CS60021: Scalable Data Mining

Similarity Search and Hashing

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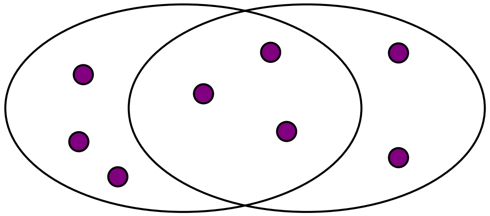
Finding Similar Items

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

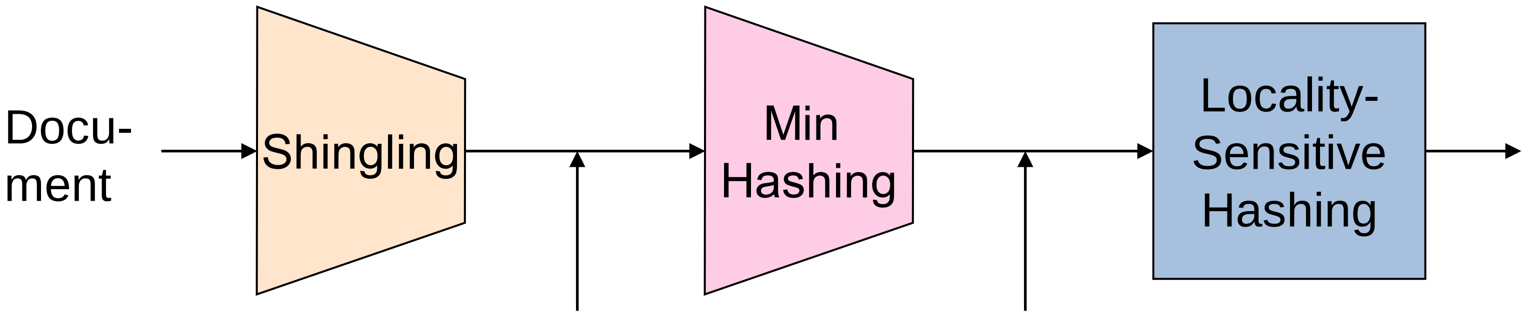
3 Essential Steps for Similar Docs

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!**

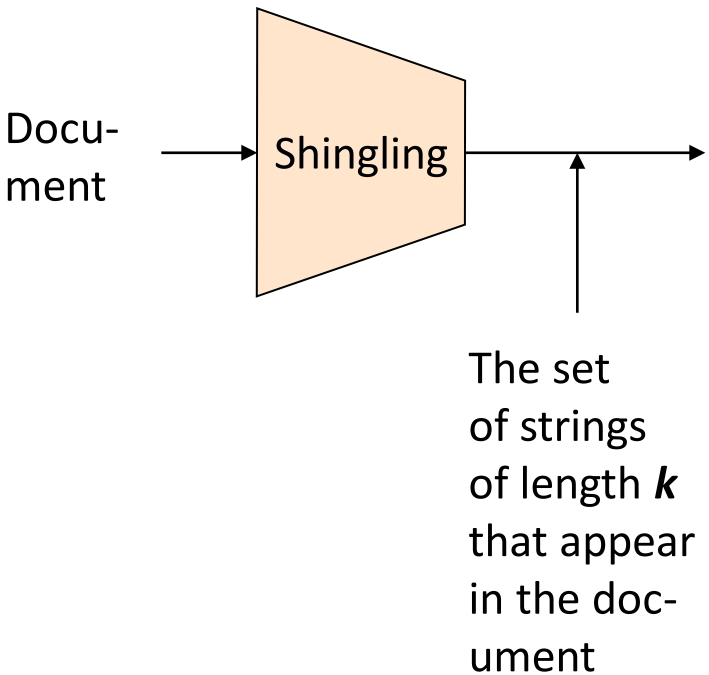
The Big Picture



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

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



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}

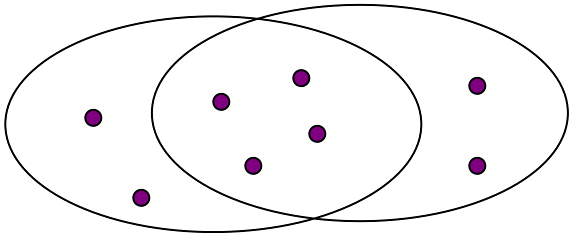
Represent Shingles

- 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:** **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**

