Low rank matrix approximation

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Plan

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Rank revealing QR factorization

Randomized algorithms for low rank approximation

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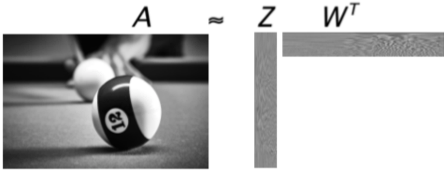
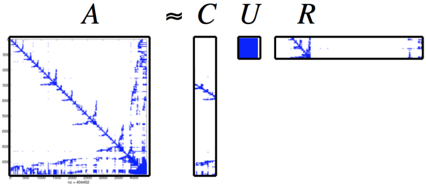
Low rank matrix approximation

- Problem: given $A \in \mathbb{R}^{m \times n}$, compute rank-k approximation ZW^T, where Z is $m \times k$ and W^T is $k \times n$.





- Problem with diverse applications
  - from scientific computing: fast solvers for integral equations, H-matrices
  - to data analytics: principal component analysis, image processing, ...

$$Ax \rightarrow ZW^T x$$

$$\textit{Flops} \quad 2mn \rightarrow 2(m+n)k$$

Singular value decomposition

Given $A \in \mathbb{R}^{m\times n}$, $m \geq n$ its singular value decomposition is

$$A = U\Sigma V^T = \begin{pmatrix} U_1 & U_2 & U_3 \end{pmatrix} \cdot \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \\ 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} V_1 & V_2 \end{pmatrix}^T$$

where

- U is $m \times m$ orthogonal matrix, the left singular vectors of A , U_1 is $m \times k$, U_2 is $m \times n - k$, U_3 is $m \times m - n$
- Σ is $m \times n$, its diagonal is formed by $\sigma_1(A) \geq \ldots \geq \sigma_n(A) \geq 0$ Σ_1 is $k \times k$, Σ_2 is $n - k \times n - k$
- V is $n \times n$ orthogonal matrix, the right singular vectors of A, V_1 is $n \times k$, V_2 is $n \times n - k$

Norms

$$
\begin{aligned}
||A||_p &= \max_{||x||_p=1} ||Ax||_p \\
||A||_F &= \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} |a_{ij}|^2} = \sqrt{\sigma_1^2(A) + \ldots \sigma_n^2(A)} \\
||A||_2 &= \sigma_{max}(A) = \sigma_1(A)
\end{aligned}
$$

Some properties:

$$||A||_2 \leq ||A||_F \leq \sqrt{min(m,n)}||A||_2$$

Orthogonal Invariance: If $Q \in \mathbb{R}^{m\times m}$ and $Z \in \mathbb{R}^{n\times n}$ are orthogonal, then

$$||QAZ||_F = ||A||_F$$
$$||QAZ||_2 = ||A||_2$$

Low rank matrix approximation

- Best rank-k approximation $A_k = U_k \Sigma_k V_k$ is rank-k truncated SVD of A [Eckart and Young, 1936]

$$\min_{rank(\tilde{A}_k) \leq k} ||A - \tilde{A}_k||_2 = ||A - A_k||_2 = \sigma_{k+1}(A) \quad (1)$$

$$\min_{rank(\tilde{A}_k) \leq k} ||A - \tilde{A}_k||_F = ||A - A_k||_F = \sqrt{\sum_{j=k+1}^{n} \sigma_j^2(A)} \quad (2)$$

Image, size 1190×1920

Rank-10 approximation, SVD

Rank-50 approximation, SVD

- Image source: `https://pixabay.com/photos/billiards-ball-play-number-half-4345870/`

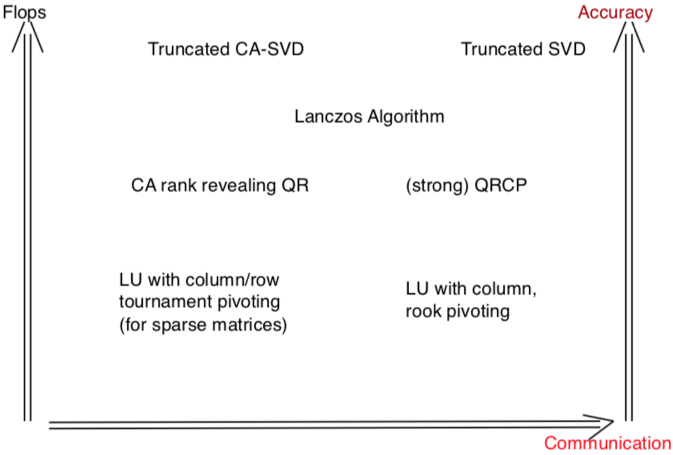
Large data sets

Matrix A might not exist entirely at a given time, rows or columns are added progressively.

- Streaming algorithm: can solve an arbitrarily large problem with one pass over the data (a row or a column at a time).
- Weakly streaming algorithm: can solve a problem with $O(1)$ passes over the data.

Matrix A might exist only implicitly, and it is never formed explicitly.

