An $\mathcal{O}(N \log N)$ Fast Direct Solver for Partial Hierarchically Semi-Separable Matrices

(Ambikasaran, Darve)

Overview

solvers for large dense linear systems mostly iterative based on Krylov subspaces
(Arnoldi, Conjugate Gradients, GMRES, MINRES, Biconjugate Gradient stabilized methods, QMR, TFQMR)

1. preconditioning
2. matrix-vector product using fast summation techniques (FMM, Barnes-Hut, panel clustering, FFT, wavelet based methods)

often used for boundary integral equations

=> methods solve systems in linear or almost linear time

Problems:
- does not scale well for multiple inversions
- good preconditioner may be hard to find

=> fast direct solvers

Hierarchical Matrices

rank of matrix A: dimension of the image of A

$\mathcal{H}$-matrices (Hackbusch): sub-divide matrix into a hierarchy of rectangular blocks and approximate them by low rank matrices

HSS (Chandrasekan): hierarchically semi-separable matrix of separability p:

(that means that A has all subblocks taken out of the matrix below a specific superdiagonal satisfying a certain rank constrain; similar for upper triangular part)

$A = L + U$ L: lower triangular, U: upper triangular $\operatorname{rank} L = \operatorname{rank} U = p$

HODLR: hierarchical off-diagonal low-rank matrix (often obtained from boundary integral equations)

$$\text{HSS} \subset p\text{-HSS} \subset \text{HODLR}$$

Chandrasekan: $\mathcal{O}(N)$ solver for HSS systems: $A = ULV^T$ U, V unitary, L lower triangular
factorization $\mathcal{O}(N^2)$

Low rank approximation

Singular value decomposition (SVD)

$$M = U \Sigma V^{*t}$$

$M \in \mathbb{R}^{m\times n}$

$U \in \mathbb{C}^{m\times m}$ unitary

Σ real, $\mathbb{R}^{m\times n}$, diagonal $\quad \Sigma = \begin{pmatrix} \sigma_1 \ldots \sigma_r & 0 \\ 0 & 0 \end{pmatrix}$

r: rank, σ_i singular values

best low rank approximation of rank p of a matrix A is given by SVD (Eckart-Young-Mirsky)

Computation: $\mathcal{O}(mn^2)$ for $m \geq n$

fast low rank approximations: adaptive cross approximation (ACA), pseudo-skeletal approximations, interpolatory decomposition, randomized algorithms, rank-revealing LU, QR

Algorithm

① Factorization

$\mathcal{O}(p^2 N \log N)$ for p-HSS

$\mathcal{O}(p^2 N \log^2 N)$ for HODLR

3D boundary element methods $\mathcal{O}(N^2)$, because rank p of interacting clusters $\mathcal{O}(\sqrt{N})$

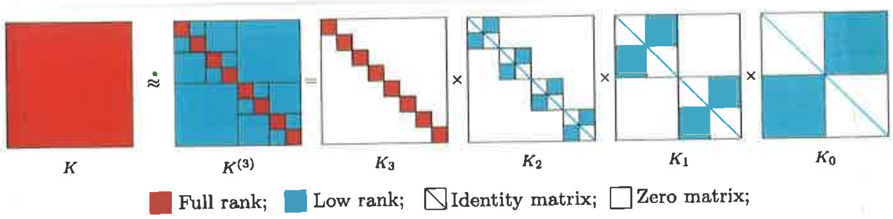

Fig. 1 Factorization of a three level HODLR/p-HSS matrix

② Calculating determinant

$$\det K \approx \det K^{(3)} = \det K_3 \det K_2 \det K_1 \det K_0$$

$$\det \begin{pmatrix} \mathbb{1} & U_{n\times p} \\ V_{n\times p} & \mathbb{1} \end{pmatrix} = \det(\mathbb{1}_n + U_{n\times p} V_{p\times n}) = \det(\mathbb{1}_p + V_{p\times n} U_{n\times p}) \qquad \mathcal{O}(p^2 n)$$