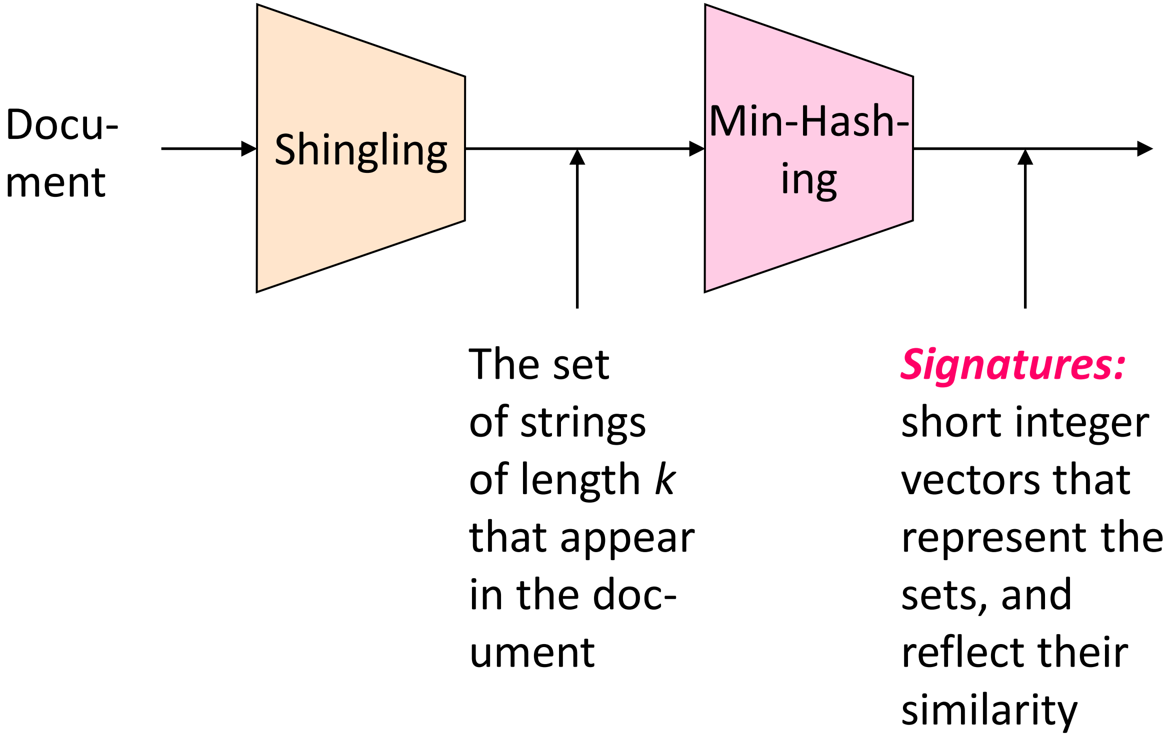
- **Caveat:** You must pick ***k*** large enough, or most documents will have most shingles
  - ***k*** = 5 is OK for short documents
  - ***k*** = 10 is better for long documents

Motivation for Minhash / LSH

- **Suppose we need to find near-duplicate documents among $\boldsymbol{N}=\mathbf{1}$ million documents**

- Naïvely, we would have to compute **pairwise Jaccard similarities** for **every pair of docs**
  - $\boldsymbol{N}(\boldsymbol{N}-\mathbf{1})/\mathbf{2}$ ≈ **$5 * 10^{11}$** comparisons
  - At 10^5 secs/day and 10^6 comparisons/sec, it would take **5 days**

