

# CSE 392: Matrix and Tensor Algorithms for Data

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## Lecture 6: Approximate matrix product and sampling

# Outline

- 1 Randomization
- 2 Approximating Matrix Multiplication
- 3 Length-squared sampling
- 4 Leverage score sampling

# Why randomization?

- *Modern data applications*: massive data, computationally expensive problems.
- *Approximate solutions* suffice in many situations.
- **Randomized sampling and sketching** allow us to design approximation algorithms with provable error guarantees.
- Probabilistic error bounds. E.g., the  $(\epsilon, \delta)$  type bounds.

# Product and norms using randomization

If a random distribution on  $\mathbf{s} \in \mathbb{R}^n$  has entries  $s_i$  with:

- $\mathbb{E}[s_i^2] = 1$  for  $i = [n]$  and  $\mathbb{E}[s_i s_j] = 0$  for  $i, j = [n], i \neq j$ .
- Then, for  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ , we have

$$\mathbb{E}[\langle \mathbf{s} \cdot \mathbf{x}, \mathbf{s} \cdot \mathbf{y} \rangle] = \mathbb{E}[(\mathbf{s}^\top \mathbf{x}) \cdot (\mathbf{s}^\top \mathbf{y})] = \mathbb{E}[\mathbf{x}^\top \mathbf{s} \mathbf{s}^\top \mathbf{y}] = \mathbf{x}^\top \mathbf{y}$$

- In particular,  $\mathbb{E}[(\mathbf{s}^\top \mathbf{y})^2] = \mathbb{E}[\mathbf{y}^\top \mathbf{s} \mathbf{s}^\top \mathbf{y}] = \mathbf{y}^\top \mathbf{y} = \|\mathbf{y}\|^2$ .

$$\mathbb{E}[\mathbf{s} \mathbf{s}^\top] = \begin{bmatrix} s_1^2 & s_1 s_2 & \cdots & s_1 s_n \\ s_2, s_1 & s_2^2 & & \vdots \\ \vdots & & \ddots & \\ s_n, s_1 & \cdots & & s_n^2 \end{bmatrix} = \mathbf{I} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & & 1 \end{bmatrix}$$

# Sketching and Sampling

## Sketching:

- Suppose  $s_i \sim \mathcal{N}(0, 1)$  and independent.
- We have  $\mathbb{E}[s_i] = 0$ ,  $\mathbb{E}[s_i^2] = \text{Var}(s_i) = 1$ .
- For  $i \neq j$ , independence implies  $\mathbb{E}[s_i s_j] = \mathbb{E}[s_i] \mathbb{E}[s_j] = 0$ .

## Sampling:

- Suppose we pick  $i \in [n]$  uniformly with probability  $\frac{1}{n}$  and set  $s_i \leftarrow \sqrt{n}$ , 0 o.w.
- We have  $\mathbb{E}[s_i^2] = \frac{1}{n} \sqrt{n^2} + (1 - \frac{1}{n}) 0 = 1$ .
- For  $i \neq j$  if  $s_i \neq 0 \implies s_j = 0$ ,  
so  $s_i s_j = 0$ .

# Randomized techniques

With repetitions and better distributions, randomization can be made highly accurate.

A random distribution on  $\mathbf{S} \in \mathbb{R}^{c \times n}$  has independent rows, each row is  $\frac{1}{\sqrt{c}}$  times a sample of  $\mathbf{s} \in \mathbb{R}^n$ , then

$$\mathbb{E}[\mathbf{S}^\top \mathbf{S}] = \mathbb{E}\left[\sum_{i \in [c]} \mathbf{s}_{i*}^\top \mathbf{s}_{i*}\right] = \sum_{i \in [c]} \mathbb{E}[\mathbf{s}_{i*}^\top \mathbf{s}_{i*}] = \sum_{i \in [c]} \frac{1}{c} \mathbf{I} = \mathbf{I},$$

so for  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ , we have  $\mathbb{E}[\langle \mathbf{S}\mathbf{x}, \mathbf{S}\mathbf{y} \rangle] = \mathbb{E}[\mathbf{x}^\top \mathbf{S}^\top \mathbf{S} \mathbf{y}] = \mathbf{x}^\top \mathbb{E}[\mathbf{S}^\top \mathbf{S}] \mathbf{y} = \mathbf{x}^\top \mathbf{y}$ .  
In particular,  $\mathbb{E}[\|\mathbf{S}\mathbf{y}\|^2] = \|\mathbf{y}\|^2$

