Data-Intensive Distributed Computing

CS 431/631 451/651 (Winter 2022)

Part 6: Data Mining (3/4)

Dan Holtby

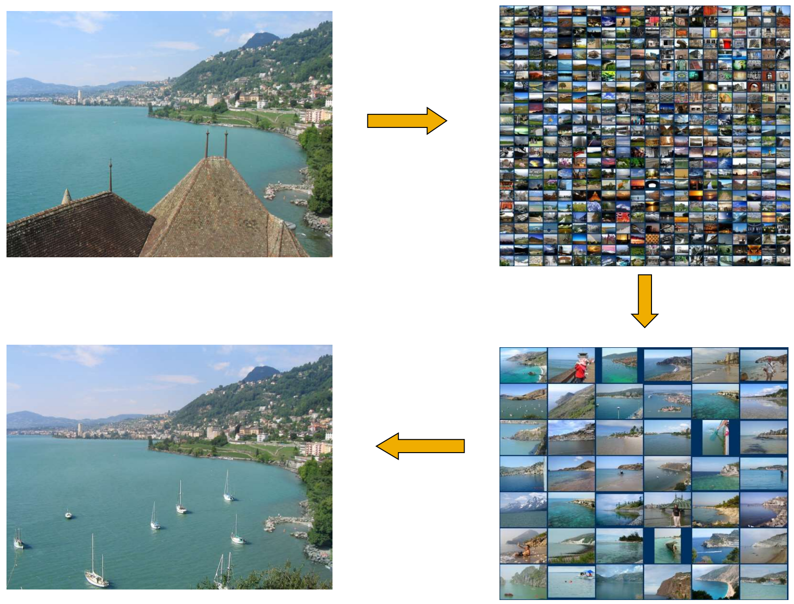
~~Ali Abedi~~

Thanks to Jure Leskovec, Anand Rajaraman, Jeff Ullman (Stanford University)

These slides are available at https://www.student.cs.uwaterloo.ca/~cs451

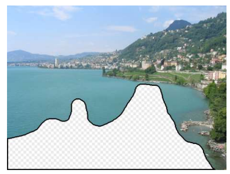
[Hays and Efros, SIGGRAPH 2007]

Scene Completion Problem



[Hays and Efros, SIGGRAPH 2007]

Scene Completion Problem

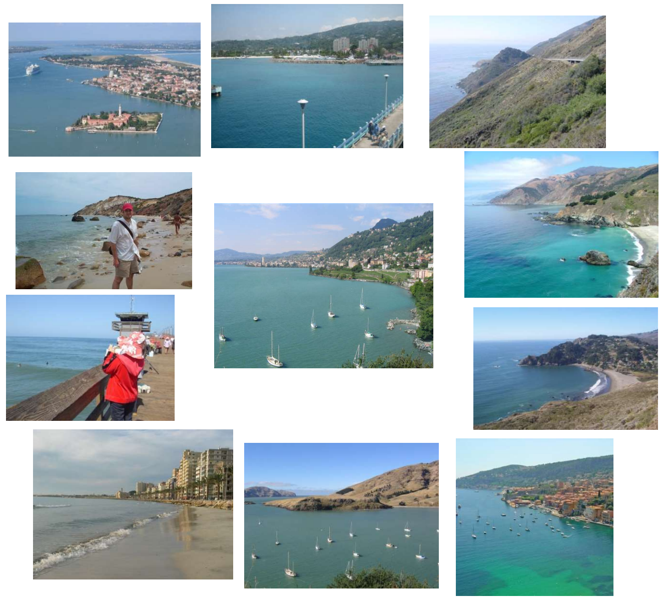


10 nearest neighbors, 20,000 image database

10 nearest neighbors, 20,000 image database

[Hays and Efros, SIGGRAPH 2007]

Scene Completion Problem

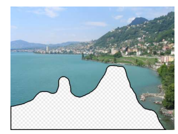


10 nearest neighbors from a collection of 2 million images

10 nearest neighbors, 2.3 million image database

A Common Metaphor

- **Many problems can be expressed as finding "similar" sets:**
  - **Find near-neighbors in high-dimensional space**
- **Examples:**
  - **Pages with similar words**
    - For duplicate detection, classification by topic
  - **Customers who purchased similar products**
    - Products with similar customer sets
  - **Images with similar features**
    - Users who visited similar websites