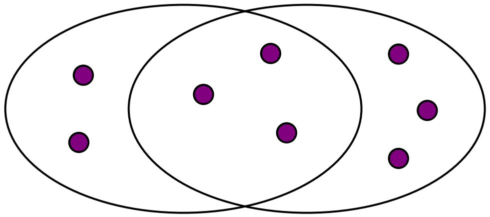
- For $\boldsymbol{N}=\mathbf{10}$ million, it takes more than a year…



MinHashing

Step 2: ***Minhashing:*** Convert **large sets** to **short signatures**, while **<u>preserving similarity</u>**

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 $h(\cdot)$ 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. $h(C_1) \neq h(C_2)$

- **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 $\boldsymbol{sim(C_1,C_2)}$ is high, then with high prob. $\boldsymbol{h(C_1) = h(C_2)}$
  - if $\boldsymbol{sim(C_1,C_2)}$ is low, then with high prob. $\boldsymbol{h(C_1) \neq h(C_2)}$
- **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), $\boldsymbol{y} \in \boldsymbol{X}$ is a shingle
  - **Then:** **$Pr[\pi(y) = \min(\pi(X))] = 1/|X|$**
    - It is equally likely that any $\boldsymbol{y} \in \boldsymbol{X}$ 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. $\boldsymbol{y} \in C_1 \cap C_2$
  - **$Pr[\min(\pi(C_1)) = \min(\pi(C_2))] = |C_1 \cap C_2| / |C_1 \cup C_2| = sim(C_1, C_2)$**

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: $\mathbf{Pr}[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
- 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*

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

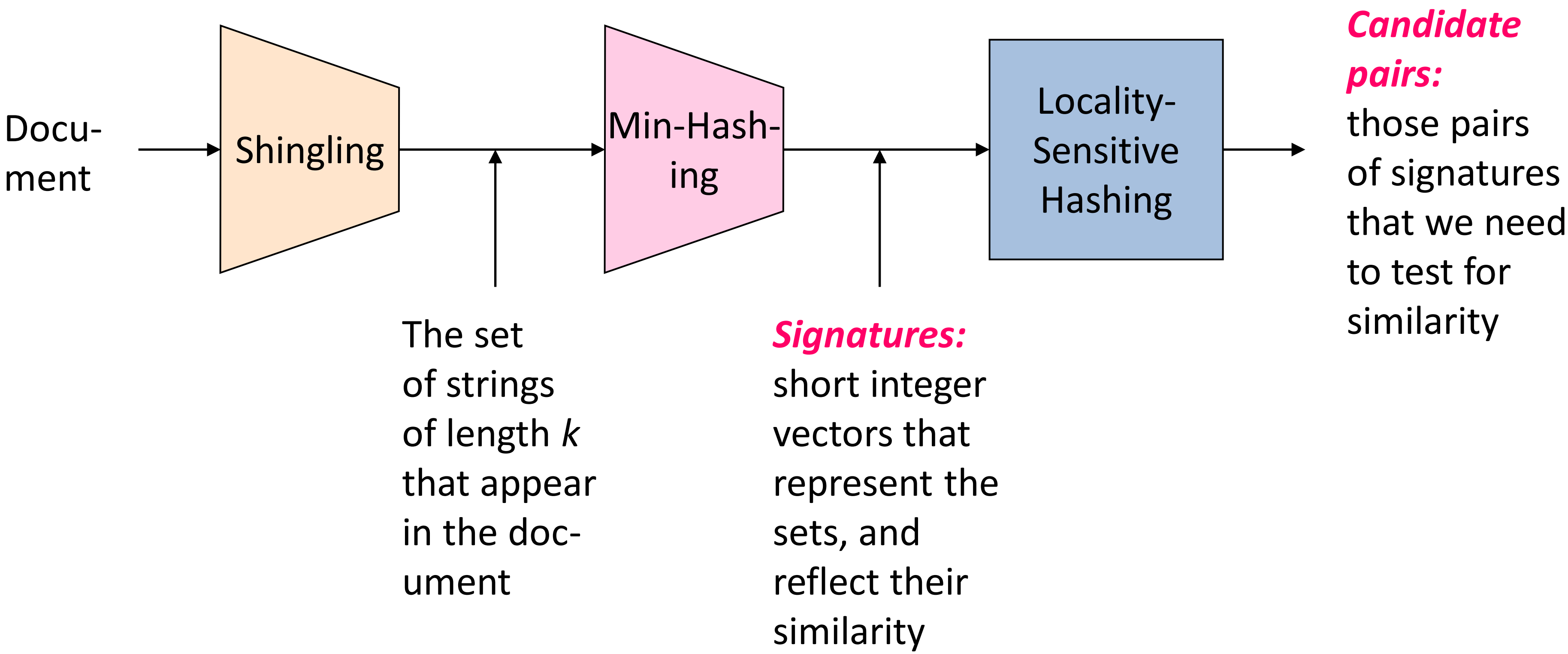
- **Note:** The sketch (signature) of document *C* is small $\sim$**100 bytes!**