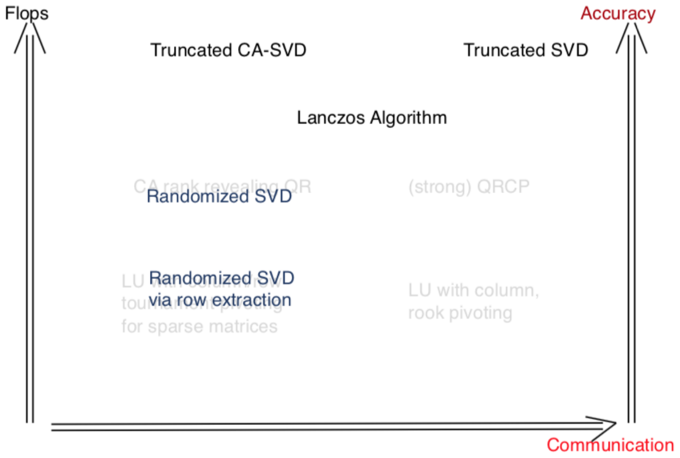
Low rank matrix approximation: trade-offs



Communication optimal if computing a rank-k approximation on P processors requires

$$\# \text{ messages} = \Omega\left(\log_2 P\right).$$

Low rank matrix approximation: trade-offs



Communication optimal if computing a rank-k approximation on P processors requires

$$\# \text{ messages} = \Omega\left(\log_2 P\right).$$

Idea underlying many algorithms

Compute $\tilde{A}_k = \mathcal{P}A$, where $\mathcal{P} = \mathcal{P}^o$ or $\mathcal{P} = \mathcal{P}^{so}$ is obtained as:

1. Construct a low dimensional subspace $X = range(A\Omega_1)$, $\Omega_1 \in \mathbb{R}^{n \times l}$ that approximates well the range of A, e.g.

$$\|A - \mathcal{P}^o A\|_2 \leq \gamma \sigma_{k+1}(A), \text{ for some } \gamma \geq 1,$$

   where Q_1 is orth. basis of $(A\Omega_1)$

$$\mathcal{P}^o = A\Omega_1(A\Omega_1)^+ = Q_1 Q_1^T, \text{ or equiv } \mathcal{P}^o a_j := arg \min_{x \in X} \|x - a_j\|_2$$

2. Select a semi-inner product $\langle \Theta_1 \cdot, \Theta_1 \cdot \rangle_2$, $\Theta_1 \in \mathbb{R}^{l' \times m}$ $l' \geq l$, define

$$\mathcal{P}^{so} = A\Omega_1(\Theta_1 A\Omega_1)^+ \Theta_1, \text{ or equiv } \mathcal{P}^{so} a_j := arg \min_{x \in X} \|\Theta_1(x - a_j)\|_2$$

Idea underlying many algorithms

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Properties of the approximations

Definitions and some of the results taken from [Demmel et al., 2019].

Definition

[low-rank approximation] A matrix A_k satisfying $\|A - A_k\|_2 \leq \gamma\sigma_{k+1}(A)$ for some $\gamma \geq 1$ will be said to be a (k, γ) *low-rank approximation of* A.

Definition

[spectrum preserving] If A_k satisfies

$$\sigma_j(A) \geq \sigma_j(A_k) \geq \gamma^{-1}\sigma_j(A)$$

for $j \leq k$ and some $\gamma \geq 1$, it is a (k, γ) *spectrum preserving*.

Definition

[kernel approximation] If A_k satisfies

$$\sigma_{k+j}(A) \leq \sigma_j(A - A_k) \leq \gamma\sigma_{k+j}(A)$$

for $1 \leq j \leq n - k$ and some $\gamma \geq 1$, it is a (k, γ) *kernel approximation of* A.

Plan

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Rank revealing QR factorization

Randomized algorithms for low rank approximation

Rank revealing QR factorization

Given A of size $m \times n$, consider the decomposition

$$AP_c = QR = Q \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix}, \tag{3}$$

where R_{11} is $k \times k$, P_c and k are chosen such that $||R_{22}||_2$ is small and R_{11} is well-conditioned.

- By the interlacing property of singular values [Golub, Van Loan, 4th edition, page 487],

  $$\sigma_i(R_{11}) \leq \sigma_i(A) \text{ and } \sigma_j(R_{22}) \geq \sigma_{k+j}(A)$$

  for $1 \leq i \leq k$ and $1 \leq j \leq n-k$.
- $\sigma_{k+1}(A) \leq \sigma_{max}(R_{22}) = ||R_{22}||$

Rank revealing QR factorization

Given A of size $m \times n$, consider the decomposition

$$AP_c = QR = Q \begin{bmatrix} R_{11} & R_{12} \\ & R_{22} \end{bmatrix}. \tag{4}$$

If $||R_{22}||_2$ is small,

- $Q(:,1:k)$ forms an approximate orthogonal basis for the range of A,

$$\begin{aligned} A(:,j) &= \sum_{i=1}^{min(j,k)} R(i,j)Q(:,i) \quad \in span\{Q(:,1), \ldots Q(:,k)\} \\ Range(A) &\in span\{Q(:,1), \ldots Q(:,k)\} \end{aligned}$$

- $P_c \begin{bmatrix} -R_{11}^{-1}R_{12} \\ I \end{bmatrix}$ is an approximate right null space of A.

Rank revealing QR factorization

The factorization from equation (5) is rank revealing if

$$1 \leq \frac{\sigma_i(A)}{\sigma_i(R_{11})}, \frac{\sigma_j(R_{22})}{\sigma_{k+j}(A)} \leq \gamma_1(n, k),$$

for $1 \leq i \leq k$ and $1 \leq j \leq \min(m, n) - k$, where

$$\sigma_{max}(A) = \sigma_1(A) \geq \ldots \geq \sigma_{min}(A) = \sigma_n(A)$$

It is **strong** rank revealing [Gu and Eisenstat, 1996] if in addition

$$||R_{11}^{-1} R_{12}||_{max} \leq \gamma_2(n, k)$$

Low rank approximation with strong RRQR

Given $A \in \mathbb{R}^{m \times n}$ and $R_{11} \in \mathbb{R}^{k \times k}$,

$$
\begin{aligned}
AP_c &= QR = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_{11} & R_{12} \\ & R_{22} \end{pmatrix}, \\
\tilde{A}_{qr} &= Q_1 \begin{pmatrix} R_{11} & R_{12} \end{pmatrix} P_c^T = Q_1 Q_1^T A = \mathcal{P}^o A
\end{aligned}
$$

