# CS60021: Scalable Data Mining 

## Similarity Search and Hashing

## Sourangshu Bhattacharya

## Finding Similar Items

## Distance Measures

- Goal: Find near-neighbors in high-dim. space
- We formally define "near neighbors" as points that are a "small distance" apart
- For each application, we first need to define what "distance" means
- Today: Jaccard distance/similarity
- The Jaccard similarity of two sets is the size of their intersection divided by the size of their union:

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

- Jaccard distance: $d\left(\mathrm{C}_{1}, \mathrm{C}_{2}\right)=1-\left|\mathrm{C}_{1} \cap \mathrm{C}_{2}\right| /\left|\mathrm{C}_{1} \cup \mathrm{C}_{2}\right|$


3 in intersection 8 in union Jaccard similarity= $3 / 8$ Jaccard distance $=5 / 8$

## Task: Finding Similar Documents

- Goal: Given a large number ( $N$ in the millions or billions) of documents, find "near duplicate" pairs
- Applications:
- Mirror websites, or approximate mirrors
- Don't want to show both in search results
- Similar news articles at many news sites
- Cluster articles by "same story"
- Problems:
- Many small pieces of one document can appear out of order in another
- Too many documents to compare all pairs
- Documents are so large or so many that they cannot fit in main memory


## 3 Essential Steps for Similar Docs

1. Shingling: Convert documents to sets
2. Min-Hashing: Convert large sets to short signatures, while preserving similarity
3. Locality-Sensitive Hashing: Focus on pairs of signatures likely to be from similar documents

- Candidate pairs!


## The Big Picture




## Shingling

## Step 1: Shingling: Convert documents to sets

## Documents as High-Dim Data

- Step 1: Shingling: Convert documents to sets
- Simple approaches:
- Document = set of words appearing in document
- Document = set of "important" words
- Don't work well for this application. Why?
- Need to account for ordering of words!
- A different way: Shingles!


## Define: Shingles

- A $k$-shingle (or $k$-gram) for a document is a sequence of $k$ tokens that appears in the doc
- Tokens can be characters, words or something else, depending on the application
- Assume tokens = characters for examples
- Example: $\mathbf{k}=\mathbf{2}$; document $\mathbf{D}_{\mathbf{1}}=\mathrm{abcab}$ Set of 2-shingles: $\mathbf{S}\left(\mathbf{D}_{1}\right)=\{a b, b c, c a\}$
- Option: Shingles as a bag (multiset), count ab twice: $\mathbf{S}^{\prime}\left(D_{1}\right)$ $=\{a b, b c, c a, a b\}$


## Represent Shingles

- To compress long shingles, we can hash them to (say) 4 bytes
- Represent a document by the set of hash values of its $k$ shingles
- Idea: Two documents could (rarely) appear to have shingles in common, when in fact only the hash-values were shared
- Example: $\mathbf{k}=\mathbf{2}$; document $\mathbf{D}_{\mathbf{1}}=\mathrm{abcab}$

Set of 2-shingles: $\mathbf{S}\left(\mathrm{D}_{1}\right)=\{a b, b c, c a\}$ Hash the singles: $\mathbf{h}\left(\mathbf{D}_{1}\right)=\{1,5,7\}$

## Similarity Metric for Shingles

- Document $D_{1}$ is a set of its $k$-shingles $C_{1}=S\left(D_{1}\right)$
- Equivalently, each document is a $0 / 1$ vector in the space of $k$-shingles
- Each unique shingle is a dimension
- Vectors are very sparse
- A natural similarity measure is the Jaccard similarity:

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



## Working Assumption

- Documents that have lots of shingles in common have similar text, even if the text appears in different order
- Caveat: You must pick $\boldsymbol{k}$ large enough, or most documents will have most shingles
$-\boldsymbol{k}=5$ is OK for short documents
$-\boldsymbol{k}=10$ is better for long documents


## Motivation for Minhash / LSH

- Suppose we need to find near-duplicate documents among $N=\mathbf{1}$ million documents
- Naïvely, we would have to compute pairwise Jaccard similarities for every pair of docs
$-N(N-1) / 2 \approx 5 * 10^{11}$ comparisons
- At $10^{5}$ secs/day and $10^{6}$ comparisons $/ \mathrm{sec}$, it would take 5 days
- For $\boldsymbol{N}=\mathbf{1 0}$ million, it takes more than a year...



