

Algorithmic Machine Learning + Data Science

CS-GY 6763/CS-UY 3943: Lecture 1

Course introduction, concentration of random variable, applications

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Algorithmic Machine Learning and Data Science

Statistics, machine learning, and data science study how to use data to make better decisions or discoveries.

In this class, we study how to do so **as quickly as possible, or with limited computational resources.**

- **Twitter** receives 6,000 tweets every second.
- **Google** receives $\approx 10,000$ Maps queries every second.
- **NASA** collects 6.4 TB of satellite images every day.
- **Large Synoptic Survey Telescope** will collect 20 TB of images every night.
- **MIT/Harvard Broad Institute** sequences 24 TB of genetic data every day.

Growing demands of data science and machine learning have ushered in a new “golden age” for algorithms research.

- Bolstered by our limited ability to build faster computers (or to access computational resources with a limited financial budget).
- Typical data applications require combining a diverse set of algorithmic tools. Most are not heavily covered in your traditional algorithms curriculum.

- (1) Randomized methods.
- (2) Optimization.
- (3) Spectral methods and linear algebra.
- (4) Fourier methods.

Section 1: Randomized Algorithms.

It is hard to find an algorithms paper in 2021 that does not use randomness in some way, but this wasn't always the case!

- Probability tools and concentration of random variables (Markovs, Chebyshev, Chernoff/Bernstein inequalities).
- Random hashing for fast data search, load balancing, and more. Locality sensitive hashing, MinHash, SimHash, etc.
- Sketching and streaming algorithms for compressing and processing data on the fly.
- High-dimensional geometry and the Johnson-Lindenstrauss lemma for compressing high dimensional vectors.

Section 2: Optimization.

Optimization has become the algorithmic workhorse of modern machine learning.

- Gradient descent, stochastic gradient descent, coordinate descent, and how to analyze these methods.
- Acceleration, conditioning, preconditioning, adaptive gradient methods.
- Constrained optimization, linear programming. Ellipsoid and interior point methods.
- Discrete optimization, relaxation, submodularity and greedy methods.

Section 3: Spectral methods and linear algebra.

“Complex math operations (machine learning, clustering, trend detection) [are] mostly specified as linear algebra on array data” – Michael Stonebraker, Turing Award Winner

- How to compute singular value decompositions and eigendecomposition.
- Spectral graph theory: i.e. how to use linear algebra to understanding large graphs through linear algebra (social networks, interaction graphs, etc.).
- Spectral clustering and non-linear dimensionality reduction.
- Random sampling and sketching methods for matrix computations.

Section 4: Fourier methods.

- Compressed sensing, sparse recovery, and their applications.
- Fast Fourier Transform inspired methods in linear algebra and dimensionality reduction.
- Fourier perspective on machine learning techniques like kernel methods, and the algorithmic benefits.

WHAT WE WON'T COVER

Software tools or frameworks. MapReduce, Tensorflow, Spark, etc. If you are interested CS-GY 6513 might be a good course.

Machine Learning Models + Techniques. Neural nets, reinforcement learning, Bayesian methods, unsupervised learning, etc. I assume you have already had a course in ML and the focus of this class is on computational considerations.

But if your research is in machine learning, I think you will find the theoretical tools we learn are more broadly applicable than in designing faster algorithms.

OUR APPROACH

This is primarily a **theory** course.

- Emphasis on proofs of correctness, bounding asymptotic runtimes, convergence analysis, etc. *Why?*
- Learn how to model complex problems in simple ways.
- Learn general mathematical tools that can be applied in a wide variety of problems (in your research, in industry, etc.)
- The homework requires **creative problem solving** and thinking beyond what was covered in class. You will not be able to solve many problems on your first try!

You will need a good background in **probability** and **linear algebra**. See the syllabus for more details. Ask me if you are still unsure.

All of this information is on the course webpage <https://www.chrismusco.com/amlds2021/> and in the syllabus posted there! Please take a look.

Class structure:

- Lecture once a week. You can attend on Zoom, but I recommend coming in person.
- Office hours from me and TAs once a week.

Tech tools:

- **Website** for up-to-date info, lecture notes, readings.
- **Ed discussion** for questions about material.
- **NYU Brightspace** for turning in assignments.