- It can be shown that

$$\sigma_j(R_{22}) = \sigma_j(A - \tilde{A}_{qr})$$

- [Gu and Eisenstat, 1996] show that given k and f, there exists permutation $V \in \mathbb{R}^{n \times n}$ such that the factorization satisfies,

$$
\begin{aligned}
1 \leq \frac{\sigma_i(A)}{\sigma_i(R_{11})}, \frac{\sigma_j(R_{22})}{\sigma_{k+j}(A)} &\leq \gamma(n,k), \quad \gamma(n,k) = \sqrt{1 + f^2 k(n-k)} \\
||R_{11}^{-1} R_{12}||_{max} &\leq f
\end{aligned}
$$

  for $1 \leq i \leq k$ and $1 \leq j \leq \min(m,n) - k$.
- Cost: $4mnk$ (QRCP) plus $O(mnk)$ flops and $O(k \log_2 P)$ messages.

$\rightarrow$ $\tilde{A}_{qr}$ with strong RRQR is $(k, \gamma(n,k))$ spectrum preserving and kernel approximation of A

QR with column pivoting [Businger and Golub, 1965]

Idea:

- At first iteration, trailing columns decomposed into parallel part to first column (or e_1) and orthogonal part (in rows $2:m$).
- The column of maximum norm is the column with largest component orthogonal to the first column.

Implementation:

- Find at each step of the QR factorization the column of maximum norm.
- Permute it into leading position.
- If rank(A) = k, at step $k+1$ the maximum norm is 0.
- No need to compute the column norms at each step, but just update them since

$$Q^T v = w = \begin{bmatrix} w_1 \\ w(2:n) \end{bmatrix}, \;\; ||w(2:n)||_2^2 = ||v||_2^2 - w_1^2$$

QR with column pivoting [Businger and Golub, 1965]

Sketch of the algorithm

column norm vector: $colnrm(j) = ||A(:,j)||_2, j = 1:n$.

for j = 1 : n **do**

Find column p of largest norm

if $colnrm[p] > \epsilon$ **then**

1. Pivot: swap columns j and p in A and modify $colnrm$.
2. Compute Householder matrix H_j s.t. $H_j A(j:m,j) = \pm ||A(j:m,j)||_2 e_1$.
3. Update $A(j:m, j+1:n) = H_j A(j:m, j+1:n)$.
4. Norm downdate $colnrm(j+1:n)^2 -= A(j, j+1:n)^2$.

else Break

end if

end for

If algorithm stops after k steps

$$\sigma_{max}(R_{22}) \leq \sqrt{n-k} \max_{1 \leq j \leq n-k} ||R_{22}(:,j)||_2 \leq \sqrt{n-k}\,\epsilon$$

Strong RRQR [Gu and Eisenstat, 1996]

Since

$$det(R_{11}) = \prod_{i=1}^{k} \sigma_i(R_{11}) = \sqrt{det(A^T A)} / \prod_{i=1}^{n-k} \sigma_i(R_{22})$$

a stron RRQR is related to a large $det(R_{11})$. The following algorithm interchanges columns that increase $det(R_{11})$, given f and k.

Compute a strong RRQR factorization, given k:

Compute $A\Pi = QR$ by using QRCP
while there exist i and j such that $det(\tilde{R}_{11})/det(R_{11}) > f$, where
$R_{11} = R(1:k, 1:k)$, $\Pi_{i,j+k}$ permutes columns i and $j+k$,
$R\Pi_{i,j+k} = \tilde{Q}\tilde{R}, \tilde{R}_{11} = \tilde{R}(1:k, 1:k)$ **do**
Find i and j
Compute $R\Pi_{i,j+k} = \tilde{Q}\tilde{R}$ and $\Pi = \Pi\Pi_{i,j+k}$
end while

Strong RRQR (contd)

It can be shown that

$$\frac{det(\tilde{R}_{11})}{det(R_{11})} = \sqrt{\left(R_{11}^{-1}R_{12}\right)_{i,j}^{2} + \omega_i^2\left(R_{11}\right)\chi_j^2\left(R_{22}\right)} \tag{5}$$

for any $1 \leq i \leq k$ and $1 \leq j \leq n-k$ (the 2-norm of the j-th column of A is $\chi_j(A)$, and the 2-norm of the j-th row of A^{-1} is $\omega_j(A)$).

Compute a strong RRQR factorization, given k:

Compute $A\Pi = QR$ by using QRCP

while $\max_{1\leq i\leq k, 1\leq j\leq n-k} \sqrt{\left(R_{11}^{-1}R_{12}\right)_{i,j}^{2} + \omega_i^2\left(R_{11}\right)\chi_j^2\left(R_{22}\right)} > f$ **do**

Find i and j such that $\sqrt{\left(R_{11}^{-1}R_{12}\right)_{i,j}^{2} + \omega_i^2\left(R_{11}\right)\chi_j^2\left(R_{22}\right)} > f$

Compute $R\Pi_{i,j+k} = \tilde{Q}\tilde{R}$ and $\Pi = \Pi\Pi_{i,j+k}$

end while

Strong RRQR (contd)

- $det(R_{11})$ strictly increases with every permutation, no permutation repeats, hence there is a finite number of permutations to be performed.

Strong RRQR (contd)

Theorem

[Gu and Eisenstat, 1996] If the QR factorization with column pivoting as in equation (5) *satisfies inequality*

$$\sqrt{\left(R_{11}^{-1}R_{12}\right)_{i,j}^{2} + \omega_i^2\left(R_{11}\right)\chi_j^2\left(R_{22}\right)} < f$$

for any $1 \le i \le k$ *and* $1 \le j \le n-k$, *then*

$$1 \le \frac{\sigma_i(A)}{\sigma_i(R_{11})}, \frac{\sigma_j(R_{22})}{\sigma_{k+j}(A)} \le \sqrt{1 + f^2 k(n-k)},$$

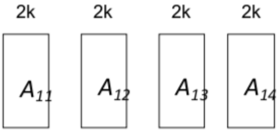
for any $1 \le i \le k$ *and* $1 \le j \le \min(m,n) - k$.

