COMPSCI 614: Randomized Algorithms with Applications to Data Science

Prof. Cameron Musco University of Massachusetts Amherst. Spring 2024. Lecture 11

Logistics

- The midterm is the Thursday after break.
- Tuesday that week I will do midterm review (not cover any new material).
- · Midterm study material will be posted shortly.
- · Pset 3 posted tonight. Will be shorter than Pset 2.
- · Project proposal due today.

Summary

Last Time:

- · Approximate matrix multiplication via importance sampling.
- · Application to fast low-rank approximation via sampling.

Summary

Last Time:

- · Approximate matrix multiplication via importance sampling.
- · Application to fast low-rank approximation via sampling.

Today:

- · Finish up fast low-rank approximation.
- · Stochastic trace estimation. Htchinson's estimation

2

Quiz Review

Question 6

Not complete Points out of 1.00

Flag question

Edit question

Considering estimating the sum of a set of numbers $\{x_1,\dots,x_n\}$ via importance sampling. You take t independent samples i_1,\dots,i_t according to probability distribution $\{p_1,\dots,p_n\}$, multiply each sample by $1/p_{i_t}$, and then average together these samples.

Which of the following distributions minimizes the variance of your estimate. **To Think About:** Is sampling according to this probability distribution likely feasible?

Check

Quiz Review

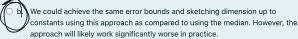
Question 5

Not complete Points out of 100

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Edit question Consider a version of Count-Sketch where instead of returning the median of our t independent estimates as the final estimate, we return the estimate which is at the 95th percentile of the t estimates. How would this change the theoretical bounds for the algorithm? How do you think it would effect the practical performance?

 \bigcirc a. We are not be able to obtain error $\varepsilon ||x||_2$ using this approach.



 c. We could achieve the same error bounds and sketching dimension up to constants using this approach as compared to using the median. Further, the approach will likely work significantly better in practice.

 We could obtain the same error bounds using this approach, but would require a much larger sketching dimension as compared to taking the median. Further, the approach will likely work significantly worse in practice.

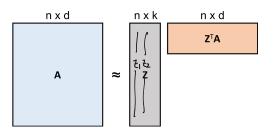
x(i)-Ellyll, X(i) K(i)+ 5/1x/1,

Randomized Low-Rank approximation

Low-rank Approximation

Consider a matrix $A \in \mathbb{R}^{n \times d}$. We would like to compute an optimal low-rank approximation of A. I.e., for $k \ll \min(n,d)$ we would like to find $Z \in \mathbb{R}^{n \times k}$ with orthonormal columns satisfying:

$$\|A-ZZ^TA\|_F=\min_{Z:Z^TZ=I}\|A-ZZ^TA\|_F.$$



Solving this exactly requires computing the top k left singular vectors of A in $O(nd^2)$ time. We will give an approximation algorithm running in $O(nd + nk^2)$ time.

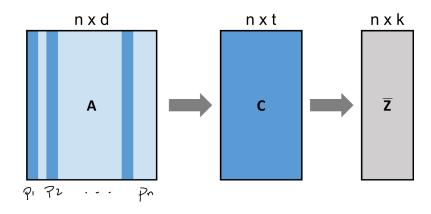
6

Sampling Based Algorithm

Linear Time Low-Rank Approximation:

- Fix sampling probabilities p_1, \ldots, p_n with $p_i = \frac{\|A_{:,i}\|_2^2}{\|A\|_F^2}$.
- Select $i_1, \ldots, i_t \in [n]$ independently, according to the distribution $\Pr[i_i = k] = p_k$ for sample size $t \ge k$.
- Let $C = \sqrt{\frac{1}{t}} \cdot \sum_{j=1}^{t} \frac{1}{\sqrt{p_{i_j}}} \cdot A_{:,i_j}$. $Cc^{\mathsf{T}} : \frac{1}{t} : \sum_{j=1}^{t} C_{i,j} : C_{$
- Let $\overline{Z} \in \mathbb{R}^{n \times k}$ consist of the top k left singular vectors of C. $e^{1 = \frac{\mathcal{E}}{\sqrt{K}}}$
- By our approximate matrix multiplication analysis, if $t = O(\frac{k}{\delta\epsilon^2})$, $\|\mathbf{CC}^\mathsf{T} AA^\mathsf{T}\|_F \le \epsilon/\sqrt{k} \cdot \|A\|_F^2$ with probability at least 1δ .
- We will use this to show that an optimal basis for C (i.e., \overline{Z}) is nearly optimal for A.