Class work:

- **Weekly online quiz** (10% of course grade) posted after Tuesday lecture. Due following Tuesday before class.
- **4 problem sets** (45% of course grade).
 - These are challenging, and the most effective way to learn the material. I recommend you start early, work with others, ask questions on Ed, etc.
 - You must write-up solutions on your own.¹
- **Midterm** (15% of course grade).
 - **Need permission from department to take remotely.**

¹10% bonus on first problem set for using Markdown or LaTeX. It should save you time in the long run!

Final project or final exam (20% of grade):

- Final exam will be similar to midterm and problem sets.
- Final project can be based on a recent algorithms paper, and can be either an experimental or theoretical project. Work alone or in a pair.
- We will hold a **reading group** outside of class for those who decide to complete a final project to workshop topics and papers.
- Others can join as well – it's a great opportunity to get better at reading and presenting papers.

Class participation (10% of grade):

- My goal is to know you all individually by the end of this course.
- Lots of ways to earn the full grade: participation in lecture, office hours, or Ed discussion. Participation in the reading group. Effort on the project.

COURSE STRUCTURE AND LOGISTICS

Important note:

- This is a mixed undergraduate/graduate course.
- Workload is the same, but undergraduates are graded on a different “curve”.
- Tandon Ph.D. student Teal Witter will be offering undergraduate only office hours for extra support.



Course Assistant
Aarshvi Gajjar



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QUESTIONS?

Goal: Demonstrate how even the simplest tools from probability can lead to a powerful algorithmic results.

Lecture applications:

- Estimating set size from samples.
- Finding frequent items with small space.

Problem set applications:

- Group testing for COVID-19.
- Smarter load balancing.
- Testing uniformity.

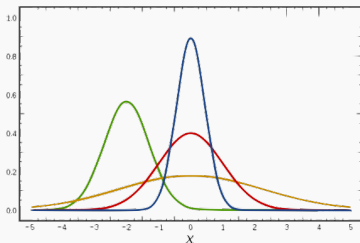
PROBABILITY REVIEW

Let X be a random variable taking value in some set \mathcal{S} . I.e. for a dice, $\mathcal{S} = \{1, \dots, 6\}$. For a continuous r.v., we might have $\mathcal{S} = \mathbb{R}$.

- **Expectation:** $\mathbb{E}[X] = \sum_{s \in \mathcal{S}} \Pr[X = s] \cdot s$

For continuous r.v., $\mathbb{E}[X] = \int_{s \in \mathcal{S}} \Pr(s) \cdot s \, ds$.

- **Variance:** $\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2]$



Exercise: For any scalar α , $\mathbb{E}[\alpha X] = \alpha \mathbb{E}[X]$. $\text{Var}[\alpha X] = \alpha^2 \text{Var}[X]$.

PROBABILITY REVIEW

Let A and B be random events.

- **Joint Probability:** $\Pr(\underline{A \cap B})$. Probability that both events happen.
- **Conditional Probability:** $\underline{\Pr(A \mid B)} = \frac{\Pr(A \cap B)}{\Pr(B)}$. Probability A happens conditioned on the event that B happens.
- **Independence:** A and B are independent events if:
 $\underline{\Pr(A \mid B)} = \underline{\Pr(A)}$.

Alternative definition of independence:

$$\underline{\Pr(A \cap B)} = \Pr(A) \cdot \Pr(B).$$

Example: What is the probability that for two independent dice rolls taking values uniformly in $\{1, 2, 3, 4, 5, 6\}$, the first roll comes up odd and the second is < 3 ?

$$\frac{3}{6} \cdot \frac{2}{6} = \frac{1}{2} \cdot \frac{1}{3} = \frac{1}{6}$$

Let X and Y be random variables. X and Y are independent if, for all events s, t , the random events $[X = s]$ and $[Y = t]$ are independent.

THE MOST POWERFUL THEOREM IN ALL OF PROBABILITY?

Linearity of expectation:

$$\underline{\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]}$$

Always, sometimes, or never?

