## 2 Announcements

Colab 0/1 Due Today
Due at 11:59 PM
We will also be releasing Colab 2
Due in 1 week (1/20 at 11:59 PM)

Note to other teachers and users of these slides: We would be delighted if you found our material useful for giving your own lectures. Feel free to use these slides verbatim, or to modify them to fit your own needs. If you make use of a significant portion of these slides in your own lecture, please include this message, or a link to our web site: http://www.mmds.org

## Theory of <br> Locality Sensitive Hashing

CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
Mina Ghashami, Amazon
http://cs246.stanford.edu


## Recap: Finding similar documents

- Task: Given a large number ( $\boldsymbol{N}$ in the millions or billions) of documents, find "near duplicates"
- Problem:
- Too many documents to compare all pairs
- Solution: Hash documents so that similar documents hash into the same bucket
- Documents in the same bucket are then candidate pairs whose similarity is then evaluated


## Recap: The Big Picture



## Recap 1: Shingles

- A $k$-shingle (or $k$-gram) is a sequence of $k$ tokens that appears in the document
- Example: $\mathbf{k}=\mathbf{2} ; \mathbf{D}_{\mathbf{1}}=\mathrm{abcab}$

Set of 2-shingles: $C_{1}=S\left(D_{1}\right)=\{a b, b c, c a\}$

- Represent a doc by a set of hash values of its $k$-shingles
- A natural similarity measure is then the Jaccard similarity:

$$
\operatorname{sim}\left(D_{1}, D_{2}\right)=\left|C_{1} \cap C_{2}\right| /\left|C_{1} \cup C_{2}\right|
$$

- Similarity of two documents is the Jaccard similarity of their shingles


## Recap 2: Minhashing

- Min-Hashing: Convert large sets into short signatures, while preserving similarity: $\operatorname{Pr}\left[h\left(\mathrm{C}_{1}\right)=h\left(\mathrm{C}_{2}\right)\right]=\operatorname{sim}\left(\mathrm{D}_{1}, \mathrm{D}_{2}\right)$

Permutation $\pi$

| 2 | 4 | 3 |
| :--- | :--- | :--- | :--- |
| 3 | 2 | 4 |
| 7 | 1 | 7 |
| 6 | 3 | 2 |
| 1 | 6 | 2 |
| 5 | 7 | 1 |
| 4 | 7 | 1 |

Input matrix (Shingles x Documents)

| 1 | 0 | 1 | 0 |
| :--- | :--- | :--- | :--- |
| 1 | 0 | 0 | 1 |
| 0 | 1 | 0 | 1 |
| 0 | 1 | 0 | 1 |
| 0 | 1 | 0 | 1 |
| 1 | 0 | 1 | 0 |
| 1 | 0 | 1 | 0 |

Signature matrix $M$

| 2 | 1 | 2 | 1 |
| :--- | :--- | :--- | :--- |
| 2 | 1 | 4 | 1 |
| 1 | 2 | 1 | 2 |

Similarities of columns and signatures (approx.) match!

|  | $1-3$ | $2-4$ | $1-2$ | $3-4$ |
| :--- | :--- | :--- | :--- | :--- |
| Col/Col | 0.75 | 0.75 | 0 | 0 |

$\begin{array}{lllll}\text { Sig/Sig } & 0.67 & 1.00 & 0 & 0\end{array}$

## Recap 3: LSH

- Hash columns of the signature matrix M: Similar columns likely hash to same bucket
- Divide matrix $M$ into $\boldsymbol{b}$ bands of $\boldsymbol{r}$ rows ( $M=b \cdot r$ )
- Candidate column pairs are those that hash to the same bucket for $\geq 1$ band



## Today: Generalizing Min-hash



# Design a locality sensitive hash function (for a given distance metric) 

Apply the
"Bands" technique

## The S-Curve

## - The S-curve is where the "magic" happens

Similarity $s$ of two sets
This is what 1 hash-code gives you
$\operatorname{Pr}\left[h_{\pi}\left(\mathrm{C}_{1}\right)=h_{\pi}\left(\mathrm{C}_{2}\right)\right]=\operatorname{sim}\left(\mathrm{D}_{1}, \mathrm{D}_{2}\right)$
Similarity $s$ of two sets
This is what we want!
How to get a step-function?
By choosing $r$ and $b$ !

