COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor
Lecture 25
This Class:

- Course wrap up.
PART III: OPTIMIZATION
• Foundational concepts like convexity (line between any two points on curve is above the curve), convex sets (line between any two points in set in the set), directional derivative (slope of curve if we move in particular direction), and Lipschitzness (slope is bounded).
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• Gradient descent greedily tries to find the min value of function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ by maintaining a vector $\vec{\theta} \in \mathbb{R}^d$ and at each step moving $\vec{\theta}$ “downhill”, i.e., in the direction that minimizes directional derivative.
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• Bounded the number of steps required if $f$ is convex and Lipschitz.
CONTINUOUS OPTIMIZATION

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• Simple extension for optimization over a convex constraint set.
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Bounded the number of steps required if $f$ is convex and Lipschitz.

Simple extension for optimization over a convex constraint set.

Lots that we didn’t cover: accelerated methods, adaptive methods, second order methods (quasi-Newton methods). Gave mathematical tools to understand these methods. See CS 690OP for more!
**Goal:** Find $\hat{\theta} \in \mathbb{R}^d$ that (nearly) minimizes convex function $f : \mathbb{R}^d \to \mathbb{R}$. 

**Algorithm/Analysis:** We analyzed the update step:

$$\hat{\theta}(i+1) = \hat{\theta}(i) - \eta \cdot \nabla f(\hat{\theta}(i))$$

and showed that after a certain number of steps depending on $\epsilon$, the max gradient of $f$, and how far the initial point is from the optimal point, $\hat{\theta} = \arg \min_{\theta} f(\theta)$ ensures $f(\hat{\theta}) \leq \min_{\theta} f(\theta) + \epsilon$.

**Projected Gradient Descent:** If we want to find $\hat{\theta} \in S$ that (nearly) minimizes convex function $f$ for some convex set $S$, we just modify the update rule to

$$\hat{\theta}(i+1) = P_S(\hat{\theta}(i) - \eta \cdot \nabla f(\hat{\theta}(i)))$$

where $P_S$ is the projection function that maps the input to the closest point in $S$. 


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$$\hat{\theta} = \arg \min_{\vec{\theta}_1, \ldots, \vec{\theta}_t} f(\vec{\theta}_i)$$

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**Goal:** Back to finding $\vec{\theta} \in \mathbb{R}^d$ that (nearly) minimizes convex function $f : \mathbb{R}^d \to \mathbb{R}$. 

**Idea for Stochastic Gradient Descent:**

Instead of computing $\vec{\nabla} f (\vec{\theta}(i))$ in the update step:

$$\vec{\theta}(i+1) = \vec{\theta}(i) - \eta \cdot \vec{\nabla} f (\vec{\theta}(i))$$

we do something randomized:

$$\vec{\theta}(i+1) = \vec{\theta}(i) - \eta \cdot D(\vec{\theta}(i))$$

where $D(\vec{\theta}(i))$ is faster to compute and approximates $\vec{\nabla} f (\vec{\theta}(i))$ in expectation.

This may increase the number of iterations but each iteration may be much cheaper depending on $f$ and how we generate $D$. 

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Online Optimization: In place of a single function $f$, we see a different objective function at each step: $f_1, f_2, \ldots, f_t : \mathbb{R}^d \rightarrow \mathbb{R}$ where we make no assumptions on how the functions are related to each other.
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- At each step, first pick (play) a parameter vector $\theta^{(i)}$. 

$$\text{Regret} = \sum_{i=1}^{t} f_i(\theta^{(i)}) - \sum_{i=1}^{t} f_i(\theta^{\text{off}})$$

where $\theta^{\text{off}} = \arg\min_{\theta} \sum_{i=1}^{t} f_i(\theta)$.
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- At each step, first pick (play) a parameter vector $\vec{\theta}(i)$.
- Then are told $f_i$ and incur cost $f_i(\vec{\theta}(i))$.
- Minimize “Regret” $= \sum_{i=1}^{t} f_i(\vec{\theta}(i)) - \sum_{i=1}^{t} f_i(\vec{\theta}^{off})$ where

$$\vec{\theta}^{off} = \arg\min_{\vec{\theta}} \sum_{i=1}^{t} f_i(\vec{\theta})$$
**Online Optimization**