Problem for Today's Lecture

- **Given: High dimensional data points $x_1, x_2, \ldots$**
  - **For example:** Image is a long vector of pixel colors

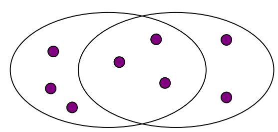
$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{bmatrix} \rightarrow [1\ 2\ 1\ 0\ 2\ 1\ 0\ 1\ 0]$$

- **And some distance function $d(x_1, x_2)$**
  - Which quantifies the "distance" between x_1 and x_2
- **Goal:** Find **all pairs of data points** (x_i, x_j) that are within some distance threshold $d(x_i, x_j) \leq s$
- **Note:** Naïve solution would take $O(N^2)$ ☹ where N is the number of data points
- **MAGIC: This can be done in $O(N)$!! How?**

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



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

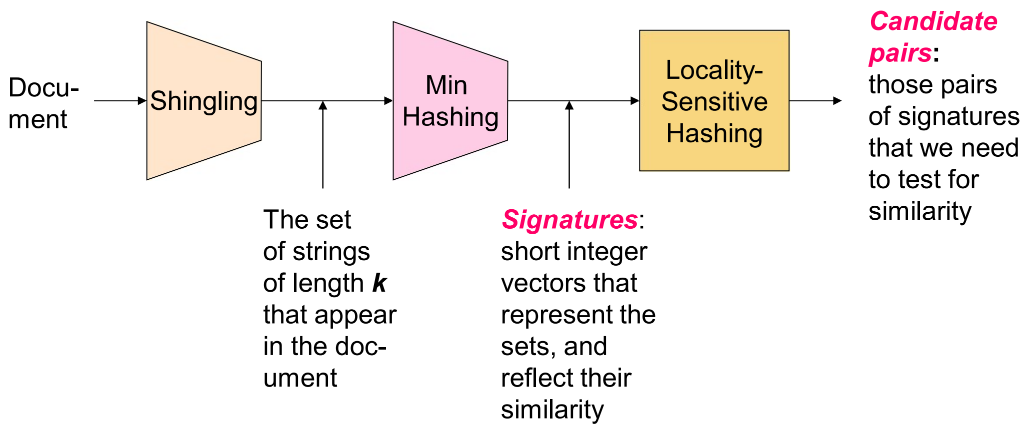
Task: Finding Similar Documents

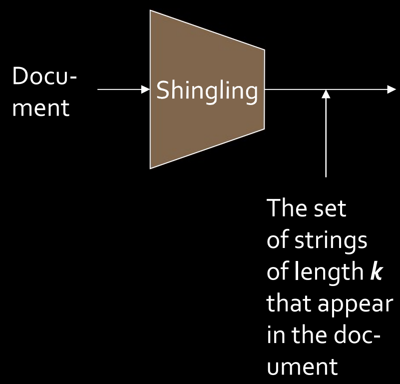
- **Goal: Given a large number (N in the millions or billions) of documents, find "near duplicate" pairs**
- **Applications:**
  - Mirror websites, or approximate mirrors
    - Don't want to show both in search results
  - Similar news articles at many news sites
    - Cluster articles by "same story"
- **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





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!**

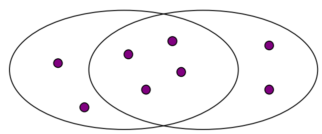
Define: Shingles

- 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}

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:**

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



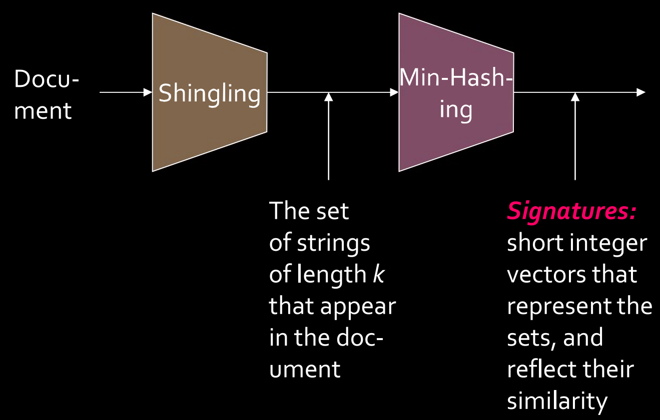
Working Assumption

- **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

Here the k is for letter shingles
The k for word shingles is 2-3 for short documents like emails and 3-4 for longer documents.

