An introduction to fractional calculus

Fundamental ideas and numerics

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Sylvester with quasiseparable matrices

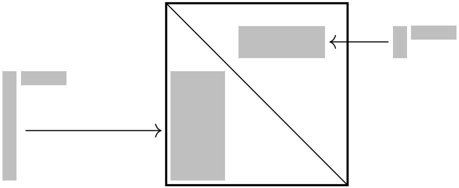
Let's start again from the problem we wanted to solve

$$AX + XB^T = C, \qquad A \in \mathbb{R}^{n\times n},\ \ B \in \mathbb{R}^{m\times m},\ \ X, C \in \mathbb{R}^{n\times m},$$

with A, B, and C **quasiseparable**

Quasiseparable matrix

A matrix A is *quasiseparable* of order k if the maximum of the ranks of all its submatrices contained in the strictly upper or lower part is less or equal than k.



💡 We have seen that A, B, and C quasiseparable $\Rightarrow$ X with decay of the singular values of off-diagonal blocks of C.

Sylvester with quasiseparable matrices

Theorem (Massei, Palitta, and Robol 2018, Theorem 2.12)

Let A, B be matrices of quasiseparable rank k_A and k_B respectively and such that $W(A) \subseteq E$ and $W(-B) \subseteq F$. Consider the Sylvester equation $AX + XB = C$, with C of quasiseparable rank k_C. Then a generic off-diagonal block Y of the solution X satisfies

$$\frac{\sigma_{1+k\ell}(Y)}{\sigma_1(Y)} \leq \mathcal{C}^2 \cdot Z_\ell(E, F), \qquad k := k_A + k_B + k_C.$$

Where $Z_\ell(E, F)$ is the solution of the **Zolotarev problem**

$$Z_\ell(E, F) \triangleq \inf_{r(x) \in \mathcal{R}_{\ell,\ell}} \frac{\max_{x \in E} |r(x)|}{\min_{y \in F} |r(y)|}, \qquad \ell \geq 1,$$

for $\mathcal{R}_{\ell,\ell}$ is the set of rational functions of degree at most (ℓ, ℓ), and $\mathcal{C}$ is the Crouzeix universal constant.

Sylvester with quasiseparable matrices

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ϵ-quasiseparable matrices of rank k (ε-qsrank k)

We say that A has *ϵ-quasiseparable rank k* if, for every off-diagonal block Y, $\sigma_{k+1}(Y) \leq \epsilon$. If the property holds for the lower (respectively upper) offdiagonal blocks, we say that A has lower (respectively upper) ϵ-quasiseparable rank k.

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Submatrices and off-diagonal blocks

If a matrix A has ϵ-quasiseparable rank k, then any of its principal submatrix A' has ϵ-quasiseparable rank k.

Any off-diagonal block Y of A' is also an off-diagonal block of $A \Rightarrow \sigma_{k+1}(Y) \leq \epsilon$.

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For $\oplus$ the direct sum

Technical lemma

Let A be a matrix with ϵ-quasiseparable rank k, Q any $(k+1) \times (k+1)$ unitary matrix. Then, $(I_{n-k-1} \oplus Q)A$ also has ϵ-quasiseparable rank k.

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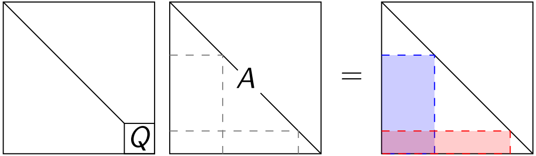

Q acts on the tall block of A without changing its singular values, while the small one has small rank thanks to the small number of rows.

Sylvester with quasiseparable matrices

Theorem (Massei, Palitta, and Robol 2018, Theorem 2.16)

Let A be of ϵ-quasiseparable rank k, for $\epsilon > 0$. Then, there exists a matrix δA of norm bounded by $\|\delta A\|_2 \leq 2\sqrt{n} \cdot \epsilon$ so that $A + \delta A$ is k-quasiseparable.

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- **Reduced cost** for BLAS-like operations,
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How can we operate efficiently with these matrix structures?

- **Reduced cost** for BLAS-like operations,
- *Contained storage cost.*
- Hierarchical matrix formats!

Hierarchical matrix formats

There exist **many hierarchical matrix formats**:

- $\mathcal{H}$-Matrices,
- $\mathcal{H}^2$-Matrices,
- **H**ierarchical **O**ff-**D**iagonal **L**ow-**R**ank (HODLR),
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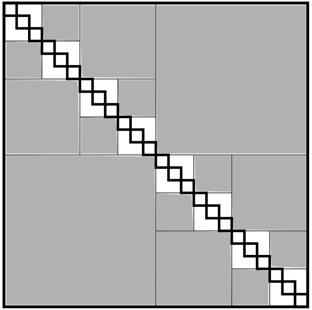

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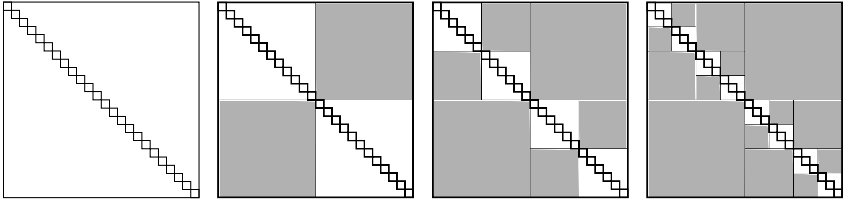
HODLR-matrices

The **general idea**:



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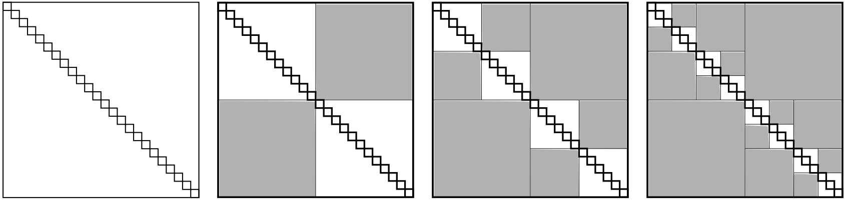

- The **grey blocks** are **low rank matrices** represented **in** a **compressed form**,
- the *diagonal blocks* in the last step are *stored as dense matrices*.
- We need now a **formal definition** and a way to **define operations**.

HODLR-matrices: trees

Cluster tree

Given $n \in \mathbb{N}$, let $\mathcal{T}_p$ be a completely balanced binary tree of depth p whose nodes are subsets of $\{1, \dots, n\}$. We say that $\mathcal{T}_p$ is a *cluster tree* if it satisfies:

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- The nodes at level ℓ, denoted by $I_1^\ell, \ldots, I_{2^\ell}^\ell$, form a partitioning of $\{1, \ldots, n\}$ into consecutive indices:
$$I_i^\ell = \{n_{i-1}^{(\ell)} + 1 \ldots, n_i^{(\ell)} - 1, n_i^{(\ell)}\}$$
for some integers $0 = n_0^{(\ell)} \leq n_1^{(\ell)} \leq \cdots \leq n_{2^\ell}^{(\ell)} = n$, $\ell = 0, \ldots p$. In particular, if $n_{i-1}^{(\ell)} = n_i^{(\ell)}$ then $I_i^\ell = \emptyset$.

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- The node I_i^ℓ has children $I_{2i-1}^{\ell+1}$ and $I_{2i}^{\ell+1}$, for any $1 \leq \ell \leq p - 1$. The children form a partitioning of their parent.

