Matrix-free construction of HSS representations using adaptive randomized sampling

Xiaoye Sherry Li
xsli@lbl.gov

Gustavo Chavez, Pieter Ghysels, Chris Gorman, Yang Liu
Lawrence Berkeley National Laboratory

Chris Gorman, UC Santa Barbara

Randomized Numerical Linear Algebra and Applications

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Hierarchical matrix approximation

- Same mathematical foundation as FMM (Greengard-Rokhlin'87), put in matrix form:
  - Diagonal block ("near field") represented exactly
  - Off-diagonal block ("far field") approximated via low-rank format

FMM
separability of Green's function

$$G(x, y) \approx \sum_{\ell=1}^{r} f_\ell(x) g_\ell(y)$$

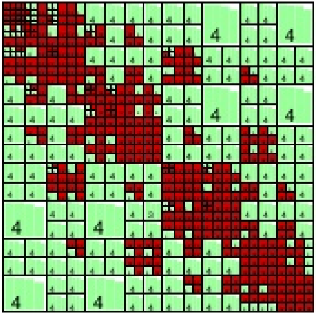
$$x \in X, y \in Y$$

Algebraic
low rank off-diagonal

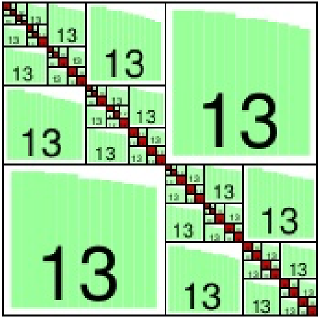
$$A = \left[\begin{array}{c|c} D_1 & U_1 B_1 V_2^T \\ \hline U_2 B_2 V_1^T & D_2 \end{array}\right]$$

- Algebraic power: matrix multiplication, factorization, inversion, tensors, ...

Hierarchical matrix formats



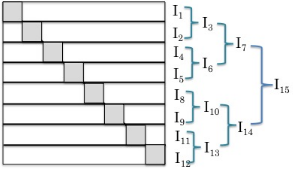
H-matrix (W. Hackbusch et al.)
O(r N log N)



HSS matrix (J Xia et al.)
O(r N)

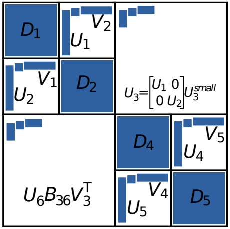
Block cluster tree and nested bases

Example: Hierarchically Semi-Separable matrices (HSS)



- Diagonal blocks are full rank: $D_\tau = A(I_\tau, I_\tau)$
- Off-diagonal blocks as low-rank:

$$A_{\nu_1,\nu_2} = A(I_{\nu_1}, I_{\nu_2}) = U_{\nu_1} B_{\nu_1,\nu_2} V_{\nu_2}^*$$



- **Column bases U and row bases V^* are nested:**

$$U_\tau = \begin{bmatrix} U_{\nu_1} & 0 \\ 0 & U_{\nu_2} \end{bmatrix} U_\tau^{\text{small}}, \; V_\tau = \begin{bmatrix} V_{\nu_1} & 0 \\ 0 & V_{\nu_2} \end{bmatrix} V_\tau^{\text{small}}$$

HSS matrix – ULV factorization

ULV-like factored form (U and V^* unitary, L triangular)

$$\Gamma_{1;b\leftrightarrow 2;t}\begin{bmatrix} I & & & \\ & \Omega_1 & & \\ & & I & \\ & & & \Omega_2 \end{bmatrix}\begin{bmatrix} \Gamma_{3;b\leftrightarrow 4;t} & \\ & \Gamma_{5;b\leftrightarrow 6;t} \end{bmatrix}\begin{bmatrix} \Omega_3 & & & \\ & \Omega_4 & & \\ & & \Omega_5 & \\ & & & \Omega_6 \end{bmatrix} A \begin{bmatrix} Q_3^* & & & \\ & Q_4^* & & \\ & & Q_5^* & \\ & & & Q_6^* \end{bmatrix}\begin{bmatrix} \Gamma^T_{3;b\leftrightarrow 4;t} & \\ & \Gamma^T_{5;b\leftrightarrow 6;t} \end{bmatrix}\begin{bmatrix} I & & & \\ & Q_1^* & & \\ & & I & \\ & & & Q_2^* \end{bmatrix}\Gamma^T_{1;b\leftrightarrow 2;t}$$