## Applications:

- Approximating matrix multiplication
- Least squares regression
- Low rank approximation

# Approximating Matrix Multiplication (AMM)

## Problem Statement:

Given an  $m \times n$  matrix  $\mathbf{A}$  and an  $n \times p$  matrix  $\mathbf{B}$ , approximate the product  $\mathbf{A} \cdot \mathbf{B}$ ,

**OR, equivalently,**

Approximate the sum of  $n$  rank-one matrices.

$$\mathbf{A} \cdot \mathbf{B} = \sum_{i=1}^n \underbrace{\begin{bmatrix} \mathbf{A}_{*i} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{B}_{i*} \end{bmatrix}}_{m \times p}$$

where  $\mathbf{A}_{*i}$  is the  $i$ th column of  $\mathbf{A}$  and  $\mathbf{B}_{i*}$  is the  $i$ th row of  $\mathbf{B}$ .



## Sampling rows of a matrix

- If  $\mathbf{S} \in \mathbb{R}^{c \times n}$  is a random row sampling matrix, then  $\mathbf{SA}$ :

$$\begin{bmatrix} 0 & s_{12} & 0 & 0 & \cdots & 0 \\ s_{21} & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & s_{33} & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \cdots & s_{cn} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{1*} \\ \mathbf{A}_{2*} \\ \vdots \\ \mathbf{A}_{n*} \end{bmatrix} = \begin{bmatrix} s_{12}\mathbf{A}_{2*} \\ s_{21}\mathbf{A}_{1*} \\ s_{33}\mathbf{A}_{3*} \\ \vdots \\ s_{cn}\mathbf{A}_{n*} \end{bmatrix}$$

- As above, for a single sampling vector  $\mathbf{s}$ , *uniform sampling* would pick  $i \in [n]$  uniformly with probability  $\frac{1}{n}$  and set  $s_i \leftarrow \sqrt{n}$ .
- Generally, given  $\mathbf{p} \in [0, 1]^n$ ,  $\sum_i p_i = 1$ . Pick  $i \in [n]$  with probability  $p_i$ ,  $s_i \leftarrow \sqrt{1/p_i}$ . We have  $\mathbb{E}[s_i^2] = p_i \sqrt{1/p_i}^2 + (1 - p_i)0 = 1$ .
- In some instances, by choosing appropriate  $p_i$ 's, we can get improved results.

$$\begin{aligned}
 \mathbf{A} \cdot \mathbf{B} &= \sum_{i=1}^n \underbrace{\begin{bmatrix} \mathbf{A}_{*i} \end{bmatrix}}_{m \times p} \cdot \begin{bmatrix} \mathbf{B}_{i*} \end{bmatrix} \\
 &\approx \frac{1}{c} \sum_{t=1}^c \frac{1}{p_{j_t}} \underbrace{\begin{bmatrix} \mathbf{A}_{*j_t} \end{bmatrix}}_{m \times p} \cdot \begin{bmatrix} \mathbf{B}_{j_t*} \end{bmatrix}
 \end{aligned}$$

Pick  $c$  terms of the sum, with replacement, with respect to the  $p_i$ 's. I.e. set  $j_t = i$ , where  $\Pr(j_t = i) = p_i$ .

$$\underbrace{\begin{bmatrix} A \end{bmatrix}}_{m \times n} \cdot \underbrace{\begin{bmatrix} B \end{bmatrix}}_{n \times p} \approx \underbrace{\begin{bmatrix} C \end{bmatrix}}_{m \times c} \cdot \underbrace{\begin{bmatrix} R \end{bmatrix}}_{c \times p}$$