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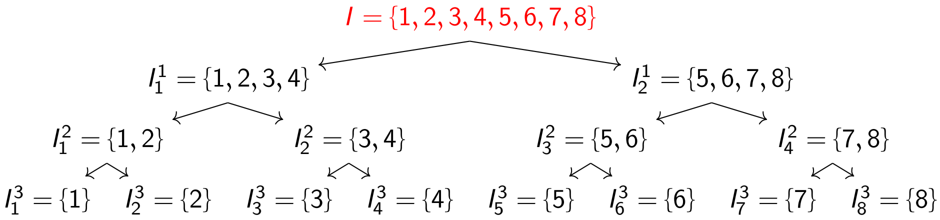
Nodes at a level ℓ partition A into a $2^\ell \times 2^\ell$ block matrix with blocks $\{A(I_i^\ell, I_j^\ell)\}_{i,j=1}^{2^\ell}$.

HODLR-matrices: trees



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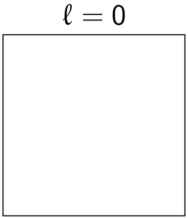

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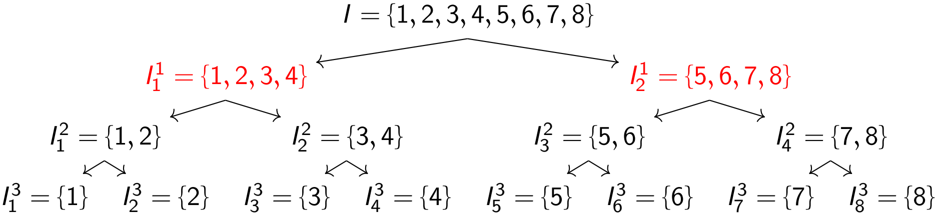

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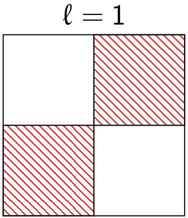

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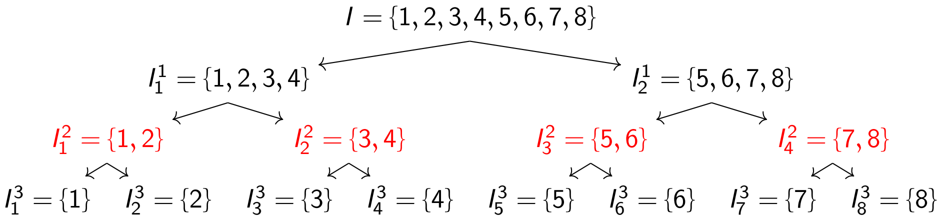

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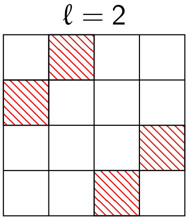

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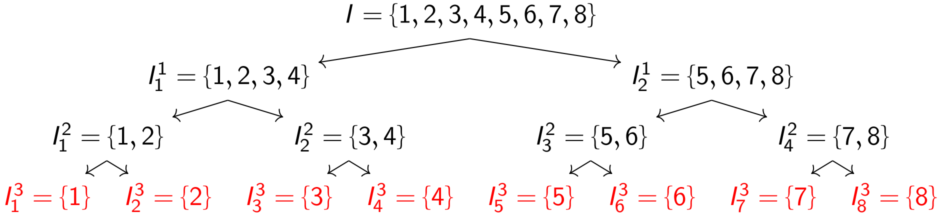

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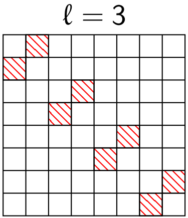

HODLR-matrices: definition

HODLR matrix

Let $A \in \mathbb{R}^{n \times n}$ and consider a cluster tree $\mathcal{T}_p$.

1. Given $k \in \mathbb{N}$, A is said to be a $(\mathcal{T}_p, k)$-HODLR matrix if every off-diagonal block

$$A(I_i^\ell, I_j^\ell) \quad \text{such that } I_i^\ell \text{ and } I_j^\ell \text{ are siblings in } \mathcal{T}_p, \quad \ell = 1, \dots, p,$$

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- $\mathcal{T}_p$ is often chosen to be as balanced as possible, i.e., cardinalities of I_i^ℓ are nearly equal for a given ℓ, with a dept determined by a minimal diagonal block size $n_{\min}$.
- The classical choice is to have a **binary tree**, i.e., $n = 2^p n_{\min}$.

HODLR-matrices: occupied space

If we assume **identical ranks** k and a **balanced partitioning** then

- Storage for off-diagonal blocks $A(I_i^\ell, I_j^\ell) = U_i^{(\ell)} (V_j^{(\ell)})^T,\ U_i^{(\ell)}, V_j^{(\ell)} \in \mathbb{R}^{m_\ell \times k}$:
  On level $\ell > 0$ there are 2^ℓ off-diagonal blocks

$$2k \sum_{\ell=1}^{p} 2^\ell m_\ell = 2kn_0 \sum_{\ell=1}^{p} 2^\ell 2^{p-\ell} 2kn_0 p 2^p = 2knp = 2kn \log_2(n/n_0),$$

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$$2k \sum_{\ell=1}^{p} 2^\ell m_\ell = 2kn_0 \sum_{\ell=1}^{p} 2^\ell 2^{p-\ell} 2kn_0 p 2^p = 2knp = 2kn \log_2(n/n_0),$$

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HODLR-matrices: occupied space

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- Both requirements on ranks and partitioning can be relaxed to obtain similar results.

HODLR-matrices: building the representation

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If A is **sparse**:

- Use a **two sided Lanczos method** only requiring matrix-vector multiplications with an off-diagonal block and its transpose, combined with recompression to each off-diagonal block.

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If A is **structured** use an *ad-hoc* constructor!

HODLR of Grünwald–Letnikov

Theorem (Fiedler 2010, Theorem A)

Let $\mathbf{x}, \mathbf{y}$ two real vectors of length N, with ascending and descending ordered entries, respectively. Moreover, we denote with $C(\mathbf{x}, \mathbf{y})$ the Cauchy matrix defined by

$$C_{ij} = \frac{1}{x_i - y_j}, \qquad i, j = 1, \dots, N.$$

If $C(\mathbf{x}, \mathbf{y}) = C(\mathbf{x}, \mathbf{y})^T$, $x_i \in [a, b]$, $y_j \in [c, d]$ with $a > d$, then $C(\mathbf{x}, \mathbf{y})$ is positive definite.

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Theorem (Beckermann and Townsend 2019, Theorem 5.5)

Let H be a positive semidefinite Hankel matrix of size N. Then, the ϵ-rank of H is bounded by

$$\mathrm{rank}_\epsilon(H) \leq 2 + 2\left\lceil \frac{2}{\pi^2} \log\left(\frac{4}{\pi}N\right) \log\left(\frac{16}{\epsilon}\right) \right\rceil \triangleq \mathfrak{B}(N, \epsilon).$$

HODLR of Grünwald–Letnikov

We need to work with $G_N \in \mathbb{R}^{N\times N}$

$$G_N = -\begin{bmatrix} g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 & 0 \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ g_{N-1}^{(\alpha)} & \ddots & \ddots & \ddots & g_1^{(\alpha)} & g_0^{(\alpha)} \\ g_N^{(\alpha)} & g_{N-1}^{(\alpha)} & \cdots & \cdots & g_2^{(\alpha)} & g_1^{(\alpha)} \end{bmatrix}$$

Lemma (Massei, Mazza, and Robol 2019)

Consider the Hankel matrix H defined as

$$H = (h_{ij}), \qquad h_{ij} = g_{i+j}^{(\alpha)},$$

for $1 \leq \alpha \leq 2$. Then, H is positive semidefinite.