## How Do We Make the S-curve?

- Remember: $\boldsymbol{b}$ bands, $\boldsymbol{r}$ rows/band
- Let $\operatorname{sim}\left(\boldsymbol{C}_{1}, \boldsymbol{C}_{2}\right)=\boldsymbol{s}$

What's the prob. that at least 1 band is equal?

- Pick some band (r rows)
- Prob. that elements in a single row of columns $\mathbf{C}_{1}$ and $\mathbf{C}_{2}$ are equal $=\boldsymbol{s}$
- Prob. that all rows in a band are equal $=s^{r}$
- Prob. that some row in a band is not equal =1-sr
- Prob. that all bands are not equal $=\left(1-s^{r}\right)^{b}$
- Prob. that at least 1 band is equal =1-(1-s $)^{r}$
$P\left(C_{1}, C_{2}\right.$ is a candidate pair $)=1-\left(1-s^{r}\right)^{b}$


## Picking $r$ and $b$ : The S-curve

Picking $r$ and $b$ to get the best S-curve

- 50 hash-functions ( $r=5, b=10$ )



## S-curves as a func. of $b$ and $r$

Given a fixed threshold $\boldsymbol{t}$.

We want choose $\boldsymbol{r}$ and $\boldsymbol{b}$ such that the P(Candidate pair) has a "step" right around $\boldsymbol{t}$.




## Visualizing S-Curves

Visualization of the effect of threshold, band size, and \# of rows in LSH by Trenton Chang (Thank you!!) https://www.desmos.com/calculator/Izzvfiiuin


Candidate pairs: those pairs of signatures that we need to test for similarity

## Theory of LSH

general hashing
locality-sensitive hashing


## Theory of LSH

- We have used LSH to find similar documents
- More generally, we found similar columns in large sparse matrices with high Jaccard similarity
- Can we use LSH for other distance measures?
- e.g., Euclidean distances, Cosine distance
- Let's generalize what we've learned!


## Distance Measures

- d( $)$ is a distance measure if it is a function from pairs of points $\mathbf{x}, \mathbf{y}$ to real numbers such that:
- $d(x, y) \geq 0$
- $d(x, y)=0$ iff $x=y$
- $d(x, y)=d(y, x)$
- $d(x, y) \leq d(x, z)+d(z, y)$ (triangle inequality)
- Jaccard distance for sets = 1 - Jaccard similarity
- Cosine distance for vectors = angle between the vectors
- Euclidean distances:
- $L_{2}$ norm: $\mathrm{d}(\mathrm{x}, \mathrm{y})=$ square root of the sum of the squares of the differences between $x$ and $y$ in each dimension
- The most common notion of "distance"
- $L_{1}$ norm: sum of absolute value of the differences in each dimension
- Manhattan distance = distance if you travel along axes only


## Families of Hash Functions

- A "hash function" is any function that allows us to say whether two elements are "equal"
- Shorthand: $\boldsymbol{h}(x)=\boldsymbol{h}(y)$ means " $h$ says $x$ and $y$ are equal"
- A family of hash functions is any set of hash functions from which we can efficiently pick one at random
- Example: The set of Min-Hash functions generated from permutations of rows


## Locality-Sensitive (LS) Families

- Suppose we have a space $S$ of points with a distance measure $d(x, y)$

Critical assumption
A family $H$ of hash functions is said to be $\left(d_{1}, d_{2}, p_{1}, p_{2}\right)$-sensitive if for any $x$ and $y$ in $S$ :