Sampling Based Algorithm



Let $Z_* \in \mathbb{R}^{n \times k}$ contain the top left singular vectors of A – i.e. $Z_* = \arg\min \|A - ZZ^TA\|_F^2$. Similarly, $\overline{\mathbf{Z}} = \arg\min \|\mathbf{C} - ZZ^T\mathbf{C}\|_F^2$.

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Claim 1: For any orthonormal $Z \in \mathbb{R}^{n \times k}$, and any matrix B,

$$||B - ZZ^TB||_F^2 = \operatorname{tr}(BB^T) - \operatorname{tr}(Z^TBB^TZ).$$

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Claim 2: If $\|AA^T - CC^T\|_F \le \frac{\epsilon}{\sqrt{k}} \|A\|_F^2$, then for any orthonormal $Z \in \mathbb{R}^{n \times k}$, $\operatorname{tr}(Z^T(AA^T - CC^T)Z) \le \epsilon \|A\|_F^2$.

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Claim 2: If $||AA^T - CC^T||_F \le \frac{\epsilon}{\sqrt{k}} ||A||_F^2$, then for any orthonormal $Z \in \mathbb{R}^{n \times k}$, $tr(Z^T(AA^T - CC^T)Z) \le \epsilon ||A||_F^2$.

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$$\|\mathbf{C} - \overline{\mathbf{Z}}\overline{\mathbf{Z}}^{\mathsf{T}}\mathbf{C}\|_{F}^{2} \leq \|\mathbf{C} - \mathbf{Z}_{*}\mathbf{Z}_{*}^{\mathsf{T}}\mathbf{C}\|_{F}^{2} \implies \mathsf{tr}(\overline{\mathbf{Z}}^{\mathsf{T}}\mathbf{C}\mathbf{C}^{\mathsf{T}}\overline{\mathbf{Z}}) \geq \mathsf{tr}(\mathbf{Z}_{*}^{\mathsf{T}}\mathbf{C}\mathbf{C}^{\mathsf{T}}\mathbf{Z}_{*})$$

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$$||B - ZZ^TB||_F^2 = \operatorname{tr}(BB^T) - \operatorname{tr}(Z^TBB^TZ).$$

Claim 2: If $||AA^T - CC^T||_F \le \frac{\epsilon}{\sqrt{h}} ||A||_F^2$, then for any orthonormal $Z \in \mathbb{R}^{n \times k}, |\operatorname{tr}(Z^T(AA^T - CC^T)Z)| \leq \epsilon ||A||_{E}^{2}.$

$$\begin{split} \|C - \overline{Z}\overline{Z}^{\mathsf{T}}C\|_{F}^{2} &\leq \|C - Z_{*}Z_{*}^{\mathsf{T}}C\|_{F}^{2} \implies \operatorname{tr}(\overline{Z}^{\mathsf{T}}CC^{\mathsf{T}}\overline{Z}) \geq \operatorname{tr}(Z_{*}^{\mathsf{T}}CC^{\mathsf{T}}Z_{*}) \\ &\implies \operatorname{tr}(\overline{Z}^{\mathsf{T}}AA^{\mathsf{T}}\overline{Z}) \geq \operatorname{tr}(Z_{*}^{\mathsf{T}}AA^{\mathsf{T}}Z_{*}) - 2\epsilon \|A\|_{F}^{2} \\ & - (1 \text{ in } 2) + 1 \text{ true for } 1$$

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$$Z_* = \arg\min \|A - ZZ^TA\|_F^2. \text{ Similarly, } \overline{Z} = \arg\min \|C - ZZ^TC\|_F^2. \|B\|_F^2 = \sum_{i=1}^{\infty} \|B_{i,i}\|_L^2$$

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$$\|\underline{B} - ZZ^TB\|_F^2 = \operatorname{tr}(BB^T) - \operatorname{tr}(Z^TBB^TZ). \qquad \begin{bmatrix} \sigma & \sigma & \sigma \\ \sigma & \sigma & \sigma \end{bmatrix}$$
Claim 2: If $\|AA^T - CC^T\|_F \le \frac{\epsilon}{\sqrt{R}} \|A\|_F^2$, then for any orthonormal $\|AB\|_F^2 = \|B\|_F^2$

$$Z \in \mathbb{R}^{n \times R}, \operatorname{tr}(Z^T(AA^T - CC^T)Z) \le \epsilon \|A\|_F^2. \qquad \qquad +, (BB) = \|B\|_F^2$$

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I project of P to Z has similar (ext to project of Z).