- Show that H is obtained as the sum of a positive definite Cauchy matrix and a positive semidefinite matrix.
- Use the result by Beckermann and Townsend 2019.

HODLR of Grünwald–Letnikov

Proof. For $k \geq 2$ we rewrite $g_k^{(\alpha)}$ as

$$\begin{aligned} g_k^{(\alpha)} &= \frac{(-1)^k}{k!}\alpha(\alpha-1)\dots(\alpha-k+1) \\ &= \frac{\alpha(\alpha-1)}{k!}(k-\alpha-1)(k-\alpha-2)\dots(2-\alpha) \\ &= \alpha(\alpha-1)\frac{\Gamma(k-\alpha)}{\Gamma(k+1)\Gamma(2-\alpha)}. \end{aligned}$$

HODLR of Grünwald–Letnikov

Proof. For $k \geq 2$ we rewrite $g_k^{(\alpha)}$ as

$$g_k^{(\alpha)} = \alpha(\alpha-1)\frac{\Gamma(k-\alpha)}{\Gamma(k+1)\Gamma(2-\alpha)}.$$

Use the Gauss representation of the Euler Γ

$$\Gamma(z) = \lim_{m\to\infty} \frac{m!m^z}{z(z+1)(z+2)\dots(z+m)}, \quad z \neq \{0,-1,-2,\dots\},$$

we rewrite

$$g_k^{(\alpha)} = \alpha(\alpha-1)\lim_{m\to\infty}\frac{1}{m!m^3}\prod_{p=0}^{m}\frac{k+1+p}{k-\alpha+p}(2-\alpha+p).$$

HODLR of Grünwald–Letnikov

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$$g_k^{(\alpha)} = \alpha(\alpha-1)\frac{\Gamma(k-\alpha)}{\Gamma(k+1)\Gamma(2-\alpha)}.$$

We rewrite

$$H = \lim_{m\to+\infty} H_0 \circ \ldots \circ H_m, \qquad (H_p)_{ij} = \frac{i+j+1+p}{i+j-\alpha+p}$$

for $\circ$ the Hadamard product, $\{H_j\}_{j=0}^m$ Hankel matrices.

HODLR of Grünwald–Letnikov

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for $\circ$ the Hadamard product, $\{H_j\}_{j=0}^{m}$ Hankel matrices. Schur Product Theorem tells us that "*the Hadamard product of two positive definite matrices is also a positive definite matrix*" $\Rightarrow$ If $H_0 \circ \ldots \circ H_m$ is positive semidefinite for every m then H is also positive semidefinite.

HODLR of Grünwald–Letnikov

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$$(H_p)_{ij} = \frac{i+j+1+p}{i+j-\alpha+p} = 1 + \frac{\alpha+1}{i+j-\alpha+p}$$

HODLR of Grünwald–Letnikov

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for $\circ$ the Hadamard product, $\{H_j\}_{j=0}^m$ Hankel matrices. Rewrite

$$(H_p)_{ij} = 1 + \frac{\alpha+1}{i+j-\alpha+p}, \quad H_p = \mathbf{1}\mathbf{1}^T + (\alpha+1)\cdot C(\mathbf{x}, -\mathbf{x}), \quad \mathbf{x} = \begin{bmatrix} 1 \\ \vdots \\ N \end{bmatrix} + \frac{p-\alpha}{2}\mathbf{1},$$

$\mathbf{x} \geq 0$ for $\alpha < 2$, thus $C(\mathbf{x}, -\mathbf{x})$ is PD. Then H_p is positive semidefinite as the sum of a PD and positive semidefinite matrix. □

HODLR of Grünwald–Letnikov

Proposition (Massei, Mazza, and Robol 2019, Lemma 3.15)

For every $\epsilon > 0$, the ϵ-qsrank of G_N is bounded by

$$\mathrm{qsrank}_\epsilon(G_N) \leq \mathfrak{B}\left(N, \frac{\epsilon}{2}\right) = 2 + 2\left\lceil \frac{2}{\pi^2}\log\left(\frac{4}{\pi}N\right)\log\left(\frac{32}{\epsilon}\right)\right\rceil.$$

Proof.

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Proof. We just need to work on the lower triangle, for the upper the rank is at most 1 (Hessenberg).

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Proof. Let $Y \in \mathbb{R}^{s\times t}$ be any lower off-diagonal block of G_N. *Without loss of generality* we assume that Y is maximal, i.e. $s + t = N$.

HODLR of Grünwald–Letnikov

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Proof. Let $Y \in \mathbb{R}^{s \times t}$ be any lower off-diagonal block of G_N. *Without loss of generality* we assume that Y is maximal, i.e. $s + t = N$. (If $\operatorname{rank}(Y + \delta Y) = k$ and $\|\delta Y\|_2 \leq \epsilon \| G_N \|_2$ then the submatrices of δY verify the analogous claim for the corresponding ones of Y.)

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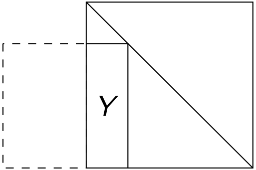
Entries Y are given by $Y_{ij} = -g^{(\alpha)}_{1+i-j+t}$. Call $h = \max\{s, t\}$, and A the $h \times h$ matrix defined by $A_{ij} = -g^{(\alpha)}_{1+i-j+h}$.

HODLR of Grünwald–Letnikov

$A =$ 

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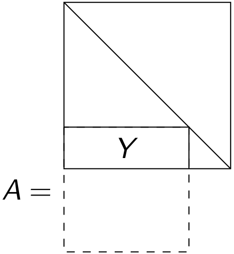
HODLR of Grünwald–Letnikov



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$$A = \begin{bmatrix} A^{(11)} & A^{(12)} \\ A^{(21)} & A^{(22)} \end{bmatrix}, \qquad A^{(ij)} \in \mathbb{C}^{m_{ij} \times n_{ij}}, \qquad \begin{cases} m_{1j} = n_{i1} = \lceil \frac{h}{2} \rceil \\ m_{2j} = n_{i2} = \lfloor \frac{h}{2} \rfloor \end{cases}, \quad \begin{cases} h \leq N - 1, \\ m_{i,j} + n_{i,j} \leq N, \end{cases}$$

HODLR of Grünwald–Letnikov

Proof. and consider the subdiagonal block $T^{(ij)}$ of G_N defined by

$$T^{(ij)} = G_N(N-m_{ij}+1 : N, N-m_{ij}-n_{ij}+1 : N-m_{ij}), \qquad i,j = 1,2, \qquad \begin{array}{l} T^{(ij)} \in \mathbb{R}^{m_{ij} \times n_{ij}}, \\ m_{ij} + n_{ij} \leq N. \end{array}$$

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- 👁 Since $g_j^{(\alpha)} > g_{j+1}^{(\alpha)} > 0$, $|T^{(ij)}| \ge |A^{(ij)}|$ for every $i,j = 1,2$,

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HODLR of Grünwald–Letnikov

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- Being $T^{(ij)}$ and $A^{(ij)}$ nonpositive and the 2 norm monotonous, $\|A^{(ij)}\|_2 \leq \|T^{(ij)}\|_2$.
- By exploiting

$$\begin{aligned} \|A\|_2 &\leq \left\| \begin{bmatrix} A^{(11)} & \\ & A^{(22)} \end{bmatrix} \right\|_2 + \left\| \begin{bmatrix} & A^{(12)} \\ A^{(21)} & \end{bmatrix} \right\|_2 \\ &= \max\{\|A^{(11)}\|_2, \|A^{(22)}\|_2\} + \max\{\|A^{(12)}\|_2, \|A^{(21)}\|_2\} \end{aligned} \qquad \Rightarrow \quad \|A\|_2 \leq 2\|G_N\|_2.$$

HODLR of Grünwald–Letnikov

Proof. and consider the subdiagonal block $T^{(ij)}$ of G_N defined by

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- Conclude by the result on Hankel matrices!

