nu}(x) = \begin{cases} \mathcal{L}_{\tau,\nu}(x) & \text{if } \tau \text{ is a leaf,} \\ \sum_{\nu'=0}^{m'} \mathcal{L}_{\tau,\nu}(\xi_{\tau',\nu'}) \widetilde{\mathcal{L}}_{\tau',\nu'}(x) & \text{if } x \in \tau',\ \tau' \in \operatorname{sons}(\tau). \end{cases}$$



Re-interpolation error

Challenge: Given $[a,b] \subsetneq [-1,1]$, find $q < 1$ such that

$$\|p - \mathfrak{I}_{[a,b],m}[p]\|_{\infty,[a,b]} \leq q\|p\|_{\infty,[-1,1]} \qquad \text{for all } p \in \Pi_{m+\beta}.$$



Bernstein estimate:

$$\|p\|_{\infty,\mathcal{B}_\zeta} \leq \zeta^{m+\beta}\|p\|_{\infty,[-1,1]}.$$

Approximation: $\mathcal{B}_{[a,b],\varrho} = \Phi(\mathcal{B}_\varrho)$

$$\|p - \mathfrak{I}_{[a,b],\infty}[p]\|_{\infty,[a,b]} \leq C\varrho^{-m}\|p\|_{\infty,\mathcal{B}_{[a,b],\varrho}}$$

Error bound

Let $[a,b] \subsetneq [-1,1]$, let $\delta := (b-a)/2 < 1$.

Geometric argument: With $\sigma := \delta(\varrho + 1/\varrho) + 2(1-\delta)$ we have

$$\mathcal{B}_{[a,b],\varrho} \subseteq \mathcal{B}_\sigma.$$

Bernstein estimate: Using $\varrho := 3m/\delta$, we find

$$\begin{aligned}
&\|p - \mathfrak{I}_{[a,b],m}[p]\|_{\infty,[a,b]} \\
&\quad \leq C\varrho^{-m}\|p\|_{\infty,\mathcal{B}_{[a,b],\varrho}} \leq C\varrho^{-m}\|p\|_{\infty,\mathcal{B}_\sigma} \\
&\quad \leq C\frac{\sigma^{m+\beta}}{\varrho^m}\|p\|_{\infty,[-1,1]} \leq C\sigma^\beta\left(\delta + \frac{3}{\varrho}\right)^m \|p\|_{\infty,[-1,1]} \\
&\quad \leq C(3m+2)^\beta e\,\delta^m\|p\|_{\infty,[-1,1]} \qquad \text{for all } p \in \Pi_{m+\beta}.
\end{aligned}$$

Error bound

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$$\begin{aligned}
&\|p - \mathfrak{I}_{[a,b],m}[p]\|_{\infty,[a,b]} \\
&\quad \leq C\varrho^{-m}\|p\|_{\infty,\mathcal{B}_{[a,b],\varrho}} \leq C\varrho^{-m}\|p\|_{\infty,\mathcal{B}_\sigma} \\
&\quad \leq C\frac{\sigma^{m+\beta}}{\varrho^m}\|p\|_{\infty,[-1,1]} \leq C\sigma^\beta\left(\delta + \frac{3}{\varrho}\right)^m\|p\|_{\infty,[-1,1]} \\
&\quad \leq C(3m+2)^\beta e\,\delta^m\|p\|_{\infty,[-1,1]} \qquad \text{for all } p \in \Pi_{m+\beta}.
\end{aligned}$$

Result: Error arbitrarily small, as long as m large enough.

Overview

Experiment: One-dimensional model problem

Task: Approximate matrix of the one-dimensional model problem by $\mathcal{H}$- or $\mathcal{H}^2$-matrices and interpolation.