1. If $\boldsymbol{d}(\boldsymbol{x}, \boldsymbol{y}) \leq \boldsymbol{d}_{\boldsymbol{1}}$, then the probability over all $\boldsymbol{h} \in \boldsymbol{H}$, that $\boldsymbol{h}(x)=\boldsymbol{h}(\boldsymbol{y})$ is at least $p_{1}$
2. If $d(x, y) \geq d_{2}$, then the probability over all $\boldsymbol{h} \in \boldsymbol{H}$, that $\boldsymbol{h}(\boldsymbol{x})=\boldsymbol{h}(\boldsymbol{y})$ is at most $\boldsymbol{p}_{\mathbf{2}}$

## With a LS Family we can do LSH!

## $\mathrm{A}\left(d_{11} d_{21} p_{11} p_{2}\right)$-sensitive function



Distance d(x,y)

## Example of LS Family: Min-Hash

- Let:
- S = space of all sets,
- d = Jaccard distance,
- $\boldsymbol{H}$ is family of Min-Hash functions for all permutations of rows
- Then for any hash function $\boldsymbol{h} \in \boldsymbol{H}$ :

$$
\operatorname{Pr}[h(x)=h(y)]=1-d(x, y)
$$

- Simply restates theorem about Min-Hashing in terms of distances rather than similarities


## Example: LS Family - (2)

- Claim: Min-hash $\boldsymbol{H}$ is a (1/3, 2/3,2/3, 1/3)sensitive family for $\boldsymbol{S}$ and $\boldsymbol{d}$.

If distance $\leq 1 / 3$
(so similarity $\geq 2 / 3$ )

Then probability that Min-Hash values agree is $\geq 2 / 3$

- For Jaccard similarity, Min-Hashing gives a $\left(d_{1}, d_{2},\left(1-d_{1}\right),\left(1-d_{2}\right)\right)$-sensitive family for any $d_{1}<d_{2}$


## Amplifying a LS-Family

- Can we reproduce the "S-curve" effect we saw before for any LS family?

- The "bands" technique we learned for signature matrices carries over to this more general setting
- Can do LSH with any ( $d_{1}, d_{2}, p_{1}, p_{2}$ )-sensitive family!
- Two constructions:
- AND construction like "rows in a band"
- OR construction like "many bands"

Amplifying Hash Functions: AND and OR

## AND of Hash Functions

- Given family $\boldsymbol{H}$, construct family $\boldsymbol{H}^{\prime}$ consisting of $r$ functions from $\boldsymbol{H}$
- For $\boldsymbol{h}=\left[\boldsymbol{h}_{1}, \ldots, \boldsymbol{h}_{r}\right]$ in $\mathbf{H}^{\prime}$, we say $h(x)=h(y)$ if and only if $h_{i}(x)=h_{i}(y)$ for all $\boldsymbol{i}_{1 \leq i \leq r}$
- Note this corresponds to creating a band of size $\mathbf{r}$
- Theorem: If $\boldsymbol{H}$ is $\left(d_{1}, d_{2}, p_{1}, p_{2}\right)$-sensitive, then $\mathbf{H}^{\prime}$ is $\left(d_{1}, d_{2},\left(p_{1}\right)^{r},\left(p_{2}\right)^{r}\right)$-sensitive
- Proof: Use the fact that $\bar{h}_{i}^{\prime}$ 's are independent

Also lowers probability
for small distances (Bad)

Lowers probability for
large distances (Good)

## Subtlety Regarding Independence

- Independence of hash functions (HFs) really means that the prob. of two HFs saying "yes" is the product of each saying "yes"
- But two particular hash functions could be highly correlated
- For example, in Min-Hash if their permutations agree in the first one million entries
- However, the probabilities in definition of a LSH-family are over all possible members of $\boldsymbol{H}, \boldsymbol{H}^{\prime}$ (i.e., average case and not the worst case)