HODLR of Grünwald–Letnikov

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Proof. We call J the $h \times h$ flip matrix, so that $-AJ$ is Hankel and positive semidefinite:

$$\mathrm{rank}_{\frac{\epsilon}{2}}(A) = \mathrm{rank}_{\frac{\epsilon}{2}}(AJ) \le \mathfrak{B}\left(N, \frac{\epsilon}{2}\right).$$

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Y is a submatrix of A, thus there exists δY such that

$$\|\delta Y\|_2 \leq \varepsilon \|G_N\|_2 \text{ and } \mathrm{rank}(Y + \delta Y) \leq \mathfrak{B}\left(N, \frac{\epsilon}{2}\right).$$

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$\Rightarrow \mathrm{qsrank}_{\epsilon}(G_N) \leq \mathfrak{B}\left(N, \frac{\epsilon}{2}\right).$ $\square$

HODLR of Grünwald–Letnikov

Let's do some experiments with the `hm-toolbox` (Massei, Robol, and Kressner 2020).

```
function G = glhodlrmatrix(N,alpha,tol)
%%GLMATRIX produces the GL discretization of
% the Riemann-Liouville derivative in HODLR
% format
g = gl(N,alpha);
c = zeros(N,1);
r = zeros(1,N);
r(1:2) = g(2:-1:1);
c(1:N) = g(2:end);
hodlroption( 'threshold', tol);
G = hodlr('toeplitz',c,r);
end
```

HODLR of Grünwald–Letnikov

Let's do some experiments with the `hm-toolbox` (Massei, Robol, and Kressner 2020).

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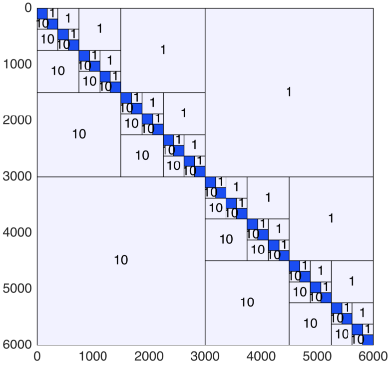

```
G = glhodlrmatrix(6000,1.5,1e-6);
```

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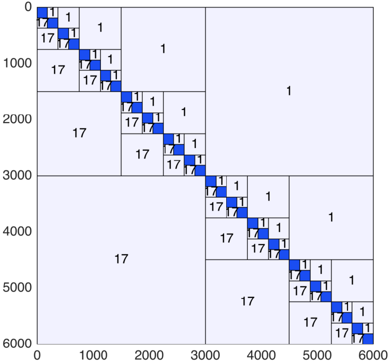

```
G = glhodlrmatrix(6000,1.5,1e-9);
```

HODLR of Grünwald–Letnikov

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```
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% format
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r = zeros(1,N);
r(1:2) = g(2:-1:1);
c(1:N) = g(2:end);
hodlroption( 'threshold', tol);
G = hodlr('toeplitz',c,r);
end
```

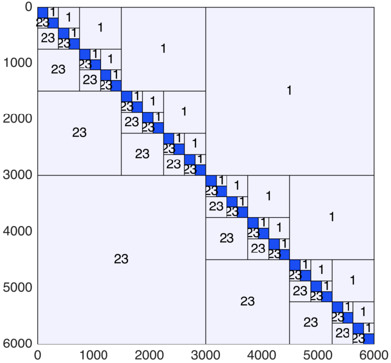

```
G = glhodlrmatrix(6000,1.5,1e-12);
```

HODLR Matrix: the whole discretization

Matrix G_N was only a piece of the whole discretization matrix

$$A_N = I_N + \frac{\Delta t}{h^\alpha}\left(D^{+}_{(m)} G_N + D^{-}_{(m)} G_N^T\right),$$

does it share the same structure?

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Corollary (Massei, Mazza, and Robol 2019, Corollary 3.16)

$$\operatorname{qsrank}_{\epsilon}(A_N) \leq 3 + 2 \left\lceil \frac{2}{\pi^2} \log\left(\frac{4}{\pi} N\right) \log\left(\frac{32}{\hat{\epsilon}}\right) \right\rceil, \quad \hat{\epsilon} \triangleq \frac{\|A_N\|}{\|G_N\| \cdot \max\{\|D^{+}_{(m)}\|, \|D^{-}_{(m)}\|\}} \epsilon.$$

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Proof. Result is invariant under scaling, so assume wlog that $\frac{\Delta t}{h^{\alpha}} = 1$.

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Proof. Result is invariant under scaling, so assume wlog that $\frac{\Delta t}{h^\alpha} = 1$. A generic off-diagonal block Y, wlog in the lower triangular part, If Y does not intersect the first subdiagonal, is a subblock of $D^+_{(m)} G_N$, so there exists a perturbation δY with norm bounded by $\|\delta Y\| \leq \|D^+_{(m)}\| \|G_N\| \cdot \hat{\epsilon}$ such that $Y + \delta Y$ has rank at most $\mathfrak{B}(N, \hat{\epsilon}/2)$. In particular, δY satisfies $\|\delta Y\| \leq \|A_N\| \cdot \epsilon$.

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Proof. Result is invariant under scaling, so assume wlog that $\frac{\Delta t}{h^\alpha} = 1$. Since we have excluded one subdiagonal, a generic off-diagonal block Y we can find a perturbation with norm bounded by $\|A_N\| \cdot \epsilon$ such that $Y + \delta Y$ has rank $1 + \mathfrak{B}(N, \hat{\epsilon}/2)$. $\square$

A HODLR right-hand side

❓ What are right-hand sides functions $f(x, y, t)$ so that the matrix C has a HODLR structure?

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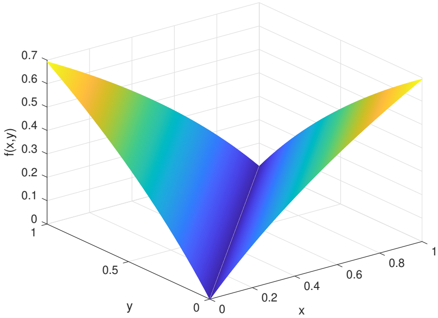
Consider the function

$$f(x, y) = \log(\tau + |x - y|), \quad \tau > 0.$$



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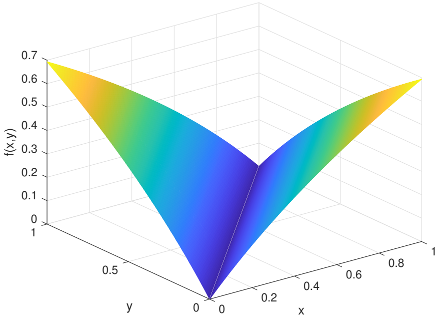

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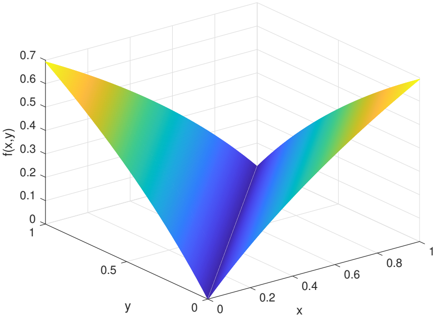

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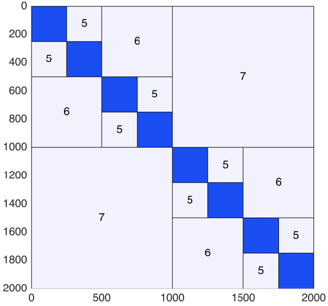
- We can use again Chebyshev basis to approximate it in a separable fashion.