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**Algorithm/Analysis:** We analyzed the update step:

$$\vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \cdot \nabla f_i(\vec{\theta}^{(i)})$$

and showed that $\frac{\text{Regret}}{t} \rightarrow 0$ as $t \rightarrow \infty$
EXAMPLE OF GRADIENTS

• Suppose $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ where $f(\bar{\theta}) = \theta_1^3 + \theta_2 \theta_3 + \theta_3^2$ then
• Suppose $f : \mathbb{R}^3 \to \mathbb{R}$ where $f(\vec{\theta}) = \theta_1^3 + \theta_2 \theta_3 + \theta_3^2$ then

$$\nabla f(\vec{\theta}) = \begin{pmatrix} 3\theta_1^2 \\ \theta_3 \\ \theta_2 + 2\theta_3 \end{pmatrix}$$

and

$$\|\nabla f(\vec{\theta})\|_2 = \sqrt{(3\theta_1^2)^2 + (\theta_3)^2 + (\theta_2 + 2\theta_3)^2}$$
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\[
\nabla f(\vec{\theta}) = \begin{pmatrix}
3\theta_2^2 \\
\theta_1 \\
\theta_3 \\
\theta_2 + 2\theta_3
\end{pmatrix}
\]

and

\[
\|\nabla f(\vec{\theta})\|_2 = \sqrt{(3\theta_2^2)^2 + (\theta_3)^2 + (\theta_2 + 2\theta_3)^2}
\]

• Suppose \( f : \mathbb{R}^3 \rightarrow \mathbb{R} \) where \( f(\vec{\theta}) = 3\theta_1 + \theta_2 + 5\theta_3 \) then

\[
\nabla f(\vec{\theta}) = \begin{pmatrix}
3 \\
1 \\
5
\end{pmatrix}
\]

and \( \|\nabla f(\vec{\theta})\|_2 = \sqrt{3^2 + 1^2 + 5^2} \).
PART II: LINEAR ALGEBRA
Methods for working with (compressing) high-dimensional data
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- Started with randomized dimensionality reduction and the JL lemma: compression from *any* d-dimensions to $O(\log n/\epsilon^2)$ dimensions while preserving pairwise distances.
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• Dimensionality reduction via low-rank approximation and optimal solution with PCA/eigendecomposition/SVD.
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• Spectral graph theory – nonlinear dimension reduction and spectral clustering for community detection.
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- Started with randomized dimensionality reduction and the JL lemma: compression from any d-dimensions to $O(\log n/\epsilon^2)$ dimensions while preserving pairwise distances.
- Dimensionality reduction via low-rank approximation and optimal solution with PCA/eigendecomposition/SVD.
- Spectral graph theory – nonlinear dimension reduction and spectral clustering for community detection.
- In the process covered linear algebraic tools that are very broadly useful in ML and data science: eigendecomposition, singular value decomposition.
• Let $\vec{\pi} \in \mathbb{R}^d$ have random $\mathcal{N}(0, 1)$ entries. Then for any $\vec{x} \in \mathbb{R}^d$,

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Proof just uses linearity of expectation and variance.

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Proof just uses linearity of expectation and variance.