- We would like to estimate  $AB \approx AS^\top SB$ .
- Suppose  $S$  has just one row  $s_i$ . Then, we just get  $A_{i*}s_i^2 B_{*i} = A_{*i}B_{i*}/p_i$  with probability  $p_i$ .
- If we pick uniformly with  $p_i = 1/n$ , and suppose one of the row norms  $\|B_{1*}\|^2$  is much  $\gg$  norms of other rows, then the estimate will be poor, if we miss the row  $i = 1$ .
- One idea : catch the rows with large norms by setting  $p_i \propto \|B_{1*}\|^2$ . This is called **Length-squared sampling**.

$$\underbrace{\begin{bmatrix} A \end{bmatrix}}_{m \times n} \cdot \underbrace{\begin{bmatrix} B \end{bmatrix}}_{n \times p} \approx \underbrace{\begin{bmatrix} C \end{bmatrix}}_{m \times c} \cdot \underbrace{\begin{bmatrix} R \end{bmatrix}}_{c \times p}$$

- Create  $C$  and  $R$  by picking columns  $A_{*j_t}$  and rows  $B_{j_t*}$  with probability

$$\Pr(j_t = i) = \frac{\|A_{*i}\|_2 \|B_{i*}\|_2}{\sum_{j=1}^n \|A_{*j}\|_2 \|B_{j*}\|_2}$$

- Include  $A_{*j_t}/\sqrt{cp_{j_t}}$  as a column of  $C$ , and  $B_{j_t*}/\sqrt{cp_{j_t}}$  as a row of  $R$ .

# Length-squared sampling

Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\mathbf{B} \in \mathbb{R}^{n \times p}$ . Let  $\mathbf{S} \in \mathbb{R}^{c \times n}$  be the length squared sampling matrix. Then,  $\mathbb{E}[\mathbf{C}\mathbf{R}] = \mathbf{A}\mathbf{B}$  (unbiased estimator), where  $\mathbf{C} = \mathbf{A}\mathbf{S}^\top$ ,  $\mathbf{R} = \mathbf{S}\mathbf{B}$ , and

$$\mathbb{E}[\|\mathbf{C}\mathbf{R} - \mathbf{A}\mathbf{B}\|_F^2] \leq \frac{1}{c} \|\mathbf{A}\|_F^2 \|\mathbf{B}\|_F^2$$

# Length-squared sampling

Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\mathbf{B} \in \mathbb{R}^{n \times p}$ . Let  $\mathbf{S} \in \mathbb{R}^{c \times n}$  be the length squared sampling matrix. Then,  $\mathbb{E}[\mathbf{CR}] = \mathbf{AB}$  (unbiased estimator), where  $\mathbf{C} = \mathbf{AS}^\top$ ,  $\mathbf{R} = \mathbf{SB}$ , and

$$\mathbb{E}[\|\mathbf{CR} - \mathbf{AB}\|_F^2] \leq \frac{1}{c} \|\mathbf{A}\|_F^2 \|\mathbf{B}\|_F^2$$

**Proof:** First, for any probability  $p_i$ , we know that  $\mathbb{E}[\mathbf{CR}_{ij}] = \mathbf{AB}_{ij}$ . Elementwise is an unbiased estimator.

Next, note that for a single vector  $\mathbf{s}$ ,  $\mathbb{E}[\|\mathbf{Ass}^\top \mathbf{B} - \mathbf{AB}\|_F^2]$  is the sum of entry-wise variances.

Since  $\text{Var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2$ , we have  $\mathbb{E}[\|\mathbf{Ass}^\top \mathbf{B} - \mathbf{AB}\|_F^2] \leq \mathbb{E}[\|\mathbf{Ass}^\top \mathbf{B}\|_F^2]$

$$\begin{aligned}
\mathbb{E}[\|\mathbf{A}\mathbf{s}\mathbf{s}^\top\mathbf{B}\|_F^2] &= \sum_{j,k} \mathbb{E}[(\mathbf{A}_{j*}\mathbf{s}\mathbf{s}^\top\mathbf{B}_{*k})^2] = \sum_{j,k} \mathbb{E}[(\sum_i a_{ji}s_i^2 b_{ik})^2] \\
&= \sum_{j,k} \sum_i a_{ji}^2 p_i \frac{1}{p_i^2} b_{ik}^2 = \sum_i \sum_j a_{ji}^2 \frac{1}{p_i} \sum_k b_{ik}^2 = \sum_i \|\mathbf{A}_{*i}\|^2 \frac{1}{p_i} \|\mathbf{B}_{i*}\|^2 \\
&= \|\mathbf{A}\|_F^2 \|\mathbf{B}\|_F^2.
\end{aligned}$$

