Randomized low rank approximation

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Extreme-scale
Mathematically-based
Computational
Chemistry

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Plan

Randomization for least-squares problem

Low rank matrix approximation

Randomized algorithms for low rank approximation

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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

$$|\langle \Omega_1 x_i, \Omega_1 x_j \rangle - \langle x_i, x_j \rangle| \leq \epsilon \|x_i\|_2 \|x_j\|_2 \tag{1}$$

- 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:

$$\|\Omega_1 x_i\|_2^2 = (1 \pm \epsilon)\|x_i\|_2^2 \tag{2}$$
$$\|\Omega_1 (x_i + x_j)\|_2^2 = (1 \pm \epsilon)\|x_i + x_j\|_2^2 \tag{3}$$

Proof that we obtain relation (4):

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

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

$$|\langle \Omega_1 x_i, \Omega_1 x_j \rangle - \langle x_i, x_j \rangle| \leq \epsilon \|x_i\|_2 \|x_j\|_2 \tag{4}$$

Source: Theorem 6 in [Woodruff, 2014]

Least squares problems

Given $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^n$, with $m \ll n$, solve

$$y := arg \min_{x \in \mathbb{R}^n} \|Ax - b\|_2$$

1. Solve by computing QR factorization of A or using normal equations,

$$A^T A x = A^T b.$$

2. Solve by using randomization, with $\Omega_1 \in \mathbb{R}^{k \times m}$

$$y^* := arg \min_{x \in \mathbb{R}^n} \|\Omega_1(Ax - b)\|_2$$

Least squares problems with randomization

Solve by using randomization, with $\Omega_1 \in \mathbb{R}^{k \times m}$, $k = O(\epsilon^{-2}(n + \log(1/\delta))$, being OSE with parameters (n, ϵ, δ) for $\mathbf{V} = range(A) + span(b)$

$$y^* := arg \min_{x \in \mathbb{R}^n} \|\Omega_1(Ax - b)\|_2$$

We obtain with probability $1 - \delta$:

$$\|Ay^* - b\|_2^2 \leq (1 + O(\epsilon))\|Ay - b\|_2^2$$

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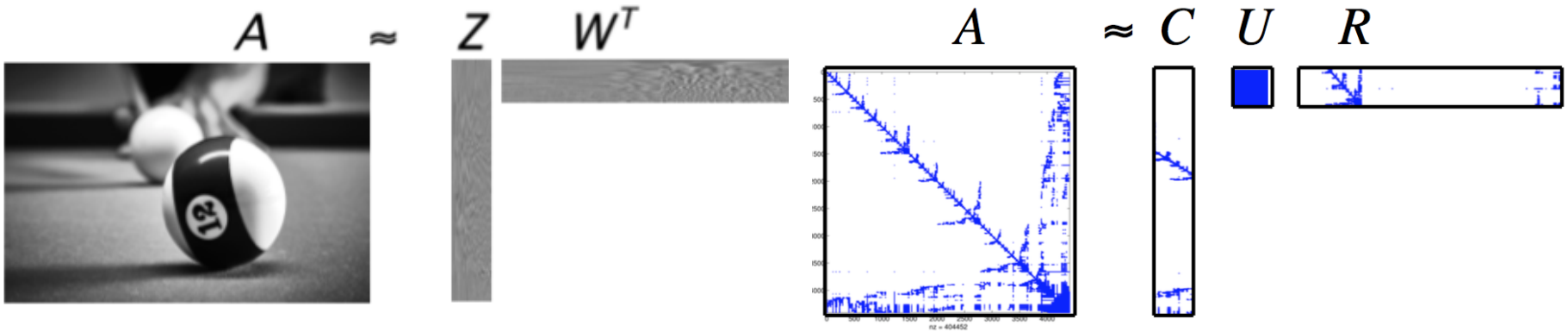
Low rank matrix approximation

- 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, ...

$$Ax \to ZW^T x$$

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

Singular value decomposition

For any 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

- $U \in \mathbb{R}^{m \times m}$ is orthogonal matrix, the left singular vectors of A , U_1 is $m \times k$, U_2 is $m \times n - k$, U_3 is $m \times m - n$
- $\Sigma \in \mathbb{R}^{m \times n}$, 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 $n - k \times n - k$
- $V \in \mathbb{R}^{n \times n}$ is orthogonal matrix, the right singular vectors of A, V_1 is $n \times k$, V_2 is $n \times n - k$

Properties of SVD

Given $A = U\Sigma V^T$, we have

- $A^TA = V\Sigma^T\Sigma V^T$,
  the right singular vectors of A are a set of orthonormal eigenvectors of A^TA.
- $AA^T = U\Sigma^T\Sigma U^T$,
  the left singular vectors of A are a set of orthonormal eigenvectors of AA^T.
- The non-negative singular values of A are the square roots of the non-negative eigenvalues of A^TA and AA^T.
- If $\sigma_k \neq 0$ and $\sigma_{k+1}, \ldots, \sigma_n = 0$, then
  $Range(A) = span(U_1)$, $Null(A) = span(V_2)$,
  $Range(A^T) = span(V_1)$, $Null(A) = span(U_2\ U_3)$.