## MinHashing

Step 2: Minhashing: Convert large sets to short signatures, while preserving similarity

## Encoding Sets as Bit Vectors

- Many similarity problems can be formalized as finding subsets that have significant intersection

- Encode sets using 0/1 (bit, boolean) vectors
- One dimension per element in the universal set
- Interpret set intersection as bitwise AND, and set union as bitwise OR
- Example: $\mathbf{C}_{1}=10111 ; \mathbf{C}_{\mathbf{2}}=10011$
- Size of intersection $=3$; size of union $=4$,
- Jaccard similarity (not distance) = 3/4
- Distance: $d\left(C_{1}, C_{2}\right)=1$ - (Jaccard similarity) $=1 / 4$


## From Sets to Boolean Matrices

- Rows = elements (shingles)
- Columns = sets (documents)
- 1 in row $\boldsymbol{e}$ and column $s$ if and only if $\boldsymbol{e}$ is a member of $s$
- Column similarity is the Jaccard similarity of the corresponding sets (rows with value 1)
- Typical matrix is sparse!
- Each document is a column:
- Example: $\operatorname{sim}\left(\mathrm{C}_{1}, \mathrm{C}_{2}\right)=$ ?
- Size of intersection $=3$; size of union $=6$, Jaccard similarity (not distance) $=3 / 6$
- $d\left(C_{1}, C_{2}\right)=1$ - (Jaccard similarity) $=3 / 6$

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

## Outline: Finding Similar Columns

- So far:
- Documents $\rightarrow$ Sets of shingles
- Represent sets as boolean vectors in a matrix
- Next goal: Find similar columns while computing small signatures
- Similarity of columns == similarity of signatures


## Outline: Finding Similar Columns

- Next Goal: Find similar columns, Small signatures
- Naïve approach:
- 1) Signatures of columns: small summaries of columns
- 2) Examine pairs of signatures to find similar columns
- Essential: Similarities of signatures and columns are related
- 3) Optional: Check that columns with similar signatures are really similar
- Warnings:
- Comparing all pairs may take too much time: Job for LSH
- These methods can produce false negatives, and even false positives (if the optional check is not made)


## Hashing Columns (Signatures)

- Key idea: "hash" each column $\boldsymbol{C}$ to a small signature $\boldsymbol{h}(\boldsymbol{C})$, such that:
- (1) $h(C)$ is small enough that the signature fits in RAM
- (2) $\operatorname{sim}\left(\boldsymbol{C}_{1}, C_{2}\right)$ is the same as the "similarity" of signatures $\boldsymbol{h}\left(\boldsymbol{C}_{1}\right)$ and $\boldsymbol{h}\left(\boldsymbol{C}_{2}\right)$
- Goal: Find a hash function $h(\cdot)$ such that:
- If $\operatorname{sim}\left(\boldsymbol{C}_{1} \boldsymbol{C}_{2}\right)$ is high, then with high prob. $\boldsymbol{h}\left(\boldsymbol{C}_{1}\right)=\boldsymbol{h}\left(\boldsymbol{C}_{2}\right)$
- If $\operatorname{sim}\left(C_{1}, C_{2}\right)$ is low, then with high prob. $\boldsymbol{h}\left(\boldsymbol{C}_{1}\right) \neq \boldsymbol{h}\left(\boldsymbol{C}_{2}\right)$
- Hash docs into buckets. Expect that "most" pairs of near duplicate docs hash into the same bucket!