Next, for the case of  $c$  rows, the expected Frobenius norm error is sum of variance of the form

$$\text{Var}[\sum_{i \in [c]} \mathbf{x}^{(i)} / c] = \sum_{i \in [c]} \text{Var}[\mathbf{x}^{(i)} / c] = \text{Var}[\mathbf{x}^{(1)}] / c.$$

Thus, we get the result

$$\mathbb{E}[\|\mathbf{C}\mathbf{R} - \mathbf{A}\mathbf{B}\|_F^2] \leq \frac{1}{c} \|\mathbf{A}\|_F^2 \|\mathbf{B}\|_F^2.$$

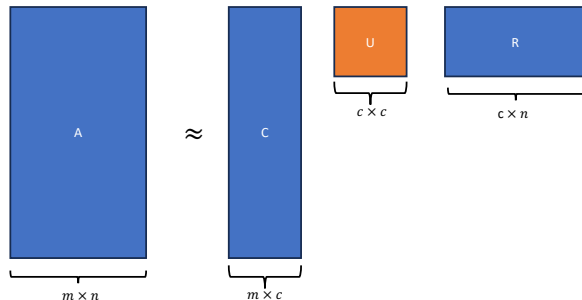
Using Markov's inequality, we can show that for  $c \geq 1/\epsilon^2\delta$ ,

$$\Pr(\|\mathbf{C}\mathbf{R} - \mathbf{A}\mathbf{B}\|_F \geq \epsilon \|\mathbf{A}\|_F \|\mathbf{B}\|_F) \leq \delta.$$

# CUR decomposition

Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , a particular type of low rank approximation:

- A row sampling matrix  $\mathbf{S}_1 \in \mathbb{R}^{c \times m}$ , and  $\mathbf{R} = \mathbf{S}_1 \mathbf{A} \in \mathbb{R}^{c \times n}$
- A column sampling matrix  $\mathbf{S}_2 \in \mathbb{R}^{n \times c}$ , and  $\mathbf{C} = \mathbf{A} \mathbf{S}_2 \in \mathbb{R}^{m \times c}$
- A matrix  $\mathbf{U} \in \mathbb{R}^{c \times c}$ , such that  $\mathbf{A} \approx \mathbf{C} \mathbf{U} \mathbf{R}$  and  $c \ll \{m, n\}$ .





# CUR decomposition

- We can compute  $\mathbf{U} = (\mathbf{A}\mathbf{S}_2)^\dagger \mathbf{S}_1^\top = (\mathbf{C}^\top \mathbf{C})^{-1} (\mathbf{S}_1 \mathbf{A} \mathbf{S}_2)^\top$ .
- $\mathbf{U}$  can be ill-conditioned.
- Typically, in applications, we are interested in random columns  $\mathbf{C}$  and rows  $\mathbf{R}$  of  $\mathbf{A}$ .
- We can also consider,  $\mathbf{S}_1 \in \mathbb{R}^{r \times m}$  and  $\mathbf{S}_2 \in \mathbb{R}^{n \times c}$ , for different  $c, r$ .

Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , row sampler  $\mathbf{S}_1 \in \mathbb{R}^{r \times m}$ , column  $\mathbf{S}_2 \in \mathbb{R}^{n \times c}$ , and with  $\mathbf{C} = \mathbf{A}\mathbf{S}_2$ ,  $\mathbf{R} = \mathbf{S}_1 \mathbf{A}$ ,  $\mathbf{U} = (\mathbf{A}\mathbf{S}_2)^\dagger \mathbf{S}_1^\top$ , then

$$\mathbb{E}[\|\mathbf{CUR} - \mathbf{A}\|_F^2] \leq 2\|\mathbf{A}\|_F^2 \left( \frac{1}{\sqrt{c}} + \frac{c}{r} \right) \leq \epsilon \|\mathbf{A}\|_F^2,$$

for  $c = 16/\epsilon^2, r = 64/\epsilon^3$ .

# Matrix (low rank) approximations

- We can also consider sampling only the columns as  $\mathbf{A} \approx \mathbf{C}\mathbf{X}$ , or
- Sample only the rows  $\mathbf{A} \approx \mathbf{X}\mathbf{R}$ .
- More flexible structure can give better-conditioned  $\mathbf{X}$ .
- We need fast decaying spectrum.
- For

$$\Pr(\|\mathbf{C}\mathbf{U}\mathbf{R} - \mathbf{A}\|_F \geq \epsilon \|\mathbf{A}\|_F) \leq \delta,$$

we need  $c = O(\delta^{-2}\epsilon^{-4})$ ,  $r = O(\delta^{-3}\epsilon^{-6})$ .

- Cost =?

## Better variance reduction

- We want  $\mathbf{S}$  such that  $\|\mathbf{S}\mathbf{A}\mathbf{x}\|$  is a good estimator of  $\|\mathbf{A}\mathbf{x}\|$ .
- Length-squared sampling :  $p_i \propto \|\mathbf{A}_{i*}\|^2$  is good, but for some  $\mathbf{x}$ , we could have  $\mathbf{A}_{i*}\mathbf{x} = 0$  even if  $\|\mathbf{A}_{i*}\|^2$  is large.
- We want  $(\frac{1}{\sqrt{p_i}}\mathbf{A}_{i*}\mathbf{x})^2$  to be “well-behaved” for all  $i$  and  $\mathbf{x}$ .
- “well-behaved” in one sense : bounded relative contribution to  $\|\mathbf{A}\mathbf{x}\|^2 = \sum_i (\mathbf{A}_{i*}\mathbf{x})^2$ .
- sampling using information related to  $\text{span}(\mathbf{A})$ .

# Leverage scores

- **Leverage scores:** Given a linear subspace  $L \subset \mathbb{R}^n$ , for  $i \in [n]$ , the  $i$ th *leverage score*  $\ell_i(L) = \sup_{\mathbf{y} \in L} y_i^2 / \|\mathbf{y}\|^2$ .
- The leverage scores of  $\mathbf{A} \in \mathbb{R}^{m \times n}$  are  $\ell_i(\mathbf{A}) = \ell_i(\text{span}(\mathbf{A}))$ .

Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , and an orthonormal basis  $\mathbf{U}$  for  $\text{span}(\mathbf{A})$ , for  $i \in [n]$ , the  $i$ th *leverage score*

$$\ell_i(\mathbf{A}) = \sup_{\mathbf{x}} \frac{(\mathbf{A}_{i*} \mathbf{x})^2}{\|\mathbf{A} \mathbf{x}\|^2} = \|\mathbf{U}_{i*}\|^2.$$

# Leverage scores

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$$\ell_i(\mathbf{A}) = \sup_{\mathbf{x}} \frac{(\mathbf{A}_{i*}\mathbf{x})^2}{\|\mathbf{A}\mathbf{x}\|^2} = \|\mathbf{U}_{i*}\|^2.$$

For  $L = \text{span}(\mathbf{A}) = \text{span}(\mathbf{U})$ , and  $\mathbf{z} \in L$  has  $\mathbf{z} = \mathbf{A}\mathbf{x} = \mathbf{U}\mathbf{y}$  for some  $\mathbf{x}, \mathbf{y}$ . So,

$$\sup_{\mathbf{x}} \frac{(\mathbf{A}_{i*}\mathbf{x})^2}{\|\mathbf{A}\mathbf{x}\|^2} = \sup_{\mathbf{y}} \frac{(\mathbf{U}_{i*}\mathbf{y})^2}{\|\mathbf{U}\mathbf{y}\|^2} = \sup_{\mathbf{y}} \frac{(\mathbf{U}_{i*}\mathbf{y})^2}{\|\mathbf{y}\|^2} = \|\mathbf{U}_{i*}\|^2.$$

We have  $\ell_i(\mathbf{A}) \in [0, 1]$  and  $\sum_i \ell_i(\mathbf{A}) = \text{rank}(\mathbf{A})$ .

