CS60021: Scalable Data Mining

Similarity Search and Hashing

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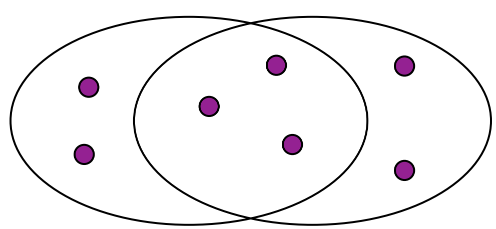
Finding Similar Items

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:
    $\boldsymbol{sim(C_1, C_2) = |C_1 \cap C_2| / |C_1 \cup C_2|}$
  - **Jaccard distance:** $\boldsymbol{d(C_1, C_2) = 1 - |C_1 \cap C_2| / |C_1 \cup C_2|}$



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

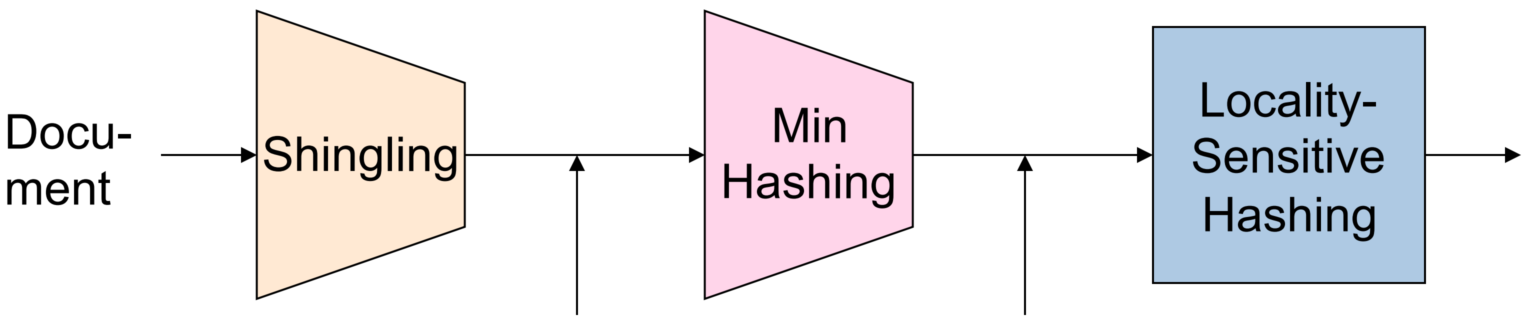
3 Essential Steps for Similar Docs

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!**

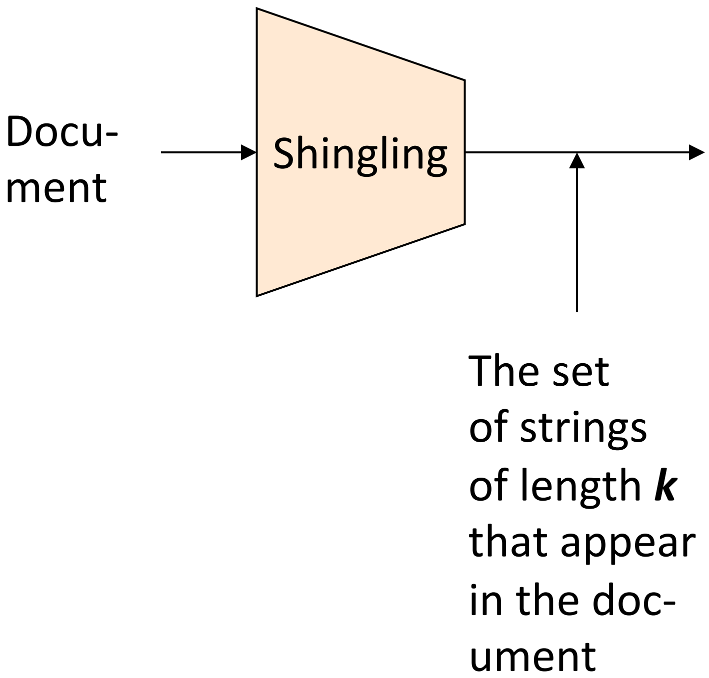
The Big Picture



The set of strings of length ***k*** that appear in the doc-ument

Signatures: short integer vectors that represent the sets, and reflect their similarity

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



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:** **k=2**; document $\mathbf{D_1}$ = abcab
  Set of 2-shingles: $\mathbf{S(D_1)}$ = {ab, bc, ca}
  - **Option:** Shingles as a bag (multiset), count ab twice: $\mathbf{S'(D_1)}$ **=** {ab, bc, ca, ab}

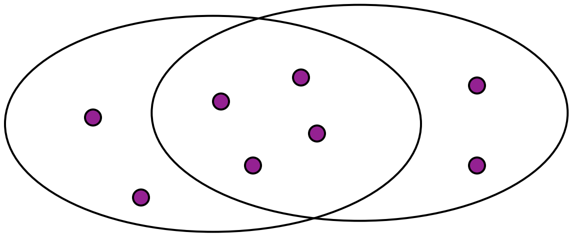
Compressing Shingles

- 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:** **k=2**; document $\mathbf{D_1}$= abcab
  Set of 2-shingles: $\mathbf{S(D_1)}$ = {ab, bc, ca}
  Hash the singles: $\mathbf{h(D_1)}$ = {1, 5, 7}

Similarity Metric for Shingles

- **Document D_1 is a set of its k-shingles C_1=S(D_1)**
- 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:**

$$sim(D_1, D_2) = |C_1 \cap C_2| / |C_1 \cup C_2|$$



Working Assumption

- **Documents that have lots of shingles in common have similar text, even if the text appears in different order**

