

# Randomized Numerical Linear Algebra: Review and Progresses

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- An interdisciplinary among Theoretical Computer Science (TCS), Numerical Linear Algebra (NLA), and Modern Data Analysis
- Many data mining and machine learning algorithms involve matrix decomposition, matrix inverse and matrix determinant; and some methods are based on low-rank matrix approximation.
- The Big Data phenomenon brings new challenges and opportunities to machine learning and data mining.

# Singular Value Decomposition (SVD)

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- Input: an  $m \times n$  data matrix  $\mathbf{A}$  of rank  $r$  and an integer  $k$  less than  $r$ .
- The (condensed) SVD:  $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$  where  $\mathbf{U}^T\mathbf{U} = \mathbf{I}_r$ ,  $\mathbf{V}^T\mathbf{V} = \mathbf{I}_r$ , and  $\mathbf{\Sigma} = \text{diag}(\sigma_1, \dots, \sigma_r)$  with  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$ .
  - time complexity:  $\mathcal{O}(mn \min(m, n))$
- The truncated SVD:  $\mathbf{A}_k = \mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k^T$  where  $\mathbf{U}_k$  and  $\mathbf{V}_k$  are the first  $k$  columns of  $\mathbf{U}$  and  $\mathbf{V}$ , and  $\mathbf{\Sigma}_k$  is the  $k \times k$  top sub-block of  $\mathbf{\Sigma}$ .
  - $\mathbf{A}_k$  is the “closest” rank- $k$  approximation to  $\mathbf{A}$ . That is,

$$\mathbf{A}_k = \underset{\text{rank}(\mathbf{X}) \leq k}{\text{argmin}} \|\mathbf{A} - \mathbf{X}\|_{\xi}.$$

where “ $\xi = 2$ ” is the matrix spectral norm and “ $\xi = F$ ” is the matrix Frobenius norm.

- time complexity:  $\mathcal{O}(mnk)$

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# The CUR Decomposition

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A CUR decomposition algorithm seeks to find a subset of  $c$  columns of  $\mathbf{A}$  to form a matrix  $\mathbf{C} \in \mathbb{R}^{m \times c}$ , a subset of  $r$  rows to form a matrix  $\mathbf{R} \in \mathbb{R}^{r \times n}$ , and an intersection matrix  $\mathbf{U} \in \mathbb{R}^{c \times r}$  such that  $\|\mathbf{A} - \mathbf{CUR}\|_{\xi}$  is minimized.

- The CUR decomposition results in an interpretable matrix approximation to  $\mathbf{A}$ .
- There are  $\binom{n}{c}$  possible choices of constructing  $\mathbf{C}$  and  $\binom{m}{r}$  possible choices of constructing  $\mathbf{R}$ , so selecting the best subsets is a hard problem.

# Kernel Methods

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- **K**:  $n \times n$  kernel matrix.
- Matrix inverse  $\mathbf{b} = (\mathbf{K} + \alpha \mathbf{I}_n)^{-1} \mathbf{y}$ 
  - time complexity:  $\mathcal{O}(n^3)$
  - performed by Gaussian process regression, least square SVM, kernel ridge regression
- Partial eigenvalue decomposition of **K**
  - time complexity:  $\mathcal{O}(n^2 k)$
  - performed by kernel PCA and some manifold learning methods
- Space complexity:  $\mathcal{O}(n^2)$ 
  - the iterative algorithms go many passes through the data
  - you had better put the entire kernel matrix in RAM
  - if the data does not fit in the RAM, one swap between RAM and disk in each pass.

# Approaches for Large Scale Matrix Computations

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- Two typical approaches: incremental and distributed
- Randomized algorithms have been also used.



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# The Johnson and Lindenstrauss Lemma

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- This lemma has been given by Johnson and Lindenstrauss (1984), but the proof was not constructive.
- Indyk and Motwani (1998) and Dasgupta and Gupta (2003) constructed a result based on Gaussian random projection matrix  $\mathbf{R} = [r_{ij}]$  where  $r_{ij} \stackrel{iid}{\sim} N(0, 1)$ .
- Matoušek (2008) generalized the result to the case that  $r_{ij}$ 's are any subgaussian random variables; that is,

$$r_{ij} \stackrel{iid}{\sim} \mathcal{G}(\nu^2) \text{ for } \nu \geq 1.$$

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## Definition ( $\epsilon$ -isometry)

Given  $\epsilon \in (0, 1)$ , a map  $f : \mathbb{R}^p \rightarrow \mathbb{R}^q$  where  $p > q$  is called an  $\epsilon$ -isometry on set  $\mathcal{X} \subset \mathbb{R}^p$  if for every pair  $\mathbf{x}, \mathbf{y} \in \mathcal{X}$ , we have

$$(1 - \epsilon)\|\mathbf{x} - \mathbf{y}\|_2^2 \leq \|f(\mathbf{x}) - f(\mathbf{y})\|_2^2 \leq (1 + \epsilon)\|\mathbf{x} - \mathbf{y}\|_2^2.$$