For random variables X, Y :

- $\mathbb{E}[XY] = \mathbb{E}[X] \cdot \mathbb{E}[Y]$. Sometimes. When X, Y are independent.
- $\text{Var}[X + Y] = \text{Var}[X] + \text{Var}[Y]$. Sometimes. When covariances is zero.
When X, Y are independent.
- $\text{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$.

$$\begin{aligned}\mathbb{E}[(X - \mathbb{E}[X])^2] &= \mathbb{E}[X^2 - 2X(\mathbb{E}[X]) + (\mathbb{E}[X])^2] \\ &= \mathbb{E}[X^2] - 2\mathbb{E}[X] \cdot \mathbb{E}[X] + (\mathbb{E}[X])^2\end{aligned}$$

FIRST APPLICATION

You run a web company that is considering contracting with a vendor that provides CAPTCHAs for logins.



They claim to have a data base of $n = 1,000,000$ unique CAPTCHAs in their database, and a random one will be shown on each API call to their service. They give you access to a test API so you can try it out.

Question: Roughly how many queries to the API, m , would you need to independently verify the claim that there are ~ 1 million unique puzzles?

First attempt: Count how many unique CAPTCHAs you see, until you find 1,000,000 or close to it. Declare that you are satisfied.

As a function of n , roughly how many API queries m do you need?

$$m = O(n)$$

$$O(\sqrt{n})$$

A DIFFERENT APPROACH

Clever alternative: Count how many duplicate CAPTCHAs you see. If you see the same CAPTCHA on query i and j that's one duplicate. If you see the same CAPTCHA on queries i , j , and k , that's three duplicates: (i, j) , (i, k) , (j, k) .



FORMALIZING THE PROBLEM

Question: How many duplicates do we expect to see?

Let $D_{i,j} = 1$ if queries i, j return the same CAPTCHA, and 0 otherwise.

$m = \# \text{ of queries}$

This is called an **indicator random variable**.

$D_{i,j} = \mathbb{1}[\text{CAPTCHA } i \text{ equals CAPTCHA } j].$ ≈ 1 if event is true
 ≈ 0 otherwise

Number of duplicates D is :

$$\underline{D} = \sum_{\substack{i,j \in \{1, \dots, m\} \\ i < j}} \underline{D_{i,j}}.$$

What is $\underline{\mathbb{E}[D]}$?

FORMALIZING THE PROBLEM

Question: How many duplicates do we expect to see? Formally, what is $\mathbb{E}[D]$?

$$D = \sum_{i < j} \mathbb{1}(\text{captcha } i = \text{captcha } j)$$

$$\mathbb{E}[D] =$$

$$\begin{aligned} & \sum_{i < j} \mathbb{E}[\mathbb{1}(\text{captcha } i = \text{captcha } j)] \\ &= \sum_{i < j} 1/n = \frac{m(m-1)}{2} \cdot \frac{1}{n} \end{aligned}$$

n = number of CAPTCHAS in database, m = number of test queries.
 $D_{i,j}$ = indicator for event CAPTCHA i and j collide.

SOME HARD NUMBERS

Suppose you take $m = 1000$ queries and see 10 duplicates. How does this compare to the expectation if the database actually has $n = 1,000,000$ unique CAPTCHAs?

$$\mathbb{E}[D] = \frac{m(m-1)}{2n} = .4995.$$

Something seems wrong... this random variable D came up much larger than its expectation.

Can we say something formally?

n = number of CAPTCHAS in database, m = number of test queries.

CONCENTRATION INEQUALITY

One of the most important tools in analyzing randomized algorithms. Tell us how likely it is that a random variable X deviates a certain amount from its expectation $\mathbb{E}[X]$.

We will learn three fundamental concentration inequalities:

1. **Markov's Inequality.**

- Applies to non-negative random variables.

2. Chebyshev's Inequality.

- Applies to random variables with bounded variance.

3. Hoeffding/Bernstein/Chernoff bounds.

- Applies to sums of random variables with bounded variance.

