Introduction to Data Mining

Lecture #5: Finding Similar Items

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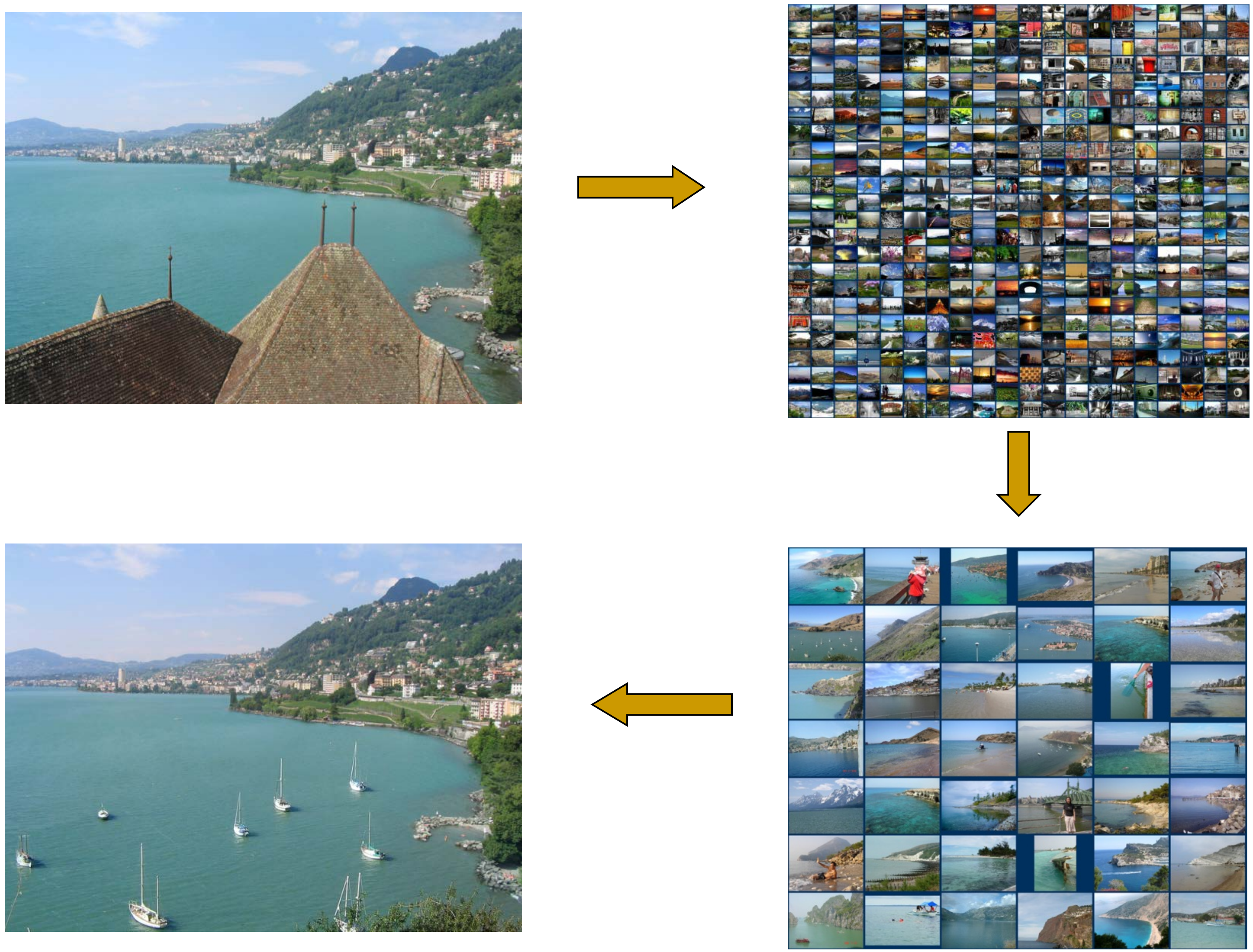
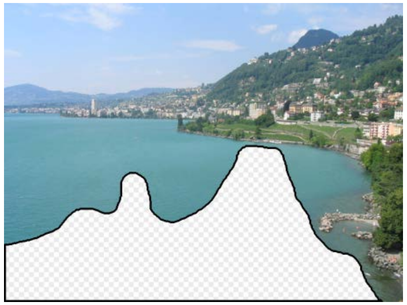
Outline