We consider the case that  $f$  is defined as a linear map  $\mathbf{R} \in \mathbb{R}^{q \times p}$ . The Basic idea is to construct a random projection  $\mathbf{R} \in \mathbb{R}^{q \times p}$  that is an exact isometry "in expectation;" that is, for every  $\mathbf{x} \in \mathbb{R}^p$ ,

$$\mathbb{E}[\|\mathbf{R}\mathbf{x}\|_2^2] = \|\mathbf{x}\|_2^2.$$

# The Johnson and Lindenstrauss Lemma

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## Theorem (The Johnson and Lindenstrauss Lemma)

*Let  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^p$ , and let  $\epsilon, \delta \in (0, 1)$ . Assume that  $\mathbf{R} \in \mathbb{R}^{q \times p}$  ( $p > q$ ) where  $r_{ij} \in \mathcal{G}(\nu^2)$  for some  $\nu \geq 1$ . If  $q \geq 100\nu^2\epsilon^{-2} \log(n/\sqrt{\delta})$ , then with probability at least  $1 - \delta$ ,  $\mathbf{R}$  is an  $\epsilon$ -isometry on  $\mathcal{X}$*

$$\Pr \left\{ \sup_{\mathbf{y} \in \mathcal{Y}} \left| \|\mathbf{R}\mathbf{y}\|_2^2 - 1 \right| \geq \epsilon \right\} \leq \delta.$$

*where  $\mathcal{Y} = \left\{ \frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|_2} : \mathbf{x}_i, \mathbf{x}_j \in \mathcal{X}, \mathbf{x}_i \neq \mathbf{x}_j \right\}$ .*

# Prototype for Randomized SVD

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Given an  $m \times n$  matrix  $\mathbf{A}$ , a target number  $k$  of singular vectors, and an integer  $c$  such that  $k < c < \min(m, n)$ , a proto-algorithm based on random projection for Singular Value Decomposition (SVD) of  $\mathbf{A}$  is as follows.

- 1 Construct an  $m \times c$  column-orthonormal matrix  $\mathbf{Q}$  and form  $\mathbf{B} = \mathbf{Q}^T \mathbf{A}$ ;
- 2 Compute SVD of the small matrix:  $\mathbf{B} = \mathbf{U}_B \mathbf{\Sigma}_B \mathbf{V}_B^T$ ;
- 3 Set  $\tilde{\mathbf{U}} = \mathbf{Q} \mathbf{U}_B$ ;
- 4 Return  $\tilde{\mathbf{U}} \mathbf{\Sigma}_B \mathbf{V}_B^T$  as an approximate SVD of  $\mathbf{A}$ , and  $\mathbf{U}_{B,k} \mathbf{\Sigma}_{B,k} \mathbf{V}_{B,k}^T$  as a truncated SVD of  $\mathbf{A}$ .

# A Proto-Algorithm for Construction of Random Projection Matrix $\mathbf{Q}$

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Let  $\mathbf{A}$  be an  $m \times n$  matrix, and  $k$  be a target number of singular vectors.

- 1 Generate an  $m \times 2k$  Gaussian test matrix  $\mathbf{\Omega}$ .
- 2 Form  $\mathbf{Y} = (\mathbf{A}\mathbf{A}^T)^\gamma \mathbf{A}\mathbf{\Omega}$  where  $\gamma = 1$  or  $\gamma = 2$ .
- 3 Construct a matrix  $\mathbf{Q}$  whose columns form an orthonormal basis for the range of  $\mathbf{Y}$ .

# Computational Complexity for the Randomized SVD

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- The randomized SVD procedure requires only  $2(\gamma + 1)$  passes over the matrix.
- The flop count is

$$(2\gamma + 2)kT_{mult} + O(k^2(m + n)),$$

where  $T_{mult}$  is the flop count of a matrix-vector multiply with  $\mathbf{A}$  or  $\mathbf{A}^T$ .



# Theoretical Analysis for the Randomized SVD

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## Theorem (Halko et al., 2011)

Let  $\mathbf{A} \in \mathbb{R}^{m \times n}$ . Give an exponent  $\gamma$  and a target number  $k$  of singular vectors, where  $2 \leq k \leq \frac{1}{2} \min(m, n)$ , running the Randomized SVD algorithm obtains a rank- $2k$  factorization  $\tilde{\mathbf{U}}_{2k} \tilde{\Sigma}_{2k} \tilde{\mathbf{V}}_{2k}^T$ . Then

$$\mathbb{E} \|\mathbf{A} - \tilde{\mathbf{U}}_{2k} \tilde{\Sigma}_{2k} \tilde{\mathbf{V}}_{2k}^T\|_2 \leq \left[ 1 + 4 \sqrt{\frac{2 \min(m, n)}{k-1}} \right]^{1/(2\gamma+1)} \sigma_{k+1}.$$

where  $\mathbb{E}$  is taken w.r.t. the random test matrix and  $\sigma_{k+1}$  is the top  $(k+1)$ th singular value of  $\mathbf{A}$ .