Deterministic column selection: tournament pivoting

1D tournament pivoting (1Dc-TP)

- 1D column block partition of A, select k cols from each block with strong RRQR

$$\begin{array}{cccc} (A_{11} & A_{12} & A_{13} & A_{14}) \\ \| & \| & \| & \| \\ (Q_{00}R_{00}P_{c00}^T & Q_{10}R_{10}P_{c10}^T & Q_{20}R_{20}P_{c20}^T & Q_{30}R_{30}P_{c30}^T \\ \downarrow & \downarrow & \downarrow & \downarrow \\ I_{00} & I_{10} & I_{20} & I_{30} \end{array}$$



- Reduction tree to select k cols from sets of $2k$ cols,

$$\begin{array}{cc} (A(:, I_{00} \cup I_{10}) & A(:, I_{20} \cup I_{30});) \\ \| & \| \\ (Q_{01}R_{01}P_{c01}^T & Q_{11}R_{11}P_{c11}^T) \\ \downarrow & \downarrow \\ I_{01} & I_{11} \end{array}$$

$$A(:, I_{01} \cup I_{11}) = Q_{02}R_{02}P_{c02}^T \rightarrow I_{02}$$

- Return selected columns $A(:, I_{02})$

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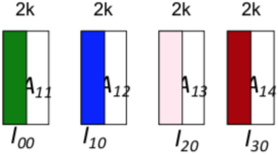
$$
\begin{array}{cccc}
(A_{11} & A_{12} & A_{13} & A_{14}) \\
\| & \| & \| & \| \\
(Q_{00} R_{00} P_{c00}^T & Q_{10} R_{10} P_{c10}^T & Q_{20} R_{20} P_{c20}^T & Q_{30} R_{30} P_{c30}^T \\
\downarrow & \downarrow & \downarrow & \downarrow \\
I_{00} & I_{10} & I_{20} & I_{30}
\end{array}
$$



- Reduction tree to select k cols from sets of $2k$ cols,

$$
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(A(:, I_{00} \cup I_{10}) & A(:, I_{20} \cup I_{30});) \\
\| & \| \\
(Q_{01} R_{01} P_{c01}^T & Q_{11} R_{11} P_{c11}^T) \\
\downarrow & \downarrow \\
I_{01} & I_{11}
\end{array}
$$

$$A(:, I_{01} \cup I_{11}) = Q_{02} R_{02} P_{c02}^T \rightarrow I_{02}$$

- Return selected columns $A(:, I_{02})$

Deterministic column selection: tournament pivoting

1D tournament pivoting (1Dc-TP)

- 1D column block partition of A, select k cols from each block with strong RRQR

$$\begin{array}{cccc} (A_{11} & A_{12} & A_{13} & A_{14}) \\ \| & \| & \| & \| \\ (Q_{00}R_{00}P_{c00}^T & Q_{10}R_{10}P_{c10}^T & Q_{20}R_{20}P_{c20}^T & Q_{30}R_{30}P_{c30}^T) \\ \downarrow & \downarrow & \downarrow & \downarrow \\ I_{00} & I_{10} & I_{20} & I_{30} \end{array}$$

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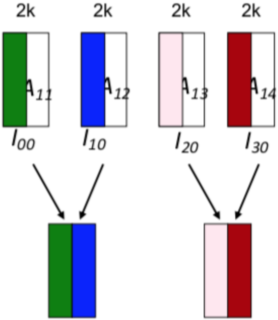
$$A(:, I_{01} \cup I_{11}) = Q_{02}R_{02}P_{c02}^T \rightarrow I_{02}$$

- Return selected columns $A(:, I_{02})$



Deterministic column selection: tournament pivoting

1D tournament pivoting (1Dc-TP)

- 1D column block partition of A, select k cols from each block with strong RRQR

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\| & \| & \| & \| \\
(Q_{00}R_{00}P_{c00}^T & Q_{10}R_{10}P_{c10}^T & Q_{20}R_{20}P_{c20}^T & Q_{30}R_{30}P_{c30}^T) \\
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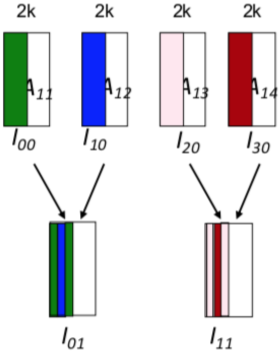

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\| & \| \\
(Q_{01}R_{01}P_{c01}^T & Q_{11}R_{11}P_{c11}^T) \\
\downarrow & \downarrow \\
I_{01} & I_{11}
\end{array}
$$

$$A(:, I_{01} \cup I_{11}) = Q_{02}R_{02}P_{c02}^T \rightarrow I_{02}$$

- Return selected columns $A(:, I_{02})$

Deterministic column selection: tournament pivoting

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- 1D column block partition of A, select k cols from each block with strong RRQR

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ \| & \| & \| & \| \\ Q_{00}R_{00}P_{c00}^T & Q_{10}R_{10}P_{c10}^T & Q_{20}R_{20}P_{c20}^T & Q_{30}R_{30}P_{c30}^T \\ \downarrow & \downarrow & \downarrow & \downarrow \\ I_{00} & I_{10} & I_{20} & I_{30} \end{pmatrix}$$

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$$A(:, I_{01} \cup I_{11}) = Q_{02}R_{02}P_{c02}^T \rightarrow I_{02}$$