## OR of Hash Functions

- Given family $\boldsymbol{H}$, construct family $\boldsymbol{H}^{\prime}$ consisting of $\boldsymbol{b}$ functions from $\boldsymbol{H}$
- For $\boldsymbol{h}=\left[\boldsymbol{h}_{1}, \ldots, \boldsymbol{h}_{b}\right]$ in $\boldsymbol{H}^{\prime}$, $h(x)=h(y)$ if and only if $h_{i}(x)=h_{i}(y)$ for at least $1 \boldsymbol{i}$
- Theorem: If $\boldsymbol{H}$ is $\left(d_{1}, d_{2}, p_{1}, p_{2}\right)$-sensitive, then $H^{\prime}$ is $\left.\left.\left.\left(d_{1}, d_{2}, \mathbf{1 - ( 1 - p}\right)_{1}\right)^{b}, \mathbf{1 - ( 1 - p}\right)^{b}\right)$-sensitive
- Proof: Use the fact that $h_{i}$ 's are îhdependent

Raises probability for
small distances (Good)

Raises probability for
large distances (Bad)

## Effect of AND and OR Constructions

- AND makes all probs. shrink, but by choosing $r$ correctly, we can make the lower prob. approach 0 while the higher does not
- OR makes all probs. grow, but by choosing b correctly, we can make the higher prob. approach 1 while the lower does not


Similarity of a pair of items


Similarity of a pair of items

## Combine AND and OR Constructions

- By choosing $\boldsymbol{b}$ and $r$ correctly, we can make the lower probability approach 0 while the higher approaches 1
- As for the signature matrix, we can use the AND construction followed by the OR construction
- Or vice-versa
- Or any sequence of AND's and OR's alternating


## Composing Constructions

- r-way AND followed by b-way OR construction
- Exactly what we did with Min-Hashing
- AND: If bands match in all $r$ values hash to same bucket
- OR: Cols that have $\geq 1$ common bucket $\rightarrow$ Candidate
- Take points $x$ and $y$ s.t. $\operatorname{Pr}[h(x)=h(y)]=s$
- $\boldsymbol{H}$ will make ( $\mathbf{x}, \mathrm{y}$ ) a candidate pair with prob. s
- Construction makes ( $\mathbf{x}, \mathbf{y}$ ) a candidate pair with probability 1-(1-s $\left.s^{r}\right)^{b} \quad$ The S-Curve!
- Example: Take $\mathbf{H}$ and construct $\mathbf{H}^{\prime}$ by the AND construction with $r=4$. Then, from $\mathbf{H}^{\prime}$, construct $\mathbf{H}^{\prime \prime}$ by the OR construction with $b=4$


## Table for Function 1-(1-s $\left.{ }^{4}\right)^{4}$

| $\mathbf{s}$ | $\mathbf{p}=\mathbf{1}-\left(1-\mathbf{s}^{4}\right)^{4}$ |
| :--- | :--- |
| .2 | .0064 |
| .3 | .0320 |
| .4 | .0985 |
| .5 | .2275 |
| .6 | .4260 |
| .7 | .6666 |
| .8 | .8785 |
| .9 | .9860 |


$r=4, b=4$ transforms a
(.2,.8,.8,.2)-sensitive family into a
(.2,.8,.8785,.0064)-sensitive family.

## How to choose $r$ and $b$

## Picking $r$ and $b$ : The S-curve

- Picking $r$ and $b$ to get desired performance
- 50 hash-functions ( $r=5, \boldsymbol{b}=10$ )


Similarity s

Blue area $X$ : False Negative rate These are pairs with sim > $\boldsymbol{t}$ but the $\boldsymbol{X}$ fraction won't share a band and then will never become candidates. This means we will never consider these pairs for (slow/exact) similarity calculation!
Green area Y: False Positive rate These are pairs with sim <t but we will consider them as candidates. This is not too bad, we will consider them for (slow/exact) similarity computation and discard them.