Motivation for Minhash/LSH

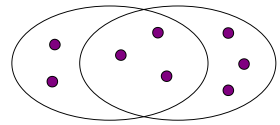
- **Suppose we need to find near-duplicate documents among $N = 1$ million documents**
- Naïvely, we would have to compute **pairwise Jaccard similarities** for **every pair of docs**
  - $\boldsymbol{N(N-1)/2}$ **≈ 5*10¹¹** comparisons
  - At 10^5 secs/day and 10^6 comparisons/sec, it would take **5 days**
- For $\boldsymbol{N = 10}$ 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 $\rightarrow$ 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 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. $h(C_1) \neq h(C_2)$

Min-Hashing

- **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. $h(C_1) \neq h(C_2)$
- **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 $y \in C_2$

    One of the two cols had to have 1 at position ***y***
  - So the prob. that **both** are true is the prob. $y \in C_1 \cap C_2$
  - $\Pr[\min(\pi(C_1)) = \min(\pi(C_2))] = |C_1 \cap C_2| / |C_1 \cup C_2| = sim(C_1, C_2)$

Size of the universe of all possible vals of $\min(\pi(C_1 \cup C_2))$ is $|C_1 \cup C_2|$ and in $|C_1 \cap C_2|$ of cases it can be that $\min(\pi(C_1)) = \min(\pi(C_2))$ which exactly the jaccard between C1 and C2

For two columns A and B, we have h_π(A) = h_π(B) exactly when the minimum hash value of the union A ∪ B lies in the intersection A ∩ B. Thus Pr[h_π(A) = h_π(B)] = |A ∩ B| / |A ∪ B|.

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 **~400 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)

Dan's commentary

Prohibitive why? Each permutation is of n rows, where n is the number of different shingles. Take for example, letter-level 10-grams. 26^10 = 141167095653376. Specifying such a permutation requires n log n bits = 2TB. That's…not small. And we need 100 of them. Note that's just the number of bits required to specify WHICH permutation you've selected. Even with that, it's still computationally expensive to compute the permutation.

Alternative? We could restrict ourself to a minimal family of permutations that will still have the property we want. However, information theory tells us that's still going to need Ω(n) bits, and still going to be computationally expensive to compute given that specification.

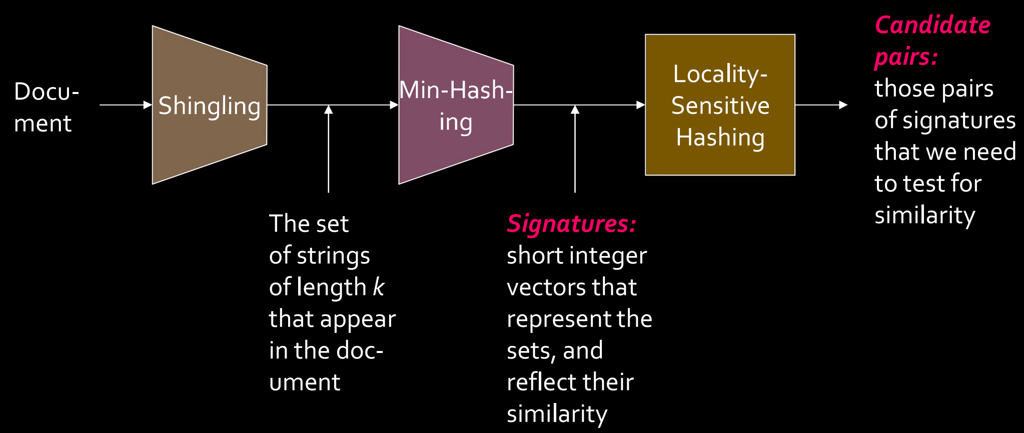
So, we need something called "k-wise independent hash functions" or "k-universal hash functions".
These are hash functions with the property that if you select a random k-universal function, then for any set of k values v1 … vk, then h(v1), … h(vk) will be k independent random variables.