## Min-Hashing

- Goal: Find a hash function $h(\cdot)$ such that:
- if $\operatorname{sim}\left(C_{1}, C_{2}\right)$ is high, then with high prob. $\boldsymbol{h}\left(\boldsymbol{C}_{1}\right)=\boldsymbol{h}\left(\boldsymbol{C}_{2}\right)$
- if $\operatorname{sim}\left(\boldsymbol{C}_{1}, C_{2}\right)$ is low, then with high prob. $\boldsymbol{h}\left(\boldsymbol{C}_{1}\right) \neq \boldsymbol{h}\left(\boldsymbol{C}_{2}\right)$
- Clearly, the hash function depends on the similarity metric:
- Not all similarity metrics have a suitable hash function
- There is a suitable hash function for the Jaccard similarity: It is called Min-Hashing


## Min-Hashing

- Imagine the rows of the boolean matrix permuted under random permutation $\pi$
- Define a "hash" function $h_{\pi}(C)=$ the index of the first (in the permuted order $\pi$ ) row in which column $\boldsymbol{C}$ has value 1:

$$
h_{\pi}(C)=\min _{\pi} \pi(C)
$$

- Use several (e.g., 100) independent hash functions (that is, permutations) to create a signature of a column


## Min-Hashing Example

$2^{\text {nd }}$ element is the first to map


## The Min-Hash Property

- Choose a random permutation $\pi$
- Claim: $\operatorname{Pr}\left[h_{\pi}\left(\mathrm{C}_{1}\right)=h_{\pi}\left(\mathrm{C}_{2}\right)\right]=\operatorname{sim}\left(\mathrm{C}_{1}, \mathrm{C}_{2}\right)$
- Why?
- Let $\boldsymbol{X}$ be a doc (set of shingles), $\boldsymbol{y} \in \boldsymbol{X}$ is a shingle
- Then: $\operatorname{Pr}[\pi(y)=\min (\pi(X))]=1 /|X|$
- It is equally likely that any $\boldsymbol{y} \in \boldsymbol{X}$ is mapped to the $\boldsymbol{m i n}$ element

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

- Let $\boldsymbol{y}$ be s.t. $\pi(\mathrm{y})=\min \left(\pi\left(\mathrm{C}_{1} \cup \mathrm{C}_{2}\right)\right)$
- Then either: $\quad \pi(y)=\min \left(\pi\left(C_{1}\right)\right)$ if $y \in C_{1}$, or

$$
\pi(y)=\min \left(\pi\left(C_{2}\right)\right) \text { if } y \in C_{2}
$$

- So the prob. that both are true is the prob. $\boldsymbol{y} \in \mathrm{C}_{1} \cap \mathrm{C}_{2}$
$-\operatorname{Pr}\left[\min \left(\pi\left(C_{1}\right)\right)=\min \left(\pi\left(C_{2}\right)\right)\right]=\left|C_{1} \cap C_{2}\right| /\left|C_{1} \cup C_{2}\right|=\operatorname{sim}\left(C_{1}, C_{2}\right)$

One of the two cols had to have 1 at position $y$

## Four Types of Rows

- Given cols $\mathrm{C}_{1}$ and $\mathrm{C}_{2}$, rows may be classified as:

|  | $\underline{C}_{1}$ | $C_{2}$ |
| :--- | :--- | :--- |
| A | 1 | 1 |
| B | 1 | 0 |
| C | 0 | 1 |
| D | 0 | 0 |

- $\mathbf{a}=$ \# rows of type $A$, etc.
- Note: $\operatorname{sim}\left(C_{1}, C_{2}\right)=a /(a+b+c)$
- Then: $\operatorname{Pr}\left[h\left(\mathrm{C}_{1}\right)=h\left(\mathrm{C}_{2}\right)\right]=\operatorname{Sim}\left(\mathrm{C}_{1}, \mathrm{C}_{2}\right)$
- Look down the cols $\mathrm{C}_{1}$ and $\mathrm{C}_{2}$ until we see a 1
- If it's a type-A row, then $h\left(\mathrm{C}_{1}\right)=h\left(\mathrm{C}_{2}\right)$ If a type- $B$ or type- $C$ row, then not


## Similarity for Signatures

- We know: $\operatorname{Pr}\left[h_{\pi}\left(\mathrm{C}_{1}\right)=h_{\pi}\left(\mathrm{C}_{2}\right)\right]=\operatorname{sim}\left(\mathrm{C}_{1}, \mathrm{C}_{2}\right)$
- Now generalize to multiple hash functions
- The similarity of two signatures is the fraction of the hash functions in which they agree
- Note: Because of the Min-Hash property, the similarity of columns is the same as the expected similarity of their signatures