MARKOV'S INEQUALITY

Theorem (Markov's Inequality): For any random variable X which only takes non-negative values any positive t ,

$$\Pr[X \geq t] \leq \frac{\mathbb{E}[X]}{t}. \quad t = \alpha \mathbb{E}[X]$$

Equivalently,

$$\Pr[X \geq \alpha \cdot \mathbb{E}[X]] \leq \frac{1}{\alpha}.$$

Proof:

$$\mathbb{E}[X] = \sum_{s \in S} \Pr[X=s] \cdot s$$

$$= \sum_{s < t} \Pr[X=s] \cdot s + \sum_{s \geq t} \Pr[X=s] \cdot s$$

$$\geq 0 + t \cdot \sum_{s \geq t} \Pr[X=s]$$

$$= t \cdot \Pr[X \geq t]$$

APPLICATION TO CAPTCHA PROBLEM

Suppose you take $m = 1000$ queries and see 10 duplicates. How does this compare to the expectation if the database actually has $n = 1,000,000$ unique CAPTCHAs?

$$\underline{\mathbb{E}[D]} = \frac{m(m-1)}{2n} = \underline{.4995.}$$

By Markov's:

$$\Pr[\underline{D} \geq 10] \leq \frac{\mathbb{E}[D]}{10} < .05 \text{ if } n \text{ actually equals 1 million.}$$

4.1/20

We can be pretty sure we're being scammed...

n = number of CAPTCHAS in database, m = number of test queries.

Alternative view: If $\mathbb{E}[D] = \frac{m(m-1)}{2n}$, then a natural estimator for n is:

$$\tilde{n} = \frac{m(m-1)}{2D}.$$

With a little more work it is possible to show the following:

Claim: If $m = \Omega\left(\frac{\sqrt{n}}{\epsilon}\right)$ queries, then with probability 9/10, $(1 - \epsilon)n \leq \tilde{n} \leq (1 + \epsilon)n$. This is a two-sided **multiplicative** error guarantee.

This is a lot better than our original method that required $O(n)$ queries!

MARK AND RECAPTCHA

Fun facts:

- Known as the “mark-and-recapture” method in ecology.
- Can also be used by webcrawlers to estimate the size of the internet, a social network, etc.



This is also closely related to the birthday paradox.

Linearity of Expectation + Markov's Inequality



Primitive but powerful toolkit, which can be applied to a wide variety of applications!

THE FREQUENT ITEMS PROBLEM

k -Frequent Items (Heavy-Hitters) Problem: Consider a stream of n items x_1, \dots, x_n with duplicates. Assume there are $u \leq n$ unique items in the stream. Return any item that appears at least $\frac{n}{k}$ times.

x_1 , x_2 , x_3 , x_4 , \dots ~~x_n~~
 v_{10} , v_{10} , v_2 , v_5 , \dots

- Finding top/viral items (i.e., products on Amazon, videos watched on Youtube, Google searches, etc.)
- Finding very frequent IP addresses sending requests (to detect DoS attacks/network anomalies).
- ‘Iceberg queries’ for all items in a database with frequency above some threshold.

Want very fast detection, without having to scan through database/logs. I.e., want to maintain a running list of frequent items that appear in a stream of data items.

THE FREQUENT ITEMS PROBLEM

k -Frequent Items (Heavy-Hitters) Problem: Consider a stream of n items x_1, \dots, x_n with duplicates. Assume there are $u \leq n$ unique items in the stream. Return any item that appears at least $\frac{n}{k}$ times.

v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9
5	12	3	3	4	5	5	10	3

- Trivial with $O(u)$ space – store the count for each item and return the one that appears $\geq n/k$ times.
- Can we do it with less space? I.e., without storing counts for all items?
- What is the maximum number of items that must be returned?

a) u b) k c) n/k d) u/k

$\sim O(u)$

FREQUENT SUBSET MINING

Association rule learning: A very common task in data mining is to identify common associations between different events.



- Identified via **frequent subset** counting. Find all sets of k items that appear many times in the same basket.
- A single basket includes many different subsets, and with many different baskets an efficient approach is critical. E.g., baskets are Twitter users and subsets are subsets of who they follow.

Issue: No algorithm using $o(u)$ space can output just the items with frequency $\geq n/k$.

Intuition: Hard to tell between an item with frequency n/k (should be output) and $n/k - 1$ (should not be output).

(ϵ, k) -Frequent Items Problem: Consider a stream of n items x_1, \dots, x_n . Return a set F of items, including all items that appear at least $\frac{n}{k}$ times and only items that appear at least $(1 - \epsilon) \cdot \frac{n}{k}$ times.

- For items with frequencies in $[(1 - \epsilon) \cdot \frac{n}{k}, \frac{n}{k}]$ no output guarantee.