## Picking $r$ and $b$ : The S-curve

- Picking $r$ and $b$ to get desired performance
- 50 hash-functions ( $\boldsymbol{r}^{*} \boldsymbol{b}=50$ )



## OR-AND Composition

- Apply a b-way OR construction followed by an $r$-way AND construction
- Transforms similarity $s$ (probability p) into (1-(1-s)b) ${ }^{r}$
- The same S-curve, mirrored horizontally and vertically
- Example: Take $\mathbf{H}$ and construct $\mathbf{H}^{\prime}$ by the OR construction with $\boldsymbol{b}=4$. Then, from $\mathbf{H}^{\prime}$, construct $\mathbf{H}^{\prime \prime}$ by the AND construction with $r=4$


## Table for Function (1-(1-s) $)^{4}$

| $\mathbf{s}$ | $\mathbf{p}=\left(1-(1-\mathbf{s})^{4}\right)^{4}$ |
| :--- | :--- |
| .1 | .0140 |
| .2 | .1215 |
| .3 | .3334 |
| .4 | .5740 |
| .5 | .7725 |
| .6 | .9015 |
| .7 | .9680 |
| .8 | .9936 |



The example transforms a (.2,.8,.8,.2)-sensitive family into a (.2,.8,.9936,.1215)-sensitive family

## Cascading Constructions

- Example: Apply the (4,4) OR-AND construction followed by the (4,4) AND-OR construction
- Transforms a (.2, .8, .8, .2)-sensitive family into a (.2, .8, .9999996, .0008715)-sensitive family
- Note this family uses 256 ( $=4 * 4 * 4 * 4$ ) of the original hash functions


## General Use of S-Curves

- For each AND-OR S-curve 1-(1-s $\left.{ }^{r}\right)^{b}$, there is a threshold $t$, for which 1-(1- $\left.t^{r}\right)^{b}=t$
- Above $t$, high probabilities are increased; below $t$, low probabilities are decreased
- You improve the sensitivity as long as the low probability is less than $t$, and the high probability is greater than $t$
- Iterate as you like
- Similar observation for the OR-AND type of Scurve: $\left(1-(1-s)^{b}\right)^{r}$


## Visualization of Threshold



## Summary

- Pick any two distances $\boldsymbol{d}_{\mathbf{1}}<\boldsymbol{d}_{\mathbf{2}}$
- Start with a $\left(d_{1}, d_{\mathbf{2}},\left(\mathbf{1}-d_{1}\right),\left(\mathbf{1}-d_{2}\right)\right)$-sensitive family
- Apply constructions to amplify $\left(d_{1}, d_{2}, p_{1}, p_{2}\right)$-sensitive family, where $p_{1}$ is almost 1 and $p_{2}$ is almost 0
- The closer to 0 and 1 we get, the more hash functions must be used!


## LSH for other distance metrics

## LSH for other Distance Metrics

- LSH methods for other distance metrics:
- Cosine distance: Random hyperplanes
- Euclidean distance: Project on lines



## Summary of what we will learn



## LSH for Cosine Distance

## Cosine Distance

- Cosine distance = angle between vectors from the origin to the points in question $\mathrm{d}(\mathrm{A}, \mathrm{B})=\theta=\arccos (\mathbf{A} \cdot \mathbf{B} /\|\mathbf{A}\| \cdot\|\mathrm{B}\|)$
- Has range $[\mathbf{0}, \boldsymbol{\pi}]$ (equivalently $\left[0,180^{\circ}\right]$ ) $\leftarrow \frac{A \cdot B}{\|B\| I}$
$=$ Can divide $\theta$ by $\boldsymbol{\pi}$ to have distance in range $[0,1]$ - Cosine similarity = 1-d(A,B)
- But often defined as cosine sim: $\cos (\theta)=\frac{A \cdot B}{\|A\|\|B\|}$


- Has range -1... 1 for general vectors - Range $0 . .1$ for non-negative vectors (angles up to $90^{\circ}$ )


## LSH for Cosine Distance

- For cosine distance, there is a technique called Random Hyperplanes
- Technique similar to Min-Hashing
- Random Hyperplanes method is a $\left(d_{1}, d_{2},\left(1-d_{1} / \pi\right),\left(1-d_{2} / \pi\right)\right)$-sensitive family for any $\boldsymbol{d}_{1}$ and $\boldsymbol{d}_{\mathbf{2}}$
- Reminder: $\left(d_{1}, d_{2}, p_{1}, p_{2}\right)$-sensitive