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

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:
  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

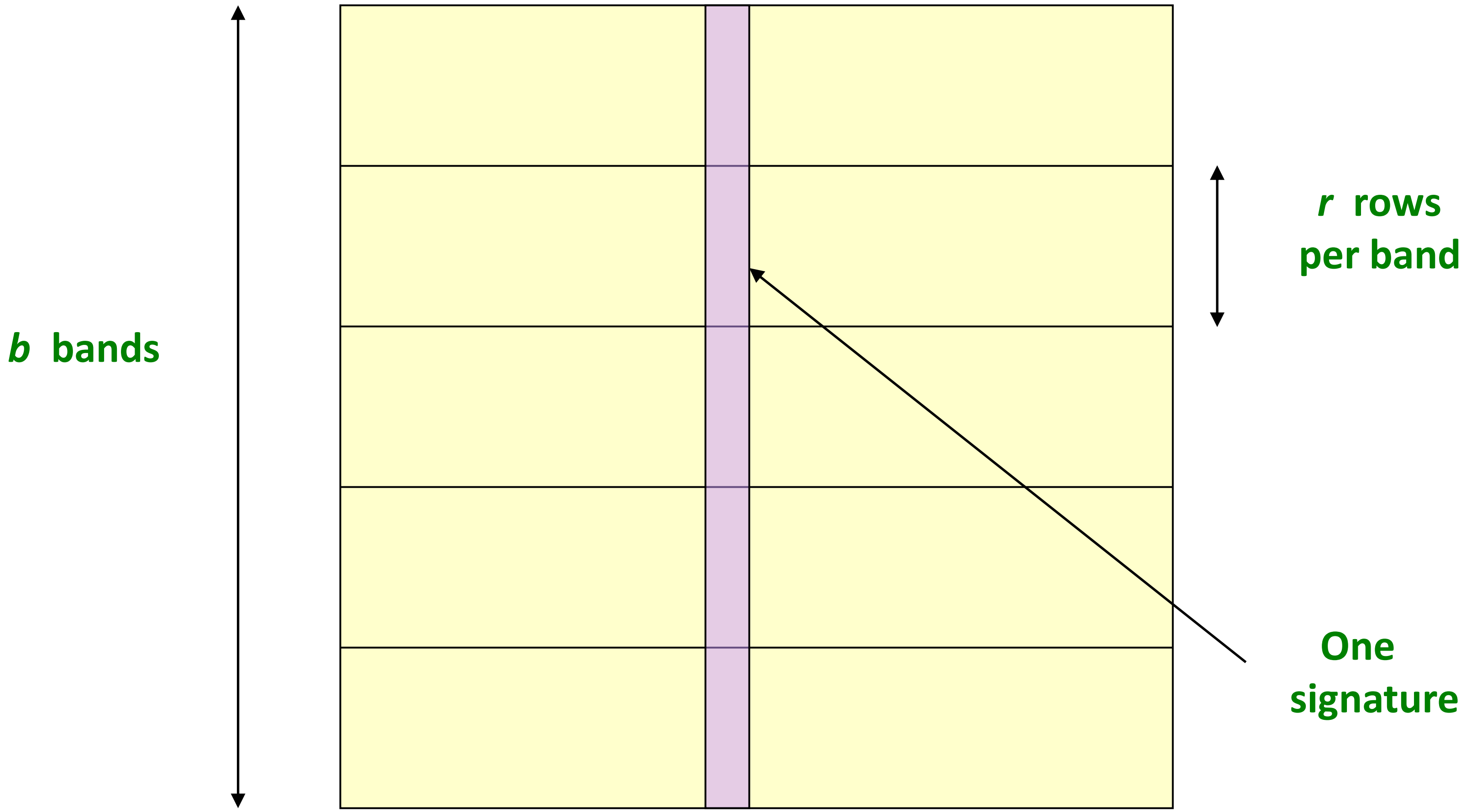
LSH for Min-Hash

- **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

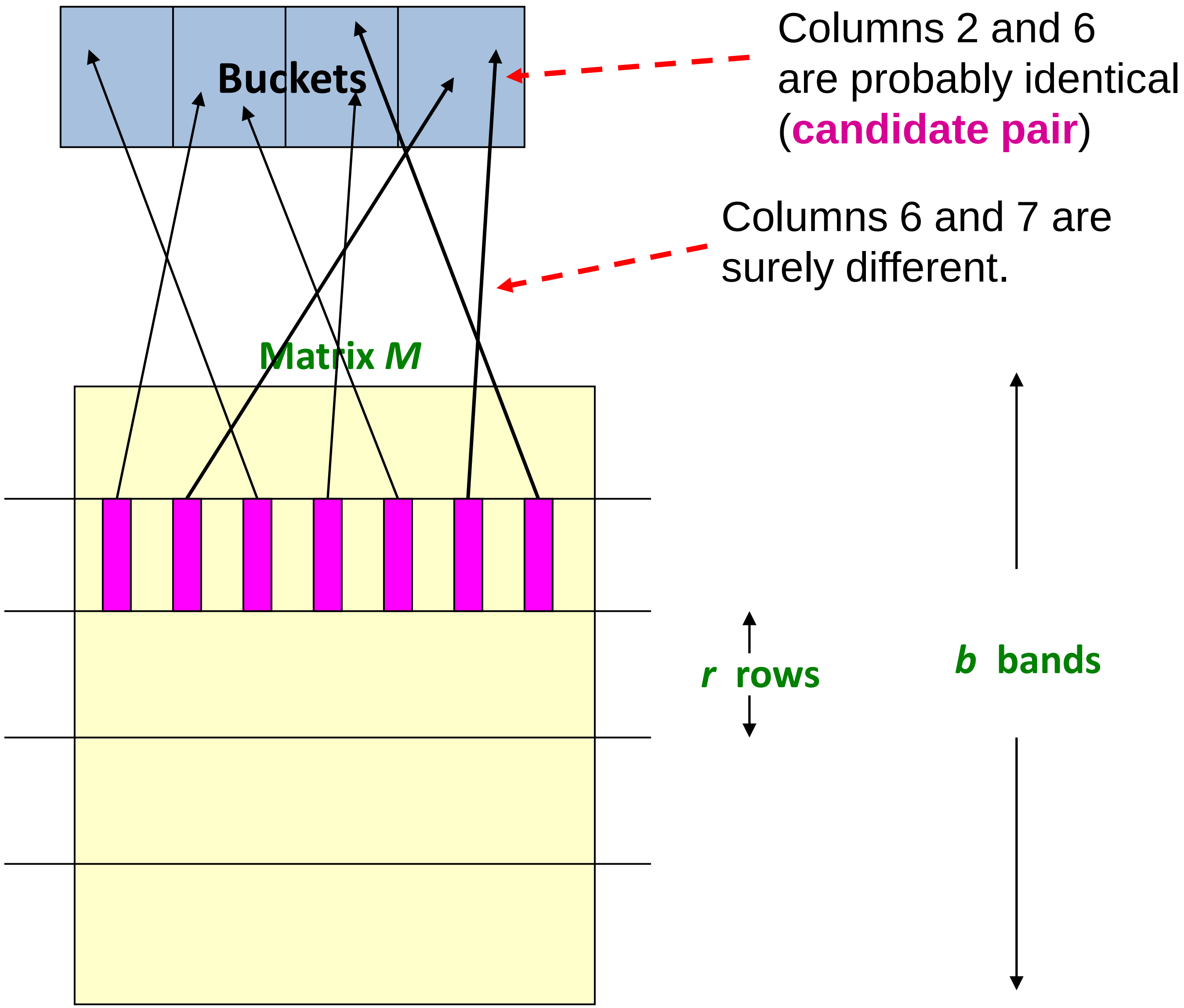


Signature matrix *M*

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: $(1-0.328)^{20} = 0.00035$
  - 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:** $\text{sim}(C_1, C_2) = 0.3$
  - Since $\text{sim}(C_1, C_2) < \mathbf{s}$ 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**