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# The Subspace Embedding Problem

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- For a fixed  $m \times n$  matrix  $\mathbf{A}$  of rank  $r$  and an error parameter  $\epsilon \in (0, 1)$ , we call  $\mathbf{S} : \mathbb{R}^m \rightarrow \mathbb{R}^k$  a *subspace embedding matrix* for  $\mathbf{A}$  if

$$(1 - \epsilon)\|\mathbf{Ax}\|_2 \leq \|\mathbf{S}\mathbf{Ax}\|_2 \leq (1 + \epsilon)\|\mathbf{Ax}\|_2$$

for all  $\mathbf{x} \in \mathbb{R}^n$ .

- The *Subspace Embedding Problem* is to find such an embedding matrix obviously. More specifically, one designs a distribution  $\pi$  over linear maps from  $\mathbb{R}^m$  to  $\mathbb{R}^k$  such that for any fixed  $m \times n$  matrix  $\mathbf{A}$ , if we choose  $\mathbf{S} \sim \pi$ , then with high probability  $\mathbf{S}$  is an embedding matrix for  $\mathbf{A}$ .

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# Sparse Embedding Matrices

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For a fixed  $m \times n$  matrix  $\mathbf{A}$  with  $m > n$ , let  $\text{nnz}(\mathbf{A})$  denote the number of non-zero entries of  $\mathbf{A}$ . Assume that  $\text{nnz}(\mathbf{A}) \geq m$  and that there are no all-zero rows or columns in  $\mathbf{A}$ . Let  $[m] = \{1, 2, \dots, m\}$ . For a parameter  $k$ , define a random linear map  $\Phi\mathbf{D} : \mathbb{R}^m \rightarrow \mathbb{R}^k$  as follows

- $h : [m] \rightarrow [k]$  is a random map so that for each  $i \in [m]$ ,  $h(i) = t$  where  $t \in [k]$  with probability  $1/k$ .
- $\Phi \in \{0, 1\}^{k \times m}$  is a  $k \times m$  binary matrix, with  $\phi_{h(i), i} = 1$  and all remaining entries 0.
- $\mathbf{D}$  is an  $m \times m$  random diagonal matrix, with each diagonal entry independently chosen to be  $+1$  or  $-1$  with equal probability.

A matrix of the form  $\mathbf{S} = \Phi\mathbf{D}$  is referred to as a *sparse embedding matrix* (Dasgupta *et al.*, 2010; Clarkson and Woodruff, 2013).

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# Subspace Embedding in Input-Sparsity Time

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## Theorem (Meng and Mahoney, 2013)

Let  $\mathbf{S} = \Phi \mathbf{D} \in \mathbb{R}^{k \times m}$  with  $k = \frac{n^2 + n}{\epsilon^2 \delta}$ . Then with probability at least  $1 - \delta$ ,

$$(1 - \epsilon) \|\mathbf{A}\mathbf{x}\|_2 \leq \|\mathbf{S}\mathbf{A}\mathbf{x}\|_2 \leq (1 + \epsilon) \|\mathbf{A}\mathbf{x}\|_2$$

for all  $\mathbf{x} \in \mathbb{R}^n$ . In addition,  $\mathbf{S}\mathbf{A}$  can be computed in  $\mathcal{O}(\text{nnz}(\mathbf{A}))$ .

# Spectral Sparsifiers

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## Theorem (Batson, Spielman and Srivastava, 2014)

Suppose  $\rho > 1$  and  $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m\} \subseteq \mathbb{R}^n$  with

$$\sum_{i \leq m} \mathbf{v}_i \mathbf{v}_i^T = \mathbf{I}_n.$$

Then there exist scalars  $d_i \geq 0$  with  $|\{i : d_i \neq 0\}| \leq \lceil \rho n \rceil$  such that

$$\left(1 - \frac{1}{\sqrt{\rho}}\right)^2 \mathbf{I}_n \preceq \sum_{i \leq m} d_i \mathbf{v}_i \mathbf{v}_i^T \preceq \left(1 + \frac{1}{\sqrt{\rho}}\right)^2 \mathbf{I}_n.$$

This theorem shows that

$$\frac{\lambda_1(\sum_{i \leq m} d_i \mathbf{v}_i \mathbf{v}_i^T)}{\lambda_n(\sum_{i \leq m} d_i \mathbf{v}_i \mathbf{v}_i^T)} \leq \frac{\rho + 1 + 2\sqrt{\rho}}{\rho + 1 - 2\sqrt{\rho}}.$$

# Outline

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- 1 Random Projection
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# Column Selection and The $CX$ Decomposition

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- Given an  $m \times n$  matrix  $\mathbf{A}$ , column selection algorithms aim to find a matrix with  $c$  columns of  $\mathbf{A}$  such that  $\|\mathbf{A} - \mathbf{C}\mathbf{C}^+\mathbf{A}\|_\xi = \|(\mathbf{I}_m - \mathbf{C}\mathbf{C}^+)\mathbf{A}\|_\xi$  achieves the minimum. Here " $\xi = 2$ ," " $\xi = F$ ," and " $\xi = *$ " respectively represent the matrix spectral norm, the matrix Frobenius norm, and the matrix nuclear norm, and  $\mathbf{C}^+$  is the Moore-Penrose inverse of  $\mathbf{C}$ .
- Let  $\mathbf{X}$  be the best rank  $k$  approximation to  $\mathbf{A}$  in the column span of  $\mathbf{C}$ . Then  $\mathbf{C}\mathbf{X}$  is called the  $CX$  Decomposition of  $\mathbf{A}$ .
- Since there are  $\binom{n}{c}$  possible choices of constructing  $\mathbf{C}$ , selecting the best subset is a hard problem.