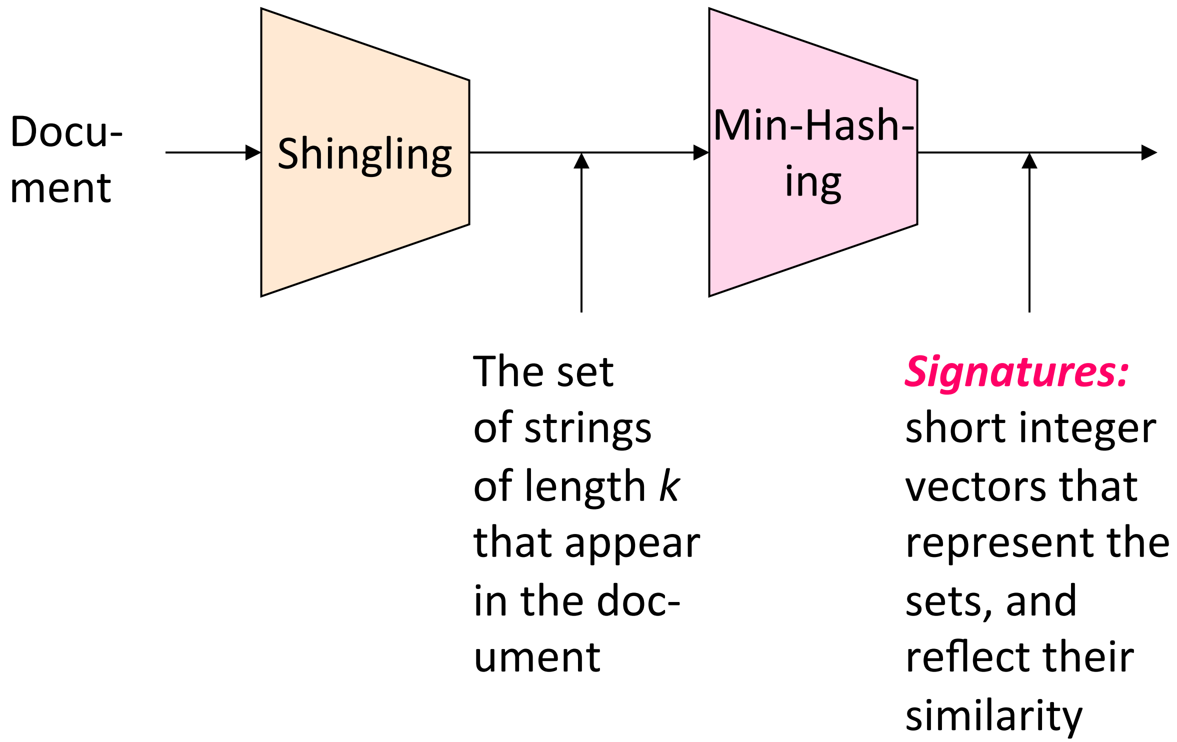
- **Caveat:** You must pick ***k*** large enough, or most documents will have most shingles
  - ***k*** = 5 is OK for short documents
  - ***k*** = 10 is better for long documents

Motivation for Minhash / LSH

- **Suppose we need to find near-duplicate documents among $N=1$ 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/sec, it would take **5 days**

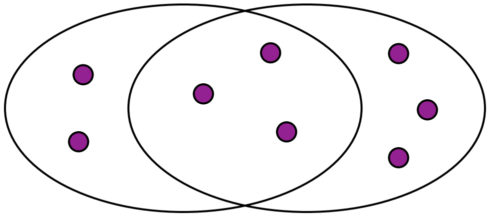
- For $N = 10$ million, it takes more than a year…



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; $\mathbf{C_2}$ = 10011
  - Size of intersection **= 3**; size of union **= 4**,
  - **Jaccard similarity** (not distance) **= 3/4**
  - **Distance: $d(C_1,C_2)$ = 1 – (Jaccard similarity) = 1/4**

From Sets to Boolean Matrices

- **Rows** = elements (shingles)
- **Columns** = sets (documents)
  - 1 in row ***e*** and column ***s*** if and only if ***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:** **sim(C_1 ,C_2) = ?**
    - Size of intersection = 3; size of union = 6, Jaccard similarity (not distance) = 3/6
    - **d(C_1,C_2) = 1 – (Jaccard similarity) = 3/6**

Documents

Shingles

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 → 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 ***C*** to a small ***signature h(C)***, such that:
  - **(1)** ***h(C)*** is small enough that the signature fits in RAM
  - **(2)** ***sim*(C_1, C_2)** is the same as the "similarity" of signatures ***h*(C_1)** and ***h*(C_2)**

- **Goal: Find a hash function *h(·)* such that:**
  - If ***sim*(C_1,C_2)** is high, then with high prob. ***h*(C_1) = *h*(C_2)**
  - If ***sim*(C_1,C_2)** is low, then with high prob. ***h*(C_1) ≠ *h*(C_2)**

- **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(·)* such that:**
  - if $sim(C_1,C_2)$ is high, then with high prob. $h(C_1) = h(C_2)$
  - if $sim(C_1,C_2)$ is low, then with high prob. $h(C_1) \neq h(C_2)$
- **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 π**
- Define a **"hash" function *$h_\pi(C)$*** = the index of the **first** (in the permuted order π) row in which column ***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

2nd element of the permutation is the first to map to a 1

Permutation π

2	4	3
3	2	4
7	1	7
6	3	2
1	6	6
5	7	1
4	5	5

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

4th element of the permutation is the first to map to a 1

The Min-Hash Property

0	0
0	0
1	**1**
0	0
0	1
1	0

- **Choose a random permutation π**
- **Claim:** $\Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
- **Why?**
  - Let **X** be a doc (set of shingles), $y \in X$ is a shingle
  - **Then:** $\Pr[\pi(y) = \min(\pi(X))] = 1/|X|$
    - It is equally likely that any $y \in X$ is mapped to the ***min*** element
  - Let y be s.t. $\pi(y) = \min(\pi(C_1 \cup C_2))$
  - **Then either:** $\pi(y) = \min(\pi(C_1))$ if $y \in C_1$, **or**