• Let $\Pi \in \mathbb{R}^{k \times d}$ where $k = O(\epsilon^{-2} \log n)$ with $\mathcal{N}(0, 1/k)$ entries, then for any $\vec{x} \in \mathbb{R}^d$,

$$(1 - \epsilon)\|\vec{x}\|_2^2 \leq \|\Pi \vec{x}\|_2^2 \leq (1 + \epsilon)\|\vec{x}\|_2^2$$
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$$(1 - \epsilon)\|\vec{x}\|_2^2 \leq \|\Pi \vec{x}\|_2^2 \leq (1 + \epsilon)\|\vec{x}\|_2^2$$

• Furthermore, for any $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n \in \mathbb{R}^d$,

$$(1 - \epsilon)\|\vec{x}_i - \vec{x}_j\|_2^2 \leq \|\Pi \vec{x}_i - \Pi \vec{x}_j\|_2^2 \leq (1 + \epsilon)\|\vec{x}_i - \vec{x}_j\|_2^2$$

i.e., random projections preserve distances between vectors.
The $\mathcal{V}$ be the $k$-dimension subspace of $\mathbb{R}^d$ and let $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix whose columns are an orthonormal basis for $\mathcal{V}$. Then,

$$\mathbf{VV}^T \tilde{x} = \arg \min_{\tilde{z} \in \mathcal{V}} \| \tilde{z} - \bar{x} \|_2$$
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• If we have $n$ points (rows of $\mathbf{X} \in \mathbb{R}^{n \times d}$), and want to project them all into a $k$-dimensional space $\mathcal{V}$, how to we chose $\mathcal{V}$ to minimizes the total error?

Best $\mathcal{V}$ is the one spanned by top $k$ eigenvectors of $\mathbf{X}^T \mathbf{X}$
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i.e., if $\mathbf{V}_k$ is the matrix with the first $k$ eigenvectors as columns,

$$\mathbf{V}_k = \arg \min_{\text{orthonormal } \mathbf{V}} \| \mathbf{X} - \mathbf{X} \mathbf{V} \mathbf{V}^T \|_F$$

and $\| \mathbf{X} - \mathbf{X} \mathbf{V}_k \mathbf{V}^T \|_F = \lambda_{k+1} + \lambda_{k+2} + \ldots$ where $\lambda_1 \geq \lambda_2 \geq \ldots$ are the eigenvalues of $\mathbf{X}^T \mathbf{X}$. 
**Power Method**: The most fundamental iterative method for approximate SVD/eigendecomposition.
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• **Goal:** Given a matrix $A \in \mathbb{R}^{d \times d}$, find an approximation to the top eigenvector $\vec{v}_1$ of $A$. 

Algorithm:

1. Choose $\vec{z}(0)$ randomly: each $\vec{z}(0)(i) \sim N(0, 1)$.
2. For $i = 1, \ldots, t$:
   - $\vec{z}(i) := A \cdot \vec{z}(i-1)$
   - $\vec{z}_i := \vec{z}(i) / \| \vec{z}(i) \|_2$
3. Return $\vec{z}_t$.

With high probability, after $t = O(\gamma^{-1} \ln(d/\epsilon))$ steps, $\| \vec{z}(t) - \vec{v}_1 \|_2 \leq \epsilon$ where $\gamma = 1 - |\lambda_2| / |\lambda_1|$. 

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• With high probability, after \( t = O(\gamma^{-1} \ln(d/\epsilon)) \) steps \( ||\vec{z}^{(t)} - \vec{v}_1||_2 \leq \epsilon \)
  where \( \gamma = 1 - |\lambda_2|/||\lambda_1|| \).
• Any symmetric matrix $A$ can be written as $V\Lambda V^T$ corresponding to eigenvectors and eigenvectors.
• The Singular Value Decomposition (SVD) extends eigendecomposition to arbitrary matrices.
• Any $X \in \mathbb{R}^{n \times d}$ with rank($X$) = $r$ can be written as $X = U\Sigma V^T$.
  • $U$ has orthonormal columns $\vec{u}_1, \ldots, \vec{u}_r \in \mathbb{R}^n$ (left singular vectors).
  • $V$ has orthonormal columns $\vec{v}_1, \ldots, \vec{v}_r \in \mathbb{R}^d$ (right singular vectors).
  • $\Sigma$ is diagonal with elements $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$ (singular values).