# A Randomized Algorithm for Column Selection

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Given an  $m \times n$  matrix  $\mathbf{A}$  and a rank parameter  $k$ , a random sampling based on the statistical leverage score is:

- Compute the importance sampling probabilities  $\{\pi_i\}_{i=1}^n$ . Here  $\pi_i = \frac{1}{k} \|\mathbf{V}_k^{(i)}\|$ , where  $\mathbf{V}_k$  is an  $n \times k$  orthonormal matrix spanning the top- $k$  right singular subspace of  $\mathbf{A}$ .
- Randomly select  $c = O(k \log(k/\epsilon^2))$  columns of  $\mathbf{A}$  according to these probabilities to form the matrix  $\mathbf{C}$ .

# Theoretical Result for the Random Column Selection (Drineas et al., 2008)

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Let  $\mathbf{C}_k$  be the best rank- $k$  approximation to the matrix  $\mathbf{C}$ , and define the projection matrix  $P_{C_k} = \mathbf{C}_k \mathbf{C}_k^+$ . Then

$$\|\mathbf{A} - P_{C_k} \mathbf{A}\|_F \leq (1 + \epsilon) \|\mathbf{A} - \mathbf{A}_k\|_F,$$

where  $\mathbf{A}_k = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T$  is the best rank  $k$  approximation to  $\mathbf{A}$ .

# The Adaptive Sampling Algorithm

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## Lemma (Deshpande et al., 2006)

*Given a matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , let  $\mathbf{C}_1 \in \mathbb{R}^{m \times c_1}$  consist of  $c_1$  columns of  $\mathbf{A}$ , and define the residual  $\mathbf{B} = \mathbf{A} - \mathbf{C}_1 \mathbf{C}_1^+ \mathbf{A}$ . Additionally, for  $i = 1, \dots, n$ , define*

$$\pi_i = \|\mathbf{b}_i\|_2^2 / \|\mathbf{B}\|_F^2.$$

*We further sample  $c_2$  columns i.i.d. from  $\mathbf{A}$ , in each trial of which the  $i$ -th column is chosen with probability  $\pi_i$ . Let  $\mathbf{C}_2 \in \mathbb{R}^{m \times c_2}$  contain the  $c_2$  sampled columns and let  $\mathbf{C} = [\mathbf{C}_1, \mathbf{C}_2] \in \mathbb{R}^{m \times (c_1 + c_2)}$ . Then, for any integer  $k > 0$ , the following inequality holds:*

$$\mathbb{E} \|\mathbf{A} - \mathbf{C} \mathbf{C}^+ \mathbf{A}\|_F^2 \leq \|\mathbf{A} - \mathbf{A}_k\|_F^2 + \frac{k}{c_2} \|\mathbf{A} - \mathbf{C}_1 \mathbf{C}_1^+ \mathbf{A}\|_F^2,$$

*where the expectation is taken w.r.t.  $\mathbf{C}_2$*





# The Near-Optimal Column Selection Algorithm

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Boutsidis et al. (2013) derived a near-optimal algorithm, which consists of three steps:

- the approximate SVD via random projection (Halko et al. 2011)
- a dual set sparsification algorithm—an extension of spectral sparsifier (BSS)
- the adaptive sampling algorithm (Deshpande et al., 2006)

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References

## Theorem (Boutsidis et al., 2013)

*Given a matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$  of rank  $\rho$ , a target rank  $k$  ( $2 \leq k < \rho$ ), and  $0 < \epsilon < 1$ , the algorithm selects*

$$c = \frac{2k}{\epsilon} (1 + o(1))$$

*columns of  $\mathbf{A}$  to form a matrix  $\mathbf{C} \in \mathbb{R}^{m \times c}$ . Then the following inequality holds:*

$$\mathbb{E} \|\mathbf{A} - \mathbf{C}\mathbf{C}^+ \mathbf{A}\|_F^2 \leq (1 + \epsilon) \|\mathbf{A} - \mathbf{A}_k\|_F^2,$$

*where the expectation is taken w.r.t.  $\mathbf{C}$ . Furthermore, the matrix  $\mathbf{C}$  can be obtained in time:*

$$O(mk^2\epsilon^{-4/3} + nk^3\epsilon^{-2/3}) + T_{\text{Multiply}}(mnk\epsilon^{-2/3}).$$



# The CUR Decomposition (Drineas et al., 2008; Mahoney and Drineas, 2009)

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Given an  $m \times n$  matrix  $\mathbf{A}$ , and integers  $c < n$  and  $r < m$ , the CUR decomposition of  $\mathbf{A}$  finds  $\mathbf{C} \in \mathbb{R}^{m \times c}$  with  $c$  columns from  $\mathbf{A}$ ,  $\mathbf{R} \in \mathbb{R}^{r \times n}$  with  $r$  rows from  $\mathbf{A}$ , and  $\mathbf{U} \in \mathbb{R}^{c \times r}$  such that  $\mathbf{A} = \mathbf{CUR} + \mathbf{E}$ . Here  $\mathbf{E} = \mathbf{A} - \mathbf{CUR}$  is the residual error matrix.

