Randomized low rank approximation

L. Grigori

Inria Paris, UPMC

November 2020









Plan

Randomization for least-squares problem

Low rank matrix approximation

Randomized algorithms for low rank approximation

Plan

Randomization for least-squares problem

Low rank matrix approximation

Randomized algorithms for low rank approximation

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 $\mathsf{JLT}(n, \epsilon, \delta)$, if with probability at least $1 - \delta$ for any n-element subset $V \subset \mathbb{R}^m$, for all $x_i, x_i \in V$, we have

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

- 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 $x_i, x_i \in V$ we require to hold:

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

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

Proof that we obtain relation (4):

$$\langle \Omega_{1}x_{i}, \Omega_{1}x_{j} \rangle = (\|\Omega_{1}(x_{i} + x_{j})\|_{2}^{2} - \|\Omega_{1}x_{i}\|_{2}^{2} - \|\Omega_{1}x_{j}\|_{2}^{2})/2$$

$$= ((1 \pm \epsilon)\|x_{i} + x_{j}\|_{2}^{2} - (1 \pm \epsilon)\|x_{i}\|_{2}^{2} - (1 \pm \epsilon)\|x_{j}\|_{2}^{2})/2$$

$$= \langle x_{i}, x_{j} \rangle \pm O(\epsilon)$$

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

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

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

$$y := arg \min_{x \in \mathbb{R}^n} \|Ax - b\|_2 = \sum_{i=1}^n (b_i - \langle A(i,:), x \rangle)^2$$

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 $1 - \delta$:

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

Plan

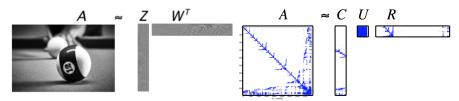
Randomization for least-squares problem

Low rank matrix approximation

Randomized algorithms for low rank approximation

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
 - $\hfill\Box$ from scientific computing: fast solvers for integral equations, H-matrices
 - $\hfill\Box$ to data analytics: principal component analysis, image processing, \dots

$$Ax \to ZW^T x$$
Flops $2mn \to 2(m+n)k$

Singular value decomposition

For any given $A \in \mathbb{R}^{m \times n}$, $m \ge n$ its singular value decomposition is

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

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 $\sigma_1(A) \ge ... \ge \sigma_n(A) \ge 0$ 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

- $A^T A = V \Sigma^T \Sigma V^T$, the right singular vectors of A are a set of orthonormal eigenvectors of $A^T A$.
- $AA^T = U\Sigma^T\Sigma U^T$, 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 $\sigma_{k+1}, \dots, \sigma_n = 0$, 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

$$||A||_{p} = \max_{||x||_{p}=1} ||Ax||_{p}$$

$$||A||_{F} = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^{2}} = \sqrt{\sigma_{1}^{2}(A) + \dots \sigma_{n}^{2}(A)}$$

$$||A||_{2} = \sigma_{max}(A) = \sigma_{1}(A)$$

Some properties:

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

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

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

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

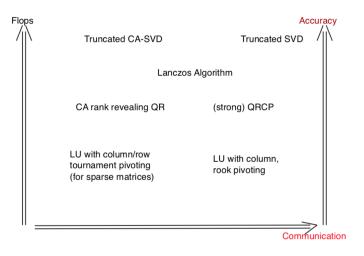
Large data sets

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.

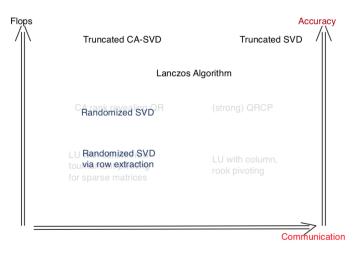
Matrix A might exist only implicitly, and it is never formed explicitly.

Low rank matrix approximation: trade-offs



Communication optimal if computing a rank-k approximation on P processors requires $\# \ \mathrm{messages} = \Omega \left(\log_2 P \right).$

Low rank matrix approximation: trade-offs



Communication optimal if computing a rank-k approximation on P processors requires $\# \ \mathrm{messages} = \Omega \left(\log_2 P \right).$

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.

$$||A - \mathcal{P}^{o}A||_{2} \leq \gamma \sigma_{k+1}(A)$$
, for some $\gamma \geq 1$,

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

$$\mathcal{P}^o = A\Omega_1(A\Omega_1)^+ = Q_1Q_1^T, \text{ or equiv } \mathcal{P}^o a_j := \arg\min_{x \in X} \|x - a_j\|_2$$

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

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

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.

$$||A - \mathcal{P}^{o}A||_{2} \leq \gamma \sigma_{k+1}(A)$$
, for some $\gamma \geq 1$,

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

$$\mathcal{P}^o = A\Omega_1(A\Omega_1)^+ = Q_1Q_1^{\mathcal{T}}, \text{ or equiv } \mathcal{P}^o a_j := \arg\min_{x \in X} \|x - a_j\|_2$$