# Leverage score sampling

**Leverage score sampling:** sample rows with probability proportional to the square of the Euclidean norms of the rows of the left singular vectors of  $\mathbf{A}$ .

$$p_i = \frac{\|\mathbf{U}_{i*}\|^2}{\|\mathbf{U}\|_F^2} = \frac{\|\mathbf{U}_{i*}\|^2}{n}$$

Column sampling is equivalent to row sampling by focusing on  $\mathbf{A}^\top$ . So, we consider the right singular vectors  $\mathbf{V}$ .

$$p_j = \frac{\|\mathbf{V}_{j*}\|^2}{m}.$$

## Leverage scores: general case

Let  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\mathbf{A}_k$  its best rank- $k$  approximation (as computed by the SVD):

$$\underbrace{\mathbf{A} \approx \begin{bmatrix} \mathbf{A}_k \end{bmatrix}}_{m \times n} \approx \underbrace{\begin{bmatrix} \mathbf{U}_k \end{bmatrix}}_{m \times k} \cdot \underbrace{\begin{bmatrix} \Sigma_k \end{bmatrix}}_{k \times k} \cdot \underbrace{\begin{bmatrix} \mathbf{V}_k^\top \end{bmatrix}}_{k \times n}$$

*Row Leverage scores and Column Leverage scores*

$$p_i = \frac{\|(\mathbf{U}_k)_{i*}\|^2}{k} \qquad p_j = \frac{\|(\mathbf{V}_k)_{j*}\|^2}{k}$$

# Leverage score sampling

Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , if we randomly sample the columns  $\mathbf{C} \in \mathbb{R}^{m \times c}$  using leverage scores, then, with probability at least 0.9,

$$\|\mathbf{A} - \mathbf{C}\mathbf{X}\|_F = \|\mathbf{A} - \mathbf{C}\mathbf{C}^\dagger \mathbf{A}\|_F \leq (1 + \epsilon) \|\mathbf{A} - \mathbf{A}_k\|_F,$$

for sampling complexity

$$c = O\left(\frac{k}{\epsilon^2} \log\left(\frac{k}{\epsilon}\right)\right)$$



# Leverage score sampling

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for sampling complexity

$$c = O\left(\frac{k}{\epsilon^2} \log\left(\frac{k}{\epsilon}\right)\right)$$

Proof uses Matrix Chernoff inequality.

Let  $\mathbf{X}_i$  for  $i \in [m]$  be i.i.d copies of symmetric random  $\mathbf{X} \in \mathbb{R}^{n \times n}$  with  $\gamma, \sigma^2 > 0$ ,  $\mathbb{E}[\mathbf{X}] = 0$ ,  $\|\mathbf{X}\|_2 \leq \gamma$ , and  $\|\mathbb{E}[\mathbf{X}^2]\|_2 \leq \sigma^2$ . Then for  $\epsilon > 0$ ,

$$\Pr\left(\left\|\frac{1}{m} \sum_i \mathbf{X}_i\right\|_2 \geq \epsilon\right) \leq 2n \exp(-m\epsilon^2/(\sigma^2 + \gamma\epsilon/3)).$$

## Further Reading

- Drineas, Petros, Ravi Kannan, and Michael W. Mahoney. “Fast Monte Carlo algorithms for matrices I: Approximating matrix multiplication.” *SIAM Journal on Computing* 36.1 (2006): 132-157.
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- Boutsidis, Christos, and David P. Woodruff. “Optimal CUR matrix decompositions.” *Proceedings of the forty-sixth annual ACM symposium on Theory of computing*. 2014.

Questions?