See next slide…

K-Universal Hashing

- A (k-1) degree polynomial is a k-universal hash function
- If we replace π with h_k then…
  - **$Pr[h_k(y) = \min(h_k(X))] = 1/|X|\ (1 \pm \varepsilon)$**
  - $\varepsilon = e^{-k}$
  - E.g. if we use degree 3 (4 random parameters) the expected value is within 2% of the Jaccard similarity
- [Dan added this slide]

If you use the universal function on the previous slide, $\varepsilon = 0.13$, which is a pretty big divergence. I think…
On the other hand, since you're doing e.g. 100 of these functions. Since it's +-, over 100 rows the expected similarity count for the signature will still be (almost) equal to the Jaccard similarity, even if individual elements
can diverge by up to 13%



Locality Sensitive Hashing

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

LSH: First Cut

2	1	4	1
1	2	1	2
2	1	2	1

- **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

2	1	4	1
1	2	1	2
2	1	2	1

- **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

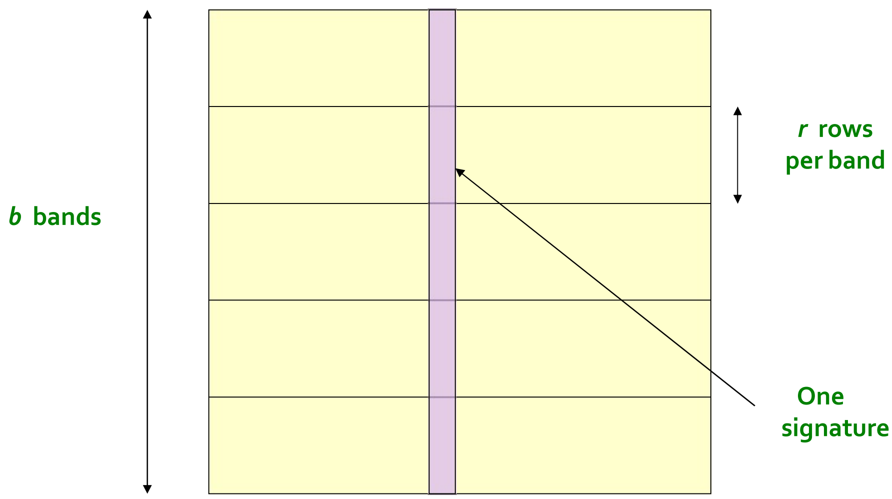
LSH for Min-Hash

2	1	4	1
1	2	1	2
2	1	2	1

- **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

2	1	4	1
1	2	1	2
2	1	2	1

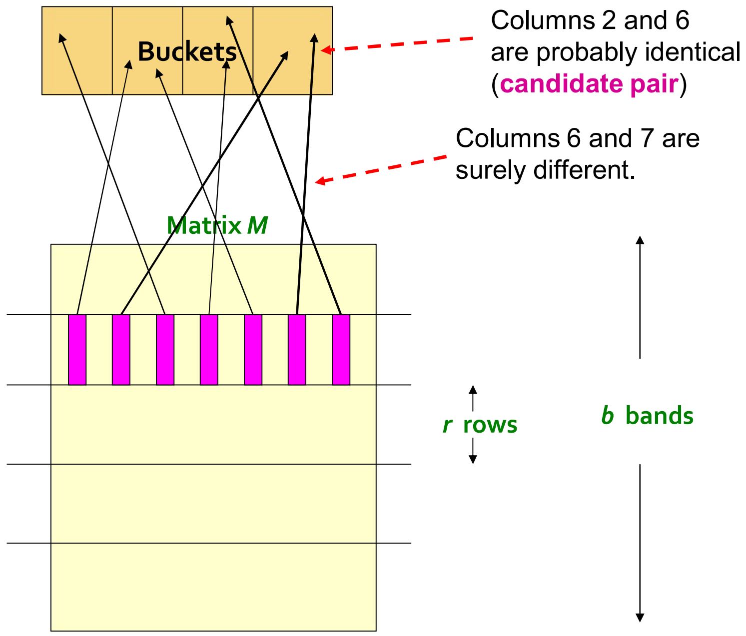


Signature matrix *M*

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 $\geq$ **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

2	1	4	1
1	2	1	2
2	1	2	1

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

2	1	4	1
1	2	1	2
2	1	2	1

- **Find pairs of** $\geq$ ***s***=0.8 similarity, set **b**=20, **r**=5
- **Assume:** sim(C_1, C_2) = 0.8
  - Since sim(C_1, C_2) $\geq$ **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

2	1	4	1
1	2	1	2
2	1	2	1

- **Find pairs of** $\geq$ ***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