• Eigen-decomposition of $X^TX$ is $V\Sigma^2V^T$
• Let $U_k, \Sigma_k, V_k$ be truncations of $U, \Sigma, V$ to first $k$ columns. The best rank $k$ approximation of $X$ is $XV_k V_k^T = U_k U_k^T X = U_k \Sigma_k V_k^T$. 

Applications include: Approximating an "incomplete" matrix $X$ by a low rank in the hope that the approximation "fills in" the missing values. LSA uses the rows of $U$ to approximate the documents in the document/term matrix.

Applications to graphs: Given adjacency matrix $A$, projecting nodes on the top $k$ eigenvalues of $A^T A$ allows us to map nodes to $k$-dimensional space such that close nodes are still close.

Spectral Clustering: Laplacian $L = D - A$ satisfies $\vec{v}^T L \vec{v} = \sum_{ij \in E} (v_i - v_j)^2$. The 2nd smallest eigenvector of $L$ gives way to decompose the graph into roughly balanced groups such that the number of cross edges is minimized: put all nodes with negative entries in one group and all nodes with positive entries in the other.
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**APPLICATIONS**

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- **Applications include:** Approximating an “incomplete” matrix $X$ by a low rank in the hope that the approximation “fills in” the missing values. LSA uses the rows of $U$ to approximate the documents in the a document/term matrix.

- **Applications to graphs:** Given adjacency matrix $A$ projecting nodes on the top $k$ eigenvalues of $A^TA$ allows us to map nodes to $k$-dimensional space such that close nodes are still close.

- **Spectral Clustering** Laplacian $L = D - A$ satisfies $\vec{v}^TL\vec{v} = \sum_{ij \in E}(v_i - v_j)^2$. The 2nd smallest eigenvector of $L$ gives way to decompose the graph into roughly balanced groups such that the number of cross edges in minimized: put all nodes with negative entries in one group and all nodes with positive entires in the other.
Stochastic Block Model is a generative model for generating graphs we could cluster: $n$ nodes are partitioned into two groups $A$ and $B$, edges between nodes in the same group are present with probability $p$ and edges between nodes in different groups are present with probability $q < p$.

We showed the second smallest eigenvector of $E[L]$ allows us to find $A$ and $B$ exactly. But the input to Spectral Clustering is $L$, not $E[L]$!

Fortunately, we could show the 2nd smallest eigenvectors of $L$ and $E[L]$ are sufficiently similar that we learn $A$ and $B$ with only a few mistakes.
• Stochastic Block Model is a **generative model** for generating graphs we could cluster: \( n \) nodes are partitioned into two groups \( A \) and \( B \), edges between nodes in same group are present with probability \( p \) and edges between nodes in different groups are present with probability \( q < p \).
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• Fortunately, we could show the 2nd smallest eigenvectors of $L$ and $\mathbb{E}[L]$ are sufficiently similar that we learn $A$ and $B$ we only a few mistakes.
PART I: RANDOMIZED TECHNIQUES
Randomization as a computational resource for massive datasets.
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- Focus on problems that are easy on small datasets but hard at massive scale – set size estimation, load balancing, distinct elements counting (MinHash), checking set membership (Bloom Filters), frequent items counting (Count-min sketch), near neighbor search (locality sensitive hashing).
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• Just the tip of the iceberg on randomized streaming/sketching/hashing algorithms.

• In the process covered probability/statistics tools that are very useful beyond algorithm design: concentration inequalities, higher moment bounds, law of large numbers, central limit theorem, linearity of expectation and variance, union bound, median as a robust estimator.
• **Linearity of Expectation**: For any random variables $X_1, \ldots, X_n$ and constants $c_1, \ldots, c_n,$

\[
\mathbb{E}[c_1 X_1 + \ldots + c_n X_n] = c_1 \mathbb{E}[X_1] + \ldots + c_n \mathbb{E}[X_n]
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• **Independent Random Variables:** $X_1, X_2, \ldots X_n$ are independent random variables if for any set $S \subset [n]$ and values $a_1, a_2, \ldots, a_n$