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:

$$
\begin{aligned}
\max_{i,j} |A(i,j)| &\leq ||A||_2 \leq \sqrt{mn} \max_{i,j} |A(i,j)| \\
||A||_2 &\leq ||A||_F \leq \sqrt{min(m,n)}||A||_2
\end{aligned}
$$

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

$$
\begin{aligned}
||QAZ||_F &= ||A||_F \\
||QAZ||_2 &= ||A||_2
\end{aligned}
$$

Low rank matrix approximation

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

$$\min_{rank(A_k) \leq k} ||A - A_k||_2 = ||A - A_{opt,k}||_2 = \sigma_{k+1}(A) \quad (5)$$

$$\min_{rank(A_k) \leq k} ||A - A_k||_F = ||A - A_{opt,k}||_F = \sqrt{\sum_{j=k+1}^{n} \sigma_j^2(A)} \quad (6)$$

Image, size 1190×1920

Rank-10 approximation, SVD

Rank-50 approximation, SVD

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

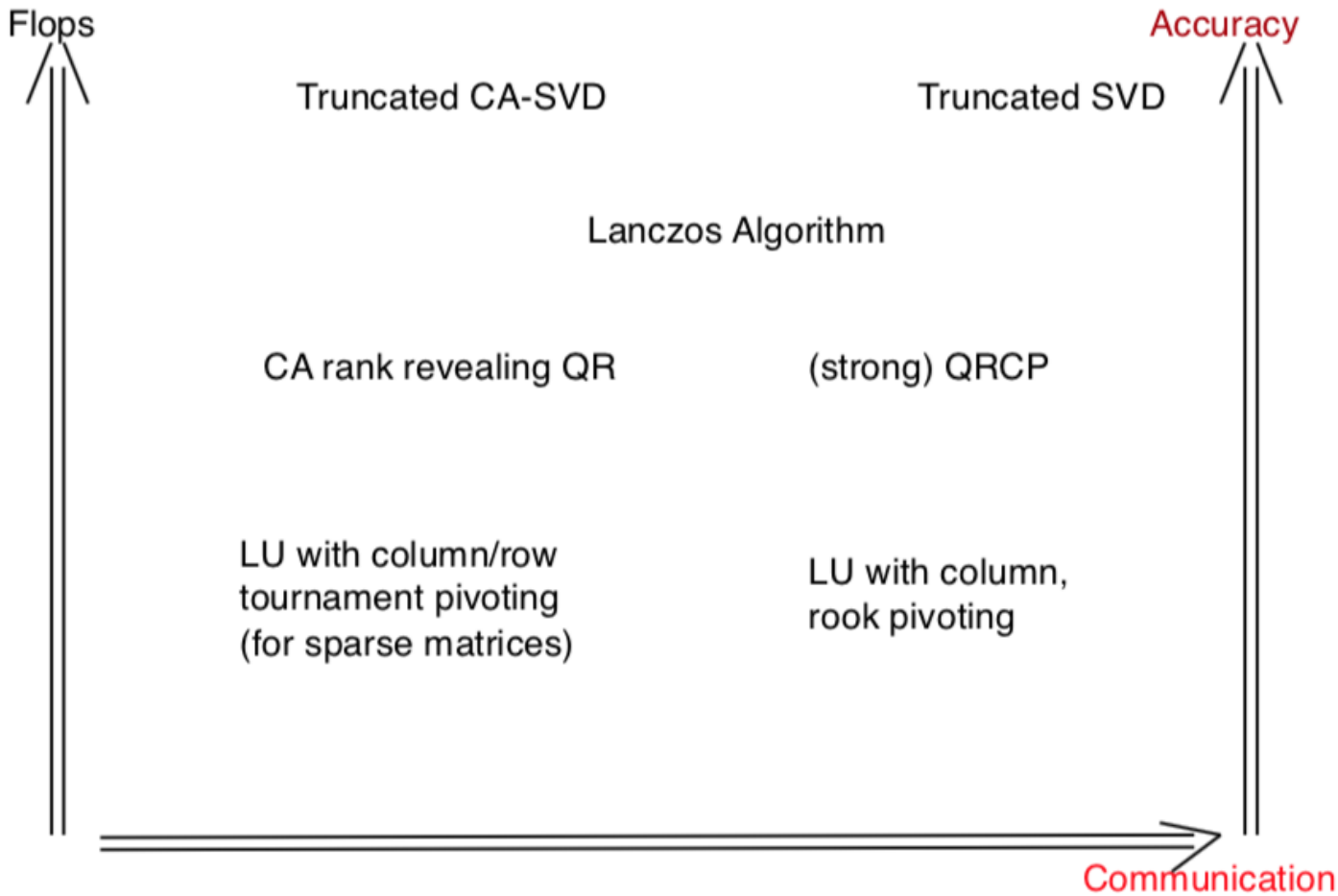
Large data sets

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.