Today: Count-min Sketch – a random hashing based method for the frequent elements problem.

Due to a 2005 paper by Graham Cormode and Muthu Muthukrishnan.

RANDOM HASH FUNCTION

Let h be a random function from $|\mathcal{U}| \rightarrow \{1, \dots, m\}$. This means that h is constructed by an algorithm using a seed of random numbers, but then the function is fixed. Given input $x \in \mathcal{U}$, it always returns the same output, $h(x)$.

Definition: Uniformly Random Hash Function. A random function $h : \mathcal{U} \rightarrow \{1, \dots, m\}$ is called uniformly random if:

- $\Pr[h(\underline{x}) = i] = \frac{1}{m}$ for all $x \in \mathcal{U}, i \in \{1, \dots, m\}$.
- $h(x)$ and $h(y)$ are independent r.v.'s for all $x, y \in \mathcal{U}$.
 - Which implies that $\Pr[h(\underline{x}) = h(y)] = \frac{1}{m}$.

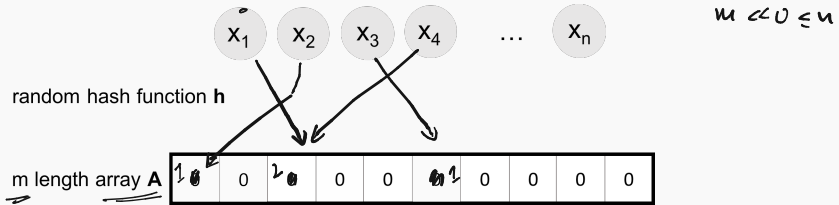
\mathcal{U} = universe of possible keys, m = number of values hashed to.

Caveat: It is not possible to efficiently implement uniform random hash functions! But:

- In practice “random looking” functions like MD5, SHA256, etc. often suffice.
- If we have time, we will discuss weaker hash functions (in particular, universal functions) which suffice for our application, and are efficient to implement.

For now, **assume** we have access to a uniformly random hash function. This is an assumption we will use in future lectures as well.

COUNT-MIN SKETCH



Count-Min Update:

- Choose random hash function h mapping to $\{1, \dots, m\}$.
- For $i = 1, \dots, n$
 - Given item x_i , set $A[h(x_i)] = A[h(x_i)] + 1$

h : random hash function. m : size of Count-Min sketch array.

COUNT-MIN SKETCH

From small space “sketch” \mathbf{A} , we can estimate the frequency of any item v , $f(v) = \sum_{i=1}^n \mathbb{1}[x_i = v]$.

In particular, we simply return $A[h(v)]$.



Claim 1: We always have $A[h(v)] \geq f(v)$. Why?

$$A(h(v)) = f(v) + \underbrace{\sum_{y \neq v} f(y) \mathbb{1}[h(y) = h(v)]}_{\geq 0}$$

$f(v)$: frequency of v in the stream. h : random hash function. m : size of Count-Min sketch array.

COUNT-MIN SKETCH ACCURACY

m = size of array

$$A[h(v)] = f(v) + \underbrace{\sum_{y \neq v} \mathbb{1}[h(y) = h(v)] \cdot f(y)}_{\text{error in frequency estimate}}$$

Expected Error:

$$\begin{aligned} \mathbb{E} \left[\sum_{y \neq v} \mathbb{1}[h(y) = h(v)] \cdot \underline{f(y)} \right] &= \sum_{y \neq v} f(y) \underbrace{\mathbb{E}[\mathbb{1}[h(y) = h(v)]]}_{1/m} \\ &= \frac{1}{m} \sum_{y \neq v} f(y) \\ &\leq \frac{1}{m} \end{aligned}$$

COUNT-MIN SKETCH ACCURACY

$$m = \frac{n}{k}$$

$$A[h(v)] = f(v) + \underbrace{\sum_{y \neq v} \mathbb{1}[h(y) = h(v)] \cdot f(y)}_{\text{error in frequency estimate}}$$

$$\frac{n}{k}$$

Expected Error:

$$\mathbb{E} \left[\sum_{y \neq v} \mathbb{1}[h(y) = h(v)] \cdot f(y) \right] \leq \frac{n}{m}$$

What is a bound on probability that the error is $\geq \frac{2n}{m}$?

