SDS 385: Stat Models for Big Data

Lecture 9: Sampling methods

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Sampling for matrix multiplication

- Goal: multiply two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$
- Used as an inner routine in many algorithms.
- Lets first try the vanilla algorithm for warmup.

The naive algorithm

Algorithm 1 Vanilla three-look matrix multiplication algorithm.

Input: An $m \times n$ matrix A and an $n \times p$ matrix B

Output: The product AB

1: **for** $i = 1$ to m **do**
2:    **for** $j = 1$ to p **do**
3:       $(AB)_{ij} = 0$
4:       **for** $k = 1$ to n **do**
5:          $(AB)_{ik} \mathrel{+}= A_{ij}B_{jk}$
6:       **end for**
7:    **end for**
8: **end for**
9: Return AB

The naive algorithm - complexity

- Step 1 has m loops
- Steo 2 has n loops
- Steo 3 has p loops
- Total mnp computation.
- When $m = n = p$ it takes $O(n^3)$ time. Too much!

Alternatives

- Strassen algorithm (1969) takes $O(n^{2.81})$ time
- Coppersmith-Winograd algorithm (2010) takes $O(n^{2.375})$ time
  - Often used as a building block in other algorithms to prove theoretical time bounds.
  - However, unlike the Strassen algorithm, it is not used in practice because it only provides an advantage for matrices so large that they cannot be processed by modern hardware
- Stother's algorithm (2011) $O(n^{2.374})$
- Vassilevska William's algorithm (2011) $O(n^{2.3728642})$
  - Le Galls improvement (2014) $O(n^{2.3728639})$

Another much simpler approach–Sample

- Notation:
  - Let $A^i \in \mathbb{R}^m$ is the ith column of A
  - $B_i \in R^p$ is the ith row of B.
- Note that
$$(AB)_{ik} = \sum_j A_{ij} B_{jk} = A_i^T B^j$$
- Instead, we will consider a matrix multiplication as the sum of outer products, i.e.
$$AB = \sum_{i=1}^{n} A^i B_i^T$$
- Why?

Take one

- Forget about matrices, say you have n real numbers and you want to calculate the sum.

- If you sample k of these uniformly at random, you can approximate the sum by:

$$\sum_i x_i \approx \sum_{j=1}^{k} (n/k) x_{j*}$$

- $P(j^* = i) = 1/n$ for $i \in \{1, \dots, n\}$

Take one

- This works because:

$$E[\sum_{j=1}^{k}(n/k)x_{j*}] = \sum_{j=1}^{k}\frac{n}{k}\sum_{i=1}^{n}\frac{1}{n}x_i = \sum_{i=1}^{n}x_i$$

- Variance is:

$$\text{var}(\sum_{j=1}^{k}(n/k)x_{j*}) = \frac{n^2}{k}\underbrace{\left(\sum_{i}x_i^2/n - \bar{x}^2\right)}_{\text{variance of the numbers}}$$

- Note that the variance of this approximation increases if the numbers are very different from each other, i.e. the variance of the numbers you are summing is large

- Solution – weighted sampling.

Take two

- Sample an element j with probability p_j
- p_j sums to one, but not necessarily uniform.
- So lets try:

$$\sum_i x_i \approx \frac{1}{k} \sum_{j=1}^{k} x_{j*}/p_{j*}$$

- The expectation is:

$$E[\frac{1}{k} \sum_{j=1}^{k} \frac{x_{j*}}{p_{j*}}] = \frac{1}{k} \sum_{j=1}^{k} \sum_{i=1}^{n} p_i \frac{x_i}{p_i} = \sum_{i=1}^{n} x_i$$

Take two

- The variance is:

$$\frac{1}{k} \left(\sum_i x_i^2 / p_i - n^2 \bar{x}^2 \right)$$

- Now if you choose $p_i = x_i^2 / \|x\|_2^2$

-
$$\frac{1}{k} \left(\sum_i x_i^2 / p_i - n^2 \bar{x}^2 \right) = \frac{1}{k} \left(\sum_i x_i^2 / p_i - n^2 \bar{x}^2 \right)$$

- How do you minimize w.r.t p_i such that $\sum_i p_i = 1$?

Take two

- Lagrange multipliers!

$$L(\pi, \lambda) = \frac{1}{k} \left(\sum_i x_i^2 / p_i - n^2 \bar{x}^2 \right) + \lambda(\sum_i p_i - 1)$$

- Differentiating w.r.t p_i and setting to zero gives:

$$\frac{x_i^2}{p_i^2} - \lambda = 0$$

$$p_i = \frac{|x_i|}{\sum_j |x_j|}$$

- The second line uses the fact that $\sum_i p_i = 1$ to solve for the λ

Take two

- So if all $x_i > 0$ then this choice of p_i gives variance 0!
- Can you explain this?
- But lets not stray from matrix multiplication

Matrix multiplication

Algorithm 2 The `BasicMatrixMultiplication` algorithm.