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Suffices to show that for any symmetric $B \in \mathbb{R}^{n \times n}$, and any orthonormal $Z \in \mathbb{R}^{n \times k}$, $|\text{tr}(Z^T B Z)| \leq \sqrt{k} \cdot ||B||_F$.

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orthonormal
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$$B_{\mathcal{T}} = \lambda_{\mathcal{T}}$$

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$$tr(Z^{T}BZ) = \sum_{i=1}^{k} z_{i}^{T}Bz_{i}$$

$$\leq \sum_{i=1}^{k} \lambda_{i}(B) \qquad \text{(By Courant-Fischer theorem)}$$

$$\leq \sqrt{k} \cdot \sqrt{\sum_{i=1}^{k} \lambda_{i}(B)^{2}} \leq \sqrt{k} \cdot \sqrt{\sum_{i=1}^{n} \lambda_{i}(B)^{2}}$$

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$$\begin{split} \left(\operatorname{tr}(Z^T B Z) \middle| = \middle| \sum_{i=1}^k z_i^T B z_i \middle| \\ & \leq \sum_{i=1}^k \middle| \lambda_i(B) \middle| \quad \text{(By Courant-Fischer theorem)} \\ & \leq \sqrt{k} \cdot \sqrt{\sum_{i=1}^k \lambda_i(B)^2} \leq \sqrt{k} \cdot \sqrt{\sum_{i=1}^n \lambda_i(B)^2} = \sqrt{k} \cdot ||B||_F. \end{split}$$

Norm based sampling gives an additive error approximation, $\|A - \overline{Z}\overline{Z}^TA\|_F^2 \leq \min_{Z:Z^TZ=I} \|A - ZZ^TA\|_F^2 + 2\epsilon \|A\|_F^2.$

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• Ideally, we would like a relative error approximation, $\|A - \overline{Z}\overline{Z}^TA\|_F^2 \le (1 + \epsilon) \cdot \min_{Z:Z^TZ=I} \|A - ZZ^TA\|_F^2$.

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- - This can be achieved with more advanced non-uniform sampling techniques, based on leverage scores or adaptive sampling.
 - · Also possible using Johnson-Lindenstrauss type random projection.

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- This can be achieved with more advanced non-uniform sampling techniques, based on leverage scores or adaptive sampling.
- Also possible using Johnson-Lindenstrauss type random projection.
- We will cover these techniques in future classes.

Stochastic Trace Estimation

Matrix Trace

The trace of a matrix $A \in \mathbb{R}^{n \times n}$ is the sum of it diagonal entries.

$$\operatorname{tr}(A) = \sum_{i=1}^{n} A_{ii}.$$

When A is diagonalizable (e.g., when it is symmetric) with eigenvalues $\lambda_1, \ldots, \lambda_n$, $\operatorname{tr}(A) = \sum_{i=1}^n \lambda_i$.

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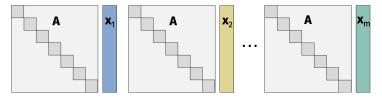
$$tr(A) = \sum_{i=1}^{n} A_{ii}.$$

When A is diagonalizable (e.g., when it is symmetric) with eigenvalues $\lambda_1, \ldots, \lambda_n$, $\operatorname{tr}(A) = \sum_{i=1}^n \lambda_i$.

How many operations does it take to compute tr(A) given explicit access to A?

Implicit Trace Estimation

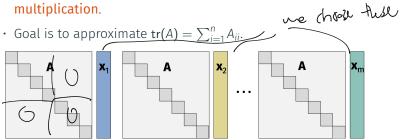
- Given implicit access to $A \in \mathbb{R}^{n \times n}$ through matrix-vector multiplication.
- Goal is to approximate $tr(A) = \sum_{i=1}^{n} A_{ii}$.



Main question: How many matrix-vector multiplication "queries" Ax_1, \ldots, Ax_m are required to approximate tr(A)?

Implicit Trace Estimation

• Given implicit access to $A \in \mathbb{R}^{n \times n}$ through matrix-vector multiplication.