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

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

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 $||A - A_k||_2 \le \gamma \sigma_{k+1}(A)$ for some $\gamma \ge 1$ 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 $1 \le j \le n-k$ and some $\gamma \ge 1$, 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, $\Theta_1 \in \mathbb{R}^{l' \times m}$, $\Omega_1 \in \mathbb{R}^{n \times l}$, $k \leq l \leq l'$.

$$\begin{split} \Theta A \Omega &= \bar{A} = \begin{pmatrix} A_{11} & A_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{pmatrix} \\ &= \begin{pmatrix} I \\ \bar{A}_{21} \bar{A}_{11}^{+} & I \end{pmatrix} \begin{pmatrix} \bar{A}_{11} & \bar{A}_{12} \\ S(\bar{A}_{11}) \end{pmatrix} = \Theta \begin{pmatrix} Q_{1} & Q_{2} \end{pmatrix} \begin{pmatrix} R_{11} & R_{12} \\ R_{22} \end{pmatrix}, \end{split}$$

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

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,

$$A_k = A\Omega_1(\Theta_1A\Omega_1)^{-1}\Theta_1A$$

| Deterministic algorithms | Randomized algorithms* |
|--|---|
| Ω_1 column permutation and | Ω_1 random matrix and |
| QR with column selection | Randomized QR |
| (a.k.a. strong rank revealing QR) | (a.k.a. randomized SVD) |
| $\Theta_1 = Q_1^{\mathcal{T}}$, $A_k = Q_1 Q_1^{\mathcal{T}} A$ | $\Theta_1 = Q_1^{T}$, $A_k = Q_1 Q_1^{T} A$ |
| $ R_{11}^{-1}R_{12} _{\it max}$ is bounded | |
| LU with column/row selection | Randomized LU with row selection |
| (a.k.a. rank revealing LU) | (a.k.a. randomized SVD via Row extraction) |
| Θ_1 row permutation s.t. $\Theta_1 Q_1 = egin{pmatrix} ar{Q}_{11} \ ar{Q}_{21} \end{pmatrix}$ | Θ_1 row permutation s.t. $\Theta_1 \mathit{Q}_1 = egin{pmatrix} ar{\mathcal{Q}}_{11} \ ar{\mathcal{Q}}_{21} \end{pmatrix}$ |
| $ ar{Q}_{21}ar{Q}_{11}^{-1} _{	extit{max}}$ is bounded | $ ar{Q}_{21}ar{Q}_{11}^{-1} _{	extit{max}}$ bounded |
| | Randomized LU approximation |
| | Θ_1 random matrix |
| Decree to the control of the control | `. · · · |

Deterministic algorithms will be discussed in a future lecture.

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

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

$$A_{k} = [\Theta_{1}^{+}(I - (\Theta_{1}A\Omega_{1})(\Theta_{1}A\Omega_{1})^{+}) + (A\Omega_{1})(\Theta_{1}A\Omega_{1})^{+}][\Theta_{1}A],$$
 (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 $Q_1Q_1^TA - A$ are identical to those of matrix $R_{22} \in \mathbb{R}^{(m-l) \times (n-l)}$. Moreover,

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

$$\sigma_j(A) \ge \sigma_j(Q_1 Q_1^T A) \ge \sigma_j(A\Omega_1)\sigma_{\min}(\Omega_1^+), \text{ for } j \le k$$
 (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

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

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

Plan

Randomization for least-squares problem

Low rank matrix approximation

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 $V_1 \in \mathbb{R}^{n \times l}$, l = p + k, with independent mean-zero, unit-variance Gaussian entries.
 - Compute $Y = AV_1$, $Y \in \mathbb{R}^{m \times l}$ expected to span column space of A.
 - □ Cost of multiplying *AV*₁: 2*mnl* 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 $Q_1^T A$: 2*mnl* 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 $Y=(AA^T)^qA\Omega_1$ /* 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 $B = Q_1^T A$, $B \in \mathbb{R}^{I \times n}$
- 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 $A=U\Sigma V^T$,

$$Q_1Q_1^TA = U(1:m,1:k+p)\Sigma(1:k+p,1:k+p)(V(1:n,1:k+p))$$
 $||A - Q_1Q_1^TA||_2 = \sigma_{k+p+1}$

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

$$\mathbb{E}(||A - Q_1Q_1^TA||_2) \leq \left(1 + \frac{4\sqrt{k+p}}{p-1}\sqrt{\textit{min}(m,n)}\right)\sigma_{k+1}(A)$$

and the probability that the error satisfies

$$||A - Q_1Q_1^TA||_2 \le \left(1 + 11\sqrt{k+p} \cdot \sqrt{\min(m,n)}\right)\sigma_{k+1}(A)$$

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.,

$$\mathbb{E}(||A - Q_1Q_1^TA||_2) \leq \left(1 + \sqrt{\frac{k}{p-1}}\right)\sigma_{k+1}(A) + \frac{e\sqrt{k+p}}{p}\left(\sum_{j=k+1}^n \sigma_j^2(A)\right)^{1/2}$$

- 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 $(AA^T)^qA$ 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 $nnz(A)/m \ge k + p$ 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

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

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

$$H_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad H_n = \begin{pmatrix} H_{n/2} & H_{n/2} \\ H_{n/2} & -H_{n/2} \end{pmatrix}.$$
 (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]):

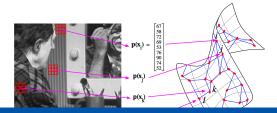
For $x \in \mathbb{R}^n$ and $\Omega_1 \in \mathbb{R}^{l \times n}$, computing $\Omega_1 x$ costs $2n \log_2(l+1)$ flops.

