CSE 392/CS 395T/M 397C: Matrix and Tensor Algorithms for Data

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University of Texas, Austin Spring 2025 Lecture 6: Approximate matrix product and sampling

Outline

- 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 (ϵ, δ) type bounds.

Product and norms using randomization

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

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

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

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

$$\mathbb{E}[oldsymbol{s}oldsymbol{s}^ op] = egin{bmatrix} \mathbf{s}_1^2 & \mathbf{s}_1\mathbf{s}_2 & \cdots & \mathbf{s}_1\mathbf{s}_n \\ \mathbf{s}_2,\mathbf{s}_1 & \mathbf{s}_2^2 & & dots \\ dots & & \ddots & & \\ \mathbf{s}_n,\mathbf{s}_1 & \cdots & & \mathbf{s}_n^2 \end{bmatrix} = oldsymbol{I} = egin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & & dots \\ dots & & \ddots & & \\ 0 & \cdots & & 1 \end{bmatrix}$$

Sketching and Sampling

Sketching:

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

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 $\mathbb{E}[\mathbf{s}_i^2] = \frac{1}{n}\sqrt{n^2} + (1 \frac{1}{n})0 = 1.$
- 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

$$\mathbb{E}[oldsymbol{S}^ op oldsymbol{S}] = \mathbb{E}[\sum_{i \in [c]} oldsymbol{S}_{i*}^ op oldsymbol{S}_{i*}] = \sum_{i \in [c]} \mathbb{E}[oldsymbol{S}_{i*}^ op oldsymbol{S}_{i*}] = \sum_{i \in [c]} rac{1}{c} oldsymbol{I} = oldsymbol{I},$$

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

Applications:

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

Approximating Matrix Multiplication (AMM)

Problem Statement:

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

Approximate the sum of n rank-one matrices.

$$oldsymbol{A} \cdot oldsymbol{B} = \sum_{i=1}^n oldsymbol{\left[A_{*i}
ight]} \cdot oldsymbol{\left[B_{i*}
ight]}{m imes p}$$

where A_{*i} is the *i*th column of A and B_{i*} is the *i*th row of B.

Sampling rows of a matrix

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

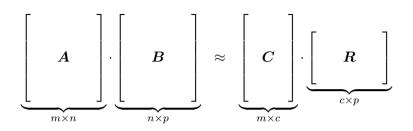
$$\begin{bmatrix} 0 & \mathbf{s}_{12} & 0 & 0 & \cdots & 0 \\ \mathbf{s}_{21} & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & \mathbf{s}_{33} & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & \mathbf{s}_{cn} \end{bmatrix} \begin{bmatrix} \boldsymbol{A}_{1*} \\ \boldsymbol{A}_{2*} \\ \vdots \\ \boldsymbol{A}_{n*} \end{bmatrix}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

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

AMM - Sampling

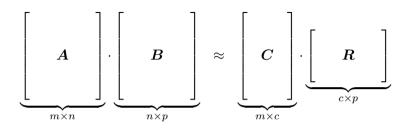
$$egin{array}{lcl} oldsymbol{A} \cdot oldsymbol{B} &=& \displaystyle \sum_{i=1}^n \left[oldsymbol{A}_{*i}
ight] \cdot \left[oldsymbol{B}_{i*}
ight] \\ &pprox & \displaystyle rac{1}{c} \displaystyle \sum_{t=1}^c rac{1}{p_{j_t}} \left[oldsymbol{A}_{*j_t}
ight] \cdot \left[oldsymbol{B}_{j_{t*}}
ight] \\ &\stackrel{m imes p}{\longrightarrow} \end{array}$$

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



- We would like to estimate $AB \approx AS^{\top}SB$.
- Suppose S has just one row s_i . Then, we just get $A_{i*}s_i^2B_{*i} = A_{*i}B_{i*}/p_i$ 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 $p_i \propto ||B_{i*}||^2$. This is called Length-squared sampling.

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

$$\Pr(j_t = i) = \frac{\|\boldsymbol{A}_{*i}\|_2 \|\boldsymbol{B}_{i*}\|_2}{\sum_{j=1}^n \|\boldsymbol{A}_{*j}\|_2 \|\boldsymbol{B}_{j*}\|_2}$$

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

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

Length-squared sampling

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

Proof: First, for any probability p_i , we know that $\mathbb{E}[CR_{ij}] = AB_{ij}$. Elementwise is an unbiased estimator.

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

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

$$\begin{split} \mathbb{E}[\|\boldsymbol{A}\boldsymbol{s}\boldsymbol{s}^{\top}\boldsymbol{B}\|_{F}^{2}] &= \sum_{j,k} \mathbb{E}[(\boldsymbol{A}_{j*}\boldsymbol{s}\boldsymbol{s}^{\top}\boldsymbol{B}_{*k})^{2}] = \sum_{j,k} \mathbb{E}[(\sum_{i} a_{ji}\mathbf{s}_{i}^{2}b_{ik})^{2}] \\ &= \sum_{j,k} \sum_{i} a_{ji}^{2}p_{i}\frac{1}{p_{i}^{2}}b_{ik}^{2} = \sum_{i} \sum_{j} a_{ji}^{2}\frac{1}{p_{i}}\sum_{k} b_{ik}^{2} = \sum_{i} \|\boldsymbol{A}_{*i}\|^{2}\frac{1}{p_{i}}\|\boldsymbol{B}_{i*}\|^{2} \\ &= \|\boldsymbol{A}\|_{F}^{2}\|\boldsymbol{B}\|_{F}^{2}. \end{split}$$