Markov's inequality: $\Pr \left[\sum_{y \neq x: h(y)=h(x)} f(y) \geq \frac{2n}{m} \right] \leq \frac{1}{2}$

$f(v)$: frequency of v in the stream. h : random hash function. m : size of Count-Min sketch array.

COUNT-MIN SKETCH ACCURACY

m length array **A**

4	2	1	6	20	1	3	41	8	2
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Claim: For any v , with probability at least $1/2$,

$$f(v) \leq \underline{\underline{A[h(v)]}} \leq f(v) + \frac{2n}{m}.$$

$\nearrow \frac{2n}{m}$

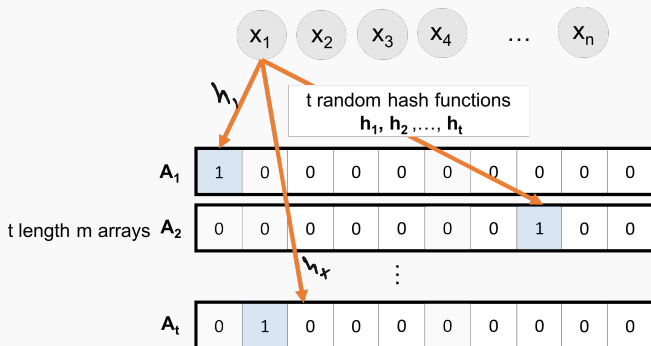
To solve the (ϵ, k) -Frequent elements problem, set $m = \frac{2k}{\epsilon}$.

How can we improve the success probability?

Repetition.

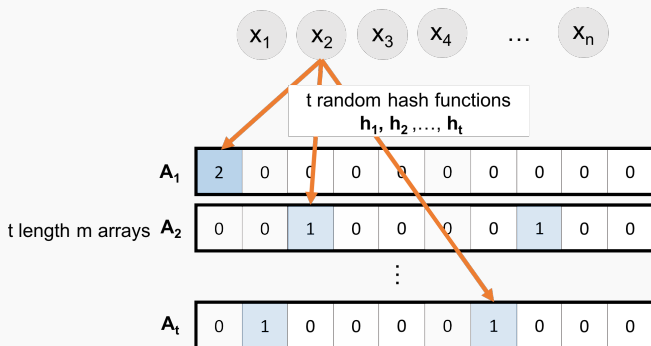
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COUNT-MIN SKETCH ACCURACY



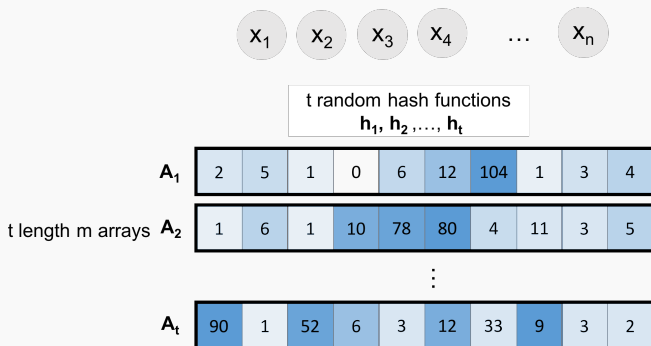
$f(v)$: frequency of v in the stream. h_1, \dots, h_t : multiple random hash functions. m : size of t Count-Min sketch arrays.

COUNT-MIN SKETCH ACCURACY



$f(v)$: frequency of v in the stream. h_1, \dots, h_t : multiple random hash functions. m : size of t Count-Min sketch arrays.

COUNT-MIN SKETCH ACCURACY



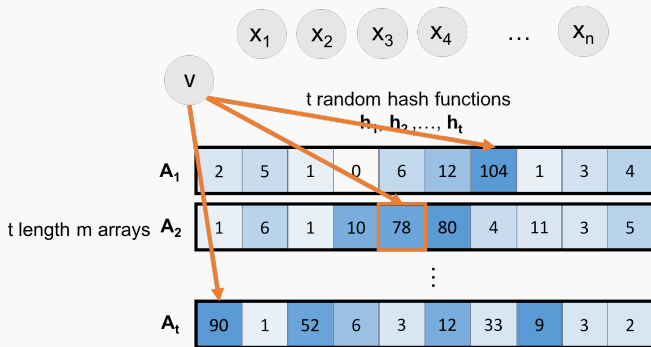
$$A_1(h_1(v)) \approx f(v)$$

$$A_2(h_2(v)) \approx f(v)$$

$$A_t(h_t(v)) \approx f(v)$$

$f(v)$: frequency of v in the stream. h_1, \dots, h_t : multiple random hash functions. m : size of t Count-Min sketch arrays.