$$= \left[\begin{array}{ccc|ccc|c}
L_3 & & & & & & \\
0 & L_4 & & & & & \\
(\Omega_1 L_{4,3})_t & (\Omega_1 L_{3,4})_t & L_1 & & & & \\
\hline
 & & & L_5 & & & \\
 & 0 & & 0 & L_6 & & \\
 & & & (\Omega_2 L_{6,5})_t & (\Omega_2 L_{5,6})_t & L_2 & \\
\hline
(\Omega_1 L_{4,3})_b & (\Omega_1 L_{3,4})_b & W_{1;b} Q^*_{1;t} & \multicolumn{3}{c|}{B_{1,2} V_2^* \begin{bmatrix} V_5^* Q^*_{5;t} & & V_5^* Q^*_{5;b} & \\ & V_6^* Q^*_{6;t} & & V_6^* Q^*_{6;b} \end{bmatrix}\begin{bmatrix} I & \\ & Q_2^* \end{bmatrix}} & \\
\multicolumn{3}{c|}{B_{2,1} V_1^* \begin{bmatrix} V_3^* Q^*_{3;t} & & V_3^* Q^*_{3;b} & \\ & V_4^* Q^*_{4;t} & & V_4^* Q^*_{4;b} \end{bmatrix}\begin{bmatrix} I & \\ & Q_1^* \end{bmatrix}} & (\Omega_2 L_{6,5})_b & (\Omega_2 L_{5,6})_b & W_{2;b} Q^*_{2;t} & D_0
\end{array}\right]$$

Low rank compression via randomized sampling (RS)

Approximate range of A:

1. Pick random matrix $\Omega_{n\times(k+p)}$, k target rank, p small, e.g. 10
2. Sample matrix $S = A\Omega$, with slight oversampling p
3. Compute $Q =$ ON-basis(S) via RRQR

Accuracy: [Halko, Martinsson, Tropp, '11]

- On average: $E(\|A - QQ^*A\|) = \left(1 + \frac{4\sqrt{k+p}}{p-1}\sqrt{\min\{m,n\}}\right)\sigma_{k+1}$
- Probabilistic bound: with *probability* $\geq 1 - 3\cdot 10^{-p}$,
  $\|A - QQ^*A\| \leq [1 + 9\sqrt{k+p}\sqrt{\min\{m,n\}}]\,\sigma_{k+1}$

(in 2-norm)

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(in 2-norm)

Benefits:

- Matrix-free, only need matvec
- When embedded in sparse frontal solver, simplifies "extend-add"

HSS compression via RS [Martinsson '11, Xia '13]

- R random matrix with $d = r + p$ columns
  - r is the **estimated maximum rank,** p is oversampling parameter
- Random sampling of matrix A
  - $S^r = AR$, columns of S^r span the column space of A
  - $S^c = A^* R$, columns of S^c span the row space of A
- Only sample off-diagonal blocks at each level (Hankel blocks):
  Block diagonal matrix at level ℓ: $D^{(\ell)} = diag(D_{\tau_1}, D_{\tau_2}, \ldots, D_{\tau_q})$

$$S^{(\ell)} = \left(A - D^{(\ell)}\right) R = S^r - D^{(\ell)} R$$

- Rank-revealing QR on $S^{(\ell)}$

Practical issues

- Need ε-rank: $\|A - QQ^* A\| \leq \varepsilon$
- Non-decay singular spectrum
- Sampling is expensive using traditional dense matvec

Solution:

1. Gradually increase sample size
   - User manually restart from scratch $\rightarrow$ costly!
   - Built-in automatic strategy $\rightarrow$ not to re-do already-compressed blocks.

     $\Rightarrow$ **Need good error estimation!**
2. Faster matvec in sampling: FFT, FMM, Gauss transform, $\mathcal{H}$-matrix, ...