- ☐ **Motivation**
- ☐ Finding Similar Items

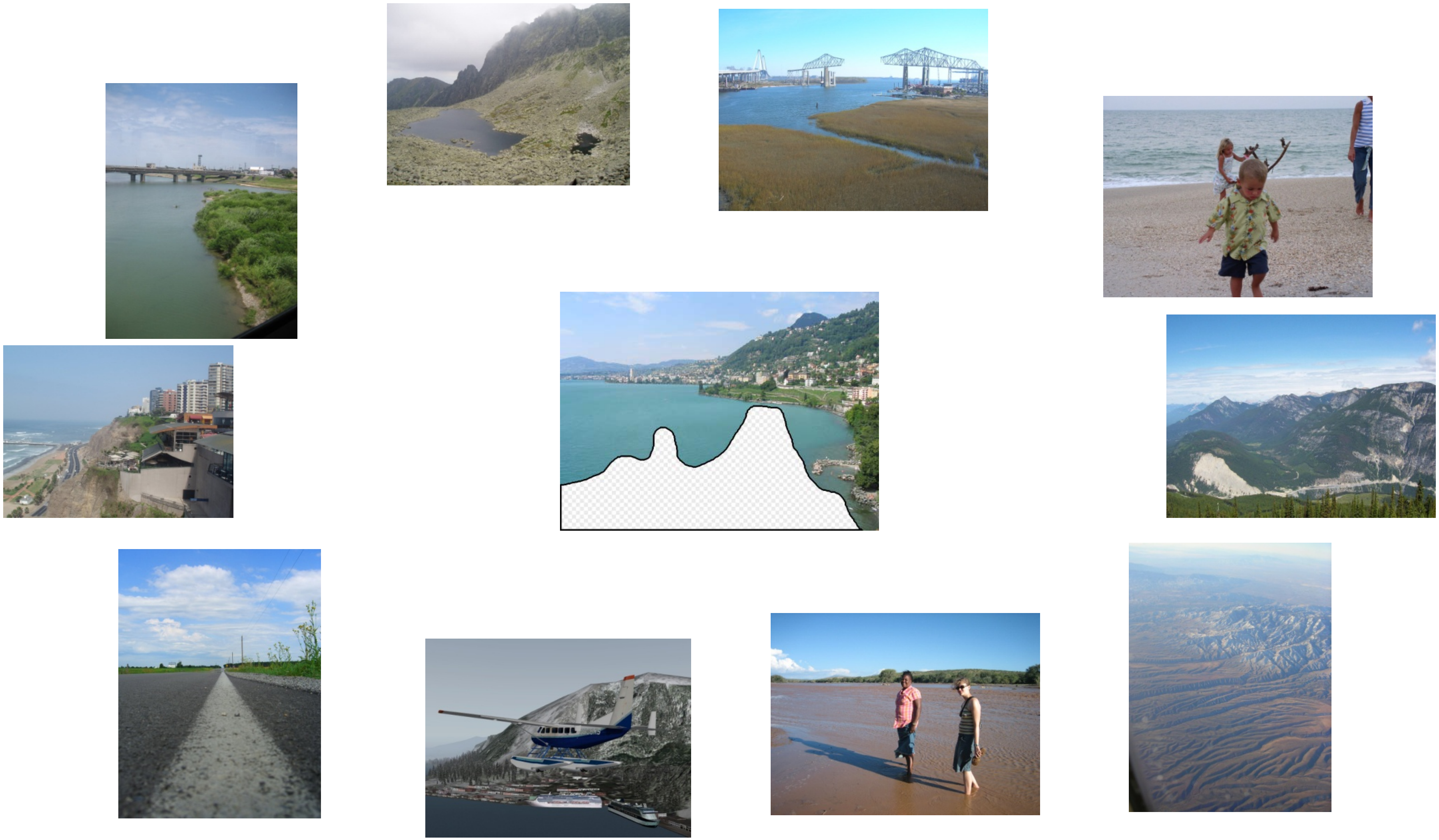
Scene Completion Problem



Scene Completion Problem

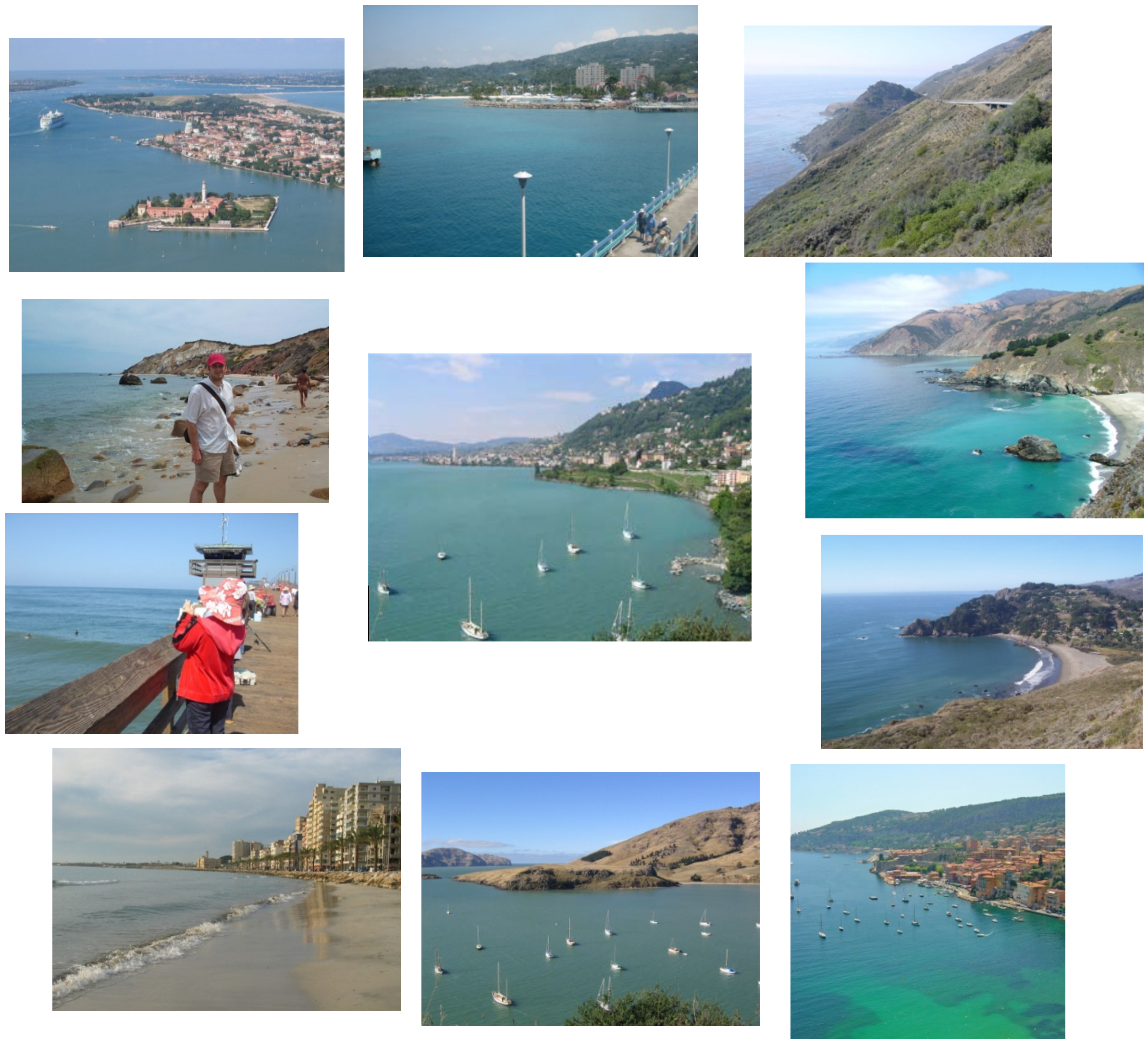


Scene Completion Problem



10 nearest neighbors from a collection of 20,000 images

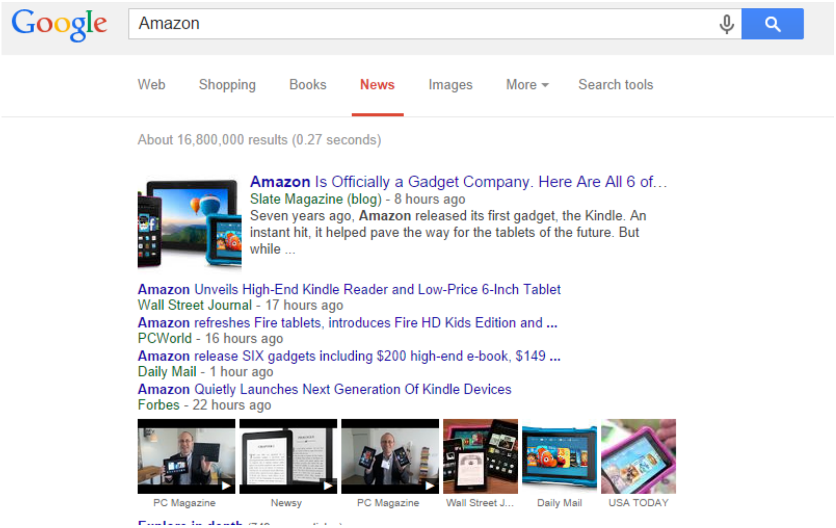
Scene Completion Problem



10 nearest neighbors from a collection of 20,000 images

