

# Hands on :Low-rank approximations and Hierarchical matrices

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# Computational Cost of Linear Algebra Routines

Given a matrix  $A$  with size  $m \times n$ ,  $B$  with size  $n \times p$  and  $x$  with size  $n \times 1$ ,

- Matrix-Vector( $Ax$ )  $\rightarrow \mathcal{O}(mn)$
- Matrix-matrix( $AB$ )  $\rightarrow \mathcal{O}(mnp)$

# Matrix Multiplication

The computational Cost for

- $A(BC) \rightarrow 108 \times 10^6$
- $(AB)C \rightarrow 450 \times 10^6$

## Condition for Matrix Multiplication

The computational Cost with general notation

- $R : A(BC) \rightarrow npl + mnl = nl(m + p)$
- $L : (AB)C \rightarrow mnp + mpl = mp(n + l)$

If  $\frac{R}{L} < 1$ , then method R is faster, so the condition for R to be faster is

$$\frac{1}{p} + \frac{1}{m} < \frac{1}{l} + \frac{1}{n}$$

$$\begin{bmatrix} 2 & 3 & 4 & 5 & 6 & 7 \\ 3 & 5 & 7 & 9 & 11 & 13 \\ 4 & 7 & 10 & 13 & 16 & 19 \\ 5 & 9 & 13 & 17 & 21 & 25 \\ 6 & 11 & 16 & 21 & 26 & 31 \\ 7 & 13 & 19 & 25 & 31 & 37 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 4 & 6 & 8 & 10 & 12 \\ 3 & 6 & 9 & 12 & 15 & 18 \\ 4 & 8 & 12 & 16 & 20 & 24 \\ 5 & 10 & 15 & 20 & 25 & 30 \\ 6 & 12 & 18 & 24 & 30 & 36 \end{bmatrix} + \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 3 & 4 & 5 & 6 & 7 \\ 3 & 5 & 7 & 9 & 11 & 13 \\ 4 & 7 & 10 & 13 & 16 & 19 \\ 5 & 9 & 13 & 17 & 21 & 25 \\ 6 & 11 & 16 & 21 & 26 & 31 \\ 7 & 13 & 19 & 25 & 31 & 37 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 3 & 4 & 5 & 6 & 7 \\ 3 & 5 & 7 & 9 & 11 & 13 \\ 4 & 7 & 10 & 13 & 16 & 19 \\ 5 & 9 & 13 & 17 & 21 & 25 \\ 6 & 11 & 16 & 21 & 26 & 31 \\ 7 & 13 & 19 & 25 & 31 & 37 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = 21 \times \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix} + 6 \times \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 27 \\ 48 \\ 69 \\ 90 \\ 111 \\ 132 \end{bmatrix}$$

# Matrix Matrix Multiplication Case 1

Consider the matrix  $A_1 \approx U_1 V_1 \in \mathbb{R}^{m \times n}$  with rank  $r$  and  $A_2 \in \mathbb{R}^{n \times p}$  which is full rank, Then  $A = A_1 \times A_2$  can be given as

Post Multiply

$$A = U_1(V_1 A_2) \rightarrow \mathcal{O}(rnp)$$

Consider the matrix  $A_1 \in \mathbb{R}^{m \times n}$  with full rank and  $A_2 \approx U_2 V_2 \in \mathbb{R}^{n \times p}$  which is rank  $r$ , Then  $A = A_1 \times A_2$  can be given as

Pre Multiply

$$A = (A_1 U_2) V_2 \rightarrow \mathcal{O}(rmn)$$



## Matrix Matrix Multiplication Case 2

Consider the matrix  $A_1 \approx U_1 V_1 \in \mathbb{R}^{m \times n}$  with rank  $r_1$  and  $A_2 \approx U_2 V_2 \in \mathbb{R}^{n \times p}$  with rank  $r_2$  Then

$$A = A_1 * A_2$$

can be given as

Representation  $r_1$

$$A = U_1 (V_1 U_2) V_2$$

$$A = U_1 S_{12} V_2, \text{ where } S_{12} = (V_1 U_2) \rightarrow \mathcal{O}(r_1 r_2 n)$$