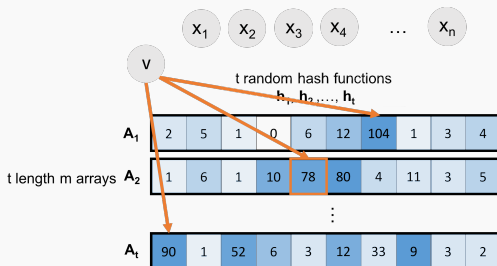
COUNT-MIN SKETCH ACCURACY



Estimate $f(v)$ with $\tilde{f}(v) = \min_{i \in [t]} \underline{A_i[h_i(v)]}$. (Count-min sketch)

Why min instead of mean or median?

COUNT-MIN SKETCH ACCURACY



$\log(1/\delta)$

Estimate $f(v)$ with $\tilde{f}(v) = \min_{i \in [t]} A_i[h_i(v)]$.

- For every v and i and $m = \frac{2k}{\epsilon}$, we know that with prob. $\geq \underline{1/2}$:

$$f(v) \leq A_i[h_i(v)] \leq f(v) + \frac{\epsilon n}{k}.$$

- $\Pr[f(x) \leq \tilde{f}(x) \leq f(x) + \frac{\epsilon n}{k}] \geq 1 - \frac{1}{2^t}$
- To get a good estimate with probability $\geq 1 - \delta$,

$$\text{set } t = \log(1/\delta)$$

Upshot: Count-min sketch lets us estimate the frequency of each item in a stream up to error $\frac{\epsilon n}{k}$ with probability $\geq 1 - \delta$ in $O(\log(1/\delta) \cdot k/\epsilon)$ space.

- Accurate enough to solve the (ϵ, k) -Frequent elements problem – distinguish between items with frequency $\frac{n}{k}$ and those with frequency $(1 - \epsilon)\frac{n}{k}$.

IDENTIFYING FREQUENT ITEMS

Count-min sketch gives an accurate frequency estimate for each item in the stream. But how do we identify the frequent items without having to store/look up the estimated frequency for all elements in the stream?

One approach:

- When a new item comes in at step i , check if its estimated frequency is $\geq i/k$ and store it if so.
- At step i remove any stored items whose estimated frequency drops below i/k .
- Store at most $O(k)$ items at once and have all items with frequency $\geq n/k$ stored at the end of the stream.

NOTE ON RANDOM HASH FUNCTIONS

Can we weaken our assumption that h is uniformly random?

Definition (~~hash~~ universal hash function)

A random hash function $h : \mathcal{U} \rightarrow \{1, \dots, m\}$ is universal if, for any fixed $x, y \in \mathcal{U}$,

$$\Pr[h(\underline{x}) = h(\underline{y})] \leq \frac{1}{m}. \quad = 1/n$$

Claim: A uniformly random hash-function is universal.

Efficient alternative: Let p be a prime number between $|\mathcal{U}|$ and $2|\mathcal{U}|$. Let a, b be random numbers in $0, \dots, p$, $a \neq 0$.

$$h(x) = \underline{[a \cdot \underline{x} + \underline{b} \pmod{p}]} \pmod{m}$$

is universal. Lecture notes with proof posted on website.

Another definition you might come across:

Definition (Pairwise independent hash function)

A random hash function $h : \mathcal{U} \rightarrow \{1, \dots, m\}$ is pairwise independent if, for any fixed $x, y \in \mathcal{U}, i, j \in \{1, \dots, m\}$,

$$\Pr[h(x) = i \cap h(y) = j] = \frac{1}{m^2}. \quad \frac{1}{m^k}$$

Can we naturally extended to k -wise independence for $k > 2$, which is strictly stronger, and needed for some applications.