## Min-Hashing Example

Permutation $\pi \quad$ Input matrix (Shingles $x$ Documents)

| 2 | 4 | 3 | 1 0 1 <br> 0   <br> 3 2 4 <br> 7 1 0 | 0 | 1 |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 7 | 1 | 7 | 0 | 1 | 0 | 1 |  |
| 6 | 3 | 2 |  | 0 | 1 | 0 | 1 |
| 1 | 6 | 6 |  | 0 | 1 | 0 | 1 |
| 5 | 7 | 1 | 1 | 0 | 1 | 0 |  |
| 4 | 5 | 5 |  | 1 | 0 | 1 | 0 |



Similarities:

|  | $1-3$ | $2-4$ | $1-2$ | $3-4$ |
| :--- | :---: | :---: | :---: | :---: |
| Col/Col | 0.75 | 0.75 | 0 | 0 |
| Sig/Sig | 0.67 | 1.00 | 0 | 0 |
|  |  |  |  |  |

## Min-Hash Signatures

- Pick K=100 random permutations of the rows
- Think of $\boldsymbol{\operatorname { s i g } ( \mathrm { C } ) \text { as a column vector }}$
- $\boldsymbol{\operatorname { s i g }}(\mathbf{C})[i]=$ according to the $i$-th permutation, the index of the first row that has a 1 in column $C$

$$
\operatorname{sig}(C)[i]=\min \left(\pi_{i}(C)\right)
$$

- Note: The sketch (signature) of document $C$ is small $\mathbf{\sim 1 0 0}$ bytes!
- We achieved our goal! We "compressed" long bit vectors into short signatures


## Implementation Trick

- Permuting rows even once is prohibitive
- Row hashing!
- Pick $\mathbf{K}=100$ hash functions $\boldsymbol{k}_{\boldsymbol{i}}$
- Ordering under $\boldsymbol{k}_{\boldsymbol{i}}$ gives a random row permutation!
- One-pass implementation
- For each column $\boldsymbol{C}$ and hash-func. $\boldsymbol{k}_{\boldsymbol{i}}$ keep a "slot" for the minhash value
- Initialize all $\operatorname{sig}(C)[i]=\infty$
- Scan rows looking for 1s
- Suppose row $\boldsymbol{j}$ has 1 in column $\boldsymbol{C}$
- Then for each $\boldsymbol{k}_{\boldsymbol{i}}$ :
- If $k_{i}(j)<\operatorname{sig}(C)[i]$, then $\operatorname{sig}(C)[i] \leftarrow k_{i}(j)$



# Locality Sensitive Hashing Step 3: Locality-Sensitive Hashing: Focus on pairs of signatures likely to be from similar documents 

## LSH: First Cut

- Goal: Find documents with Jaccard similarity at least $s$ (for some similarity threshold, e.g., $s=0.8$ )
- LSH - General idea: Use a function $f(x, y)$ that tells whether $\boldsymbol{x}$ and $\boldsymbol{y}$ is a candidate pair: a pair of elements whose similarity must be evaluated
- For Min-Hash matrices:
- Hash columns of signature matrix $\boldsymbol{M}$ to many buckets
- Each pair of documents that hashes into the same bucket is a candidate pair


## Candidates from Min-Hash

- Pick a similarity threshold $s(0<s<1)$
- Columns $\boldsymbol{x}$ and $\boldsymbol{y}$ of $\boldsymbol{M}$ are a candidate pair if their signatures agree on at least fraction $s$ of their rows:
$\boldsymbol{M}(\boldsymbol{i}, \boldsymbol{x})=\boldsymbol{M}(\boldsymbol{i}, \boldsymbol{y})$ for at least frac. $\boldsymbol{s}$ values of $\boldsymbol{i}$
- We expect documents $\boldsymbol{x}$ and $\boldsymbol{y}$ to have the same (Jaccard) similarity as their signatures