	$\mathcal{H}$-matrix			$\mathcal{H}^2$-matrix			$\mathcal{H}^2$-matrix (var.)		
n	Bld	M/n	Err	Bld	M/n	Err	Bld	M/n	Err
128	0.00	0.6	2.8_{-5}	0.00	0.5	3.0_{-5}	0.00	0.5	1.9_{-4}
256	0.01	0.8	2.7_{-5}	0.00	0.5	3.2_{-5}	0.00	0.5	1.1_{-4}
512	0.02	1.0	2.6_{-5}	0.01	0.5	3.2_{-5}	0.01	0.5	5.7_{-5}
1024	0.04	1.2	2.6_{-5}	0.01	0.5	3.2_{-5}	0.01	0.5	2.9_{-5}
2048	0.10	1.4	2.6_{-5}	0.03	0.5	3.3_{-5}	0.03	0.5	1.4_{-5}
4096	0.22	1.6	2.6_{-5}	0.05	0.5	3.3_{-5}	0.05	0.5	7.3_{-6}
8192	0.50	1.8	2.6_{-5}	0.10	0.5	3.3_{-5}	0.10	0.5	3.6_{-6}
⋮	⋮	⋮		⋮	⋮		⋮	⋮	
524288	52.97	2.9		6.62	0.5		6.62	0.5	

Experiment: Unit sphere

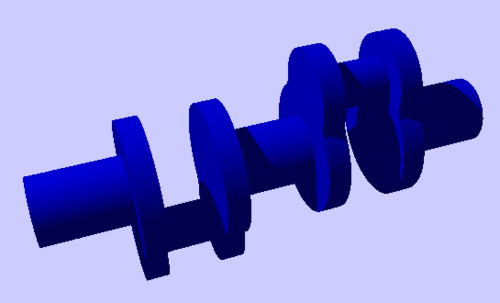
Task: Approximate matrix corresponding to single layer potential operator on the unit sphere by $\mathcal{H}^2$-matrices of variable order.

n	Bld	Mem	Mem$/n$	MVM	$\|X - \tilde{X}\|_2$
512	0.9	1.8	3.6	< 0.01	4.0_{-4}
2048	3.5	10.3	5.2	0.04	2.0_{-4}
8192	14.1	54.8	6.8	0.22	4.1_{-5}
32768	64.6	300.8	9.4	1.08	7.6_{-6}
131072	300.6	1508.3	11.8	4.60	1.3_{-6}
524288	1633.0	7181.7	14.0	20.26	1.5_{-7}
2097152	6177.5	30584.1	14.9	89.50	2.0_{-8}

Result: Error in $\mathcal{O}(h^3)$, relative error in $\mathcal{O}(h)$.

Experiment: General geometries

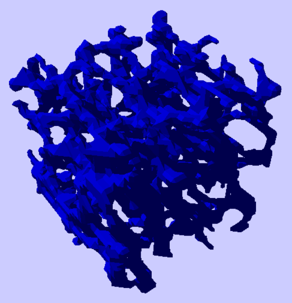
Approach: Cross approximation and $\mathcal{H}^2$-matrix recompression.



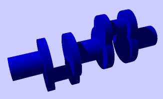
Crank shaft, from Joachim Schöberl's NetGen package

Experiment: General geometries

Approach: Cross approximation and $\mathcal{H}^2$-matrix recompression.



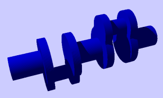
Nickle foam,
courtesy of Heiko Andrä
and Günther Of

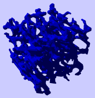


Experiment: General geometries

Approach: Cross approximation and $\mathcal{H}^2$-matrix recompression.

	$\mathcal{H}$-matrix			$\mathcal{H}^2$-matrix		
n	Bld	Mem	Err	Bld	Mem	Err
25 744	67	181	1.9_{-8}	68	135	1.4_{-8}
102 976	283	1 136	1.2_{-9}	289	551	8.4_{-10}
411 904	1 416	6 757	5.9_{-11}	1 464	2 225	5.1_{-11}
1 647 616	6 248	37 196	3.8_{-12}	6 627	9 795	3.0_{-12}
6 590 464	33 982	198 867	2.2_{-13}	36 224	41 611	1.8_{-13}
28 952	178	294	8.8_{-8}	172	387	7.0_{-8}
115 808	682	1 841	5.8_{-9}	700	1 228	3.7_{-9}
463 232	3 145	11 365	2.8_{-10}	3 176	4 933	2.2_{-10}
1 852 928	17 384	69 571	1.2_{-11}	17 629	15 905	1.3_{-11}





Current research

Algebraic recompression: Quasi-optimal compression via singular value decomposition.

Preconditioners: Arithmetic operations (multiplication, inversion, factorization) based on $\mathcal{H}^2$-matrices.

Helmholtz equation: High-frequency problems lead to oscillating kernel function, can be handled by modified interpolation.

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