    $\pi(y) = \min(\pi(C_2))$ if $y \in C_2$
  - So the prob. that **both** are true is the prob. $y \in C_1 \cap C_2$
  - $\Pr[\min(\pi(C_1)) = \min(\pi(C_2))] = |C_1 \cap C_2| / |C_1 \cup C_2| = sim(C_1, C_2)$

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

Four Types of Rows

- **Given cols C_1 and C_2, rows may be classified as:**

	C_1	C_2
A	1	1
B	1	0
C	0	1
D	0	0

  - **a** = # rows of type A, etc.
- **Note: sim(C_1, C_2) = a/(a +b +c)**
- **Then: Pr**[$h(C_1) = h(C_2)$] = $Sim(C_1, C_2)$
  - Look down the cols C_1 and C_2 until we see a 1
  - If it's a type-*A* row, then $h(C_1) = h(C_2)$
    If a type-*B* or type-*C* row, then not

Similarity for Signatures

- We know: $\Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
- 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 π

2	4	3
3	2	4
7	1	7
6	3	2
1	6	6
5	7	1
4	5	5

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:

	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 ***sig*(C)** as a column vector
- ***sig*(C)[i] =** according to the *i*-th permutation, the index of the first row that has a 1 in column *C*

$$sig(C)[i] = \min(\pi_i(C))$$

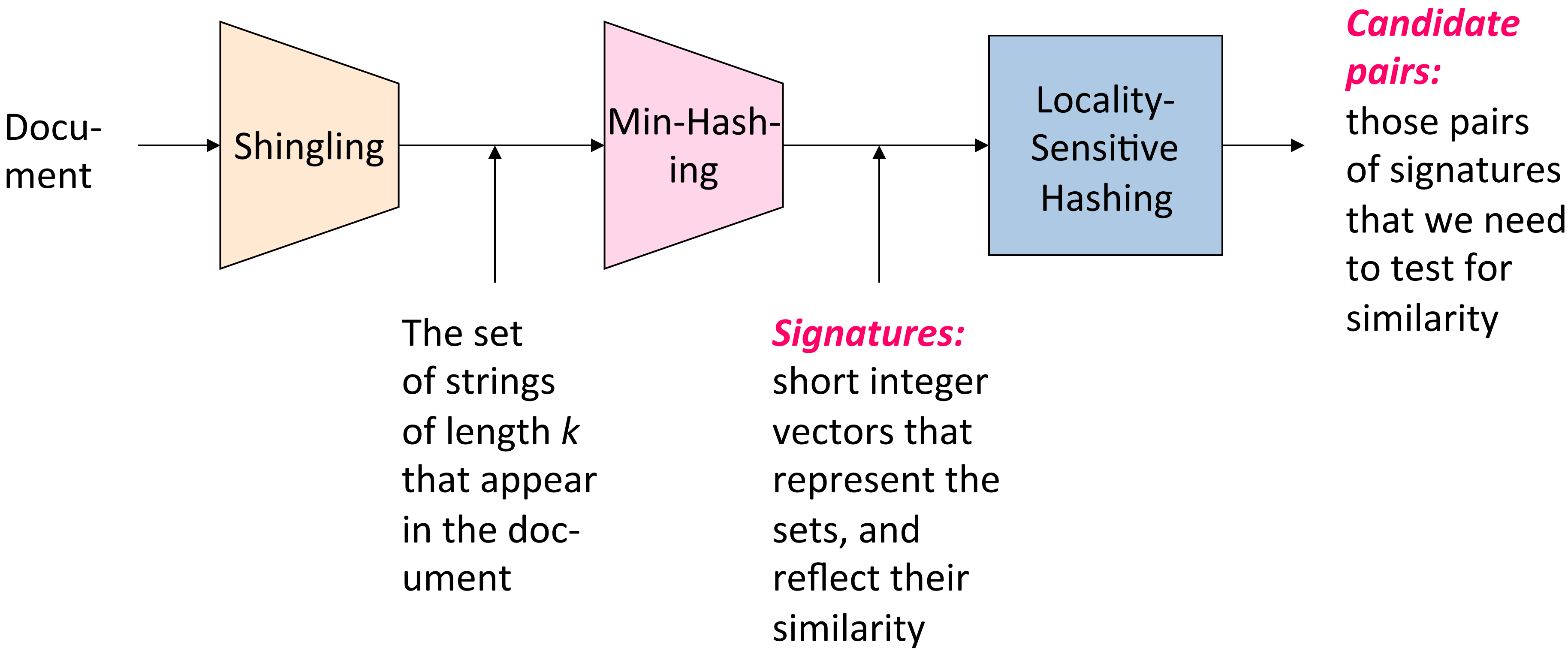
- **Note:** The sketch (signature) of document *C* is small $\sim$**100 bytes!**

- **We achieved our goal! We "compressed" long bit vectors into short signatures**

Implementation Trick

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

How to pick a random hash function h(x)?
Universal hashing:
$h_{a,b}(x)=((a \cdot x+b) \bmod p) \bmod N$
where:
a,b … random integers
p … prime number (p > N)



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 ***x*** and ***y*** is a ***candidate pair****:* a pair of elements whose similarity must be evaluated

- **For Min-Hash matrices:**
  - Hash columns of signature matrix ***M*** to many buckets
  - Each pair of documents that hashes into the same bucket is a **candidate pair**