Automatic adaptive sampling is essential for robustness

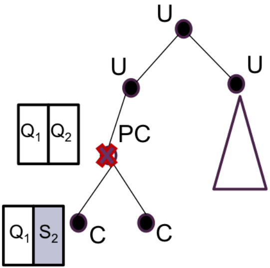
Increase sample size d, build Q incrementally **(block variant)**
$[S_1 \quad S_2 \quad S_3 \quad \dots]$

$Q \leftarrow \emptyset$;
$S_1 \leftarrow A\Omega_1$;
$i \leftarrow 1$;
WHILE (error still large) {
    $Q_i \leftarrow QR(S_i)$;   // Orthogonalize within current block
    $Q \leftarrow [Q \ Q_i]$;
    $S_{i+1} \leftarrow A\Omega_{i+1}$;   // New samples
    $S_{i+1} \leftarrow (I - QQ^*)S_{i+1}$; // Orthogonalize against previous Q
    Compute error;
    $i \leftarrow i + 1$;
}

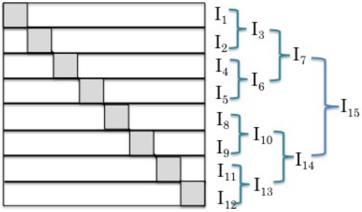
Adaptive sampling in HSS tree

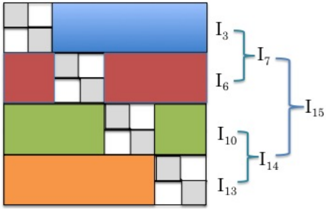
Recall:

- Only have $S = A\Omega$
- At level ℓ:
  $S^{(\ell)} = (A - D^{(\ell)})\Omega = S - D^{(\ell)}\Omega$



Node state:
U – untouched
C – compressed
PC – partially compressed





Adaptive sampling: probabilistic error estimation

- **Goal:** Bound errors for A: $||(I - QQ^*)A||$, but A is not available.
- **Approach:** Use sample S. **Need to establish a stochastic relationship between $||A||$ and $||S||$.**

Let $A \in \mathbb{R}^{m\times n}$, and $x \in \mathbb{R}^n$ with $x_i \sim \mathcal{N}(0,1)$. Consider SVD:

$$A = U\Sigma V^* = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1^* \\ V_2^* \end{bmatrix}$$

Define $\xi = V^* x$, ξ is also a Gaussian random vector.

$$||Ax||_2^2 = ||\Sigma\xi||_2^2 = \xi_1^2\sigma_1^2 + \cdots + \xi_r^2\sigma_r^2. \tag{1}$$

Here, $\sigma_1 \geq \cdots \geq \sigma_r > 0$ are positive singular values. Therefore,

$$\mathbb{E}\left(||Ax||_2^2\right) = \sigma_1^2 + \cdots + \sigma_r^2 = ||A||_F^2. \tag{2}$$

For d sample vectors: $\mathbb{E}\left(||S||_F^2\right) = d\,||A||_F^2$.

Adaptive sampling: stopping criterion

Let $[S_1\ S_2] = [AR_1\ AR_2]$, $Q = QR(S_1)$

Absolute criterion:

$$\|(I - QQ^*)A\|_F \approx \frac{1}{\sqrt{d}}\|(I - QQ^*)S_2\|_F \leq \varepsilon_a$$

Relative criterion:

$$\frac{\|(I - QQ^*)A\|_F}{\|A\|_F} \approx \frac{\|(I - QQ^*)S_2\|_F}{\|S_2\|_F} \leq \varepsilon_r$$

Cost: one reduction to compute norms of the sample vectors.

Estimation accuracy: exponential decaying tail probabilities

Define random variables:

$$X = ||Ax||_2^2 \sim \sigma_1^2 \xi_1^2 + \cdots + \sigma_r^2 \xi_r^2, \quad \overline{X}_d \sim \frac{1}{d}\left[X_1 + \cdots + X_d\right],$$

X_i are independent realizations of X, $\mathbb{E}(X) = \mathbb{E}\left(\overline{X}_d\right) = ||A||_F^2$.

Theorem [C. Gorman]

$$\mathbb{P}\left[\overline{X}_d \geq ||A||_F^2\,\tau\right] \leq \exp\left(-\frac{d\tau}{2}\right) ||A||_F^{dr} \prod_{k=1}^{r} \left(A'_k\right)^{-d} \qquad \tau > 1$$

$$\mathbb{P}\left[\overline{X}_d \leq ||A||_F^2\,\tau\right] \leq \exp\left(-\frac{d\tau}{2}\right) ||A||_F^{dr} \prod_{k=1}^{r} \left(A''_k\right)^{-d} \qquad \tau \in [0,1)$$

where, $(A'_k)^2 = ||A||_F^2 - \sigma_k^2, \quad (A''_k)^2 = ||A||_F^2 + \sigma_k^2$.