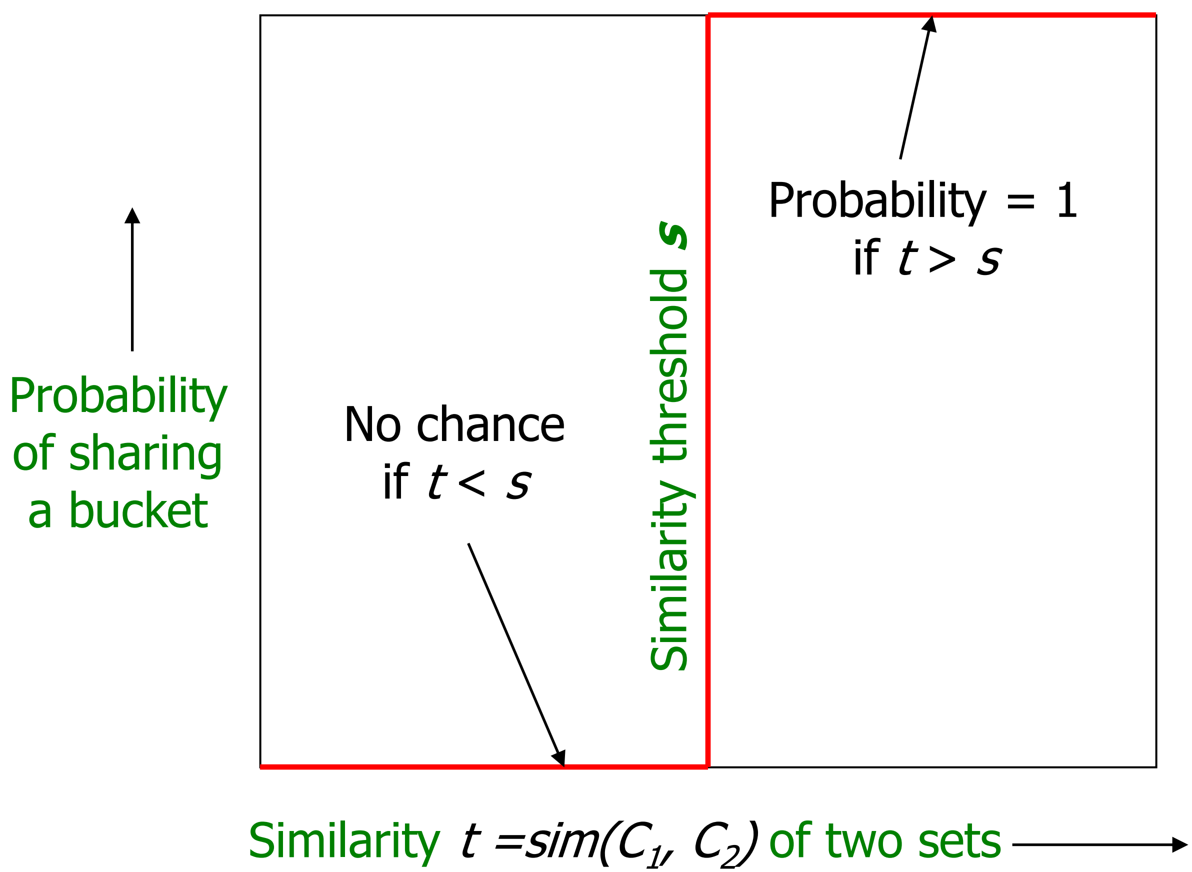
LSH Involves a Tradeoff

- **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

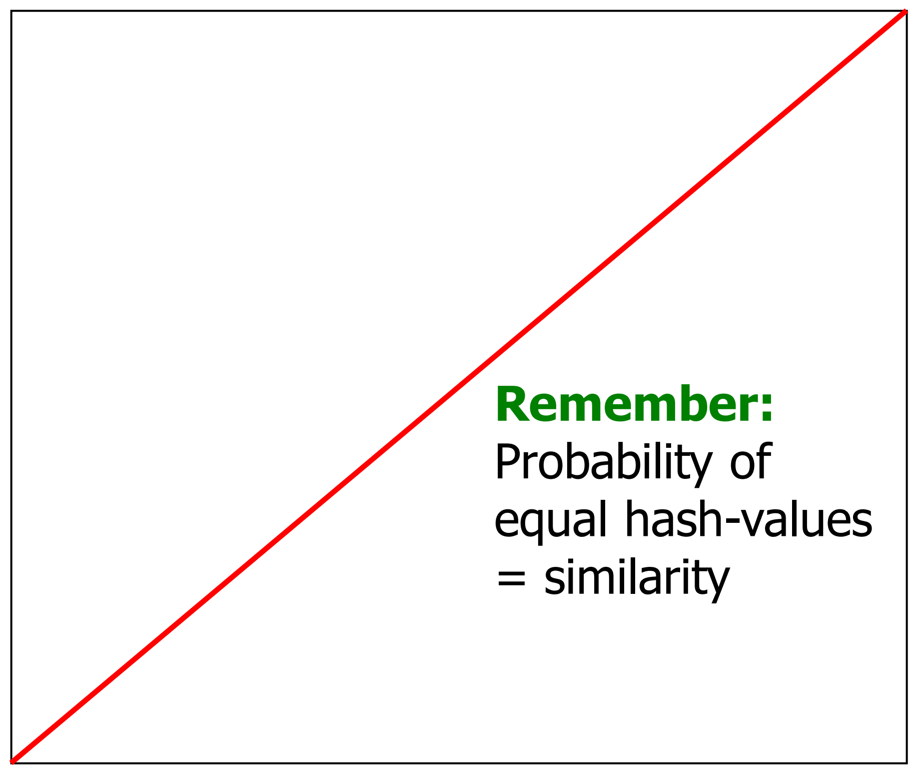
- **Example:** If we had only 15 bands of 5 rows, the number of false positives would go down, but the number of false negatives would go up