# The CUR Problem

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## Definition (The CUR Decomposition)

Given an  $m \times n$  matrix  $\mathbf{A}$  of rank  $\rho$ , a rank parameter  $k$ , and accuracy parameter  $\epsilon \in (0, 1)$ , construct a matrix  $\mathbf{C} \in \mathbb{R}^{m \times c}$  with  $c$  columns from  $\mathbf{A}$ ,  $\mathbf{R} \in \mathbb{R}^{r \times n}$  with rows from  $\mathbf{A}$ , and  $\mathbf{U} \in \mathbb{R}^{c \times r}$ , with  $c$ ,  $r$ , and  $\text{rank}(\mathbf{U})$  being as small as possible, such that

$$\|\mathbf{A} - \mathbf{CUR}\|_F^2 \leq (1 + \epsilon) \|\mathbf{A} - \mathbf{A}_k\|_F^2.$$

Here  $\mathbf{A}_k = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T \in \mathbb{R}^{m \times n}$  is the best rank  $k$  matrix obtained via the SVD of  $\mathbf{A}$ :  $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$ .

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Drineas et al., (2008) proposed a two-stage randomized CUR algorithm that called *Subspace Sampling*.

- The first stage samples  $c$  columns of  $\mathbf{A}$  to construct  $\mathbf{C}$  according to the sampling probabilities proportional to the squared  $\ell_2$ -norm of the rows of  $\mathbf{V}_k$ ;
- The second stage samples  $r$  rows from  $\mathbf{A}$  and  $\mathbf{C}$  simultaneously to construct  $\mathbf{R}$  and  $\mathbf{W}$  and let  $\mathbf{U} = \mathbf{W}^\dagger$ . The sampling probabilities in this stages are proportional to the leverage scores of  $\mathbf{A}$  and  $\mathbf{C}$ , respectively.

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## Lemma (Drineas et al., 2008)

*Given an  $m \times n$  matrix  $\mathbf{A}$  and a target rank  $k \ll \min\{m, n\}$ , the subspace sampling algorithm selects  $c = \mathcal{O}(k\epsilon^{-2} \log k \log(1/\delta))$  columns and  $r = \mathcal{O}(c\epsilon^{-2} \log c \log(1/\delta))$  rows without replacement. Then*

$$\|\mathbf{A} - \mathbf{CUR}\|_F = \|\mathbf{A} - \mathbf{CW}^+\mathbf{R}\|_F \leq (1 + \epsilon)\|\mathbf{A} - \mathbf{A}_k\|_F,$$

*holds with probability at least  $1 - \delta$ , where  $\mathbf{W}$  contains the rows of  $\mathbf{C}$  with scaling. The running time is dominated by the truncated SVD of  $\mathbf{A}$ , that is,  $\mathcal{O}(mnk)$ .*

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References

Wang and Zhang (2013) proposed an *Adaptive Sampling CUR Algorithm*.

- Select  $c = \frac{2k}{\epsilon}(1 + o(1))$  columns of  $\mathbf{A}$  to construct  $\mathbf{C} \in \mathbb{R}^{m \times c}$  using Algorithm of Boutsidis et al. (2013);
- Select  $r_1 = c$  rows of  $\mathbf{A}$  to construct  $\mathbf{R}_1 \in \mathbb{R}^{r_1 \times n}$  using Algorithm of Boutsidis et al. (2013);
- Adaptively sample  $r_2 = c/\epsilon$  rows from  $\mathbf{A}$  according to the residual  $\mathbf{A} - \mathbf{A}\mathbf{R}_1^\dagger\mathbf{R}_1$ ;
- Return  $\mathbf{C}$ ,  $\mathbf{R} = [\mathbf{R}_1^T, \mathbf{R}_2^T]^T$ , and  $\mathbf{U} = \mathbf{C}^\dagger\mathbf{A}\mathbf{R}^\dagger$ .

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## Lemma (Wang and Zhang, 2013)