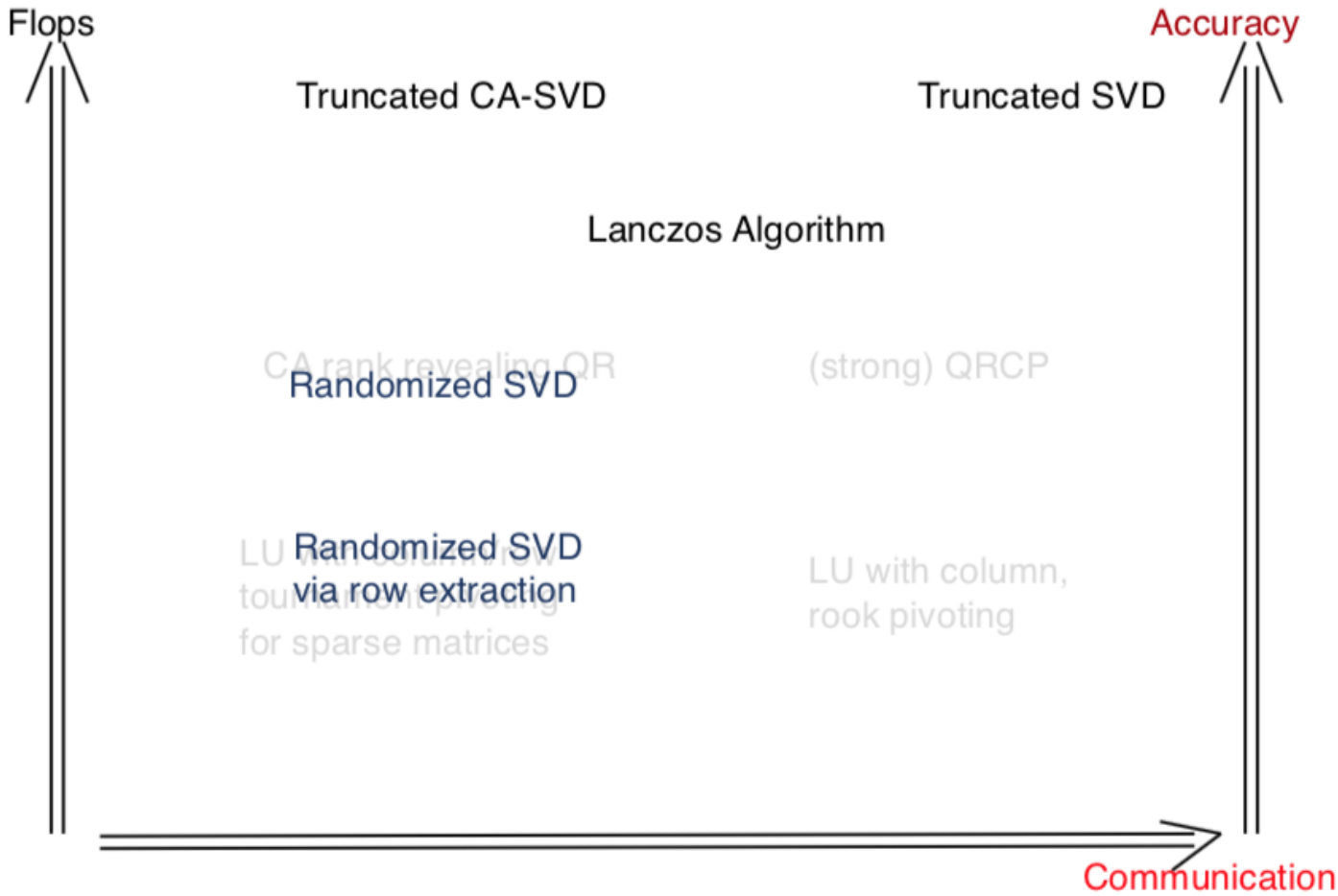
Low rank matrix approximation: trade-offs



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



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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 o f 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

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

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Properties of the approximations

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

Definition 1

[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 2

[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 3

[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.