## Matrix-Vector multiplication $y = Ax$

Consider the matrix  $A \approx UV$ ,  $U \in \mathbb{R}^{m \times r}$ ,  $V \in \mathbb{R}^{r \times n}$  and vector  $x \in \mathbb{R}^n$ , then  $Ax = y$  can be treated as  $UVx = y$

- $y = Vx \rightarrow \mathcal{O}(nr)$
- $b = Uy \rightarrow \mathcal{O}(mr)$

Total Cost  $\rightarrow \mathcal{O}((m+n)r)$

## Matrix Matrix Addition

Consider the matrix  $A_1 \approx U_1 V_1 \in \mathbb{R}^{m \times n}$  with rank  $r_1$  and  $A_2 \approx U_2 V_2 \in \mathbb{R}^{m \times n}$  with rank  $r_2$  Then

$$A = A_1 + A_2$$

can be given as

$$A = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \end{bmatrix}$$

The Matrix  $A$  can have rank at most  $r = (r_1 + r_2)$ , if rank is less than  $r$ , then a routine for rank reduction is needed.

# Matrix Rank Reduction

Consider the matrix  $A \approx UV \in \mathbb{R}^{m \times n}$  with rank  $r$  but that still can be reduced to rank  $k < r$ , then the following steps can be taken to reduce the rank,

- $U = Q_u R_u$  and  $V^T = Q_v R_v$  takes  $\rightarrow \mathcal{O}((m+n)r^2)$
- Calculate SVD for  $R_u R_v^T$  which is  $\tilde{u} \tilde{s} \tilde{v}$  takes  $\rightarrow \mathcal{O}(r^3)$
- Form  $\tilde{U} \tilde{s} \tilde{V}$  where  $\tilde{U} = Q_u \tilde{u}$   $\tilde{V} = \tilde{v} Q_v^T$  takes  $\rightarrow \mathcal{O}(rk(m+n))$

# Cross Approximation

Given a Matrix  $A \in \mathbb{R}^{n \times n}$  with rank  $r$ , Cross approximation constructs the Approximation as follows:

## Algorithm

- $A = \tilde{A}$
- while  $\|\tilde{A}\|_{\infty} > tol$ 
  - $\delta_k = |\tilde{A}_{ij}|_{max}$
  - $u^{(k)} = \frac{\tilde{A}_{:,j}}{\delta_k}$  and  $v^{(k)} = \tilde{A}_{i,:}$
  - $\tilde{A} \rightarrow \tilde{A} - u^{(k)} v^{(k)}, \rightarrow \mathcal{O}(rmn)$
- $A \approx UV$  - Computation of the decomposition  $UV$  costs as  $\mathcal{O}(rmn)$

## Example

$$A = \begin{bmatrix} 158 & 176 & 194 & 212 & 230 \\ 176 & 197 & 218 & 239 & 260 \\ 194 & 218 & 242 & 266 & 290 \\ 212 & 239 & 266 & 293 & 320 \\ 230 & 260 & 290 & 320 & 350 \end{bmatrix} \quad \text{Iteration 1: } \delta = 350 \text{ with}$$

$$(i,j) = (5,5) \quad A = \begin{bmatrix} 6.86 & 5.14 & 3.43 & 1.71 & 0.00 \\ 5.14 & 3.86 & 2.57 & 1.29 & 0.00 \\ 3.43 & 2.57 & 1.71 & 0.86 & 0.00 \\ 1.71 & 1.29 & 0.86 & 0.43 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \end{bmatrix} \quad U = \begin{bmatrix} 0.66 \\ 0.74 \\ 0.83 \\ 0.91 \\ 1.00 \end{bmatrix}$$

$$V = \begin{bmatrix} 230 & 260 & 290 & 320 & 350 \end{bmatrix}$$

## Example

Iteration 2:  $\delta = 6.86$  with  $(i, j) = (1, 1)$   $A =$

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1.24e-14 & -3.55e-15 & -1.24e-14 & 0 \\ 0 & -3.55e-15 & -7.11e-15 & -2.49e-14 & 0 \\ -2.22e-16 & 1.60e-14 & 3.19e-14 & 1.24e-14 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$U = \begin{bmatrix} 0.66 & 1.00 \\ 0.74 & 0.75 \\ 0.83 & 0.50 \\ 0.91 & 0.25 \\ 1.00 & 0.00 \end{bmatrix}$$