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

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

Thus, we get the result

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

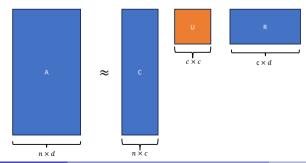
Using Markov's inequality, we can show that for $c \geq 1/\epsilon^2 \delta$,

$$\Pr(\|\boldsymbol{C}\boldsymbol{R} - \boldsymbol{A}\boldsymbol{B}\|_F > \epsilon \|\boldsymbol{A}\|_F \|\boldsymbol{B}\|_F) < \delta.$$

CUR decomposition

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

- A row sampling matrix $S_1 \in \mathbb{R}^{c \times m}$, and $R = S_1 A \in \mathbb{R}^{c \times n}$
- A column sampling matrix $S_2 \in \mathbb{R}^{n \times c}$, and $C = AS_2 \in \mathbb{R}^{m \times c}$
- A matrix $U \in \mathbb{R}^{c \times c}$, such that $A \approx CUR$ and $c \ll \{m, n\}$.



CUR decomposition

- We can compute $U = (AS_2)^{\dagger} S_1^{\top} = (C^{\top}C)^{-1} (S_1 A S_2)^{\top}$.
- \bullet U can be ill-conditioned.
- ullet Typically, in applications, we are interested in random columns C and rows R of A.
- We can also consider, $S_1 \in \mathbb{R}^{r \times m}$ and $S_2 \in \mathbb{R}^{n \times c}$, for different c, r.

Given $A \in \mathbb{R}^{m \times n}$, row sampler $S_1 \in \mathbb{R}^{r \times m}$, column $S_2 \in \mathbb{R}^{n \times c}$, and with $C = AS_2, R = S_1A, U = (AS_2)^{\dagger}S_1^{\top}$, then

$$\mathbb{E}[\|\boldsymbol{C}\boldsymbol{U}\boldsymbol{R} - \boldsymbol{A}\|_{2}^{2}] \leq 2\|\boldsymbol{A}\|_{F}^{2} \left(\frac{1}{\sqrt{c}} + \frac{c}{r}\right) \leq \epsilon \|\boldsymbol{A}\|_{F}^{2},$$

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

Matrix (low rank) approximations

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

$$\Pr(\|\boldsymbol{C}\boldsymbol{U}\boldsymbol{R} - \boldsymbol{A}\|_2 \ge \epsilon \|\boldsymbol{A}\|_F) \le \delta,$$

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

• Cost = ?

Better variance reduction

- We want S such that ||SAx|| is a good estimator of ||Ax||.
- Length-squared sampling : $p_i \propto ||A_{i*}||^2$ is good, but for some \boldsymbol{x} , we could have $A_{i*}\boldsymbol{x} = 0$ even if $||A_{i*}||^2$ 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 $\|Ax\|^2 = \sum_i (A_{i*}x)^2$.
- sampling using information related to $span(\mathbf{A})$.

Leverage scores

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

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

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

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

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

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

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} .

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

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

$$p_j = \frac{\|\boldsymbol{V}_{j*}\|^2}{n}.$$

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):

$$oldsymbol{A} pprox egin{bmatrix} oldsymbol{A}_k & oldsymbol{A} & oldsymbol{\otimes} oldsymbol{U}_k & oldsymbol{\otimes} oldsymbol{U}_k & oldsymbol{\otimes} oldsymbol{\otimes} oldsymbol{\Sigma}_k & oldsymbol{\otimes} oldsymbol{V}_k^ op & oldsymbol{\otimes} oldsymbol{\otimes} oldsymbol{V}_k^ op & oldsymbol{\otimes} oldsymbol{\otimes} oldsymbol{\otimes} oldsymbol{W}_k^ op & oldsymbol{\otimes} oldsy$$

Row Leverage scores and Column Leverage scores

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

Leverage score sampling

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

$$\|A - CX\|_F = \|A - CC^{\dagger}A\|_F \le (1 + \epsilon)\|A - A_k\|_F,$$

for sampling complexity

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

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Proof uses Matrix Chernoff inequality.

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

$$\Pr(\|\frac{1}{c}\sum_{i} \boldsymbol{X}_{i}\|_{2} \ge \epsilon) \le 2n \exp(-c\epsilon^{2}/(\sigma^{2} + \gamma\epsilon/3)).$$

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.
- Drineas, Petros, Ravi Kannan, and Michael W. Mahoney. "Fast Monte Carlo algorithms for matrices II: Computing a low-rank approximation to a matrix." SIAM Journal on computing 36.1 (2006): 158-183.
- Kannan, Ravindran, and Santosh Vempala. "Randomized algorithms in numerical linear algebra." Acta Numerica 26 (2017): 95-135.
- Boutsidis, Christos, and David P. Woodruff. "Optimal CUR matrix decompositions." Proceedings of the forty-sixth annual ACM symposium on Theory of computing. 2014.

Questions?