Input: An $m \times n$ matrix A, an $n \times p$ matrix B, a positive integer c, and probabilities $\{p_i\}_{i=1}^n$.

Output: Matrices C and R such that $CR \approx AB$.

  1: **for** $t = 1$ to c **do**

  2:      Pick $i_t \in \{1, \ldots, n\}$ with probability $\mathbf{Pr}\left[i_t = k\right] = p_k$, in i.i.d. trials, with replacement

  3:      Set $C^{(t)} = A^{(i_t)}/\sqrt{cp_{i_t}}$ and $R_{(t)} = B_{(i_t)}/\sqrt{cp_{i_t}}$.

  4: **end for**

  5: Return C and R.

Analogy to the sum

- For the sum we wanted to compute $\sum_i x_i$

- Here we want to compute $\sum_i A^i B_i^T$

- So the analog of x_i is the rank one outer product matrix $A^i B_i^T$

- Note that $\|A^i B_i^T\|_2^2 = \|A^i\|_2^2 \|B_i^T\|_2^2$

- Use $p_i := \dfrac{\|A^i\|_2 \|B_i\|_2}{\sum_i \|A^i\|_2 \|B_i\|_2}$

Initial results

- $E[(CR)_{ij}] = (AB)_{ij}$

- $\text{var}((CR)_{ij}) = \dfrac{1}{c} \left(\displaystyle\sum_{k=1}^{n} \dfrac{A_{ik}^2 B_{kj}^2}{p_k} - (AB)_{ij}^2 \right)$

- Now the x_k's are the same as $A_{ik} B_{kj}$. Remember our formula for mean?

  - The mean of $\dfrac{1}{c} \displaystyle\sum_{j=1}^{c} \dfrac{x_{j*}}{p_{j*}}$ was $\displaystyle\sum_{k=1}^{n} x_k$

  - Plug in $x_k = A_{ik} B_{kj}$ to get the mean as $\displaystyle\sum_{k} A_{ik} B_{kj}$

- How about variance?

  - Variance was: $\dfrac{1}{c} \left(\displaystyle\sum_{k} \dfrac{x_k^2}{p_k} - (\sum_{k} x_k)^2 \right)$

  - Variance of $(CR)_{ij}$ is $\dfrac{1}{c} \left(\displaystyle\sum_{k} \dfrac{x_k^2}{p_k} - (\sum_{k} x_k)^2 \right)$

  - Plug in $x_k = A_{ik} B_{kj}$ to get the right expression.

Error bounds

- $E[\|AB - CR\|_F^2] = \dfrac{1}{c}\left(\displaystyle\sum_{k=1}^{n}\dfrac{\|A^k\|^2\|B_k\|^2}{p_k} - \|AB\|_F^2\right)$

- Why?

$$
\begin{aligned}
E\left[\|AB - CR\|_F^2\right] &= \sum_{ij} E[(CR)_{ij} - (AB)_{ij}]^2 \\
&= \sum_{ij} \mathrm{var}((CR)_{ij}) \\
&= \frac{1}{c}\sum_{ij}\left(\sum_{k=1}^{n}\frac{A_{ik}^2 B_{kj}^2}{p_k} - (AB)_{ij}^2\right)
\end{aligned}
$$

- Exchange the two sums and get the answer.

Optimal weights

- The optimal $p_k = \dfrac{\|A^k\|\|B_k\|}{\sum_k \|A^k\|\|B_k\|}$
- Same Lagrange multiplier trick to see $p_k = |x_k|/\sum_i |x_i|$
- Plug in $x_k = \|A^k\|\|B_k\|$
- Plug in to get

$$E[\|CR - AB\|_F^2] = \frac{1}{c}\left(\left(\sum_{k=1}^{n} \|A^k\|\|B_k\|\right)^2 - \|AB\|_F^2\right)$$

- Calculate p_k in $O(n(m + p))$ time.
- Computational saving from $mnp \rightarrow \max(mn, np)$
- What if I did a sub-optimal weighted sampling?
- Take $p_i = \|A_i\|_F^2 / \|A\|_F^2$
- Now the error becomes $\frac{1}{c}(\|A\|_F^2 \|B\|_F^2 - \|AB\|_F^2)$

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