Deterministic rank-k matrix approximation

Given $A \in \mathbb{R}^{m\times n}$, $\Theta = \begin{pmatrix}\Theta_1\\ \Theta_2\end{pmatrix} \in \mathbb{R}^{m\times m}$, $\Omega = \begin{pmatrix}\Omega_1 & \Omega_2\end{pmatrix} \in \mathbb{R}^{n\times n}$, Θ, Ω invertible, $\Theta_1 \in \mathbb{R}^{l'\times m}$, $\Omega_1 \in \mathbb{R}^{n\times l}$, $k \le l \le l'$.

$$\begin{aligned}\Theta A\Omega &= \bar{A} = \begin{pmatrix}\bar{A}_{11} & \bar{A}_{12}\\ \bar{A}_{21} & \bar{A}_{22}\end{pmatrix}\\ &= \begin{pmatrix} I & \\ \bar{A}_{21}\bar{A}_{11}^{+} & I\end{pmatrix}\begin{pmatrix}\bar{A}_{11} & \bar{A}_{12}\\ & S(\bar{A}_{11})\end{pmatrix} = \Theta\begin{pmatrix}Q_1 & Q_2\end{pmatrix}\begin{pmatrix}R_{11} & R_{12}\\ & R_{22}\end{pmatrix},\end{aligned}$$

where $\bar{A}_{11} \in \mathbb{R}^{l',l}$, $\bar{A}_{11}^{+}\bar{A}_{11} = I$, $S(\bar{A}_{11}) = \bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^{+}\bar{A}_{12}$.

- Generalized LU computes the approximation

$$A_k = \Theta^{-1}\begin{pmatrix} I \\ \bar{A}_{21}\bar{A}_{11}^{+}\end{pmatrix}\begin{pmatrix}\bar{A}_{11} & \bar{A}_{12}\end{pmatrix}\Omega^{-1}$$

- QR computes the approximation

$A_k = Q_1\begin{pmatrix}R_{11} & R_{12}\end{pmatrix}V^{-1} = Q_1 Q_1^T A$, where Q_1 is orth basis for $(A\Omega_1)$

Unified perspective: generalized LU factorization

Given Θ_1, A, Ω_1, Q_1 orth. basis of $(A\Omega_1)$, $k = l = l'$, rank-k approximation,

$$A_k = A\Omega_1(\Theta_1 A\Omega_1)^{-1}\Theta_1 A$$

Deterministic algorithms Ω_1 column permutation and ...	**Randomized algorithms*** Ω_1 random matrix and ...
QR with column selection (a.k.a. strong rank revealing QR) $\Theta_1 = Q_1^T$, $A_k = Q_1 Q_1^T A$ $\|\|R_{11}^{-1}R_{12}\|\|_{max}$ is bounded	Randomized QR (a.k.a. randomized SVD) $\Theta_1 = Q_1^T$, $A_k = Q_1 Q_1^T A$
LU with column/row selection (a.k.a. rank revealing LU) Θ_1 row permutation s.t. $\Theta_1 Q_1 = \begin{pmatrix}\bar{Q}_{11}\\ \bar{Q}_{21}\end{pmatrix}$ $\|\|\bar{Q}_{21}\bar{Q}_{11}^{-1}\|\|_{max}$ is bounded	Randomized LU with row selection (a.k.a. randomized SVD via Row extraction) Θ_1 row permutation s.t. $\Theta_1 Q_1 = \begin{pmatrix}\bar{Q}_{11}\\ \bar{Q}_{21}\end{pmatrix}$ $\|\|\bar{Q}_{21}\bar{Q}_{11}^{-1}\|\|_{max}$ bounded
	Randomized LU approximation Θ_1 random matrix

Deterministic algorithms will be discussed in a future lecture.

Generalized LU factorization $k \leq l \leq l'$ (contd)

Given Θ_1, A, Ω_1, Q_1 orth. basis of $(A\Omega_1)$, $k \leq l \leq l'$, rank-k approximation,

$$A_k = [\Theta_1^+(I - (\Theta_1 A\Omega_1)(\Theta_1 A\Omega_1)^+) + (A\Omega_1)(\Theta_1 A\Omega_1)^+][\Theta_1 A], \qquad (7)$$

where Θ_1 and $(\Theta_1 A\Omega_1)$ are of dimensions $l' \times m$ and $l' \times l$ respectively.

Remark Given that only Θ_1 and Ω_1 are required for computing A_k, Θ and Ω are used only for the analysis, Θ_2 and Ω_2 are chosen to be the orthogonal of Θ_1 and Ω_1 respectively.