## LSH for Min-Hash

- Big idea: Hash columns of signature matrix $M$ several times
- Arrange that (only) similar columns are likely to hash to the same bucket, with high probability
- Candidate pairs are those that hash to the same bucket


## Partition $M$ into $b$ Bands



## Partition M into Bands

- Divide matrix $\boldsymbol{M}$ into $\boldsymbol{b}$ bands of $\boldsymbol{r}$ rows
- For each band, hash its portion of each column to a hash table with $\boldsymbol{k}$ buckets
- Make $\boldsymbol{k}$ as large as possible
- Candidate column pairs are those that hash to the same bucket for $\geq 1$ band
- Tune $\boldsymbol{b}$ and $\boldsymbol{r}$ to catch most similar pairs, but few non-similar pairs


## Hashing Bands



## Simplifying Assumption

- There are enough buckets that columns are unlikely to hash to the same bucket unless they are identical in a particular band
- Hereafter, we assume that "same bucket" means "identical in that band"
- Assumption needed only to simplify analysis, not for correctness of algorithm


## Example of Bands

Assume the following case:

- Suppose 100,000 columns of $M$ (100k docs)
- Signatures of 100 integers (rows)
- Therefore, signatures take 40 Mb
- Choose $\boldsymbol{b}=20$ bands of $\boldsymbol{r}=5$ integers/band
- Goal: Find pairs of documents that are at least $\boldsymbol{s}=0.8$ similar


## $C_{1}, C_{2}$ are 80\% Similar

- Find pairs of $\geq s=0.8$ similarity, set $b=20, r=5$
- Assume: $\operatorname{sim}\left(C_{1}, C_{2}\right)=0.8$
- Since $\operatorname{sim}\left(C_{1}, C_{2}\right) \geq \mathbf{s}$, we want $C_{1}, C_{2}$ to be a candidate pair: We want them to hash to at least 1 common bucket (at least one band is identical)
- Probability $\mathrm{C}_{1}, \mathrm{C}_{2}$ identical in one particular band: $(0.8)^{5}=0.328$
- Probability $\mathrm{C}_{1}, \mathrm{C}_{2}$ are not similar in all of the 20 bands: $(1-0.328)^{20}=0.00035$
- i.e., about $1 / 3000$ th of the $80 \%$-similar column pairs are false negatives (we miss them)
- We would find $99.965 \%$ pairs of truly similar documents


## $\mathrm{C}_{1}, \mathrm{C}_{2}$ are $30 \%$ Similar

- Find pairs of $\geq s=0.8$ similarity, set $b=20, r=5$
- Assume: $\operatorname{sim}\left(C_{1}, C_{2}\right)=0.3$
- Since $\operatorname{sim}\left(C_{1}, C_{2}\right)<s$ we want $C_{1}, C_{2}$ to hash to NO common buckets (all bands should be different)
- Probability $\mathrm{C}_{1}, \mathrm{C}_{2}$ identical in one particular band: $(0.3)^{5}=0.00243$
- Probability $\mathrm{C}_{1}, \mathrm{C}_{2}$ identical in at least 1 of 20 bands: $1-(1-0.00243)^{20}=0.0474$
- In other words, approximately $4.74 \%$ pairs of docs with similarity $0.3 \%$ end up becoming candidate pairs
- They are false positives since we will have to examine them (they are candidate pairs) but then it will turn out their similarity is below threshold $\mathbf{s}$


## LSH Involves a Tradeoff

- Pick:
- The number of Min-Hashes (rows of $\boldsymbol{M}$ )
- The number of bands $\boldsymbol{b}$, and
- The number of rows $r$ per band
to balance false positives/negatives
- Example: If we had only 15 bands of 5 rows, the number of false positives would go down, but the number of false negatives would go up