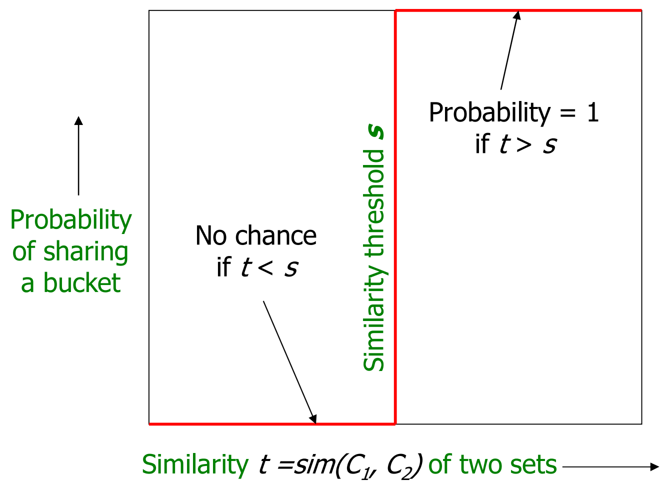
2	1	4	1
1	2	1	2
2	1	2	1

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

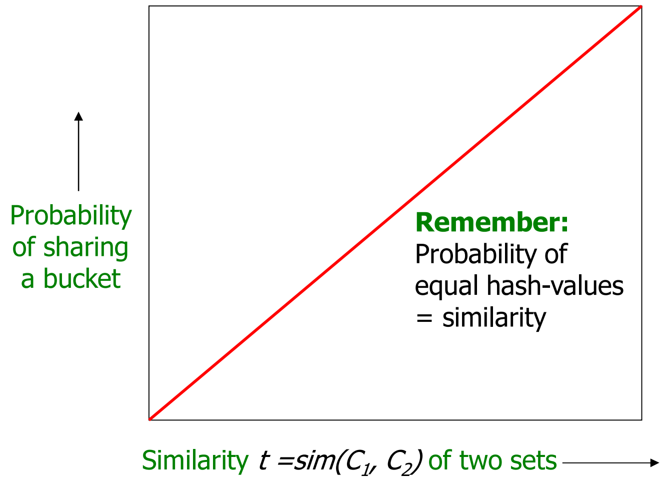
  to balance false positives/negatives

- **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



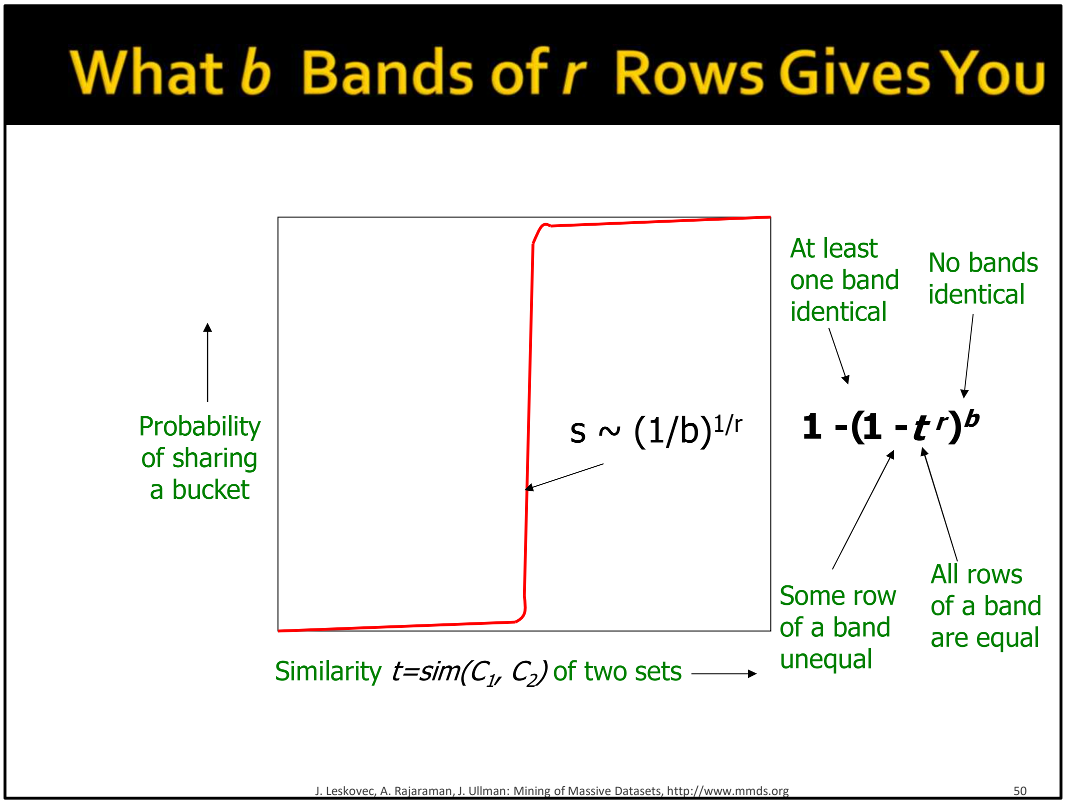
What 1 Band of 1 Row Gives You



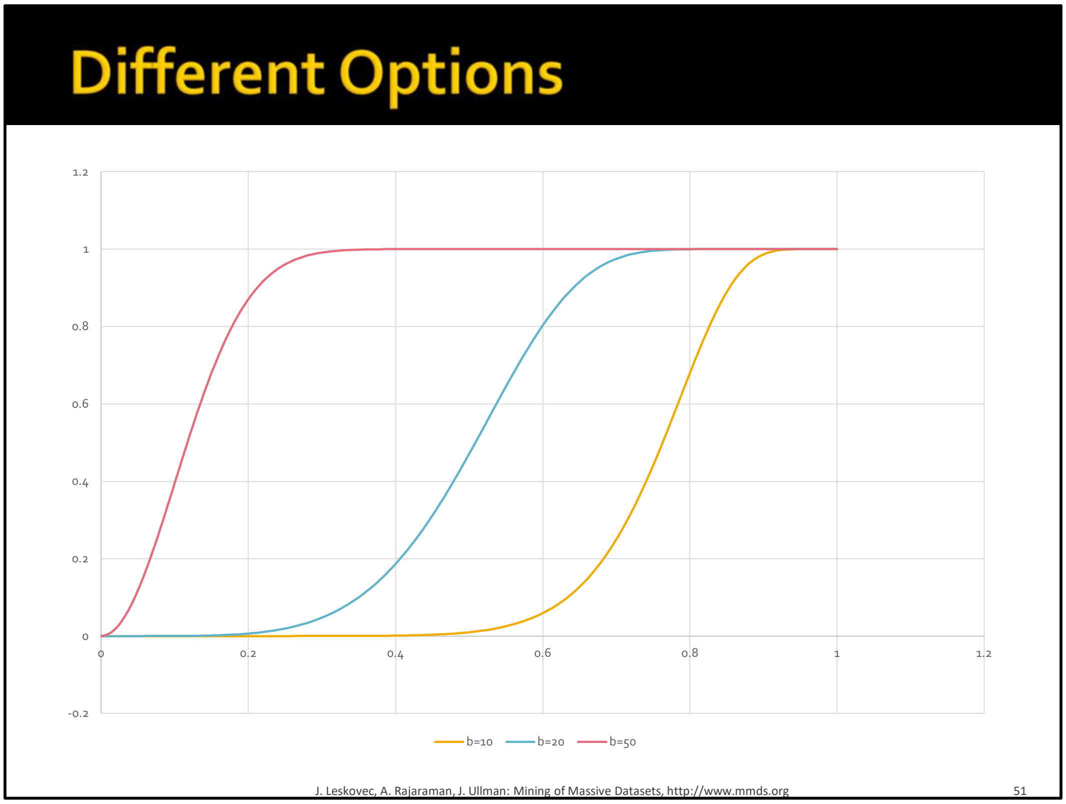
b bands, r rows/band

- 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 =

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



That bump at the top is because drawing is hard. It's an S curve, similar to the sigmoid functions we've seen before



Different values for b, given 100 elements in the signatures. (b * r = 100)

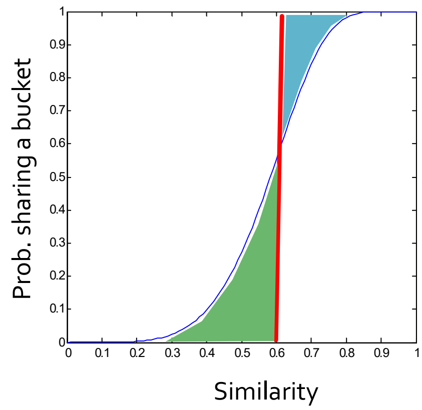
Example: $b = 20$; $r = 5$

- 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**