*Given a matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and a matrix  $\mathbf{C} \in \mathbb{R}^{m \times c}$  such that  $\text{rank}(\mathbf{C}) = \text{rank}(\mathbf{C}\mathbf{C}^\dagger \mathbf{A}) = \rho$  ( $\rho \leq c \leq n$ ), let  $\mathbf{R}_1 \in \mathbb{R}^{r_1 \times n}$  consist of  $r_1$  rows of  $\mathbf{A}$  and define the residual  $\mathbf{B} = \mathbf{A} - \mathbf{A}\mathbf{R}_1^\dagger \mathbf{R}_1$ . Additionally, for  $i = 1, \dots, m$ , we define*

$$\pi_i = \|\mathbf{b}^{(i)}\|_2^2 / \|\mathbf{B}\|_F^2.$$

*We further sample  $r_2$  rows i.i.d. from  $\mathbf{A}$ , in each trial of which the  $i$ -th row is chosen with probability  $p_i$ . Let  $\mathbf{R}_2 \in \mathbb{R}^{r_2 \times n}$  contain the  $r_2$  sampled rows and let  $\mathbf{R} = [\mathbf{R}_1^T, \mathbf{R}_2^T]^T \in \mathbb{R}^{(r_1+r_2) \times n}$ . Then we have*

$$\mathbb{E} \|\mathbf{A} - \mathbf{C}\mathbf{C}^\dagger \mathbf{A}\mathbf{R}^\dagger \mathbf{R}\|_F^2 \leq \|\mathbf{A} - \mathbf{C}\mathbf{C}^\dagger \mathbf{A}\|_F^2 + \frac{\rho}{r_2} \|\mathbf{A} - \mathbf{A}\mathbf{R}_1^\dagger \mathbf{R}_1\|_F^2,$$

*where the expectation is taken w.r.t  $\mathbf{R}_2$*





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## Theorem (Wang and Zhang, 2013)

*Given a matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and a positive integer  $k \ll \min\{m, n\}$ , the Adaptive Sampling CUR algorithm randomly selects  $c = \frac{2k}{\epsilon}(1+o(1))$  columns of  $\mathbf{A}$  to construct  $\mathbf{C} \in \mathbb{R}^{m \times c}$ , and then selects  $r = \frac{c}{\epsilon}(1+\epsilon)$  rows of  $\mathbf{A}$  to construct  $\mathbf{R} \in \mathbb{R}^{r \times n}$ . Then we have*

$$\mathbb{E} \|\mathbf{A} - \mathbf{CUR}\|_F = \mathbb{E} \|\mathbf{A} - \mathbf{C}(\mathbf{C}^\dagger \mathbf{A} \mathbf{R}^\dagger) \mathbf{R}\|_F \leq (1 + \epsilon) \|\mathbf{A} - \mathbf{A}_k\|_F.$$

*The algorithm costs time  $\mathcal{O}((m+n)k^3\epsilon^{-2/3} + mk^2\epsilon^{-2} + nk^2\epsilon^{-4}) + T_{\text{Multiply}}(mnk\epsilon^{-1})$  to compute matrices  $\mathbf{C}$ ,  $\mathbf{U}$  and  $\mathbf{R}$ .*

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Boutsidis and Woodruff (2014) proposed *Optimal CUR Algorithm*.

- Construction **C** with  $O(k + \frac{k}{\epsilon})$  columns:
  - Compute the top  $k$  singular vectors of **A**:  $\mathbf{Z}_1$
  - Sample  $O(k \log k)$  columns from  $\mathbf{Z}_1^T$  with the leverage scores
  - Down-sample columns to  $c_1 = O(k)$  columns with the sampling algorithm of Boutsidis et al. (2013)
  - Adaptively sample  $c_2 = O(\frac{k}{\epsilon})$  columns of **A**
- Construction **R** with  $O(k + \frac{k}{\epsilon})$  rows:
  - Find  $\mathbf{Z}_2$  in the span of **C** such that:  
$$\|\mathbf{A} - \mathbf{Z}_2 \mathbf{Z}_2^T \mathbf{A}\|_F^2 \leq (1 + \epsilon) \cdot \|\mathbf{A} - \mathbf{A}_k\|_F^2$$
  - Sample  $O(k \log k)$  rows from  $\mathbf{Z}_2$  with the leverage scores
  - Down-sample rows to  $r_1 = O(k)$  rows with the sampling algorithm of Boutsidis et al. (2013)
  - Sample  $r_2 = O(\frac{k}{\epsilon})$  rows with adaptive sampling

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## Lemma (Boutsidis and Woodruff, 2014)

*Given a matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$ ,  $\mathbf{V} \in \mathbb{R}^{m \times c}$  and an integer  $k$ , let  $\mathbf{V} = \mathbf{Y}\Psi$  be a QR decomposition of  $\mathbf{V}$ ,  $\Gamma = \mathbf{Y}^T \mathbf{A}$ ,  $\Gamma_k = \Delta \Sigma_k \mathbf{V}_k^T$  be a rank  $k$  SVD of  $\Gamma$ ,  $\Delta \in \mathbb{R}^{c \times k}$ . Then  $\mathbf{Y}\Delta\Delta^T\mathbf{Y}^T$  satisfies:*

$$\|\mathbf{A} - \mathbf{Y}\Delta\Delta^T\mathbf{Y}^T\mathbf{A}\|_F^2 \leq \|\mathbf{A} - \mathbf{Y}\Delta\Sigma_k\mathbf{V}_k^T\|_F^2 = \|\mathbf{A} - \Pi_{V,k}^F(\mathbf{A})\|_F^2.$$

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## Theorem (Boutsidis and Woodruff, 2014)