This shows the probability tails of X and $\overline{X}_d$ decay exponentially away from the mean $||A||_F^2$.

Adaptive sampling example: decay singular value

$A = \alpha I + UDV^*$, U, V $rank = 120$, $D_{k,k} = 2^{-24(k-1)/r}$

$\varepsilon_r \backslash \varepsilon_a$	1e-2	1e-4	1e-6	1e-8	1e-10	1e-12	1e-14
1e-1	24; 64	24; 64	24; 64	24; 64	24; 64	24; 64	24; 64
1e-2	42; 80	42; 80	42; 80	42; 80	42; 80	42; 80	42; 80
1e-3	59; 96	59; 96	59; 96	59; 96	59; 96	59; 96	59; 96
1e-4	77; 112	77; 112	77; 112	77; 112	77; 112	77; 112	77; 112
1e-5	94; 128	94; 128	94; 128	94; 128	94; 128	94; 128	94; 128
1e-6	111; 128	111; 128	111; 128	111; 128	111; 128	111; 128	111; 128
1e-7	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128
1e-8	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128

Table 10: Size: 100000; Alpha: 100000; Rank: 120; Decay-value: 24; d-start: 16; d-add: 16. These numbers are "(Computed HSS Rank); (Random Samples Used)". Here, we are using $\text{fl}\left[\left(I - Q_1 Q_1^*\right) S_2\right] = \left(I - Q_1 Q_1^*\right)^2 S_2$, with the products computed intelligently.

Adaptive sampling: non-decay singular values

$A = \alpha I + UDV^*$, U, V $rank = 120$, $D_{k,k} = 1$

$\varepsilon_r \backslash \varepsilon_a$	1e-2	1e-4	1e-6	1e-8	1e-10	1e-12	1e-14
1e-1	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128
1e-2	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128
1e-3	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128
1e-4	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128
1e-5	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128	120; 128
1e-6	120; 128	120; 128	120; 128	120; 128	120; 768	120; 768	120; 768
1e-7	120; 128	120; 128	120; 128	120; 128	120; 768	120; 768	120; 768
1e-8	120; 128	120; 128	120; 128	120; 128	120; 768	120; 768	120; 768

Table 8: Size: 100000; Alpha: 100000; Rank: 120; Decay-value: 0; d-start: 16; d-add: 16. These numbers are "(Computed HSS Rank); (Random Samples Used)". Here, we are using $\mathrm{fl}\left[\left(I - Q_1 Q_1^*\right) S_2\right] = \left(I - Q_1 Q_1^*\right)^2 S_2$, with the products computed intelligently.

Adaptivity cost is small

$A = \alpha I + UDV^*$, U, V $rank = 1200$, $D_{k,k} = 2^{-24(k-1)/r}$, $N = 60,000$, $P = 1024$, $\varepsilon_a = \varepsilon_r = 10^{-14}$

		"Known-rank"	Adaptive	"Hard-restart"
$d_0 = 128$ $\Delta d = 64$	Compr. time	36.5	37.2	100.3
	HSS-rank	1162	1267	1165
	Num. adapt.	0	17	4

Mitigate dense sampling cost

- HSS compression cost = sampling cost + $O(r^2 N)$.
- Sampling cost:
  - Traditional matvec: $O(rN^2)$
  - FFT: $O(rN \log N)$ (e.g., Toeplitz)
  - FMM: $O(rN)$

Mitigate dense sampling cost

- Kernel Rdge Regression for classification [IPDPS ParLearning Workshop 2018]
  - Kernel matrix: $K_{ij} = exp(-\frac{1}{2}\frac{||x_i - x_j||^2}{h^2})$
  - Need to solve $w := (K + \lambda I)^{-1} y$; **a few digits suffice** $\rightarrow$ use HSS
- **Use $\mathcal{H}$-matrix to perform sampling for HSS construction.**
  UCI dataset; parallel runtime on Intel Haswell at NERSC.