$$V = \begin{bmatrix} 230.00 & 260.00 & 290.00 & 320.00 & 350.00 \\ 6.86 & 5.14 & 3.43 & 1.71 & 0.00 \end{bmatrix}$$

$$\|A - UV\|_{\infty} = 3.190e-14$$

# Adaptive Cross Approximation

Given a Matrix  $A \in \mathbb{R}^{n \times n}$  with rank  $r$ , Adaptive Cross approximation constructs the Approximation as follows:

## Algorithm - Initialize

- $i_1 = 1$  and  $Z = \{\text{set of Vanishing Rows}\}$
- $v = A(i_1, :)$
- $j_1 = \text{index of } \max |v| \text{ and } \delta_1 = \frac{1}{v(j_1)}$
- $V(1, :) = \delta_1 v$
- $U(:, 1) = A(:, j_1)$  and  $Z = Z \cup i_1$
- $A \approx UV$



# Adaptive Cross Approximation(Contd..)

## Algorithm

- while  $k=2,3,\dots$
- $i_k = \text{index of } \max |U(:, k-1)| \text{ and } i_k \notin Z$
- $v = A(i_k, :) - \sum_{l=1}^{k-1} U(l, i_k) V(l, :)$  and  $Z = Z \cup i_k$
- $j_k = \text{index of } \max |v| \text{ and } \delta_k = \frac{1}{v(j_k)}$
- $V(k, :) = \delta_k v$
- $U(:, k) = A(:, j_k) - \sum_{l=1}^{k-1} V(j_k, l) U(:, l)$

$A \approx UV$  - Computation of the decomposition  $UV$  costs as  
 $\mathcal{O}(r^2(m+n))$

## Example

$$A = \begin{bmatrix} 158 & 176 & 194 & 212 & 230 \\ 176 & 197 & 218 & 239 & 260 \\ 194 & 218 & 242 & 266 & 290 \\ 212 & 239 & 266 & 293 & 320 \\ 230 & 260 & 290 & 320 & 350 \end{bmatrix} \quad \text{Iteration 1: } \delta = 230 \text{ with}$$

$$i_1 = 1, j_1 = 5 \quad U = \begin{bmatrix} 230 \\ 260 \\ 290 \\ 320 \\ 350 \end{bmatrix} \quad V = [0.69 \quad 0.77 \quad 0.84 \quad 0.92 \quad 1.00]$$

## Example

$$\text{Iteration 2: } \delta = -10.438 \text{ with } i_1 = 5, j_1 = 1 \quad U = \begin{bmatrix} 230 & 0 \\ 260 & -2.61 \\ 290 & -5.22 \\ 320 & -7.83 \\ 350 & -10.43 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.69 & 0.77 & 0.84 & 0.92 & 1.00 \\ 1.00 & 0.75 & 0.50 & 0.25 & 0.00 \end{bmatrix}$$

$$\|A - UV\|_{\infty} = 6.5036e - 14$$

The partially pivoted ACA produces Low-rank decomposition in roughly  $\mathcal{O}(n)$  and the most attractive feature is the non requirement of target rank as the case with randomized method.

# Low-rank approximation through Chebyshev Interpolation

## Definition

Given a Kernel Matrix  $K_{ij} = f(x_i, y_j)$  then Low rank approximation can be given as

$$K(x, y) = U(x, \tilde{X})\tilde{K}(\tilde{X}, \tilde{Y})V(y, \tilde{Y})$$

$A \approx U\tilde{K}V$  where,

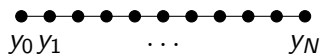
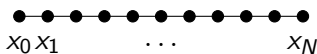
- $x_i$  be distributed along a domain  $[a,b]$  of length  $n$
- $y_i$  be distributed along a domain  $[c,d]$  of length  $n$
- $\tilde{X}$  be Chebyshev nodes on the domain  $[a,b]$  of length  $r$ (Rank of approximation)
- $\tilde{Y}$  be Chebyshev nodes on the domain  $[c,d]$  of length  $r$ (Rank of approximation)
- $K \in \mathbb{R}^{n \times n}, U \in \mathbb{R}^{n \times r}, V \in \mathbb{R}^{r \times n}$  and  $\tilde{K} \in \mathbb{R}^{r \times r}$