Properties of projection based approximations

Proposition 4 (Proposition 4.3 from [Demmel et al., 2019])

Let $A \in \mathbb{R}^{m\times n}$ matrix with SVD $A = U\Sigma V^T$. Set $[Q, R] = \mathbf{QR}(A\Omega)$, where $\Omega \in \mathbb{R}^{n\times n}$ matrix, $\Omega = (\Omega_1, \Omega_2)$, Ω_1 is full column rank and Ω_2 is the orthogonal of Ω_1. Then the singular values of $Q_1 Q_1^T A - A$ are identical to those of matrix $R_{22} \in \mathbb{R}^{(m-l)\times(n-l)}$. Moreover,

$$\|R_{22}\|_F^2 \leq \|\Sigma_{1,2}\|_F^2 + \|\Sigma_{1,2}(V^T\Omega)_{21}(V^T\Omega)_{11}^+\|_F^2$$

$$\sigma_j(A) \geq \sigma_j(Q_1 Q_1^T A) \geq \sigma_j(A\Omega_1)\sigma_{\min}(\Omega_1^+), \quad \text{for } j \leq k \tag{8}$$

as well as for any given $j \leq \min(m, n) - k$, there is an orthogonal $n \times (n - j)$ matrix $\tilde{V}$ independent of Ω such that

$$\sigma_j^2(R_{22}) \quad \leq \quad \sigma_{j+k}^2(A) + \|\Sigma_{j,2}(\tilde{V}^T\Omega)_{21}(\tilde{V}^T\Omega)_{11}^+\|_2^2 \tag{9}$$

with $(\tilde{V}^T\Omega)_{11} \in \mathbb{R}^{k\times l}$, and $\Sigma_{j,2} := \mathbf{diag}(\sigma_{k+j}(A), \ldots, \sigma_n(A), 0, \ldots, 0)$, and $\Sigma_{j,2} \in \mathbb{R}^{(m-k)\times(n-k)}$, where **diag** *denotes the diagonal matrix.*

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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_1 $(m \times k)$ with orthonormal columns and approximate A by the projection of its columns onto the space spanned by Q_1:

$$A \approx Q_1 Q_1^T A$$

2. Use Q_1 to compute a standard factorization of A

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

Typical randomized SVD

1. Compute an approximate basis for the range of $A \in \mathbb{R}^{m \times n}$
   Sample $\Omega_1 \in \mathbb{R}^{n \times l}$, $l = p + k$, with independent mean-zero, unit-variance Gaussian entries.
   Compute $Y = A\Omega_1$, $Y \in \mathbb{R}^{m \times l}$ expected to span column space of A.
   - Cost of multiplying $A\Omega_1$: $2mnl$ flops
2. With Q_1 being orthonormal basis of Y, approximate A as:

$$\tilde{A}_k = Q_1 Q_1^T A = \mathcal{P}^o A$$

   - Cost of multiplying $Q_1^T A$: $2mnl$ flops

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

Typical randomized SVD

Algorithm

Input: matrix $A \in \mathbb{R}^{m \times n}$, desired rank k, $l = p + k$.

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 $Q_1 \in \mathbb{R}^{m \times l}$ with columns forming an orthonormal basis for the range of Y.
4. Compute $B = Q_1^T A$, $B \in \mathbb{R}^{l \times n}$
5. Compute the rank-k truncated SVD of B as $\hat{U}\Sigma V^T$, $\hat{U} \in \mathbb{R}^{l \times k}$, $V^T \in \mathbb{R}^{k \times n}$

Return the approximation $\tilde{A}_k = Q_1 \hat{U} \cdot \Sigma \cdot V^T$

Randomized SVD ($q = 0$)

The best approximation is when Q_1 equals the first $k + p$ left singular vectors of A. Given $A = U\Sigma V^T$,

$$\begin{aligned} Q_1 Q_1^T A &= U(1:m, 1:k+p)\Sigma(1:k+p, 1:k+p)(V(1:n, 1:k+p \\ ||A - Q_1 Q_1^T A||_2 &= \sigma_{k+p+1} \end{aligned}$$

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

$$\mathbb{E}(||A - Q_1 Q_1^T A||_2) \leq \left(1 + \frac{4\sqrt{k+p}}{p-1}\sqrt{min(m,n)}\right)\sigma_{k+1}(A)$$

and the probability that the error satisfies

$$||A - Q_1 Q_1^T A||_2 \leq \left(1 + 11\sqrt{k+p} \cdot \sqrt{min(m,n)}\right)\sigma_{k+1}(A)$$

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

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

Randomized SVD

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

$$\mathbb{E}(||A - Q_1 Q_1^T A||_2) \leq \left(1 + \sqrt{\frac{k}{p-1}}\right) \sigma_{k+1}(A) + \frac{e\sqrt{k+p}}{p} \left(\sum_{j=k+1}^{n} \sigma_j^2(A)\right)^{1/2}$$