Candidates from Min-Hash

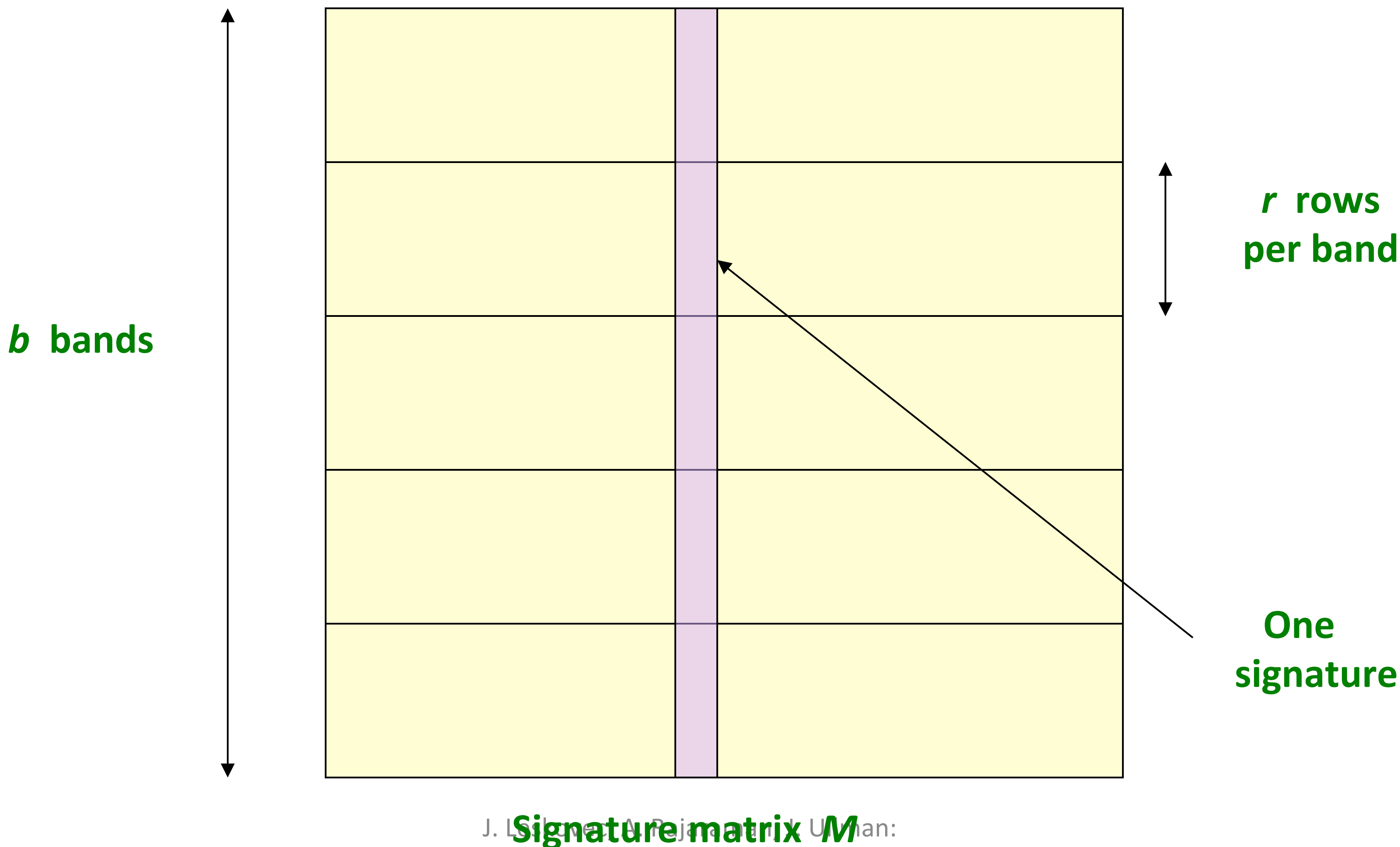
- **Pick a similarity threshold *s* (0 < s < 1)**

- Columns ***x*** and ***y*** of ***M*** are a **candidate pair** if their signatures agree on at least fraction ***s*** of their rows:
  $\boldsymbol{M(i, x) = M(i, y)}$ for at least frac. ***s*** values of ***i***
  - We expect documents ***x*** and ***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**