```
x = linspace(0,1,N); y = linspace(0,1,N);
[X,Y] = meshgrid(x,y); tau = 1;
C = log(tau + abs(X-Y)); hC = hodlr(C);
```

Separability (a bit more formally)

Separable expansion (Hackbusch 2015, Definition 4.4)

Take a function $\chi(x, y) : X \times Y \to \mathbb{R}$, we call

$$\chi(x,y) = \sum_{\nu=1}^{r} \phi_{\nu}^{(r)}(x)\psi_{\nu}^{(r)}(y) + R_r(x,y), \qquad \text{for } x \in X,\ y \in Y,$$

a *separable expansion* of χ with r terms in $X \times Y$ with remainder R_r.

- 🔧 To have an idea of the **goodness** of the *separable expansion*, we would like to have $\{\|R_r\|_{\infty}, \|R_r\|_{\mathbb{L}^p}\} \xrightarrow{r \to 0} 0$ as fast as possible, e.g., **exponentially**.

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- If $\|R_r\| \leq c_1 \exp(-c_2 r^\alpha) \Rightarrow \|R_r\| \leq \varepsilon$ if $r \geq \left\lceil \left(\frac{1}{c_2} \log^{1/\alpha} \frac{c_1}{\varepsilon} \right) \right\rceil = O(\log^{1/\alpha} 1/\varepsilon)$ $\varepsilon \to 0$.

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- We can use Taylor expansions, Chebyshev expansion, Hermite/Lagrange interpolation, cross approximation... In all the cases, the behavior of R_r is tied to the regularity of $\chi(x, y)$; see (Hackbusch 2015, Chapter 4).

BLAS with HODLR format

? We now have **everything represented in the right format**, but can we operate with it?

BLAS with HODLR format

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$\mathbf{y} = A\mathbf{x}$: Matrix-vector products, *recursively*:

$$\begin{aligned}
\mathbf{y}(I_1^1) &= A(I_1^1, I_1^1)\mathbf{x}(I_1^1) + A(I_1^1, I_2^1)\mathbf{x}(I_2^1),\\
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⚙ Off-diagonal blocks $A(I_1^1, I_2^1)$ and $A(I_2^1, I_1^1)$ are obtained by multiplying $n/2 \times n/2$ low-rank matrix with vector. This **cost** $c_{\mathrm{LR}\cdot\mathbf{x}}(n/2) = 2nk$.

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- ⚙ Diagonal blocks are processed recursively at a **cost**

$$c_{A\cdot\mathbf{x}}(n) = 2c_{A\cdot\mathbf{x}}(n/2) + 4kn + n.$$

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- Diagonal blocks are processed recursively at a **cost**

$$c_{A\cdot\mathbf{x}}(n) = 2c_{A\cdot\mathbf{x}}(n/2) + 4kn + n.$$

Master theorem (*divide and conquer*): $c_{A\cdot\mathbf{x}}(n) = (4k+1)\log_2(n)n.$

BLAS with HODLR format

$C = A + B$: Adding two equally partitioned HODLR matrices **increases the ranks** of off-diagonal blocks by a factor 2.

BLAS with HODLR format

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- ⚙ We need truncation $\mathfrak{T}_k(A(I_1^\ell, I_j^\ell) + B(I_1^\ell, I_j^\ell))$, costs

$$c_{\mathrm{LR+LR}} = c_{\mathrm{SVD}} \times (nk^2 + k^3),$$

  where c_{SVD} is the cost of the given low-rank truncation algorithm (SVD, rand-SVD, QR, ...)

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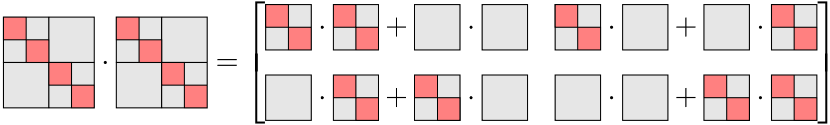
where c_{SVD} is the cost of the given low-rank truncation algorithm (SVD, rand-SVD, QR, ...)

Total cost is then:

$$\begin{aligned}\sum_{\ell=1}^{p} 2^\ell c_{\mathrm{LR+LR}}(m_\ell) =& c_{\mathrm{SVD}} \sum_{\ell=1}^{p} 2^\ell (k^3 + m_\ell k^2) \\ \leq& c_{\mathrm{SVD}} \left(2^{p+1} k^3 + \sum_{\ell=1}^{p} 2^\ell 2^{p-\ell} n_0 k^2 \right) \\ \leq& c_{\mathrm{SVD}} \left(2nk^3 + n \log_2(n) k^2 \right).\end{aligned}$$

BLAS with HODLR format

$C = AB$: Matrix-matrix multiplication can also be done recursively



where ▚ is a $n/2 \times n/2$ HODLR matrix and □ is a low-rank block.

BLAS with HODLR format

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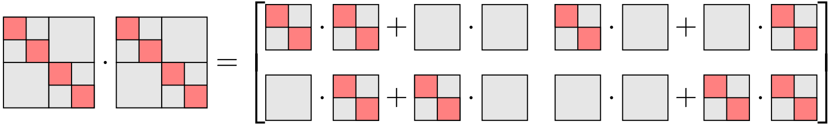

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1. ▦ · ▦ · of 2 HODLR $n/2$ matrices,

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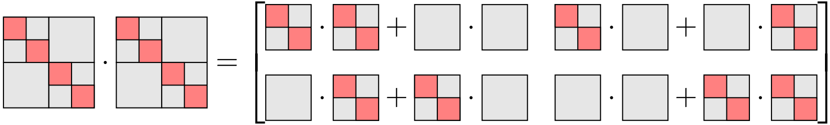

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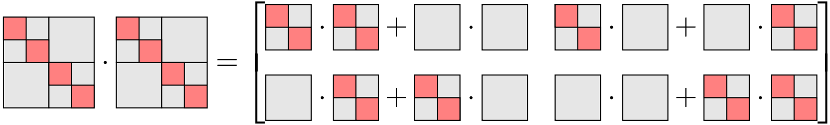

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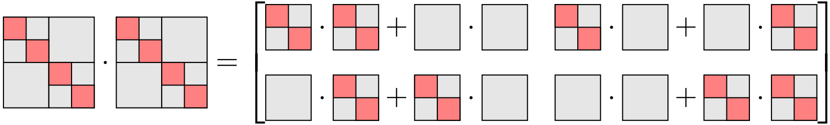

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4. □ · ⊞ · of low-rank times HODLR.

BLAS with HODLR format

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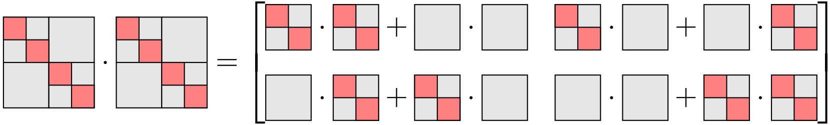

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$$\begin{aligned} c_{H\cdot H}(n) = & 2\left(c_{H\cdot H}(^{n}/_{2}) + c_{\mathrm{LR}\cdot \mathrm{LR}}(^{n}/_{2}) + c_{H\cdot \mathrm{LR}}(^{n}/_{2}) + c_{\mathrm{LR}\cdot H}(^{n}/_{2})\right. \\ & \left. + c_{H+\mathrm{LR}}(^{n}/_{2}) + c_{\mathrm{LR}+\mathrm{LR}}(^{n}/_{2})\right) \end{aligned}$$

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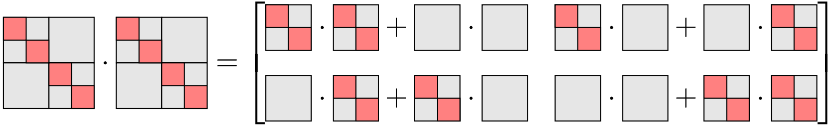

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$c_{\mathrm{LR}\cdot\mathrm{LR}}(n) = 4nk^2$

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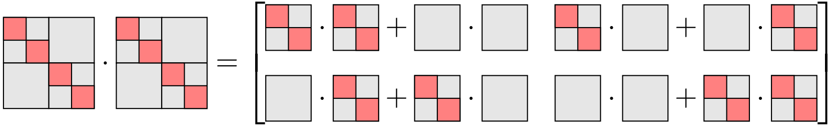

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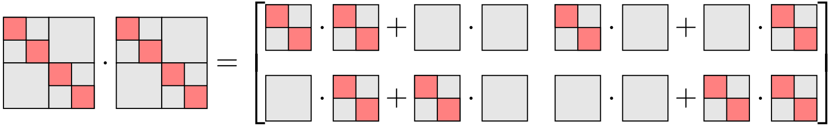