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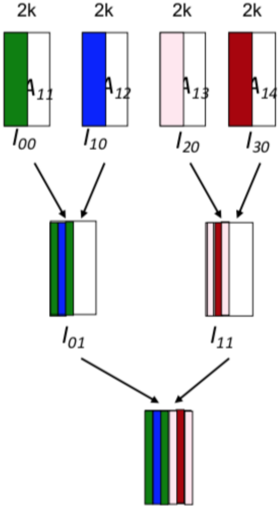

Deterministic column selection: tournament pivoting

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\begin{array}{cccc}
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\| & \| & \| & \| \\
(Q_{00}R_{00}P_{c00}^T & Q_{10}R_{10}P_{c10}^T & Q_{20}R_{20}P_{c20}^T & Q_{30}R_{30}P_{c30}^T) \\
\downarrow & \downarrow & \downarrow & \downarrow \\
I_{00} & I_{10} & I_{20} & I_{30}
\end{array}
$$

- Reduction tree to select k cols from sets of $2k$ cols,

$$
\begin{array}{cc}
(A(:, I_{00} \cup I_{10}) & A(:, I_{20} \cup I_{30});) \\
\| & \| \\
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\downarrow & \downarrow \\
I_{01} & I_{11}
\end{array}
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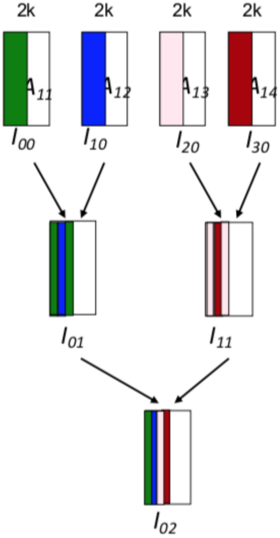
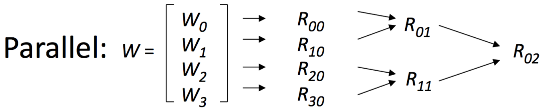


Select k columns from a tall and skinny matrix

Given W of size $m \times 2k$, $m >> k$, k columns are selected as:

$W = QR_{02}$ using TSQR
$R_{02} P_c = Q_2 R_2$ using QRCP
Return $WP_c(:, 1:k)$



Rank revealing properties of CA-RRQR

It is shown in [Demmel et al., 2015] that the column permutation computed by CA-RRQR satisfies

$$\chi_j^2\left(R_{11}^{-1}R_{12}\right)+\left(\chi_j\left(R_{22}\right)/\sigma_{\min}(R_{11})\right)^2\leq F_{TP}^2,\ \text{for } j=1,\ldots,n-k. \qquad (6)$$

where F_{TP} depends on k, f, n, the shape of reduction tree used during tournament pivoting, and the number of iterations of CARRQR.

CA-RRQR - bounds for one tournament

Selecting k columns by using tournament pivoting reveals the rank of A with the following bounds:

$$1 \leq \frac{\sigma_i(A)}{\sigma_i(R_{11})}, \frac{\sigma_j(R_{22})}{\sigma_{k+j}(A)} \leq \sqrt{1 + F_{TP}^2(n-k)},$$

$$||R_{11}^{-1}R_{12}||_{max} \leq F_{TP}$$

- Binary tree of depth $\log_2(n/k)$,

$$F_{TP} \leq \frac{1}{\sqrt{2k}} (n/k)^{\log_2\left(\sqrt{2}fk\right)}. \qquad (7)$$

  The upper bound is a decreasing function of k when $k > \sqrt{n/(\sqrt{2}f)}$.
- Flat tree of depth n/k,

$$F_{TP} \leq \frac{1}{\sqrt{2k}} \left(\sqrt{2}fk\right)^{n/k}. \qquad (8)$$

CA-RRQR : 2D tournament pivoting

- A distributed on $P_r \times P_c$ procs as e.g.

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \end{pmatrix}$$

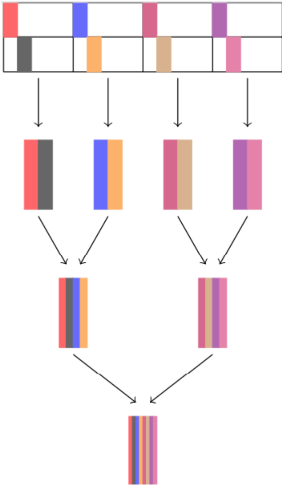
- Select k cols from each column block by 1Dr-TP,

$$\begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} \quad \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} \quad \begin{pmatrix} A_{13} \\ A_{23} \end{pmatrix} \quad \begin{pmatrix} A_{14} \\ A_{24} \end{pmatrix}$$
$$\downarrow \qquad\quad \downarrow \qquad\quad \downarrow \qquad\quad \downarrow$$
$$I_{00} \qquad I_{10} \qquad I_{20} \qquad I_{30}$$

- Apply 1Dc-TP on sets of k selected cols,

$$A(:, I_{00}) \quad A(:, I_{10}) \quad A(:, I_{20}) \quad A(:, I_{30})$$

- Return columns selected by 1Dc-TP $A(:, I_{02})$



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$$\begin{matrix} \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} & \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} & \begin{pmatrix} A_{13} \\ A_{23} \end{pmatrix} & \begin{pmatrix} A_{14} \\ A_{24} \end{pmatrix} \\ \downarrow & \downarrow & \downarrow & \downarrow \\ I_{00} & I_{10} & I_{20} & I_{30} \end{matrix}$$

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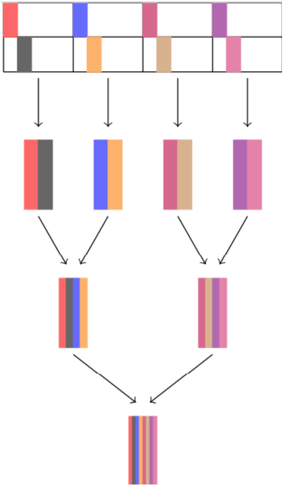