- 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 4 steps of the algorithm 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 $B = Q_1^T A$: $2nnz(A) \cdot (k+p)$
  (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

$$\Omega_1 = \sqrt{\frac{n}{l}} \cdot P \cdot H \cdot D, \text{ where} \tag{10}$$

- $D \in \mathbb{R}^{n \times n}$ 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,

$$H_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad H_n = \begin{pmatrix} H_{n/2} & H_{n/2} \\ H_{n/2} & -H_{n/2} \end{pmatrix}. \tag{11}$$

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

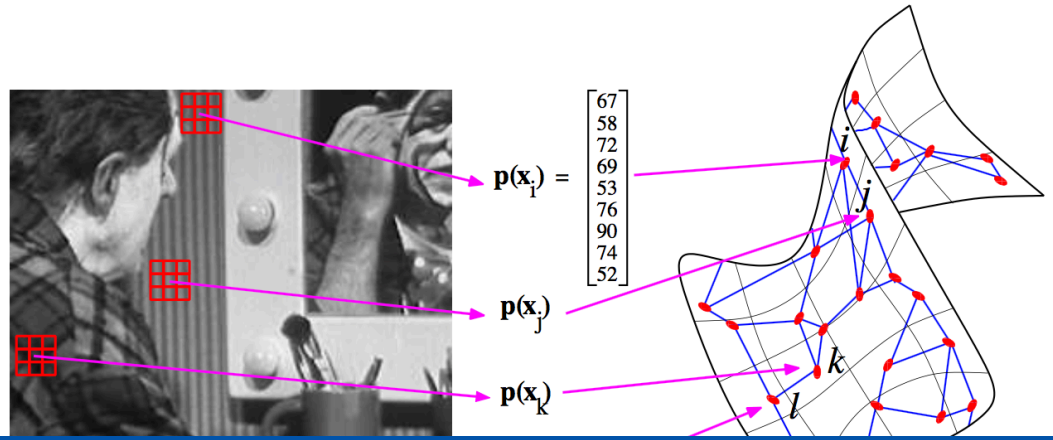
Cost of matrix vector multiplication (Theorem 2.1 in [Ailon and Liberty, 2008]):
For $x \in \mathbb{R}^n$ and $\Omega_1 \in \mathbb{R}^{l \times n}$, computing $\Omega_1 x$ costs $2n \log_2(l+1)$ flops.

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,

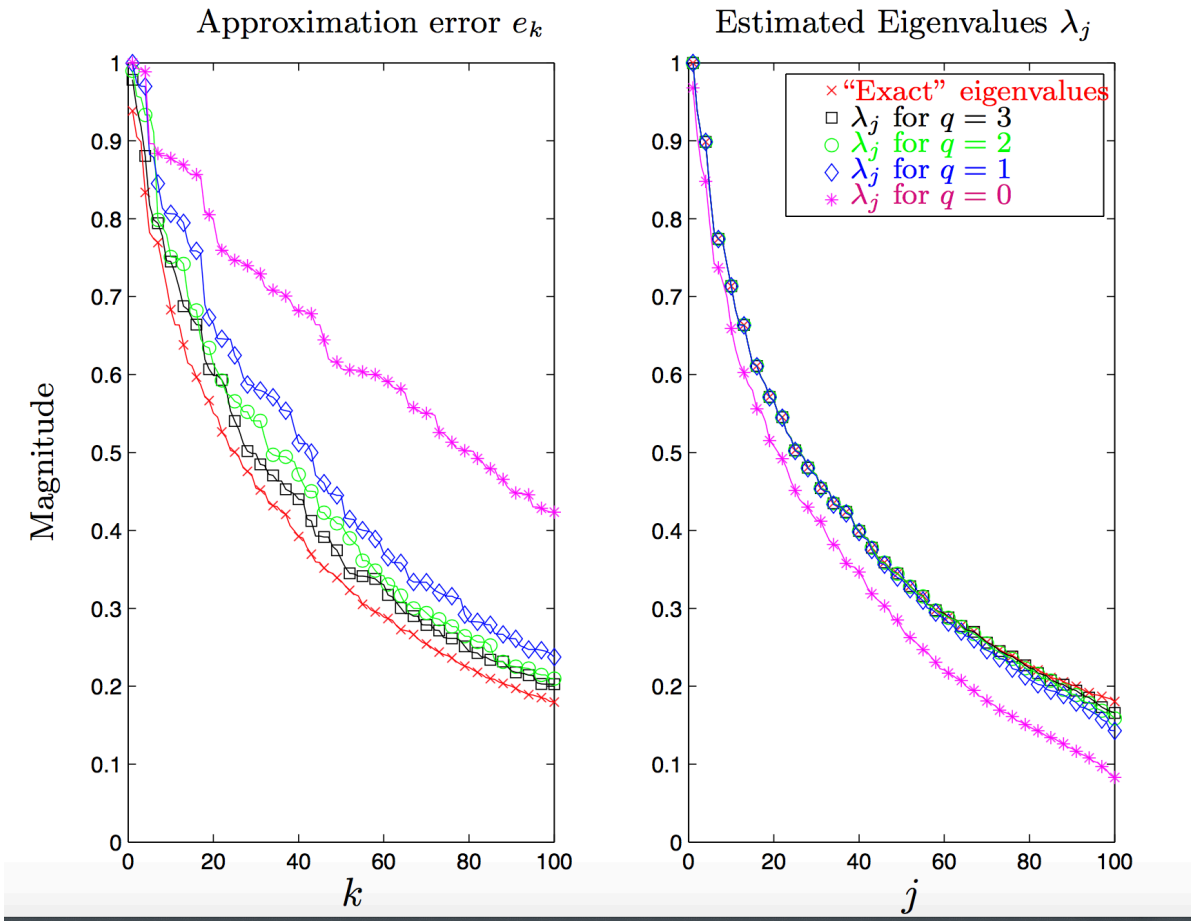
$$w_{ij} = exp\{-||x^{(i)} - x^{(j)}||^2/\sigma^2\},$$