$$c_{H\cdot H}(n) = 2\left(c_{H\cdot H}(n/2) + c_{\mathrm{LR}\cdot\mathrm{LR}}(n/2) + {\color{red}c_{H\cdot\mathrm{LR}}(n/2)} + {\color{red}c_{\mathrm{LR}\cdot H}(n/2)}\right.$$
$$\left.+{\color{red}c_{H+\mathrm{LR}}(n/2)} + c_{\mathrm{LR}+\mathrm{LR}}(n/2)\right)$$

$$c_{H\cdot\mathrm{LR}}(n) = c_{\mathrm{LR}\cdot H} = k c_{H\mathbf{v}}(n) = k(4k+1)\log_2(n)n$$

BLAS with HODLR format

$C = AB$: Matrix-matrix multiplication can also be done recursively



where ⊞ is a $n/2 \times n/2$ HODLR matrix and □ is a low-rank block.

1. ⊞ · ⊞ · of 2 HODLR $n/2$ matrices,
2. □ · □ · of 2 low-rank blocks,
3. ⊞ · □ · of HODLR times low-rank,
4. □ · ⊞ · of low-rank times HODLR.

$$\begin{aligned} c_{H\cdot H}(n) =& 2\left(c_{H\cdot H}(n/2) + c_{\mathrm{LR}\cdot \mathrm{LR}}(n/2) + c_{H\cdot \mathrm{LR}}(n/2) + c_{\mathrm{LR}\cdot H}(n/2)\right. \\ & \left. + c_{H+\mathrm{LR}}(n/2) + c_{\mathrm{LR}+\mathrm{LR}}(n/2)\right) \end{aligned}$$

$$c_{H+\mathrm{LR}}(n) = c_{H+H}(n) = c_{\mathrm{SVD}}(nk^3 + n\log(n)k^2)$$

BLAS with HODLR format

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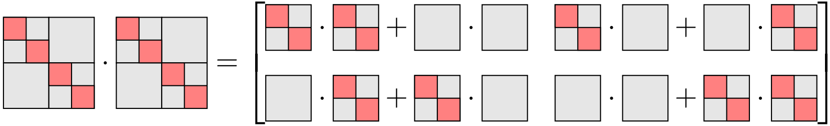

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Total cost $c_{H \cdot H}(n) \in O(k^3 n \log n + k^2 n \log^2 n)$.

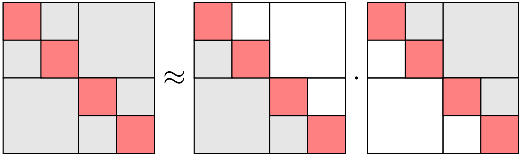
BLAS with HODLR format

Approximate solution of a linear system $A\mathbf{x} = \mathbf{b}$ with HODLR matrix A:

BLAS with HODLR format

Approximate solution of a linear system $A\mathbf{x} = \mathbf{b}$ with HODLR matrix A:

$A \approx LU$ Approximate LU-factorization $A \approx LU$ in HODLR format:



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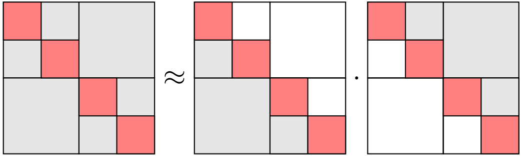

Forward substitution to solve $L\mathbf{y} = \mathbf{b}$,

Backward substitution to solve $U\mathbf{x} = \mathbf{y}$.

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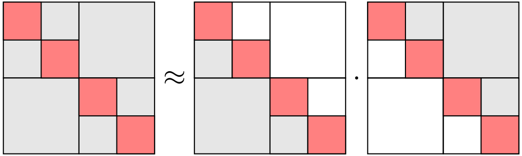

Forward substitution to solve $L\mathbf{y} = \mathbf{b}$,

Backward substitution to solve $U\mathbf{x} = \mathbf{y}$.

We need to analyze the two steps separately.

BLAS with HODLR format

Approximate LU factorization, on level $\ell = 1$:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad L = \begin{bmatrix} L_{11} & O \\ L_{21} & L_{22} \end{bmatrix}, \quad U = \begin{bmatrix} U_{11} & U_{12} \\ O & U_{22} \end{bmatrix}$$

It is done in four steps

BLAS with HODLR format

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4. Compute LU factors L_{22}, U_{22} of $A_{22} - L_{21} U_{12}$.

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The analysis of the cost is *analogous to the matrix-matrix multiplication case*, **but** we need to know how to do and how-much does forward/backward substitution costs.

BLAS with HODLR format

Forward substitution with lower triangular L in HODLR format: $\mathbf{y} = L^{-1}\mathbf{b}$

$$L = \begin{bmatrix} L_{11} & O \\ L_{21} & L_{22} \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}$$

with L_{21} low-rank, and L_{11}, L_{22} HODLR.

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Cost recursively:

$$c_{\text{forw}} = 2c_{\text{forw}}(n/2) + (2k+1)n.$$

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On level $\ell = p$, we have the direct solution of $2^p = n/n_0$ linear systems of size $n_0 \times n_0$.

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Total cost $c_{\mathrm{forw}} \in O(kn\log(n))$, and analogously for backward substitution.

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- Total cost $c_{\text{forw}} \in O(kn\log(n))$, and analogously for backward substitution.
- Total cost $c_{\text{LU}}(n) \lesssim c_{H\cdot H}(n) \in O(k^3 n \log n + k^2 n \log^2 n)$.

BLAS with HODLR format

The `hm-toolbox` (Massei, Robol, and Kressner 2020) contains all the routines.

- They *overload* the standard MATLAB operation by the same name, i.e., if you have variables in the right class you operate directly in this format.
- One can use different **cluster tree** $\mathcal{T}_p$ to get smaller ranks. They are determined by the partitioning of the index set on the leaf level and represented as the vector $\mathbf{c} = [n_1^{(p)}, \dots, n_{2^p}^{(p)}]$, change it to change the HODLR matrix.

Operation	HODLR complexity
`A*v`	$\mathcal{O}(kn\log n)$
`A\v`	$\mathcal{O}(k^2 n\log^2 n)$
`A+B`	$\mathcal{O}(k^2 n\log n)$
`A*B`	$\mathcal{O}(k^2 n\log^2 n)$
`A\B`	$\mathcal{O}(k^2 n\log^2 n)$
`inv(A)`	$\mathcal{O}(k^2 n\log^2 n)$
`A.*B`[2]	$\mathcal{O}(k^4 n\log n)$
`lu(A)`, `chol(A)`	$\mathcal{O}(k^2 n\log^2 n)$
`qr(A)`	$\mathcal{O}(k^2 n\log^2 n)$
compression	$\mathcal{O}(k^2 n\log(n))$

---

[2] The complexity of the Hadamard product is dominated by the recompression stage due to the k^2 HODLR rank of $A \circ B$. Without recompression the cost is $\mathcal{O}(k^2 n\log n)$.

HODLR solver for the 1D case

We can modify our first example to get a solution for the 1D problem in the new format.