$$\Pr(X_i = a_i \text{ for all } i \in S) = \prod_{i \in S} \Pr(X_i = a_i) .$$

They are **$k$-wise independent** if this holds for $S$ with $|S| \leq k$. 
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• **Linearity of Variance:** If $X_1, \ldots, X_n$ are independent (in fact 2-wise independent suffices) then for any constants $c_1, \ldots, c_n$

$$\text{Var}[c_1 X_1 + \ldots + c_n X_n] = c_1^2 \text{Var}[X_1] + \ldots + c_n^2 \text{Var}[X_n]$$
• **Union Bound**: For any events $A_1, A_2, A_3, \ldots$

$$\Pr \left[ \bigcup A_i \right] \leq \sum_i \Pr[A_i] .$$

• An indicator random variable $X$ just takes the values 0 or 1:

$$\mathbb{E}[X] = p \quad \text{Var}[X] = p(1 - p) \quad \text{where } p = \Pr[X = 1]$$

• If $Y = X_1 + \ldots + X_n$ where each $X_i$ are independent and $p = \Pr[X_1 = 1] = \ldots = \Pr[X_n = 1]$ then $Y$ is a binomial random variable. Using linearity of expectation and variance,

$$\mathbb{E}[X] = np \quad \text{Var}[X] = np(1 - p)$$
Most of the analysis of hash functions that we’ve considered can be abstracted as “balls and bins” problems: we throw $n$ balls and each ball is equally likely to land in one of $m$ bins.

Let $R_i$ be the number of balls in bin $i$. Then $R_i \sim \text{Bin}(n, \frac{1}{m})$ and $\mathbb{E}[R_i] = \frac{n}{m}$, $\text{Var}[R_i] = \frac{n}{m} \cdot \left(1 - \frac{1}{m}\right)$. $R_i$ and $R_j$ are not independent!

Union Bound implies $\Pr[\max(R_1, \ldots, R_m) > t] \leq \sum_i \Pr[R_i > t]$

$\Pr[\text{no collisions}] = \frac{m-1}{m} \cdot \frac{m-2}{m} \cdot \ldots \cdot \frac{m-(n-1)}{m}$

$\Pr[\text{collisions}] = \Pr[\max(R_1, \ldots, R_m) > 1] \leq 1/8$ if $m > 4n^2$

and more generally

$\Pr[\max(R_1, \ldots, R_m) \geq 2n/m] \leq m^2/n$

In the exam, you’ll be expected to do calculations like these.
• Hash function $h : U \rightarrow [n]$ is **two universal** if:

$$\Pr[h(x) = h(y)] \leq \frac{1}{n}.$$
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• Hash function $h : U \rightarrow [n]$ is fully independent if $\{h(e)\}_{e \in U}$ are independent and each $h(e)$ is uniform in $[n]$. 
• **Markov.** For any non-negative random variable \( X \) and \( t > 0 \),

\[
\Pr[X \geq t] \leq \frac{\mathbb{E}[X]}{t}.
\]
THREE MAIN CONCENTRATION BOUNDS

- **Markov.** For any non-negative random variable $X$ and $t > 0$,
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- **Chebyshev.** For any random variable $X$ and $t > 0$,
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  \Pr[|X - \mathbb{E}[X]| \geq t] \leq \frac{\text{Var}[X]}{t^2}.
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• **Chernoff.** Let $X_1, \ldots, X_n$ be independent $\{0, 1\}$ random variables with $\mu = \mathbb{E}[\sum_i X_i]$. Then for any $\delta > 0$,

$$\Pr[|\left(\sum_i X_i\right) - \mu| \geq \delta \mu] \leq 2 \exp \left(-\frac{\delta^2 \mu}{\delta + 2}\right).$$
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• Generally, Chernoff gives better results then Chebyshev and Chebyshev gives better results than Markov. So choose bound based on how much you know about $X$. 
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• **Bernstein** generalizes Chernoff to arbitrary bounded $X_i$ variables.
Want to learn a quantity $q$. Suppose you have a randomized algorithm that returns $X$ that has expectation $q$ and variance $\sigma^2$.