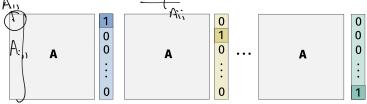
Main question: How many matrix-vector multiplication "queries" Ax_1, \ldots, Ax_m are required to approximate tr(A)?

Algorithms in this model are called matrix-free methods. Useful when A is not given explicitly, but we have an efficient algorithm for multiplying A by a vector (examples to come).

Naive Exact Algorithm

Naive solution:

- Set $x_i = e_i$ for $i = 1, \ldots, n$.
- Return $\operatorname{tr}(A) = \sum_{i=1}^{n} x_{i}^{\mathsf{T}} A x_{i}$.

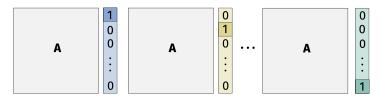


Returns exact solution, but requires *n* matrix-vector multiplies.

Naive Exact Algorithm

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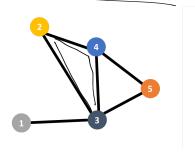
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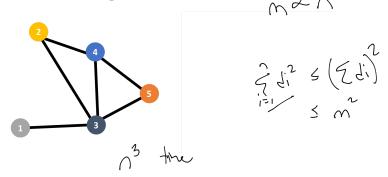
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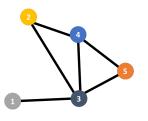
We will see how to use $m \ll n$ multiplies by using randomness and allowing for small approximation error.

The number of triangles or other small 'motifs' is an important metric of network connectivity. E.g., important in computing the network clustering coefficient

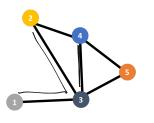


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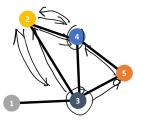


		В		
0	0	1	0	0
0	0	1	1	0
1	1	0	1	1
0	1	1	0	1
0	0	1	1	0



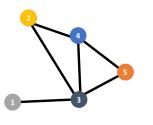
		В		
0	0	1	0	0
0	0	1	1	0
1	1	0	1	1
0	1	1	0	1
0	0	1	1	0

- B_{ij} indicates the number of 1-step paths (edges) from i, j
- $[B^2]_{ij}$ indicates the number of 2-step paths from i,j
- $[B^3]_{ij}$ indicates the number of 3-step paths from i,j



		B ²		
1	1	0	1	1
1	2	1	1	2
0	1	4	2	1
1	1	2	3	1
1	2	1	1	2

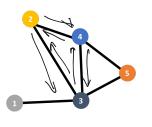
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		B^3		
0	1	4	2	1
1	2	6	5	2
4	6	4	6	6
2	5	6	4	5
1	2	6	5	2

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Can use the adjacency matrix $B \in \{0,1\}^{n \times n}$ to write the number of triangles in a linear algebraic way.



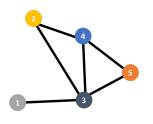
		B^3		
0	1	4	2	1
1 '	(2)	6	5	2
4	6	4	6	6
2	5	6	4	5
1	2	6	5	2

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 B_{ii} is the number of length 3-paths from i back to i. Thus,

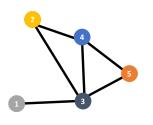
$$\cap^{\vee}$$

$$\frac{1}{6}\operatorname{tr}(B^3) = \# \operatorname{triangles}.$$



		B^3		
0	1	4	2	1
1	2	6	5	2
4	6	4	6	6
2	5	6	4	5
1	2	6	5	2

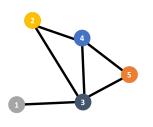
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		B^3		
0	1	4	2	1
1	2	6	5	2
4	6	4	6	6
2	5	6	4	5
1	2	6	5	2

$$\frac{1}{6}\operatorname{tr}(B^3) = \# \operatorname{triangles}.$$

• Explicitly forming B^3 and computing $\mathrm{tr}(B^3)$ takes $O(n^3)$ time.



		B^3		
0	1	4	2	1
1	2	6	5	2
4	6	4	6	6
2	5	6	4	5
1	2	6	5	2

$$\frac{1}{6}\operatorname{tr}(B^3) = \# \operatorname{triangles}.$$

- Explicitly forming B^3 and computing $tr(B^3)$ takes $O(n^3)$ time.
- Can multiply B^3 by a vector in $3 \cdot |E| = O(n^2)$ operations.
- So a trace estimation algorithm using m queries, yields an $O(m \cdot |E|)$ time approximate triangle counting algorithm.