```
%% Discretization
N = 2^7; hN = 1/(N-1);  x = 0:hN:1; dt = hN;
alpha = 1.5; % Coefficients
dplus=@(x)gamma(3-alpha).*x.^alpha;
dminus=@(x)gamma(3-alpha).*(1-x).^alpha;
w = @(x) 5*x.*(1-x);
tol = 1e-9; % HODLR building
tic;
G = glhodlrmatrix(N,alpha,tol);
Dplus = hodlr('diagonal',dplus(x));
Dminus = hodlr('diagonal',dminus(x));
I = hodlr('eye', N);
nu = hN^alpha/dt;
A = nu*I -(Dplus*G + Dminus*G');
buildtime = toc;
```

```
%% Solving
[L,U] = lu(A);
flu = @() lu(A);
timelu = timeit(flu,2);
w = w(x).';
solvetime = 0;
for i=1:N
 tic;
 w = U\(L\(nu*w));
 solvetime = solvetime + toc;
end
solvetime = solvetime/N;
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```
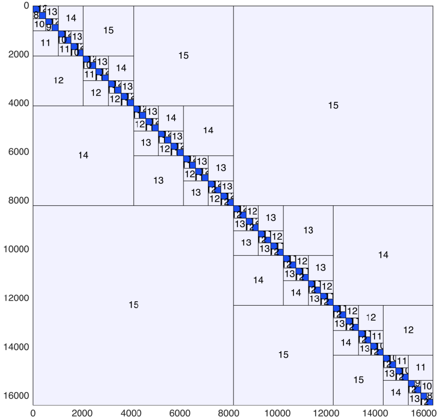

Let us try looking at the timings.

HODLR solver for the 1D case

We take $\alpha = 1.5$, and $\varepsilon = 10^{-9}$

N	Build (s)	LU (s)	Avg. Solve (s)
2^7	8.96e-03	1.44e-04	2.93e-04
2^8	1.35e-02	4.63e-04	3.33e-04
2^9	3.14e-02	2.05e-03	5.41e-04
2^{10}	7.28e-02	6.21e-03	9.35e-04
2^{11}	1.59e-01	1.63e-02	1.75e-03
2^{12}	3.85e-01	4.33e-02	3.68e-03
2^{13}	8.81e-01	1.27e-01	7.99e-03
2^{14}	2.19e+00	3.73e-01	1.55e-02



Largest matrix occupies 46.25 Mb, against the 2 Gb of the dense storage and the 0.87 Mb of storing three diagonals and $2 \times (2N - 1)$ for the Toeplitz storage.

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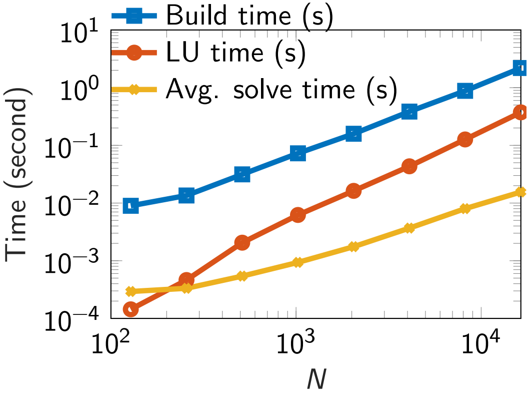

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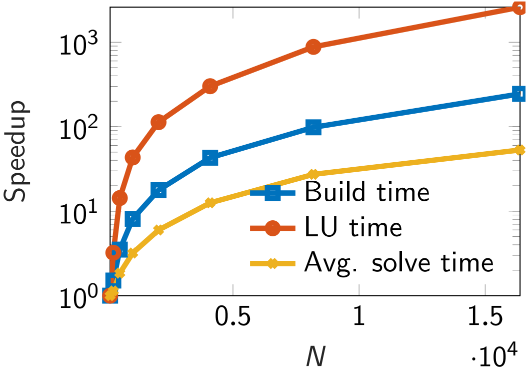

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Back to Sylvester (Massei, Palitta, and Robol 2018)

To solve the Sylvester equation with HODLR coefficients

$$AX + XB^T = C, \qquad A \in \mathbb{R}^{n\times n},\ \ B \in \mathbb{R}^{m\times m},\ \ X, C \in \mathbb{R}^{n\times m},$$

we can use the integral formulation

$$X = \int_0^{+\infty} e^{-At} C e^{-B^T t}\, \mathrm{d}t.$$

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We perform the *change of variables*: $t = f(\theta) \triangleq L \cdot \cot\left(\frac{\theta}{2}\right)^2$, rewriting the integral as

$$X = 2L \int_0^{\pi} \frac{\sin(\theta)}{(1-\cos(\theta))^2}\ e^{-Af(\theta)} C e^{-B^T f(\theta)}\,\mathrm{d}\theta,$$

with L a parameter to be optimized for convergence.

Back to Sylvester (Massei, Palitta, and Robol 2018)

We now have an integral on a finite domain $\Rightarrow$ **Gauss-Legendre quadrature**

$$X \approx \sum_{j=1}^{m} \omega_j \cdot e^{-Af(\theta_j)} C e^{-B^T f(\theta_j)},$$

for $\{\theta_j, w_j\}_{j=1}^{m}$ are the Legendre points and weights, and $\omega_j = 2Lw_j \cdot \frac{\sin(\theta_j)}{(1-\cos(\theta_j))^2}$.

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❓ The **dominant cost** is now computing $e^{-Af(\theta_j)}$ and $e^{-B^T f(\theta_j)}$, how do we do it?

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</> A **good idea** could be using *rational approximation* to $\exp(t)$

Back to Sylvester (Massei, Palitta, and Robol 2018)

We now have an integral on a finite domain ⇒ **Gauss-Legendre quadrature**

$$X \approx \sum_{j=1}^{m} \omega_j \cdot e^{-Af(\theta_j)} C e^{-B^T f(\theta_j)},$$

for $\{\theta_j, w_j\}_{j=1}^{m}$ are the Legendre points and weights, and $\omega_j = 2Lw_j \cdot \frac{\sin(\theta_j)}{(1-\cos(\theta_j))^2}$.

- The **dominant cost** is now computing $e^{-Af(\theta_j)}$ and $e^{-B^T f(\theta_j)}$, how do we do it?
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🚪 (d,d)-Padé with *scaling and squaring* $e^A = (e^{2^{-k}A})^{2^k}$ and $k = \lceil \log_2 \|A\|_2 \rceil$.

🚪 Rational Chebyshev function (Popolizio and Simoncini 2008):

$$e^x \approx \frac{r_1}{x - s_1} + \ldots + \frac{r_d}{x - s_d}.$$

requiring d inversions and additions that is uniformly accurate for every positive value of t, and thus is better in the case in which $\|A\|_2$ is large.