Median Trick: Let $t = t_1 t_2$ where $t_1 = 4 \sigma^2 \epsilon^2 q^2$ and $t_2 = O(\log(1/\delta))$. Let $A_1$ be the average of the first $t_1$ results, let $A_2$ be the average of the next $t_1$ results etc. Then, $Pr[|A_i - q| \geq \epsilon q] \leq 1/4$ and $Pr[|\text{median}(A_1, \ldots, A_{t_2}) - q| \geq \epsilon q] \leq \delta$. 
AVERAGING AND THE MEDIAN TRICK

- Want to learn a quantity \( q \). Suppose you have a randomized algorithm that returns \( X \) that has expectation \( q \) and variance \( \sigma^2 \).
- To get a good estimate of \( q \), repeat algorithm \( t \) times to get \( X_1, \ldots, X_t \) and let \( A = (X_1 + \ldots + X_t)/t \). Then, if \( t = \frac{\sigma^2}{\delta \epsilon^2 q^2} \)

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2-LEVEL HASH TABLES VS. BLOOM FILTER

• Input to both is a set of items $S$ and and both support queries of the form “$x \in S?$” in constant time.
2-Level Hash Tables vs. Bloom Filter

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  - Space is $O(|S|)$ “space required to store an element of $S$”
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• **Bloom Filter:**
  • Does not actually store the items in $S$, just a binary array from which we make various deductions.
  • Uses only $O(|S|)$ space but at the cost of sometimes answering “yes” when answer should be “no” (a false positive)
  • If the Bloom Filter array is length $m$, false positive probability is roughly $(1 - e^{-k|S|/m})^k$ where $k$ is the number of hash functions used. Picking $k = \ln 2 \cdot m / |S|$ gives probability $1/2 (\ln 2)^m / |S|$.
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• Designed a hash function for hashing sets such that for sets $A$ and $B$, 
$\Pr[MH(A) = MH(B)] = J(A, B) = \frac{|A \cap B|}{|A \cup B|}$.

$$MH(A) = \min_{x \in A} h(x) \text{ where } h : U \rightarrow [0, 1] \text{ is fully independent}$$
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• Can form signature of set $A$ using $r$ independent hash functions:

  $\text{signature}(A) = (MH_1(A), \ldots, MH_r(A))$

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• Given $rt$ independent hash functions, we can form $t$ signatures
\[ \text{signature}_1(A), \ldots, \text{signature}_t(A). \]
Then if $s = J(A, B),$
\[ \Pr[\text{signature}_{i}(A) = \text{signature}_{i}(B) \text{ for some } i] = 1 - (1 - s^r)^t. \]
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• To find all pairs of similar sets amongst $A_1, A_2, A_3, \ldots$ only compare a pair if there exists $i$, their $i$th signatures match.
• We want to compute something about the stream $x_1, x_2, \ldots, x_m$ with only one pass over the stream and limited space.
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  • **Distinct Items**: Can estimate \( D = |\{i : f_i > 0\}| \) up to a factor \( 1 + \epsilon \) with probability \( 1 - \delta \) in \( O(\epsilon^{-2} \log 1/\delta) \) space.
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  - **Frequently Elements Items**: Can return a set $S$ such that:
    
    $$f_i \geq m/k \text{ implies } i \in S \quad \text{and} \quad i \in S \text{ implies } f_i \geq m(1 - \epsilon)/k$$

    with probability $1 - \delta$ in $O(k/\epsilon \cdot \log 1/\delta)$ space.
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with probability \( 1 - \delta \) in \( O(k/\epsilon \cdot \log 1/\delta) \) space.

• **Sum of Squares:** Can estimate \( \sum f_i^2 \) up to a factor \( 1 + \epsilon \) with probability \( 1 - \delta \) in \( O(\epsilon^{-2} \log 1/\delta) \) space. Also investigated estimating \( \sum f_i^k \) for general \( k \).
Thanks for a great semester!