## Analysis of LSH - What We Want



Similarity $t=\operatorname{sim}\left(C_{1}, C_{2}\right)$ of two sets

## What 1 Band of 1 Row Gives You



Similarity $t=\operatorname{sim}\left(C_{1}, C_{2}\right)$ of two sets

## $b$ bands, $r$ rows/band

- Columns $\mathrm{C}_{1}$ and $\mathrm{C}_{2}$ have similarity $t$
- Pick any band (r rows)
- Prob. that all rows in band equal $=t^{r}$
- Prob. that some row in band unequal $=1-t^{r}$
- Prob. that no band identical $=\left(1-t^{r}\right)^{b}$
- Prob. that at least 1 band identical =

$$
1-\left(1-t^{r}\right)^{b}
$$

## What $b$ Bands of $r$ Rows Gives You



## Example: $b=20 ; r=5$

- Similarity threshold s
- Prob. that at least 1 band is identical:

| $\boldsymbol{s}$ | $\mathbf{1 - ( 1 - s}^{\mathbf{r}} \mathbf{b}^{\mathbf{b}}$ |
| :--- | :--- |
| .2 | .006 |
| .3 | .047 |
| .4 | .186 |
| .5 | .470 |
| .6 | .802 |
| .7 | .975 |
| .8 | .9996 |

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

- Picking $r$ and $b$ to get the best S-curve
-50 hash-functions ( $r=5, b=10$ )


Blue area: False Negative rate Green area: False Positive rate

## LSH Summary

- Tune $\mathbf{M}, \boldsymbol{b}, r$ to get almost all pairs with similar signatures, but eliminate most pairs that do not have similar signatures
- Check in main memory that candidate pairs really do have similar signatures
- Optional: In another pass through data, check that the remaining candidate pairs really represent similar documents


## Summary: 3 Steps

- Shingling: Convert documents to sets
- We used hashing to assign each shingle an ID
- Min-Hashing: Convert large sets to short signatures, while preserving similarity
- We used similarity preserving hashing to generate signatures with property $\operatorname{Pr}\left[h_{\pi}\left(\mathrm{C}_{1}\right)=h_{\pi}\left(\mathrm{C}_{2}\right)\right]=\operatorname{sim}\left(\mathrm{C}_{1}, \mathrm{C}_{2}\right)$
- We used hashing to get around generating random permutations
- Locality-Sensitive Hashing: Focus on pairs of signatures likely to be from similar documents
- We used hashing to find candidate pairs of similarity $\geq s$


## GENERALIZATION OF LSH

## Locality sensitive hashing

- Originally defined in terms of a similarity function [C'02]
- Given universe $U$ and a similarity $s: U \times U \rightarrow[0,1]$, does there exist a prob distribution over some hash family $H$ such that

$$
\operatorname{Pr}_{h \in H}[h(x)=h(y)]=s(x, y)
$$

$$
\begin{gathered}
s(x, y)=1 \rightarrow x=y \\
s(x, y)=s(y, x)
\end{gathered}
$$

## Locality Sensitive Hashing

- Hash family $H$ is locality sensitive if [Indyk Motwani]

$$
\begin{aligned}
& \operatorname{Pr}[h(x)=h(y)] \text { is high if } x \text { is close to } y \\
& \operatorname{Pr}[h(x)=h(y)] \text { is low if } x \text { is far from } y
\end{aligned}
$$

- Not clear such functions exist for all distance functions


## Hamming distance

- Points are bit strings of length $d$
- $H(x, y)=\left|\left\{i, x_{i} \neq y_{i}\right\}\right| \quad S_{H}(x, y)=1-\frac{H(x, y)}{d}$
- Define a hash function $h$ by sampling a set of positions
$-x=1011010001, y=0111010101$
$-S=\{1,5,7\}$
$-h(x)=100, h(y)=100$


## LSH for Hamming Distance

- The above hash family is locality sensitive, $k=$ $|S|$

$$
\operatorname{Pr}[h(x)=h(y)]=\left(1-\frac{H(x, y)}{d}\right)^{k}
$$

## LSH for angle distance

- $x, y$ are unit norm vectors
- $d(x, y)=\cos ^{-1}(x \cdot y)=\theta$
- $S(x, y)=1-\theta / \pi$
- Choose direction $v$ uniformly at random
$-h_{v}(x)=\operatorname{sign}(v \cdot x)$
$-\operatorname{Pr}\left[h_{v}(x)=h_{v}(y)\right]=1-\theta / \pi$