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/* Solves $AX + XB^T = C$ with $m$
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 accuracy!  */
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If the right-hand side C is low-rank, and the structure in the matrices A and B is HODLR, thus permitting to perform fast matrix vector multiplications and system solutions; then we can apply the *extended Krylov subspace method* we had already seen.

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A numerical test (Massei, Mazza, and Robol 2019)

We use the usual square $[0,1]^2$, and the source f

$$f(x,y,t) = 100 \cdot (\sin(10\pi x)\cos(\pi y) + \sin(10t)\sin(\pi x) \cdot y(1-y)) \,.$$

for both **constant coefficient** $d^+ = d^- = 1$, and variable coefficients

$$\begin{aligned} d_1^+(x) &= \Gamma(1.2)(1+x)^{\alpha_1}, & d_1^-(x) &= \Gamma(1.2)(2-x)^{\alpha_1}, \\ d_2^+(y) &= \Gamma(1.2)(1+y)^{\alpha_2}, & d_2^-(y) &= \Gamma(1.2)(2-y)^{\alpha_2}. \end{aligned}$$

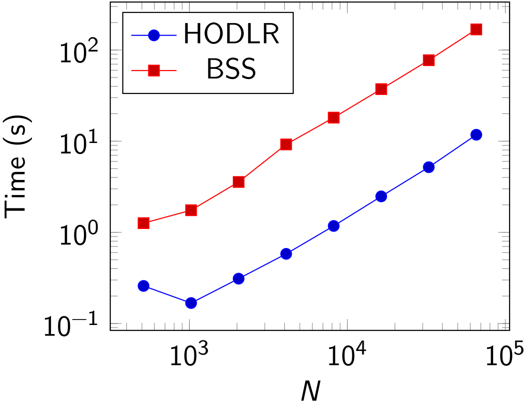
The fractional orders are $\alpha_1 = 1.3, \alpha_2 = 1.7$, and $\alpha_1 = 1.7, \alpha_2 = 1.9$. Methods are

- Sylvester by Extended-Krylov with stopping $\epsilon = 10^{-6}$ (HODLR),
  - HODLR arithmetic is set to work with a truncation of 10^{-8}.
- Sylvester by Extended-Krylov with stopping $\epsilon = 10^{-6}$ (Breiten, Simoncini, and Stoll 2016),
  - Inner solve with: GMRES with tolerance 10^{-7} and *structured preconditioners*,

A numerical test (Massei, Mazza, and Robol 2019)

Constant coefficient with $\alpha_1 = 1.3$ and $\alpha_2 = 1.7$.

N	t_{HODLR}	t_{BSS}	rank_ϵ	qsrank_ϵ
512	0.26	1.26	14	11
1,024	0.17	1.75	15	11
2,048	0.31	3.57	15	12
4,096	0.58	9.21	16	12
8,192	1.17	18.14	16	13
16,384	2.48	37.24	16	13
32,768	5.18	77.28	16	14
65,536	11.76	168.29	15	14



`FD_Example.m` from github.com/numpi/fme

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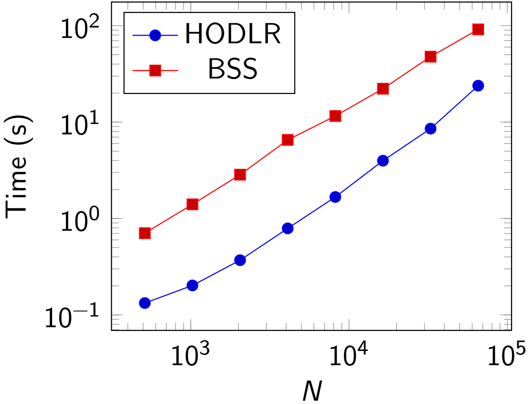
Constant coefficient with $\alpha_1 = 1.7$ and $\alpha_2 = 1.9$.

N	t_{HODLR}	t_{BSS}	rank_ϵ	qsrank_ϵ
512	0.13	0.7	17	10
1,024	0.2	1.4	18	10
2,048	0.37	2.85	19	11
4,096	0.79	6.53	20	11
8,192	1.67	11.57	20	11
16,384	3.98	22.2	21	11
32,768	8.56	47.75	22	11
65,536	23.86	91.53	23	11



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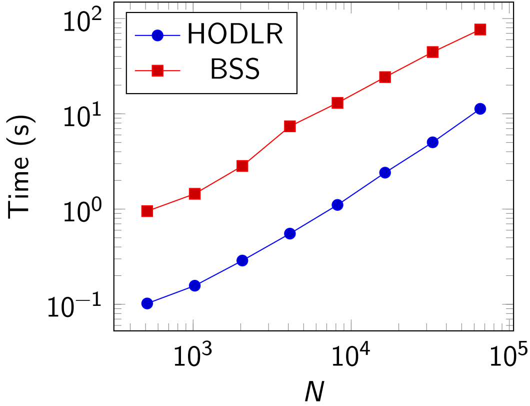
Non-constant coefficient case with $\alpha_1 = 1.3$ and $\alpha_2 = 1.7$.

N	t_{HODLR}	t_{BSS}	rank_ϵ	qsrank_ϵ
512	0.1	0.95	14	10
1,024	0.16	1.45	14	11
2,048	0.29	2.83	15	12
4,096	0.55	7.39	16	12
8,192	1.11	13.02	16	13
16,384	2.41	24.27	16	13
32,768	5.02	44.5	16	14
65,536	11.28	76.78	16	14

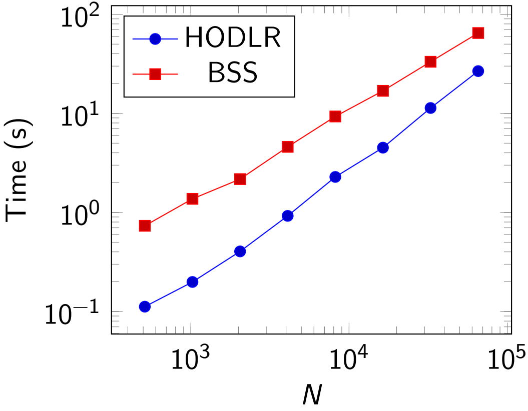


`FD_Example_vc.m` from github.com/numpi/fme

A numerical test (Massei, Mazza, and Robol 2019)

Non-constant coefficient case with $\alpha_1 = 1.7$ and $\alpha_2 = 1.9$.

N	t_{HODLR}	t_{BSS}	rank_ϵ	qsrank_ϵ
512	0.11	0.73	18	10
1,024	0.2	1.37	19	10
2,048	0.4	2.17	20	11
4,096	0.92	4.59	21	11
8,192	2.28	9.31	22	11
16,384	4.51	16.89	22	11
32,768	11.33	33.19	23	12
65,536	26.71	64.73	24	12



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here the spectrum is *fictitiously independent from the discretization*, i.e., all matrix-equation solvers perform a number of iteration independent from the system size: the cost is reduced to the extended Krylov subspace cost! **But** we still have time-stepping to do.

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- ❗ Still looking for a way to solve **everything** *all-at-once* compactly.

Conclusion and summary

- ✓ We have seen how to work with matrices in HODLR format,
- ✓ We have discussed a couple of strategy to solve Sylvester equations with HODLR coefficients,
- ✓ We have applied all the machinery to solve a time step of a 2D equation FDE.

Next up

- Back to *all-at-once* solution with respect to both space and time,
- Linear multistep formulas in boundary value form,
- Structured preconditioner for LMFs,
- Tensor-Train reformulation of the problem.

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