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



Experimental results (from Halko et al)

- Approximation error : $||A - Q_1 Q_1^T A||_2$
- Estimated eigenvalues for $k = 100$



Oblivious subspace embedding

Definition 5

A (k, ϵ, δ) oblivious subspace embedding (OSE) from $\mathbb{R}^n$ to $\mathbb{R}^l$ is a distribution $\Omega_1 \sim \mathbb{D}$ over $l \times n$ matrices. It satisfies with probability $1 - \delta$

$$1 - \epsilon \leq \sigma^2_{\min}(\Omega_1 Q) \leq \sigma^2_{\max}(\Omega_1 Q) \leq 1 + \epsilon$$

for any given orthogonal $n \times k$ matrix Q. We will assume $l \geq k$ and $\epsilon < 1/6$.

Definition 6

$\Omega_1 \in \mathbb{R}^{l \times n}$ is (ϵ, δ, n) multiplication approximating, if for any A, B having n rows, it satisfies with probability $1 - \delta$,

$$\|A^T \Omega_1^T \Omega_1 B - A^T B\|_F \leq \epsilon \|A\|_F \|B\|_F. \tag{12}$$

Properties of SRHT ensembles

Additional property of the SRHT ensemble from Lemma 4.8 of [Boutsidis and Gittens, 2013].

Lemma 7

Let Ω_1 be drawn from an SRHT of dimension $l \times n$. Then for $m \times n$ matrix A with rank ρ, with probability $1 - 2\delta$,

$$\|A\Omega_1^T\|_2^2 \leq 5\|A\|_2^2 + \frac{\log(\rho/\delta)}{l}(\|A\|_F + \sqrt{8\log(n/\delta)}\|A\|_2)^2$$

Oblivious embeddings: Let $\Omega_1 \in \mathbb{R}^{l \times n}$ be drawn from SRHT ensembles. With $l = 4\epsilon^{-1}k(1 + 2\sqrt{\ln(3/\delta)})^2(1 + \sqrt{8\ln(3n/\delta)})^2$, Ω_1 is a $(k, \sqrt{\epsilon}, 3\delta)$ OSE (Lemma 4.1 from [Boutsidis and Gittens, 2013]). It satisfies the multiplication property with $(\epsilon/k, \delta, n)$ (Lemma 4.11 from [Boutsidis and Gittens, 2013]).

Subspace embeddings

Lemma 5.4 from [Demmel et al., 2019], an extension of Lemma 4.1 of [Boutsidis and Gittens, 2013].

Lemma 8

Let Ω_1 be an $l \times n$ matrix that is a (k, ϵ, δ) OSE from $\mathbb{R}^n$ to $\mathbb{R}^l$, and Q be an $(n \times k)$ orthogonal matrix. Provided $\epsilon < 1/6$, then with probability $1 - \delta$ both of the following hold,

$$\|(\Omega_1 Q)^+ - (\Omega_1 Q)^T\|_2^2 \leq 3\epsilon \tag{13}$$

$$\|\Omega_1\|_2^2 = O\left(\frac{n}{k}\right), \tag{14}$$

where in the second of these we require the additional assumption $\delta > 2e^{-k/5}$.