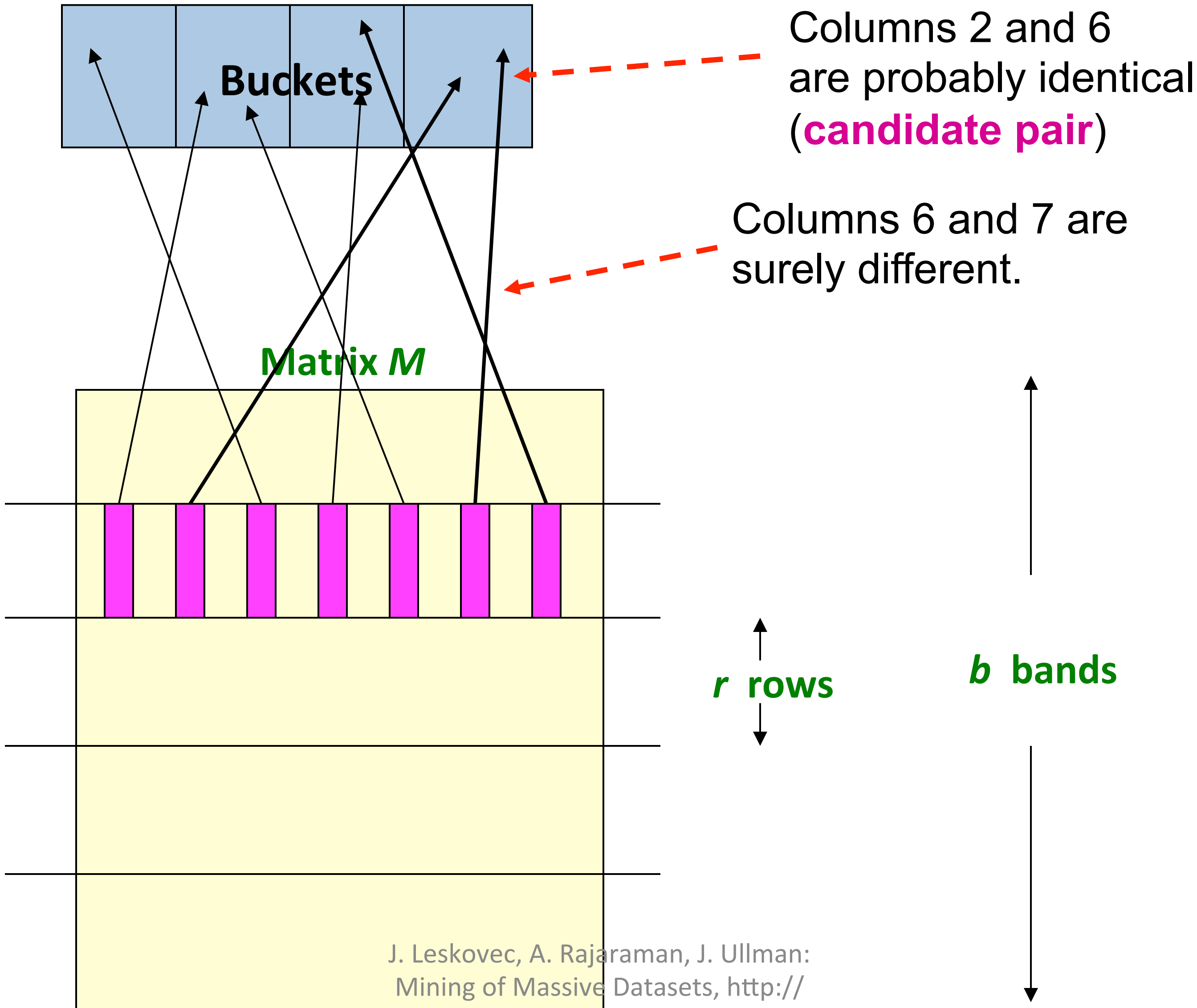
Partition *M* into *b* Bands



Partition M into Bands

- Divide matrix ***M*** into ***b*** bands of ***r*** rows
- For each band, hash its portion of each column to a hash table with ***k*** buckets
  - Make ***k*** as large as possible
- ***Candidate*** column pairs are those that hash to the same bucket for ≥ **1** band
- Tune ***b*** and ***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 40Mb
- Choose ***b*** = 20 bands of ***r*** = 5 integers/band

- **Goal:** Find pairs of documents that are at least ***s*** = *0.8* similar

C_1, C_2 are 80% Similar

- **Find pairs of ≥ *s***=0.8 similarity, set **b**=20, **r**=5
- **Assume:** sim(C_1, C_2) = 0.8
  - Since sim(C_1, C_2) ≥ **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 C_1, C_2 identical in one particular band:** $(0.8)^5 = 0.328$
- Probability C_1, C_2 are ***not*** similar in all of the 20 bands: $(1\text{-}0.328)^{20} = 0.00035$
  - i.e., about 1/3000th of the 80%-similar column pairs are **false negatives** (we miss them)
  - **We would find 99.965% pairs of truly similar documents**

C_1, C_2 are 30% Similar

- **Find pairs of ≥ *s***=0.8 similarity, set **b**=20, **r**=5
- **Assume:** sim(C_1, C_2) = 0.3
  - Since sim(C_1, C_2) < **s** we want C_1, C_2 to hash to **NO common buckets** (all bands should be different)
- **Probability C_1, C_2 identical in one particular band:** $(0.3)^5 = 0.00243$
- Probability C_1, 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 **s**