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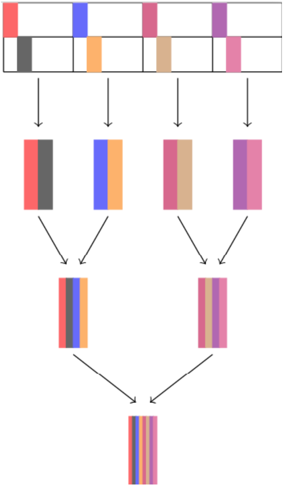
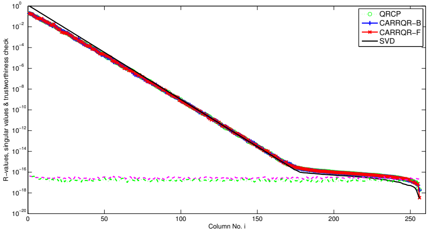
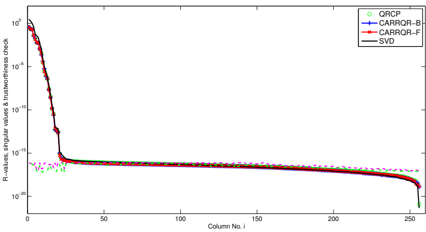


Numerical results

- Stability close to QRCP for many tested matrices.
- Absolute value of diagonals of R, L referred to as R-values, L-values.
- Methods compared
  - RRQR: QR with column pivoting
  - CA-RRQR-B with tournament pivoting based on binary tree
  - CA-RRQR-F with tournament pivoting based on flat tree
  - SVD

Numerical results (contd)





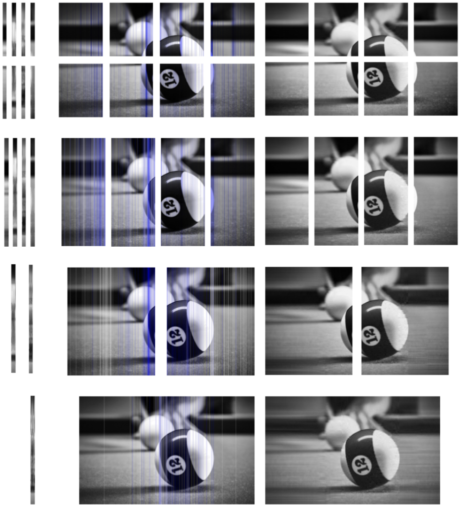
- Left: exponent - exponential Distribution, $\sigma_1 = 1$, $\sigma_i = \alpha^{i-1}$ $(i = 2, \dots, n)$, $\alpha = 10^{-1/11}$ [Bischof, 1991]
- Right: shaw - 1D image restoration model [Hansen, 2007]

$$\epsilon \min\{||(A\Pi_0)(:,i)||_2\,, ||(A\Pi_1)(:,i)||_2\,, ||(A\Pi_2)(:,i)||_2\} \tag{9}$$

$$\epsilon \max\{||(A\Pi_0)(:,i)||_2\,, ||(A\Pi_1)(:,i)||_2\,, ||(A\Pi_2)(:,i)||_2\} \tag{10}$$

where $\Pi_j (j = 0, 1, 2)$ are the permutation matrices obtained by QRCP, CARRQR-B, and CARRQR-F, and ϵ is the machine precision.

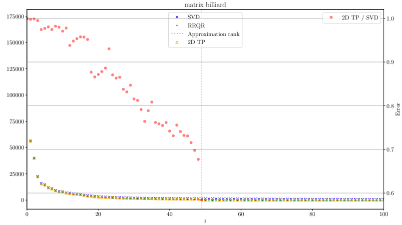
CA-RRQR : 2D tournament pivoting



Numerical experiments

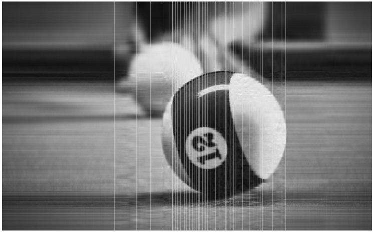
Original image, size 1190×1920

Singular values and ratios



Rank-10 approx, 2D TP 8×8 procs

Rank-50 approx, 2D TP 8×8 procs



- Image source: `https://pixabay.com/photos/billiards-ball-play-number-half-4345870/`

Plan

Low rank matrix approximation

Rank revealing QR factorization

Randomized algorithms for low rank approximation

Randomized algorithms - main idea

- Construct a low dimensional subspace that captures the action of A.
- Restrict A to the subspace and compute a standard QR or SVD factorization.

Obtained as follows:

1. Compute an approximate basis for the range of A ($m \times n$)
   find Q ($m \times k$) with orthonormal columns and approximate A by the projection of its columns onto the space spanned by Q:

$$A \approx QQ^T A$$

2. Use Q to compute a standard factorization of A

Source: Halko et al, *Finding structure with randomness: probabilistic algorithms for constructing approximate matrix decomposition*, SIREV 2011.