Randomized SVD with SRHT ensembles

Corollary 9 (Corollary 5.16 in [Demmel et al., 2019])

Let $\Omega_1 \in \mathbb{R}^{n\times l}$ *be drawn from an SHRT ensemble,* $l \geq 4\epsilon^{-1}k(1+2\sqrt{\ln(3/\delta)})^2(1+\sqrt{8\ln(3n/\delta)})^2$, Ω_1, *and for simplicity assume* $l \geq \log(n/\delta)\log(\rho/\delta)$. *Then with probability* $1-2\delta$

$$\sigma_j^2(R_{22}) \leq O(1)\sigma_{k+j}^2(A) + O(\frac{\log(\rho/\delta)}{l})(\sigma_{k+j}^2(A)+\ldots\sigma_n^2(A))\,, \tag{15}$$

for $1 \leq j \leq min(m,n)-k$ *with probability* $1-3\delta$ *for a particular* j. *We also have upper and lower bounds on the largest singular values, as for* $1 \leq j \leq k$,

$$\sigma_j(A) \geq \sigma_j(Q_1 Q_1^T A) = \Omega(\sqrt{\frac{k}{n}})\sigma_j(A) \tag{16}$$

holds with probability $1-2\max(\delta, e^{-k/5})$.

Details of proof of eq (15)

Begin by using Proposition 4 and Lemma 8,

$$\sigma_j^2(R_{22}) \leq \|\Sigma_{j,2}\|_2^2 + \|\Sigma_{j,2}(\tilde{V}^T\Omega)_{21}(\tilde{V}^T\Omega)_{11}^{+}\|_2^2 \leq \|\Sigma_{j,2}\|_2^2 + 2\|\Sigma_{j,2}(\tilde{V}^T\Omega)_{21}\|_2^2,$$

with probability $1-\delta$. Next apply Lemma 7 to the second term to get

$$\begin{aligned}
\sigma_j^2(R_{22}) &= O\left(1 + \frac{\log(\rho/\delta)\log(n/\delta)}{l}\right)\|\Sigma_{j,2}\|_2^2 + O\left(\frac{\log(\rho/\delta)}{l}\right)\|\Sigma_{j,2}\|_F^2 \\
&= O(1)\|\Sigma_{j,2}\|_2^2 + O\left(\frac{\log(\rho/\delta)}{l}\right)\|\Sigma_{j,2}\|_F^2) \qquad (17) \\
&= O(1)\sigma_{k+j}^2(A) + O(\frac{\log(\rho/\delta)}{l})(\sigma_{k+j}^2(A) + \ldots \sigma_n^2(A)), \qquad (18)
\end{aligned}$$

where ρ is the rank of A, with probability $1-2\delta$.

Probabilistic guarantees for randomized GLU

- Consider $\Theta_1 \in \mathbb{R}^{l' \times m}, \Omega_1 \in \mathbb{R}^{n \times l}$ are Subsampled Randomized Hadamard Transforms (SRHT), $l' > l$.
- Compute A_k through generalized LU as in equation (7) costs $O(mn \log_2 l' + mll')$ flops,

$$A_k = [\Theta_1^+(I - (\Theta_1 A \Omega_1)(\Theta_1 A \Omega_1)^+) + (A\Omega_1)(\Theta_1 A \Omega_1)^+][\Theta_1 A].$$

Theorem 10 (Theorem 5.9 from [Demmel et al., 2019])

Let $\Theta_1 \in \mathbb{R}^{l' \times m}$ *and* $\Omega_1 \in \mathbb{R}^{n \times l}$ *be drawn from SRHT ensembles,*
$l = 4\epsilon^{-1}k(1 + 2\sqrt{\ln(3/\delta)})^2(1 + \sqrt{8\ln(3n/\delta)})^2$,
$l' = 4\epsilon^{-1}l(1 + 2\sqrt{\ln(3/\delta)})^2(1 + \sqrt{8\ln(3m/\delta)})^2$.
With probability $1 - 5\delta$, *the* **randomized GLU** *approximation* A_k *satisfies*

$$\|A - A_k\|_2^2 = O(1)\sigma_{k+1}^2(A) + O(\frac{\log(n/\delta)}{l} + \frac{\log(m/\delta)}{l'})(\sigma_{k+1}^2(A) + \ldots \sigma_n^2(A))$$

$$\sigma_j^2(A - A_k) \leq O(1)\sigma_{k+j}^2 + O(\frac{\log(\rho/\delta)}{l} + \frac{\log(\rho/\delta)}{l'})(\sigma_{k+j}^2(A) + \ldots \sigma_n^2(A)).$$

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Results used in the proofs

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

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

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

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