## Aside: picking a direction u.a.r.

- How to sample a vector $x \in R^{d},|x|_{2}=1$ and the direction is uniform among all possible directions
- Generate $x=\left(x_{1}, \ldots . x_{d}\right), x_{i} \sim N(0,1)$ iid
- Normalize $\frac{x}{|x|_{2}}$
- By writing the pdf of the d-dimensional Gaussian in polar form, easy to see that this is uniform direction on unit sphere


## Which similarities admit LSH?

- There are various similarities and distance that are used in scientific literature
- Encyclopedia of distances DL'11
- Will there be an LSH for each one of them?
- Similarity is LSHable if there exists an LSH for it


## LSHable similarities

Thm: S is LSHable $\rightarrow 1-\mathrm{S}$ is a metric

$$
\begin{gathered}
d(x, y)=0 \rightarrow x=y \\
d(x, y)=d(y, x) \\
d(x, y)+d(y, z) \geq d(x, z)
\end{gathered}
$$

Fix hash function $h \in H$ and define

$$
\begin{gathered}
\Delta_{h}(A, B)=[h(A) \neq h(B)] \\
1-\mathrm{S}(\mathrm{~A}, \mathrm{~B})=\operatorname{Pr}_{h}\left[\Delta_{h}(A, B)\right]
\end{gathered}
$$

Also

$$
\Delta_{h}(A, B)+\Delta_{h}(B, C) \geq \Delta_{h}(A, C)
$$

## Example of non-LSHable similarities

- $d(A, B)=1-s(A, B)$
- Sorenson-Dice : $s(A, B)=\frac{2|A \cap B|}{|A|+|B|}$

$$
\begin{aligned}
& - \text { Ex: } A=\{a\}, B=\{b\}, C=\{a, b\} \\
& -s(A, B)=0, s(B, C)=s(A, C)=\frac{2}{3}
\end{aligned}
$$

- Overlap: $s(A, B)=\frac{|A \cap B|}{\min (|A|,|B|)}$

$$
-s(A, B)=0, s(A, C)=1=s(B, C)
$$

## Gap Definition of LSH

- A family is $(r, R, p, q)$ LSH if

$$
\begin{aligned}
& \operatorname{Pr}_{h \in H}[h(x)=h(y)] \geq p \text { if } d(x, y) \leq r \\
& \operatorname{Pr}_{h \in H}[h(x)=h(y)] \leq q \text { if } d(x, y) \geq R
\end{aligned}
$$

Here $p>q$.


## Gap LSH

- All the previous constructions satisfy the gap definition
- Ex: for $J S(S, T)=\frac{|S \cap T|}{|S \cup T|}$

$$
\begin{aligned}
& J D(S, T) \leq r \rightarrow J S(S, T) \geq 1-r \rightarrow \operatorname{Pr}[h(S)=h(T)]=J S(S, T) \geq 1-r \\
& J D(S, T) \geq R \rightarrow J S(S, T) \leq 1-R \rightarrow \operatorname{Pr}[h(S)=h(T)]=J S(S, T) \leq 1-R
\end{aligned}
$$

Hence is a $(r, R, 1-r, 1-R)$ LSH

## L2 norm

- $d(x, y)=\sqrt{ }\left(\sum_{i}\left(x_{i}-y_{i}\right)^{2}\right.$
- $u=$ random unit norm vector, $w \in R$ parameter, $b \sim \operatorname{Unif}[0, w]$
- $h(x)=\left\lfloor\frac{u \cdot x+b}{w}\right\rfloor$
- If $|x-y|_{2}<\frac{w}{2}, \operatorname{Pr}[h(x)=h(y)] \geq \frac{1}{3}$
- If $|x-y|_{2}>4 w, \operatorname{Pr}[h(x)=h(y)] \leq \frac{1}{4}$


## Solving the near neighbour

- $(r, c)$-near neighbour problem
- Given query point $q$, return all points $p$ such that $d(p, q)<r$ and none such that $d(p, q)>c r$
- Solving this gives a subroutine to solve the "nearest neighbour", by building a data-structure for each $r$, in powers of $(1+\epsilon)$