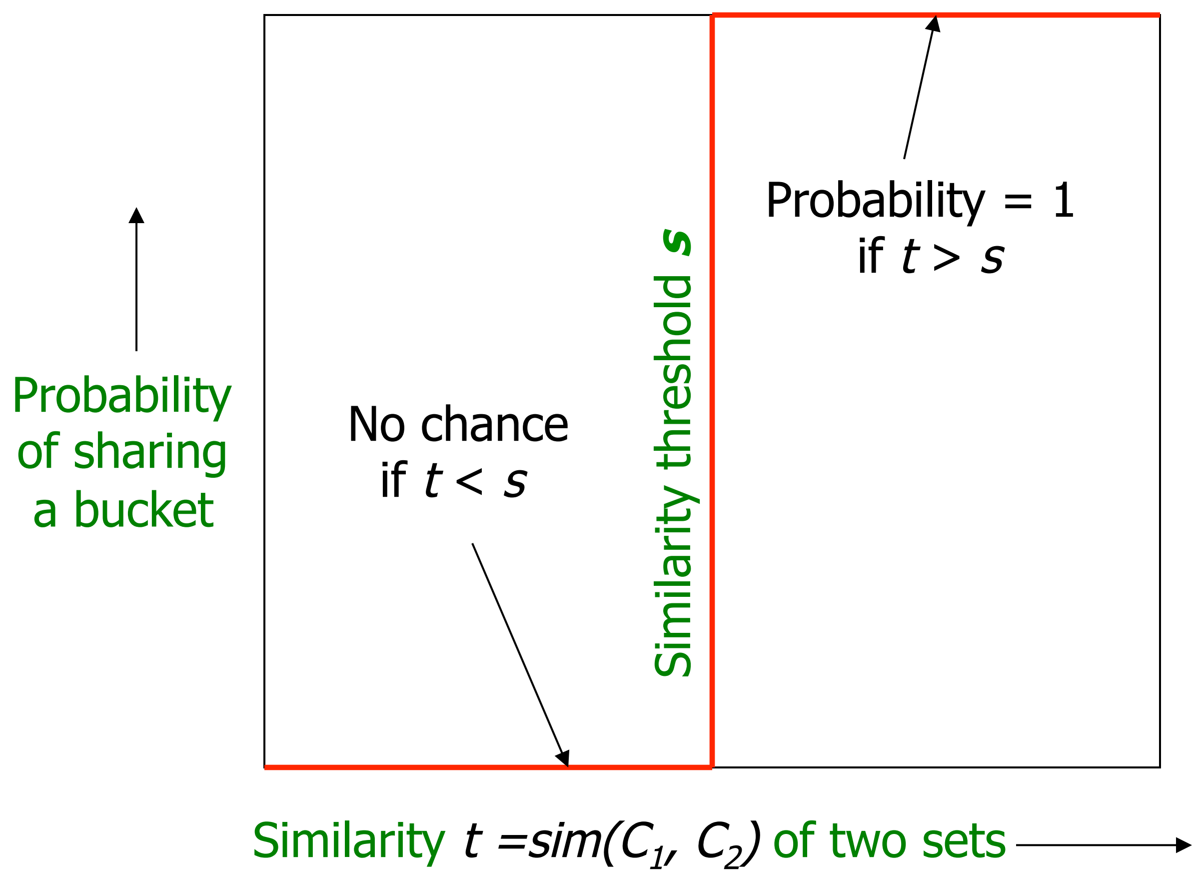
LSH Involves a Tradeoff

- **Pick:**
  - The number of Min-Hashes (rows of ***M***)
  - The number of bands ***b***, and
  - The number of rows ***r*** per band

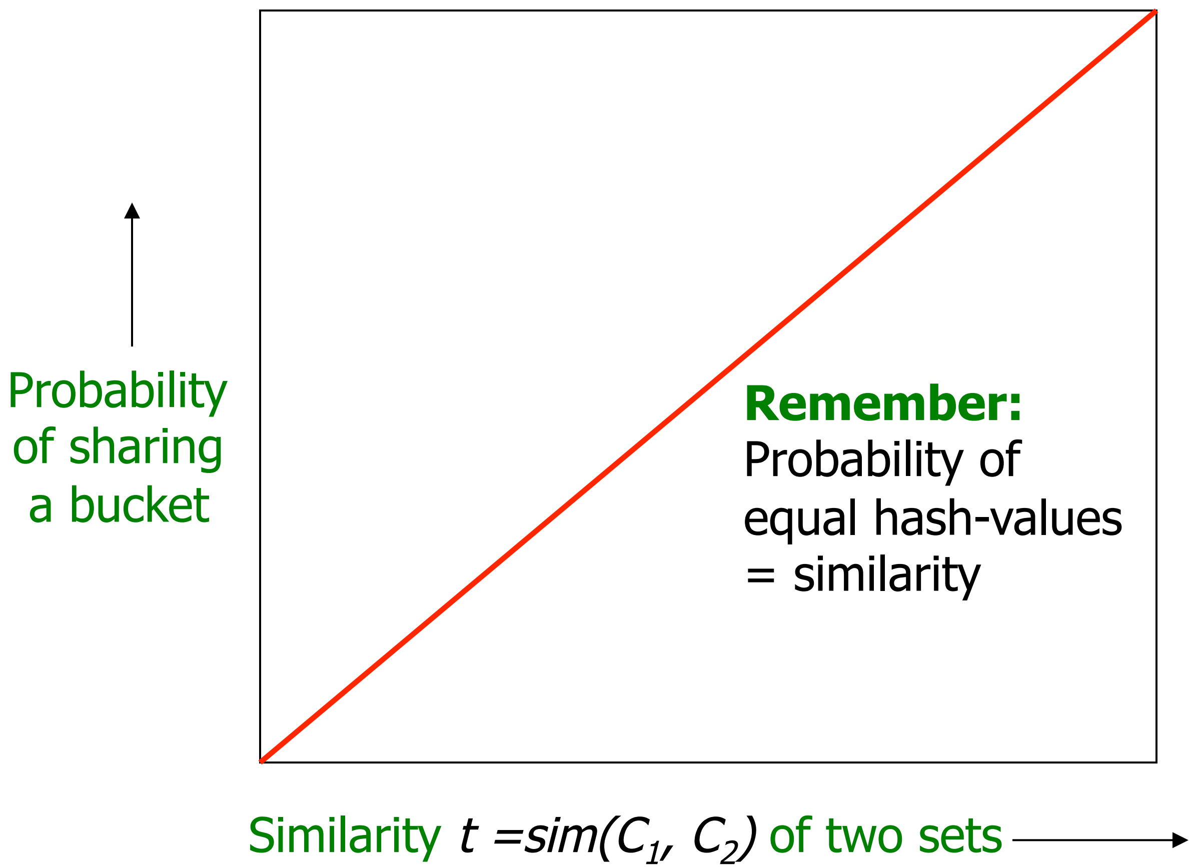
  to balance false positives/negatives

- **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



What 1 Band of 1 Row Gives You



b bands, r rows/band

- Columns C_1 and 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 = $1 - t^r$