Johnson-Lindenstrauss transform

Definition 3 from [Woodruff, 2014].
A random matrix $\Omega_1 \in \mathbb{R}^{k \times m}$ is a Johnson-Lindenstrauss transform with parameters ϵ, δ, n, or JLT(n, ϵ, δ), if with probability at least $1 - \delta$ for any n-element subset $V \subset \mathbb{R}^m$, for all $x_i, x_j \in V$, we have

$$|\langle \Omega_1 x_i, \Omega_1 x_j \rangle - \langle x_i, x_j \rangle| \leq \epsilon \|x_i\|_2 \|x_j\|_2 \tag{11}$$

- If $x_i = x_j$ we obtain $\|\Omega_1 x_i\|_2^2 = (1 \pm \epsilon)\|x_i\|_2^2$.
- It can also be expressed as: given all vectors $x_i, x_j \in V$ are rescaled to be unit vectors, then for all $x_i, x_j \in V$ we require to hold:

$$\begin{aligned} \|\Omega_1 x_i\|_2^2 &= (1 \pm \epsilon)\|x_i\|_2^2 && (12) \\ \|\Omega_1 (x_i + x_j)\|_2^2 &= (1 \pm \epsilon)\|x_i + x_j\|_2^2 && (13) \end{aligned}$$

Proof that we obtain relation (14):

$$\begin{aligned} \langle \Omega_1 x_i, \Omega_1 x_j \rangle &= \left(\|\Omega_1 (x_i + x_j)\|_2^2 - \|\Omega_1 x_i\|_2^2 - \|\Omega_1 x_j\|_2^2\right)/2 \\ &= \left((1 \pm \epsilon)\|x_i + x_j\|_2^2 - (1 \pm \epsilon)\|x_i\|_2^2 - (1 \pm \epsilon)\|x_j\|_2^2\right)/2 \\ &= \langle x_i, x_j \rangle \pm O(\epsilon) \end{aligned}$$

Johnson-Lindenstrauss transform (contd)

Let $\Omega_1 \in \mathbb{R}^{k \times m}$ be a matrix whose entries are independent standard normal random variables, multiplied by $1/\sqrt{k}$. If $k = O(\epsilon^{-2} \log(n/\delta))$, then Ω_1 is a JLT(n, ϵ, δ).

Source: Theorem 4 in [Woodruff, 2014], see also Theorem 2.1 and proof in S. Dasgupta, A. Gupta, 2003, *An Elementary Proof of a Theorem of Johnson and Lindenstrauss*

Oblivious subspace embedding

Let $\Omega_1 \in \mathbb{R}^{k\times m}$ be a matrix whose entries are independent standard normal random variables, multiplied by $1/\sqrt{k}$. If $k = O(\epsilon^{-2}(n + \log(1/\delta)))$, then Ω_1 is an oblivious subspace embedding (OSE) with parameters (n, ϵ, δ). That is, with probability at least $1 - \delta$ for any n-dimensional subspace $\mathbf{V} \subset \mathbb{R}^m$, for all $x_i, x_j \in \mathbf{V}$, we have

$$|\langle \Omega_1 x_i, \Omega_1 x_j\rangle - \langle x_i, x_j\rangle| \leq \epsilon \|x_i\|_2 \|x_j\|_2 \tag{14}$$

Source: Theorem 6 in [Woodruff, 2014]

Typical randomized truncated SVD

Algorithm

Input: $m \times n$ matrix A, desired rank k, $l = p + k$ exponent q.

1. Sample an $n \times l$ test matrix Ω_1 with independent mean-zero, unit-variance Gaussian entries.
2. Compute $Y = (AA^T)^q A\Omega_1$ /* Y is expected to span the column space of A */
3. Construct $Q \in \mathbb{R}^{m \times l}$ with columns forming an orthonormal basis for the range of Y.
4. Compute $B = Q^T A$
5. Compute the SVD of $B = \hat{U}\Sigma V^T$

Return the approximation $\tilde{A}_k = Q\hat{U} \cdot \Sigma \cdot V^T$

Randomized truncated SVD ($q = 0$)

The best approximation is when Q equals the first $k + p$ left singular vectors of A. Given $A = U\Sigma V^T$,

$$\begin{aligned} QQ^T A &= U(1:m, 1:k+p)\Sigma(1:k+p, 1:k+p)(V(1:n, 1:k+p) \\ ||A - QQ^T A||_2 &= \sigma_{k+p+1} \end{aligned}$$

Theorem 1.1 from Halko et al. If Ω_1 is chosen to be i.i.d. N(0,1), $k, p \geq 2$, $q = 1$, then the expectation with respect to the random matrix Ω_1 is

$$\mathbb{E}(||A - QQ^T A||_2) \leq \left(1 + \frac{4\sqrt{k+p}}{p-1}\sqrt{min(m,n)}\right)\sigma_{k+1}(A)$$

and the probability that the error satisfies

$$||A - QQ^T A||_2 \leq \left(1 + 11\sqrt{k+p} \cdot \sqrt{min(m,n)}\right)\sigma_{k+1}(A)$$

is at least $1 - 6/p^p$.

For $p = 6$, the probability becomes .99.

Randomized truncated SVD

Theorem 10.6, Halko et al. Average spectral norm. Under the same hypotheses as Theorem 1.1 from Halko et al.,

$$\mathbb{E}(||A - QQ^T A||_2) \leq \left(1 + \sqrt{\frac{k}{p-1}}\right)\sigma_{k+1}(A) + \frac{e\sqrt{k+p}}{p}\left(\sum_{j=k+1}^{n} \sigma_j^2(A)\right)^{1/2}$$

- Fast decay of singular values:
  If $\left(\sum_{j>k} \sigma_j^2(A)\right)^{1/2} \approx \sigma_{k+1}$ then the approximation should be accurate.
- Slow decay of singular values:
  If $\left(\sum_{j>k} \sigma_j^2(A)\right)^{1/2} \approx \sqrt{n-k}\sigma_{k+1}$ and n large, then the approximation might not be accurate.