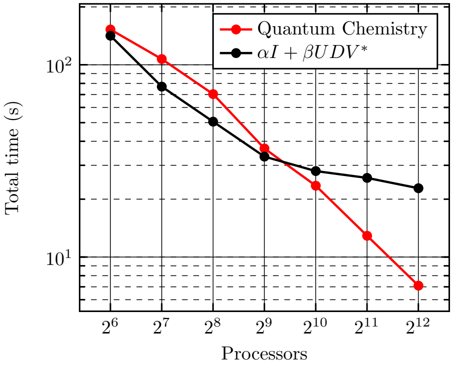
SUSY: 4.5M, dimension=8; COVTYPE: 0.5M, dimension=54

	SUSY		COVTYPE	
Cores	32	512	32	512
$\mathcal{H}$ construction	173.7	18.3	36.5	32.2
HSS construction	3344.4	726.7	432.3	239.7
$\rightarrow$ Sampling	2993.5	662.1	305.2	178.4
$\rightarrow$ Other	350.9	64.6	127.1	61.3
ULV Factorization	14.2	3.3	26.5	4.6
Solve	0.5	0.3	0.5	0.4

Dense scalability

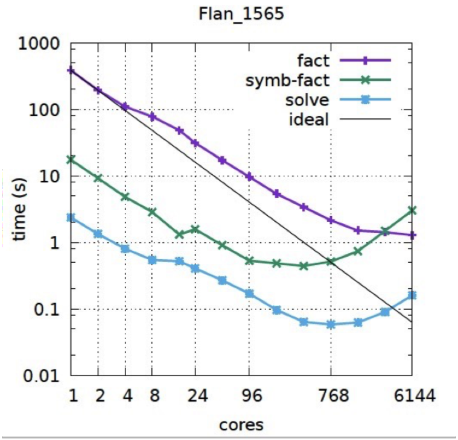
P = 4096, Cray XC40 (Cori at NERSC)

- quantum chemistry (Toeplitz): $a_{i,i} = \frac{\pi^2}{6}$ and $a_{i,j} = \frac{(-1)^{i-j}}{(i-j)^2 d^2}$
- $A = I + UDV^*$, U, V, $r = 500$, $D_{k,k} = 2^{-24(k-1)/r}$, $N = 500,000$



Sparse scalability

Matrix from SuiteSparse collection:
Flan_1565 (N = 1,564,794, NNZ = 114,165,372)



- Flat MPI on nodes with 2 12-core Intel Ivy Bridge (NERSC Edison)

STRUMPACK – STRUctured Matrices PACKage

http://portal.nersc.gov/project/sparse/strumpack/

- Two components:
  - Dense – applicable to Toeplitz, Cauchy, BEM, integral equations, etc.
  - Sparse – aim at matrices discretized from PDEs.
- Open source on Github, BSD license.
- C++, hybrid MPI + OpenMP implementation
- Real & complex datatypes, single & double precision (via template), and 64-bit indexing.
- Input interfaces:
  - Dense matrix in standard format.
  - Matrix-free, with query function to return selected entries.
  - Sparse matrix in CSR format.
- Can take user input: cluster tree & block partitioning.
- Functions:
  - HSS construction, HSS-vector product, ULV factorization, Solution.
- Available from PETSc, MFEM.
- **Extensible to include other data-sparse formats.**

Summary

- Sampling is handy, but still needs more mathematical insight to make it robust and efficient.
- Preconditioner appears to be robust [IPDPS 2017]
  - Works well for problems where AMG has slow convergence, e.g., indefinite problems.
  - More parallelizable than ILU, fewer parameters to tune.
- More research
  - Dynamic load balancing.
  - Communication analysis for sparse solvers.
  - Rank analysis of different application problems.
  - Good ordering and hierarchical clustering / partitioning to reduce off-diagonal rank.
  - Not all problems compress well in HSS, look into other formats.

THANK YOU !