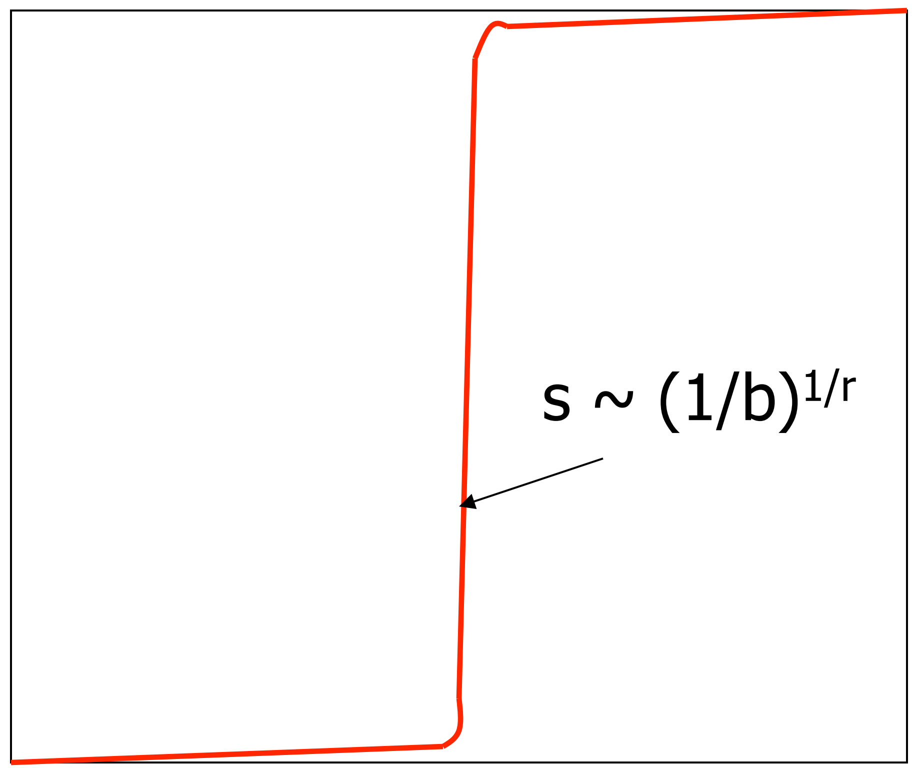
- Prob. that no band identical = $(1 - t^r)^b$

- Prob. that at least 1 band identical =

  $1 - (1 - t^r)^b$

What b Bands of r Rows Gives You

Probability of sharing a bucket



Similarity $t=sim(C_1, C_2)$ of two sets →

At least one band identical

No bands identical

$$\mathbf{1 - (1 - \mathit{t}^{\,r})^{b}}$$

Some row of a band unequal

All rows of a band are equal

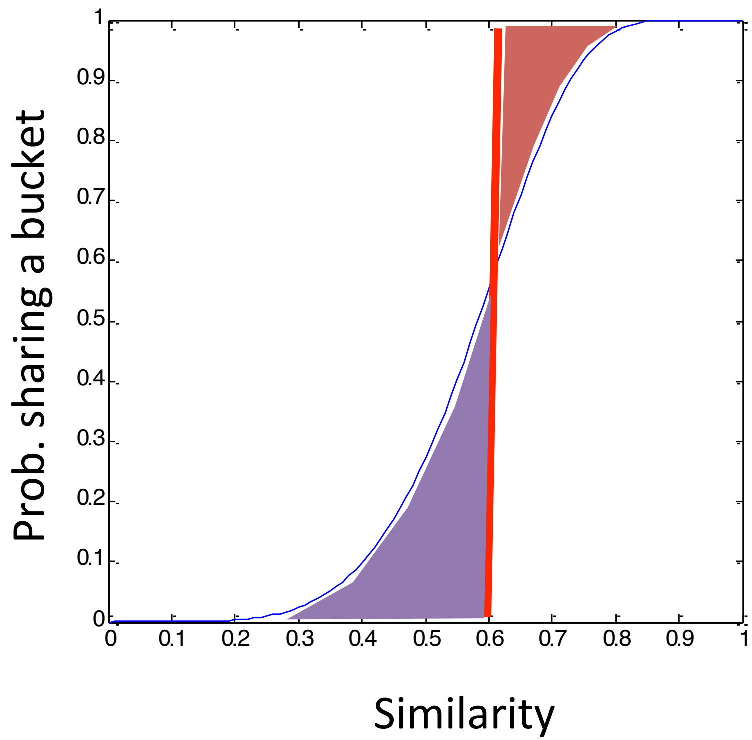
Example: $b = 20$; $r = 5$

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

s	$1-(1-s^r)^b$
.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 ***M, 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 $\mathbf{Pr}[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
  - 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

LSH: Locality Sensitive Hashing C'02

- U = Universe of objects
- S: $U \times U \to [0, 1]$ = Similarity function

An LSH for a similarity S is a probability distribution over a set $\mathcal{H}$ of hash functions such that

$$\Pr_{h \in \mathcal{H}} [h(A) = h(B)] = S(A, B)$$

for each $A, B \in U$

LSH: Gap definition IMRS'97, IM'98, GIM'99

- $S: U \times U \to [0, 1]$ = Similarity function over a universe U of objects

An (r, R, p, P)-LSH for a similarity S is a probability distribution over a set $\mathcal{H}$ of hash functions such that

- $S(A, B) \geq R \Rightarrow \Pr_{h \in \mathcal{H}} [h(A) = h(B)] > P$
- $S(A, B) < r \Rightarrow \Pr_{h \in \mathcal{H}} [h(A) = h(B)] < p$

for each $A, B \in U$; here, $r < R$ and $P > p$

Original definition implies an (r, R, r, R) gap version

Eg 1. Hamming similarity

- Given two n-bit vectors x and y

$$HS(x, y) = \#\{\, i : x_i = y_i \,\}/n$$

- Eg, disjoint vectors have similarity 0 and HS(x, x) = 1

  x = 01001, y = 10011, HS(x, y) = 2/5

- 1 – HS(x, y) is the Hamming distance metric

Sampling hash IM'98

- $\mathcal{H} = \{h_1, \ldots, h_n\}$, where $h_i(x) = x_i$
  - The i-th hash function outputs the i-th bit of x