Source: G. Martinsson's talk

Power iteration $q \geq 1$

The matrix $(AA^T)^q A$ has a faster decay in its singular values:

- has the same left singular vectors as A
- its singular values are:

$$\sigma_j((AA^T)^q A) = (\sigma_j(A))^{2q+1}$$

Cost of randomized truncated SVD

- Randomized SVD requires $2q + 1$ passes over the matrix.
- The last 3 steps of the algorithms cost:
  (2) Compute $Y = (AA^T)^q A\Omega_1$: $2(2q+1) \cdot nnz(A) \cdot (k+p)$
  (3) Compute QR of Y: $2m(k+p)^2$
  (4) Compute $B = Q^T A$: $2nnz(A) \cdot (k+p)$
  (5) Compute SVD of B: $O(n(k+p)^2)$
- If $nnz(A)/m \geq k + p$ and $q = 1$, then (2) and (4) dominate (3).
- To be faster than deterministic approaches, the cost of (2) and (4) need to be reduced.

Fast Johnson-Lindenstrauss transform

Find sparse or structured Ω_1 such that computing $A\Omega_1$ is cheap, e.g. a subsampled random Hadamard transform (SRHT).
Given $n = 2^p, l < n$, the SRHT ensemble embedding $\mathbb{R}^n$ into $\mathbb{R}^l$ is defined as

$$\Omega_1 = \sqrt{\frac{n}{l}} \cdot P \cdot H \cdot D, \text{ where} \tag{15}$$

- $D \in \mathbb{R}^{n \times n}$ is diagonal matrix of uniformly random signs, random variables uniformly distributed on ± 1
- $H \in \mathbb{R}^{n \times n}$ is the normalized Walsh-Hadamard transform
- $P \in \mathbb{R}^{l \times n}$ formed by subset of l rows of the identity, chosen uniformly at random (draws l rows at random from HD).

References: Sarlos'06, Ailon and Chazelle'06, Liberty, Rokhlin, Tygert and Woolfe'06.

Fast Johnson-Lindenstrauss transform (contd)

Definition of Normalized Walsh–Hadamard Matrix
For given $n = 2^p$, $H_n \in \mathbb{R}^{n \times n}$ is the non-normalized Walsh-Hadamard transform defined recursively as,

$$H_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad H_n = \begin{pmatrix} H_{n/2} & H_{n/2} \\ H_{n/2} & -H_{n/2} \end{pmatrix}. \tag{16}$$

The normalized Walsh-Hadamard transform is $H = n^{-1/2} H_n$.

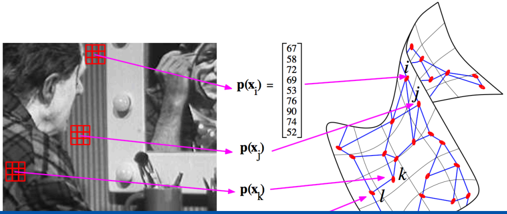
Cost of matrix vector multiplication (Theorem 2.1 in [Ailon and Liberty, 2008]):
For $x \in \mathbb{R}^n$ and $\Omega_1 \in \mathbb{R}^{l \times n}$, computing $\Omega_1 x$ costs $2n \log_2(l+1)$ flops.

Results from image processing (from Halko et al)

- A matrix A of size 9025×9025 arising from a diffusion geometry approach.
- A is a graph Lapacian on the manifold of 3×3 patches.
- 95×95 pixel grayscale image, intensity of each pixel is an integer ≤ 4095.
- Vector $x^{(i)} \in \mathbb{R}^9$ gives the intensities of the pixels in a 3×3 neighborhood of pixel i.
- W reflects similarities between patches, $\sigma = 50$ reflects the level of sensitivity,

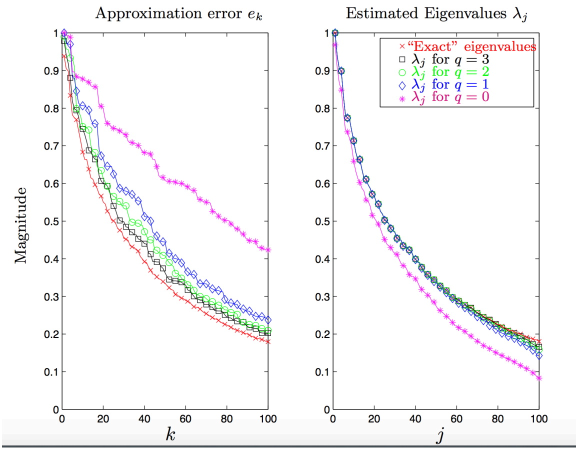
$$w_{ij} = exp\{-||x^{(i)} - x^{(j)}||^2/\sigma^2\},$$

- Sparsify W, compute dominant eigenvectors of $A = D^{-1/2} W D^{-1/2}$.



Experimental results (from Halko et al)

- Approximation error : $||A - QQ^T A||_2$
- Estimated eigenvalues for $k = 100$



More details on CA deterministic algorithms

- [Demmel et al., 2015] Communication avoiding rank revealing QR factorization with column pivoting Demmel, Grigori, Gu, Xiang, SIAM J. Matrix Analysis and Applications, 2015.
- Low rank approximation of a sparse matrix based on LU factorization with column and row tournament pivoting, with S. Cayrols and J. Demmel, Inria TR 8910.

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Results used in the proofs

- Interlacing property of singular values [Golub, Van Loan, 4th edition, page 487]
  Let $A = [a_1| \dots |a_n]$ be a column partitioning of an $m \times n$ matrix with $m \geq n$. If $A_r = [a_1| \dots |a_r]$, then for $r = 1 : n-1$

  $$\sigma_1(A_{r+1}) \geq \sigma_1(A_r) \geq \sigma_2(A_{r+1}) \geq \dots \geq \sigma_r(A_{r+1}) \geq \sigma_r(A_r) \geq \sigma_{r+1}(A_{r+1}).$$

- Given $n \times n$ matrix B and $n \times k$ matrix C, then ([Eisenstat and Ipsen, 1995], p. 1977)

  $$\sigma_{min}(B)\sigma_j(C) \leq \sigma_j(BC) \leq \sigma_{max}(B)\sigma_j(C), j = 1, \dots, k.$$