*Given a matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$  of rank  $\rho$ , a target rank  $1 \leq k \leq \rho$ , and  $0 < \epsilon < 1$ , the optimal CUR algorithm selects at most  $c = O(k/\epsilon)$  columns and at most  $r = O(k/\epsilon)$  rows from  $\mathbf{A}$  form matrices  $\mathbf{C} \in \mathbb{R}^{m \times c}$ ,  $\mathbf{R} \in \mathbb{R}^{r \times n}$ , and  $\mathbf{U} \in \mathbb{R}^{c \times r}$  with  $\text{rank}(\mathbf{U}) = k$  such that, with some probability,*

$$\|\mathbf{A} - \mathbf{CUR}\|_F^2 \leq \|(1 + O(\epsilon))\|\mathbf{A} - \mathbf{A}_k\|_F^2.$$

*The matrices  $\mathbf{C}$ ,  $\mathbf{U}$ , and  $\mathbf{R}$  can be computed in time*

$$\mathcal{O}[\text{nnz}(\mathbf{A}) \log n + (m + n) \times \text{poly}(\log n, k, 1/\epsilon)].$$

# The Nystrom Method

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## ■ Random Selection:

selects  $c (\ll n)$  columns of  $\mathbf{K}$  to construct  $\mathbf{C}$  using some randomized algorithms. After permutation we have

$$\mathbf{K} = \begin{bmatrix} \mathbf{W} & \mathbf{K}_{21}^T \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \mathbf{W} \\ \mathbf{K}_{21} \end{bmatrix}.$$

## ■ The Nystrom Approximation: $\tilde{\mathbf{K}}_c^{\text{nys}} \approx \mathbf{K}$

$$\underbrace{\tilde{\mathbf{K}}_c^{\text{nys}}}_{n \times n} = \underbrace{\mathbf{C}}_{n \times c} \underbrace{\mathbf{W}^\dagger}_{c \times c} \underbrace{\mathbf{C}^T}_{c \times n}.$$

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## ■ Random Selection:

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## ■ The Nystrom Approximation: $\tilde{\mathbf{K}}_c^{\text{nys}} \approx \mathbf{K}$

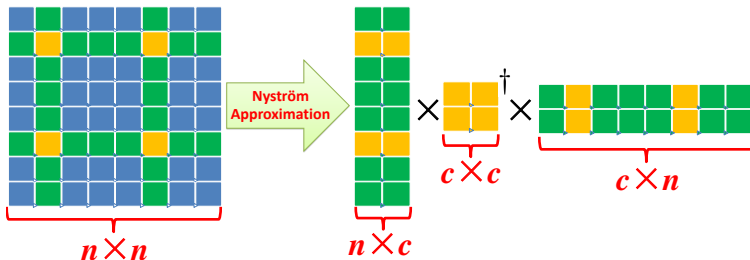
$$\underbrace{\tilde{\mathbf{K}}_c^{\text{nys}}}_{n \times n} = \underbrace{\mathbf{C}}_{n \times c} \underbrace{\mathbf{W}^\dagger}_{c \times c} \underbrace{\mathbf{C}^T}_{c \times n}.$$

# The Nyström Approximation

## ■ The Nyström Approximation:

$$\mathbf{K} \approx \tilde{\mathbf{K}}_c^{\text{nys}} = \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T$$

(A low-rank factorization).



# Problem Formulation

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Problem:

- How to select informative columns of  $\mathbf{K} \in \mathbb{R}^{n \times n}$  to construct  $\mathbf{C} \in \mathbb{R}^{n \times c}$ ?
- The approximation error  $\|\mathbf{K} - \mathbf{C}\mathbf{C}^T\|_F$  or  $\|\mathbf{K} - \mathbf{C}\mathbf{C}^T\|_2$  should be as small as possible.



# Criterion: Upper Error Bounds

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- Using approximation algorithms to find  $c$  *good* columns (not necessarily the *best*)
- Hope that  $\frac{\|\mathbf{K} - \mathbf{C}\mathbf{U}\mathbf{C}^T\|_F}{\|\mathbf{K} - \mathbf{K}_k\|_F}$  has upper bound, which is the smaller the better.

# Uniform Sampling: The Simplest Algorithm

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- Sample  $c$  columns of  $\mathbf{K}$  uniformly at random to construct  $\mathbf{C}$ .
- The simplest, but the most widely used.

# Adaptive Sampling

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The adaptive sampling algorithm [Deshpande *et al.*, 2006]:

- 1 Sample  $c_1$  columns of  $\mathbf{K}$  to construct  $\mathbf{C}_1$  using some algorithm;
- 2 Compute the residual  $\mathbf{B} = \mathbf{K} - \mathbf{C}_1 \mathbf{C}_1^\dagger \mathbf{K}$ ;
- 3 Compute sampling probabilities  $p_i = \frac{\|\mathbf{b}_i\|_2^2}{\|\mathbf{B}\|_F^2}$ , for  $i = 1$  to  $n$ ;
- 4 Sample further  $c_2$  columns of  $\mathbf{K}$  in  $c_2$  i.i.d. trials, in each trial the  $i$ -th column is chosen with probability  $p_i$ ;  
Denote the selected columns by  $\mathbf{C}_2$ ;
- 5 Return  $\mathbf{C} = [\mathbf{C}_1, \mathbf{C}_2]$ .