# Kernel Matrix in 1D

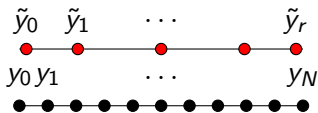
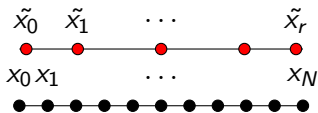
Let  $x, y$  denote the set of charges in  $[a, b]$  and  $[c, d]$  respectively.

$$x_i \in [a, b]$$

$$y_j \in [c, d]$$



$$K(x, y) = \begin{bmatrix} K(x_1, y_1) & K(x_1, y_2) & \dots & K(x_1, y_N) \\ K(x_2, y_1) & K(x_2, y_2) & \dots & K(x_2, y_N) \\ \vdots & \vdots & \ddots & \vdots \\ K(x_N, y_1) & K(x_N, y_2) & \dots & K(x_N, y_N) \end{bmatrix}$$



$$L_{ij} = \prod_{k=0:nj \neq k} \frac{(x_i - y_k)}{(y_j - y_k)}$$

$$U(x, \tilde{X}) = \begin{bmatrix} L(x_1, \tilde{x}_1) & \dots & L(x_1, \tilde{x}_r) \\ \vdots & \ddots & \vdots \\ L(x_N, \tilde{x}_1) & \dots & L(x_N, \tilde{x}_r) \end{bmatrix}, U(x, \tilde{X}) \in \mathbb{R}^{N \times r}$$

$$V(y, \tilde{Y})^T = \begin{bmatrix} L(y_1, \tilde{y}_1) & \dots & L(y_1, \tilde{y}_r) \\ \vdots & \ddots & \vdots \\ L(y_N, \tilde{y}_1) & \dots & L(y_N, \tilde{y}_r) \end{bmatrix}, V(y, \tilde{Y}) \in \mathbb{R}^{r \times N}$$

$$\tilde{K}(x, y) = \begin{bmatrix} f(\tilde{x}_1, \tilde{y}_1) & \dots & f(\tilde{x}_1, \tilde{y}_r) \\ \vdots & \ddots & \vdots \\ f(\tilde{x}_r, y_1) & \dots & f(\tilde{x}_r, \tilde{y}_r) \end{bmatrix} \tilde{K}(x, y) \in \mathbb{R}^{r \times r}$$

## Example - Chebyshev

Consider approximating kernel matrix  $K(x,y) \in \mathbb{R}^{5 \times 5}$  using rank 3 chebyshev approximation,

$$x = [-1 \quad -0.75 \quad -0.5 \quad -0.25 \quad 0] \text{ and } \tilde{X} = [-0.933 \quad -0.5 \quad -0.0670]$$

$$y = [1 \quad 1.25 \quad 1.5 \quad 1.75 \quad 2] \text{ and } \tilde{Y} = [1.0670 \quad 1.5 \quad 1.933]$$

$$U = \begin{bmatrix} 1.24 & -0.33 & 0.09 \\ 0.46 & 0.67 & -0.12 \\ 0.00 & 1.00 & 0.00 \\ -0.12 & 0.67 & 0.46 \\ 0.09 & -0.33 & 1.24 \end{bmatrix} \quad \tilde{K} = \begin{bmatrix} 0.135 & 0.209 & 0.322 \\ 0.088 & 0.135 & 0.209 \\ 0.057 & 0.088 & 0.135 \end{bmatrix}$$

$$V = \begin{bmatrix} 1.24 & 0.46 & 0.00 & -0.12 & 0.09 \\ -0.33 & 0.67 & 1.00 & 0.67 & -0.33 \\ 0.09 & -0.12 & 0.00 & 0.46 & 1.24 \end{bmatrix}$$

$$\text{Error} = 4.8e - 3$$

# well separatedness



# $\mathcal{H}$ -matrix