Analysis of LSH – What We Want



What 1 Band of 1 Row Gives You

Probability of sharing a bucket



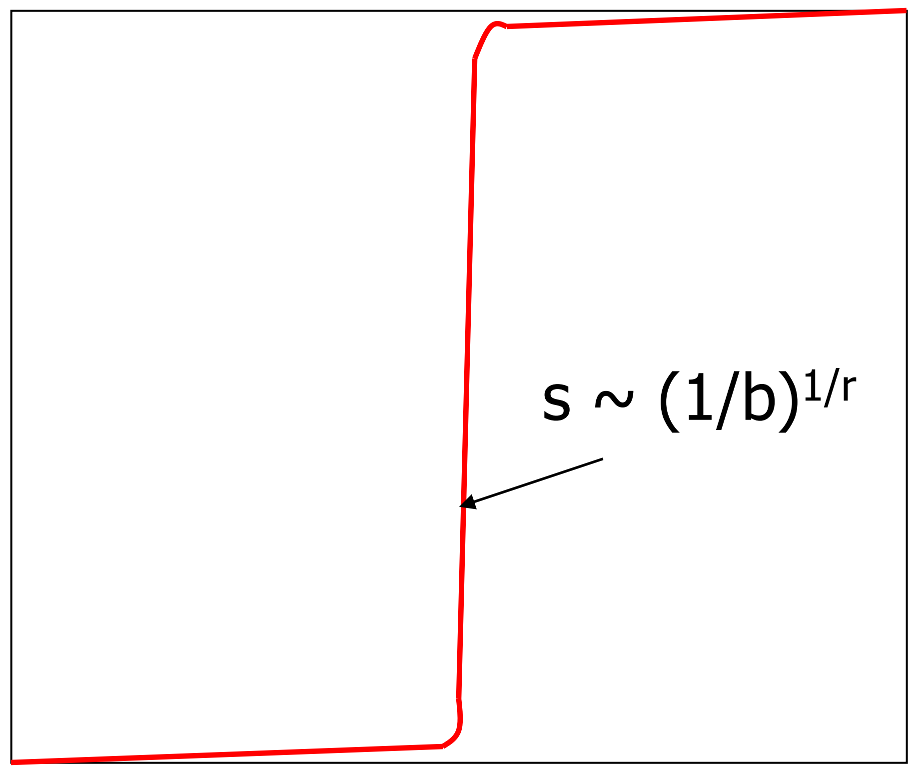
Similarity $t = sim(C_1, C_2)$ of two sets

b bands, *r* rows/band

- Columns C_1 and C_2 have similarity $\boldsymbol{t}$
- Pick any band ($\boldsymbol{r}$ rows)
  - Prob. that all rows in band equal = $\boldsymbol{t^r}$
  - Prob. that some row in band unequal = $\mathbf{1 -} \boldsymbol{t^r}$
- Prob. that no band identical = $\mathbf{(1 -} \boldsymbol{t^r}\mathbf{)}^{\boldsymbol{b}}$
- Prob. that at least 1 band identical =

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

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

$$\mathbf{1 - (1 - s^r)^b}$$

Some row of a band unequal

All rows of a band are equal

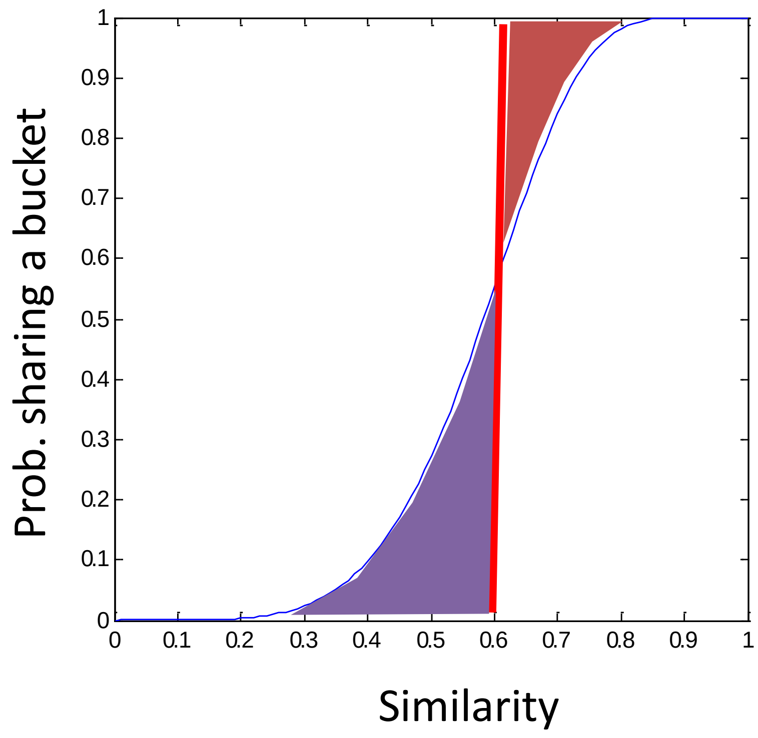
Example: $b = 20$; $r = 5$

- **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**

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