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,

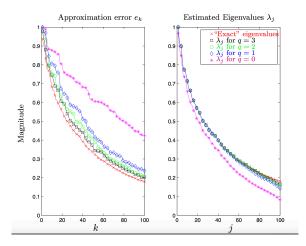
$$w_{ij} = \exp\{-||x^{(i)} - x^{(j)}||^2/\sigma^2\},\,$$

■ 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 $1 - \delta$

$$1 - \epsilon \le \sigma_{\mathsf{min}}^2(\Omega_1 Q) \le \sigma_{\mathsf{max}}^2(\Omega_1 Q) \le 1 + \epsilon$$

for any given orthogonal $n \times k$ matrix Q. We will assume $l \ge k$ 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 $1 - \delta$,

$$||A^T \Omega_1^T \Omega_1 B - A^T B||_F \le \epsilon ||A||_F ||B||_F.$$
 (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 $1 - 2\delta$,

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

Oblivious embeddings: Let $\Omega_1 \in \mathbb{R}^{I \times n}$ be drawn from SRHT ensembles. With $I = 4\epsilon^{-1}k(1+2\sqrt{\ln(3/\delta)})^2(1+\sqrt{8\ln(3n/\delta)})^2$, 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,

$$\|(\Omega_1 Q)^+ - (\Omega_1 Q)^T\|_2^2 \le 3\epsilon$$
 (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 $1-2\delta$

$$\sigma_j^2(R_{22}) \le O(1)\sigma_{k+j}^2(A) + O(\frac{\log(\rho/\delta)}{I})(\sigma_{k+j}^2(A) + \dots + \sigma_n^2(A)),$$
 (15)

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

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

$$\sigma_{j}^{2}(R_{22}) = O\left(1 + \frac{\log(\rho/\delta)\log(n/\delta)}{I}\right) \|\Sigma_{j,2}\|_{2}^{2} + O\left(\frac{\log(\rho/\delta)}{I}\right) \|\Sigma_{j,2}\|_{F}^{2}$$

$$= O(1)\|\Sigma_{j,2}\|_{2}^{2} + O\left(\frac{\log(\rho/\delta)}{I}\right) \|\Sigma_{j,2}\|_{F}^{2})$$

$$= O(1)\sigma_{k+j}^{2}(A) + O(\frac{\log(\rho/\delta)}{I})(\sigma_{k+j}^{2}(A) + \dots + \sigma_{n}^{2}(A)),$$
(18)

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, $l = 4\epsilon^{-1}k(1 + 2\sqrt{\ln(3/\delta)})^2(1 + \sqrt{8\ln(3n/\delta)})^2$.

$$I' = 4e^{-1}I(1 + 2\sqrt{\ln(3/\delta)})^2(1 + \sqrt{8\ln(3m/\delta)})^2.$$

With probability $1-5\delta$, the randomized GLU approximation A_k satisfies

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

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

References (1)



Ailon, N. and Liberty, E. (2008).

Fast dimension reduction using rademacher series on dual bch codes.

In Proceedings of the Nineteenth Annual ACM-SIAM Symposium on Discrete Algorithms, SODA '08, pages 1–9, Philadelphia, PA, USA. Society for Industrial and Applied Mathematics.



Boutsidis, C. and Gittens, A. (2013).

Improved matrix algorithms via the subsampled randomized hadamard transform.

SIAM J. Matrix Analysis Applications, 34:1301–1340.



Demmel, J., Grigori, L., and Rusciano, A. (2019).

An improved analysis and unified perspective on deterministic and randomized low rank matrix approximations.

Technical report, Inria.

available at https://arxiv.org/abs/1910.00223.



Eckart, C. and Young, G. (1936).

The approximation of one matrix by another of lower rank.

Psychometrika, 1:211-218.



Eisenstat, S. C. and Ipsen, I. C. F. (1995).

Relative perturbation techniques for singular value problems.

SIAM J. Numer. Anal., 32(6):1972-1988.



Woodruff, D. P. (2014).

Sketching as a tool for numerical linear algebra.

Found. Trends Theor. Comput. Sci., 10(1–2):1-157.

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 $m \ge n$. If $A_r = [a_1|\dots|a_r]$, then for r = 1 : n - 1

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

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

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