Claim. Sampling hash forms an LSH for Hamming similarity

$$\Pr[h(x) = h(y)] = \Pr_i[h_i(x) = h_i(y)] = HS(x, y)$$

Eg 2. Jaccard similarity

- Given two sets A and B

$$J(A, B) = |A \cap B| \ / \ |A \cup B|$$

- Eg, disjoint sets have similarity 0 and $J(A, A) = 1$

  $A = \{1, 2\}$, $B = \{2, 3\}$, $J(A, B) = 1/3$

- $1 - J(A, B)$ is a metric
- Used extensively in many scientific and sociological applications
- Paul Jaccard introduced this similarity in 1901 for comparing and clustering fields of flowers on the Alps

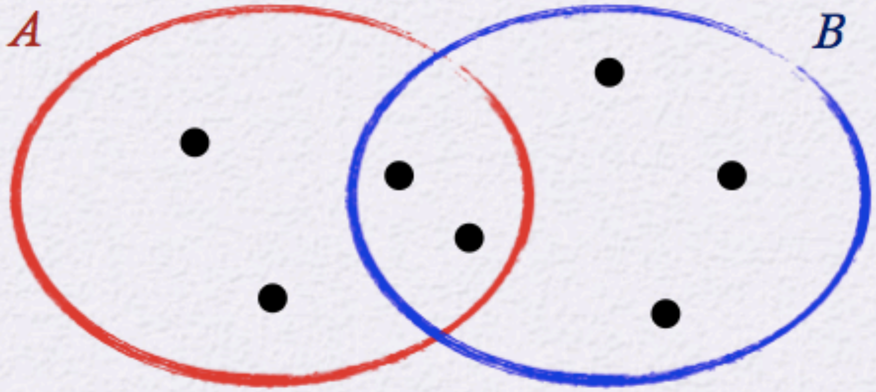
MinHash B'97, BCFM'00

- Given a universe U, pick a permutation π on U uniformly at random
- Hash each subset $S \subseteq U$ to the minimum value it contains according to π
- Eg, $A = \{1, 2\}$, $B = \{2, 3\}$

$\pi = (1 < 2 < 3)$, $h(A) = 1$, $h(B) = 2$
$\pi = (1 < 3 < 2)$, $h(A) = 1$, $h(B) = 3$
$\pi = (2 < 1 < 3)$, $h(A) = 2$, $h(B) = 2$
$\pi = (2 < 3 < 1)$, $h(A) = 2$, $h(B) = 2$
$\pi = (3 < 1 < 2)$, $h(A) = 1$, $h(B) = 3$
$\pi = (3 < 2 < 1)$, $h(A) = 2$, $h(B) = 3$

MinHash (contd)

Claim. MinHash forms an LSH for Jaccard similarity



$\Pr[h(A) = h(B)] = |A \cap B| \ / \ |A \cup B| = J(A, B)$

Eg 3. Angle similarity

- Given two unit vectors x and y

  $\theta(x, y)$ = angle between x and y

- Natural measure of similarity for high-dimensional vectors

- Eg, $\theta(x, x) = 0$ and $\theta(x, y)$ maximum at $y = -x$

  $x = (\sqrt{3}/2, 1/2)$, $y = (1/\sqrt{2}, 1/\sqrt{2})$, $\theta(x, y) = \pi/12$

- Used extensively in text processing, machine learning applications

SimHash C'02

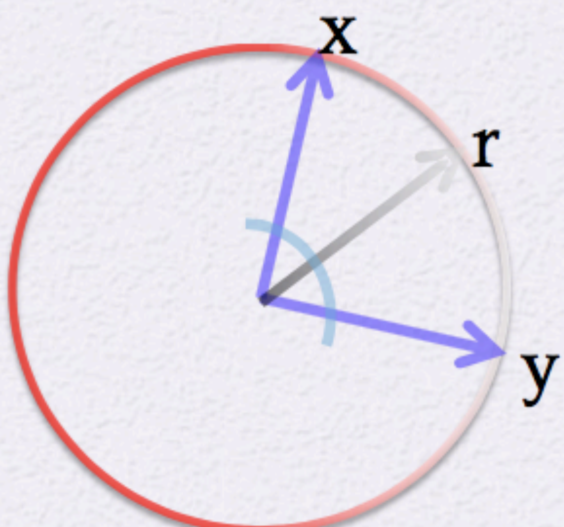
- Pick a random unit vector r
- Hash each vector x by computing $\mathrm{sgn}\langle x, r\rangle$

Eg, $x = (\sqrt{3}/2, 1/2)$, $r = (0.41, -0.91)$, $h(x) = -0.1$

- Can also pick each entry of r from $N(0, 1)$ and normalize

SimHash (contd)

Claim. SimHash forms an LSH for angle similarity



$$\Pr[h(x) = h(y)] = 1 - \theta(x, y)/\pi$$

A different set similarity measure: if x and y are characteristic vectors $\theta = \arccos(|A \cap B| / (\sqrt{A}\sqrt{B}))$

A metric condition C'02

Theorem. S is LSHable $\Rightarrow$ 1 – S is a metric

Proof. Fix a hash function h and define

$$\Delta_h(\mathrm{A}, \mathrm{B}) \equiv [\mathrm{h}(\mathrm{A}) \neq \mathrm{h}(\mathrm{B})]$$

$$1 - \mathrm{S}(\mathrm{A}, \mathrm{B}) = \mathrm{Pr}_{\mathrm{h} \in \mathcal{H}}\, \Delta_h(\mathrm{A}, \mathrm{B})$$

$\Delta_h(\mathrm{A}, \mathrm{B})$ satisfies the triangle inequality

$$\Delta_h(\mathrm{A}, \mathrm{B}) + \Delta_h(\mathrm{B}, \mathrm{C}) \geq \Delta_h(\mathrm{A}, \mathrm{C})$$