# Adaptive Sampling

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- The error term  $\|\mathbf{K} - \mathbf{C}\mathbf{C}^\dagger\mathbf{K}\|_F$  is bounded theoretically, but  $\|\mathbf{K} - \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T\|_F$  is not.
- Empirically, the adaptive sampling algorithm works very well.

# Better Sampling Algorithms?

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- We hope  $\frac{\|\mathbf{K} - \mathbf{C}\mathbf{W}^\dagger \mathbf{C}^T\|_F}{\|\mathbf{K} - \mathbf{K}_k\|_F}$  will be very small if the column sampling algorithm is good enough.
- But it cannot be arbitrarily small.
- Lower Error Bound

## Theorem (Wang & Zhang, JMLR 2013)

*Whatever column sampling is used to select  $c$  columns, there exists a bad case  $\mathbf{K}$  such that*

$$\frac{\|\mathbf{K} - \mathbf{C}\mathbf{W}^\dagger \mathbf{C}^T\|_F^2}{\|\mathbf{K} - \mathbf{K}_k\|_F^2} \geq \Omega\left(1 + \frac{nk}{c^2}\right).$$

# Different Types of Low-Rank Approximation?

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- The *Ensemble Nyström Method* [Kumar et al., JMLR 2012]:

$$\mathbf{K} \approx \sum_{i=1}^t \frac{1}{t} \mathbf{C}^{(i)} \mathbf{W}^{(i)\dagger} \mathbf{C}^{(i)T}$$

- It does not improve the lower error bound.
- Lower Error Bound

## Theorem (Wang & Zhang, JMLR 2013)

*Whatever column sampling is used to select  $c$  columns, there exists a bad case  $\mathbf{K}$  such that*

$$\frac{\|\mathbf{K} - \sum_{i=1}^t \frac{1}{t} \mathbf{C}^{(i)} \mathbf{W}^{(i)\dagger} \mathbf{C}^{(i)T}\|_F^2}{\|\mathbf{K} - \mathbf{K}_k\|_F^2} \geq \Omega\left(1 + \frac{nk}{c^2}\right).$$

# The Modified Nystrom Method

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- The *Modified Nystrom Method* [Wang & Zhang, JMLR 2013]:

$$\mathbf{K} \approx \mathbf{C} \underbrace{(\mathbf{C}^\dagger \mathbf{K} (\mathbf{C}^\dagger)^T)}_{c \times c} \mathbf{C}^T.$$

## Theorem (Wang & Zhang, JMLR 2013)

*Using a column sampling algorithm, the error incurred by the modified Nystrom method satisfies*

$$\mathbb{E} \frac{\|\mathbf{K} - \mathbf{C}(\mathbf{C}^\dagger \mathbf{K} (\mathbf{C}^\dagger)^T) \mathbf{C}^T\|_F^2}{\|\mathbf{K} - \mathbf{K}_k\|_F^2} \leq 1 + \sqrt{\frac{k}{c}}.$$

# Comparisons between the Two Methods

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- **The Standard Nyström Method: fast.**

It costs only  $T_{\text{SVD}}(c^3)$  time to compute the intersection matrix  $\mathbf{U}^{\text{nys}} = \mathbf{W}^\dagger$ .

- **The Modified Nyström Method: slow.**

It costs  $T_{\text{SVD}}(nc^2) + T_{\text{Multiply}}(n^2c)$  time to compute the intersection matrix  $\mathbf{U}^{\text{mod}} = \mathbf{C}^\dagger \mathbf{K}(\mathbf{C}^\dagger)^T$  naively.



# Comparisons between the Two Methods

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- **The Standard Nyström Method: inaccurate.**

It cannot attain  $1 + \epsilon$  Frobenius relative-error bound unless

$$c \geq \sqrt{nk/\epsilon}$$

columns are selected, whatever column selection algorithm is used. (Due to its lower error bound.)

- **The Modified Nyström Method: accurate.**

Some adaptive sampling based algorithms attain  $1 + \epsilon$  Frobenius relative-error bound when

$$c = \mathcal{O}(k/\epsilon^2).$$

( $c$  is the smaller the better.)

# Comparisons between the Two Methods

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## Theorem (Exact Recovery)

*For the symmetric matrix  $\mathbf{K}$  defined previously, the following three statements are equivalent:*

- 1  $\text{rank}(\mathbf{W}) = \text{rank}(\mathbf{K})$ ,
- 2  $\mathbf{K} = \mathbf{C}\mathbf{W}^\dagger\mathbf{C}^T$ ,  
*(i.e., the standard Nyström method is exact)*
- 3  $\mathbf{K} = \mathbf{C}(\mathbf{C}^\dagger\mathbf{K}(\mathbf{C}^\dagger)^T)\mathbf{C}^T$ ,  
*(i.e., the modified Nyström method is exact)*

# Outline

## Randomized Numerical Linear Algebra

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## Random Projection

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## Subspace Embedding

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### 1 Random Projection

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### 2 Subspace Embedding

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### 4 References

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