HSS matrix – ULV factorization

ULV-like factored form (U and V^* unitary, L triangular)

$$
\Gamma_{1;b\leftrightarrow 2;t}
\begin{bmatrix} I & & & \\ & \Omega_1 & & \\ & & I & \\ & & & \Omega_2 \end{bmatrix}
\begin{bmatrix} \Gamma_{3;b\leftrightarrow 4;t} & \\ & \Gamma_{5;b\leftrightarrow 6;t} \end{bmatrix}
\begin{bmatrix} \Omega_3 & & & \\ & \Omega_4 & & \\ & & \Omega_5 & \\ & & & \Omega_6 \end{bmatrix}
A
\begin{bmatrix} Q_3^* & & & \\ & Q_4^* & & \\ & & Q_5^* & \\ & & & Q_6^* \end{bmatrix}
\begin{bmatrix} \Gamma^T_{3;b\leftrightarrow 4;t} & \\ & \Gamma^T_{5;b\leftrightarrow 6;t} \end{bmatrix}
\begin{bmatrix} I & & & \\ & Q_1^* & & \\ & & I & \\ & & & Q_2^* \end{bmatrix}
\Gamma^T_{1;b\leftrightarrow 2;t}
$$

$$
= \left[\begin{array}{c|c|c|c|c|c|c}
L_3 & & & & & & \\
0 & L_4 & & & & & \\
(\Omega_1 L_{4,3})_t & (\Omega_1 L_{3,4})_t & L_1 & & & & \\
\multicolumn{3}{c|}{} & L_5 & & & \\
\multicolumn{3}{c|}{0} & 0 & L_6 & & \\
\multicolumn{3}{c|}{} & (\Omega_2 L_{6,5})_t & (\Omega_2 L_{5,6})_t & L_2 & \\
(\Omega_1 L_{4,3})_b & (\Omega_1 L_{3,4})_b & W_{1;b} Q^*_{1;t} & \multicolumn{3}{c|}{B_{1,2} V_2^* \begin{bmatrix} V_5^* Q^*_{5;t} & & V_5^* Q^*_{5;b} & \\ & V_6^* Q^*_{6;t} & & V_6^* Q^*_{6;b} \end{bmatrix} \begin{bmatrix} I & \\ & Q_2^* \end{bmatrix}} & \\
\multicolumn{3}{c|}{B_{2,1} V_1^* \begin{bmatrix} V_3^* Q^*_{3;t} & & V_3^* Q^*_{3;b} & \\ & V_4^* Q^*_{4;t} & & V_4^* Q^*_{4;b} \end{bmatrix} \begin{bmatrix} I & \\ & Q_1^* \end{bmatrix}} & (\Omega_2 L_{6,5})_b & (\Omega_2 L_{5,6})_b & W_{2;b} Q^*_{2;t} & D_0
\end{array}\right]
$$

Themes

Many research areas for exascale computing: **https://exascaleproject.org**

- Algorithms with lower arithmetic & communication complexity. Multilevel algorithms:
  - Multigrid
  - Fast Multipole Method (FMM)
  - **Hierarchical matrices – algebraic generalization of FMM, applicable to broader classes of problems**

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- Algorithms with lower arithmetic & communication complexity. Multilevel algorithms:
  - Multigrid
  - Fast Multipole Method (FMM)
  - **Hierarchical matrices – algebraic generalization of FMM, applicable to broader classes of problems**
- Parallel algorithms and codes for machines with million-way parallelism, hierarchical organization.
  - Distributed memory
  - **Manycore nodes: 100s of lightweight cores, accelerators, co-processors**

Why factorization?

- Target problems:
  - indefinite, ill-conditioned, nonsymmetric (e.g. those from multiphysics, multiscale simulations)
- Where can be used?
  - Stand-alone solver.
  - Good for multiple right-hand sides.
  - Precondition Krylov solvers.
  - Coarse-grid solver in multigrid. (e.g., Hypre)
  - In nonlinear solver. (e.g., SUNDIALS)
  - Solving interior eigenvalue prolems.
  - ...
- Error analysis:
  - Componentwise error bounds (**Guaranteed solution accuracy**).
  - Condition number estimation.

Arithmetic complexities – dense HSS

Let r = HSS rank, i.e., maximum rank found during the different compression steps.

Compression

- Without RS: $O(r\,N^2)$.
- With RS: sampling cost (dominant) + $O(r^2 N)$

  sampling cost:

  - Classical matvec: $O(r\,N^2)$.
  - FFT (e.g., Toeplitz matrix): $O(r\,N \log N)$.
  - FMM: $O(r\,N)$.

ULV factorization and solve: $O(r\,N)$