1. If $d(x, y) \leq d_{1}$, then prob. that $h(x)=h(y)$ is at least $p_{1}$
2. If $d(x, y) \geq d_{2}$, then prob. that $h(x)=h(y)$ is at most $p_{2}$

## Random Hyperplanes

- Each vector $\boldsymbol{v}$ determines a hash function $\boldsymbol{h}_{\boldsymbol{v}}$ with two buckets
- $h_{v}(x)=+1$ if $v \cdot x \geq 0 ;=-1$ if $v \cdot x<0$
- LS-family $\boldsymbol{H}=$ set of all functions derived from any vector
- Claim: For points $\mathbf{x}$ and $\mathbf{y}$,

$$
\operatorname{Pr}[h(x)=h(y)]=1-d(x, y) / \pi
$$

## Proof of Claim

## Look in the plane of $x$ and $y$.

Hyperplane normal to $\boldsymbol{v}$.
Here $h(x)=h(y)$


Note: what is important is that hyperplane is outside the angle, not that the vector is inside.

## Proof of Claim



## Signatures for Cosine Distance

- Pick some number of random vectors, and hash your data for each vector
- The result is a signature (sketch) of +1's and -1's for each data point
- Can be used for LSH like we used the Min-Hash signatures for Jaccard distance
- Amplify using AND/OR constructions


## How to pick random vectors?

- Expensive to pick a random vector in $\boldsymbol{M}$ dimensions for large $\boldsymbol{M}$
- Would have to generate $\boldsymbol{M}$ random numbers
- A more efficient approach
- It suffices to consider only vectors $\boldsymbol{v}$ consisting of +1 and -1 components
- Why? Assuming data is random, then vectors of +/-1 cover the entire space evenly (and does not bias in any way)


## LSH for Euclidean Distance

## LSH for Euclidean Distance

- Idea: Hash functions correspond to lines
- Partition the line into buckets of size a
- Hash each point to the bucket containing its projection onto the line
"An element of the "Signature" is a bucket id for that given projection line
- Nearby points are always close; distant points are rarely in same bucket


## Projection of Points



## Multiple Projections



# Projection of Points (1) 



Randomly chosen line
Bucket width a

## Projection of Points (2)



## A LS-Family for Euclidean Distance

- If points are distance $d \leq a / \mathbf{2}$, prob. they are in same bucket $\geq 1-d / a=1 / 2$
- If points are distance $\boldsymbol{d} \geq \mathbf{2 a}$ apart, then they can be in the same bucket only if $d \cos \theta \leq \boldsymbol{a}$
- $\cos \theta \leq 1 / 2$
- $60 \leq \theta \leq 90$, i.e., at most $1 / 3$ probability
- Yields a (a/2, 2a, 1/2, 1/3)-sensitive family of hash functions for any $a$
- Amplify using AND-OR cascades


## Summary



Data $\longrightarrow \begin{gathered}\text { Hash } \\ \text { func. }\end{gathered} \xrightarrow{ }$

Design a $\left(d_{11}, d_{21} p_{11}, p_{2}\right)$-sensitive family of hash functions (for that distance metric)

| Locality- <br> sensitive <br> Hashing | Candidate pairs: <br> those pairs of <br> signatures that <br> we need to test <br> for similarity |
| :--- | :--- |

Amplify the family using AND and $O R$


## Two Important Points

- Property $\mathrm{P}\left(\mathrm{h}\left(\mathrm{C}_{1}\right)=\mathrm{h}\left(\mathrm{C}_{2}\right)\right)=\operatorname{sim}\left(\mathrm{C}_{1}, \mathrm{C}_{2}\right)$ of hash function $h$ is the essential part of LSH, without which we can't do anything
- LS-hash functions transform data to signatures so that the bands technique (AND, OR constructions) can then be applied