## How to actually use it?

- Need to amplify the probability of collisions for "near" points


## Band construction

- AND-ing of LSH
- Define a composite function $H(x)=\left(h_{1}(x), \ldots h_{k}(x)\right)$
$-\operatorname{Pr}[H(x)=H(y)]=\Pi_{\mathrm{i}} \operatorname{Pr}\left[h_{i}(x)=h_{i}(y)\right]=\operatorname{Pr}\left[h_{1}(x)=\right.$ $\left.h_{1}(y)\right]^{k}$
- OR-ing
- Create $L$ independent hash-tables for $H_{1}, H_{2}, \ldots H_{L}$
- Given query $x$, search in $U_{j} H_{j}(x)$


## Example

|  | $\mathrm{S}_{1}$ | $\mathrm{~S}_{2}$ | $\mathrm{~S}_{3}$ | $\mathrm{~S}_{4}$ |
| :--- | :--- | :--- | :--- | :--- |
| A | 1 | 0 | 1 | 0 |
| B | 1 | 0 | 0 | 1 |
| C | 0 | 1 | 0 | 1 |
| D | 0 | 1 | 0 | 1 |
| E | 0 | 1 | 0 | 1 |
| F | 1 | 0 | 1 | 0 |
| G | 1 | 0 | 1 | 0 |


|  | S1 | S2 | S3 | S3 |
| :--- | :--- | :--- | :--- | :--- |
| h1 | 1 | 2 | 1 | 2 |
| h2 | 2 | 1 | 3 | 1 |


|  | S1 | S2 | S3 | S3 |
| :--- | :--- | :--- | :--- | :--- |
| h3 | 3 | 1 | 2 | 1 |
| h4 | 1 | 3 | 2 | 2 |

## Why is this better?

- Consider $\mathrm{x}, y$ with $\operatorname{Pr}[h(x)=h(y)]=1-d(x, y)$
- Probability of not finding $y$ as one of the candidates in $\mathrm{U}_{j} H_{j}(x)$

$$
1-\left(1-(1-d)^{k}\right)^{L}
$$

## Creating an LSH

- Query $x$
- If we have a $(r, c r, p, q)$ LSH

$$
\rho=\frac{\log (p)}{\log (q)} \quad L=n^{\rho} \quad k=\log (n) / \log \left(\frac{1}{q}\right)
$$

- For any $y$, with $|x-y|<r$,
- Prob of $y$ as candidate in $U_{j} H_{j}(x) \geq 1-\left(1-p^{k}\right)^{L} \geq 1-\frac{1}{e}$
- For any $z,|x-z|>c r$,
- Prob of $z$ as candidate in any fixed $H_{j}(x) \leq q^{k}$
- Expected number of such $z \leq L q^{k} \leq L=n^{\rho}$
$-\rho<1$


## Runtime

- Space used $=n^{1+\rho}$
- Query time $=n^{\rho} \times(k+d) \quad$ [time for $k$-hashes \& brute force comparison]
- We can show that for Hamming, angle etc, $\rho \approx \frac{1}{c}$
- Can get 2-approx near neighbors with $O(\sqrt{ } n)$ neighbour comparisons


## LSH: theory vs practice

- In order to design LSH in practice, the theoretical parameter values are only a guidance
- Typically need to search over the parameter space to find a good operating point
- Data statistics can provide some guidance.


## Summary

- Locality sensitive hashing is a powerful tool for near neighbour problems
- Trades off space with query time
- Practical for medium to large datasets with fairly large number of dimensions
- However, doesn't really work very well for sparse, very very high dimensional datasets
- LSH and extensions are an area of active research and practice


## References:

- Primary references for this lecture
- Modern Massive Datasets, Rajaraman, Leskovec, Ullman.
- Survey by Andoni et al. (CACM 2008) available at www.mit.edu/~andoni/LSH


## References:

- Primary references for this lecture
- Modern Massive Datasets, Rajaraman, Leskovec, Ullman.
- Survey by Andoni et al. (CACM 2008) available at www.mit.edu/~andoni/LSH