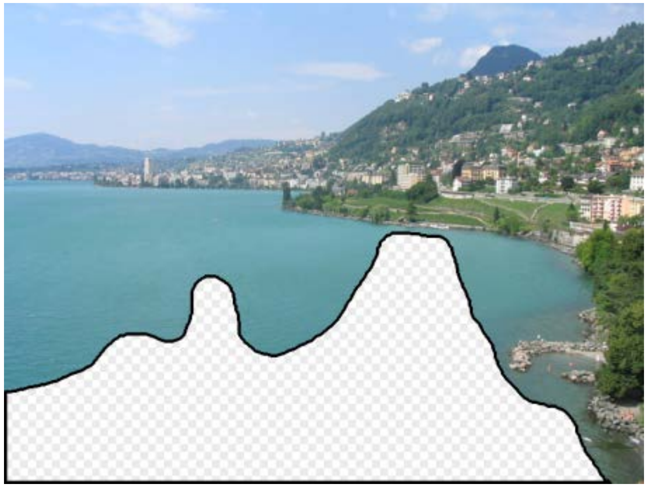
A Common Metaphor

- **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



A Common Metaphor

- **Examples (cont.):**
  - **Customers who purchased similar products**
    - Products with similar customer sets
  - **Images with similar features**
    - Scene completion



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

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

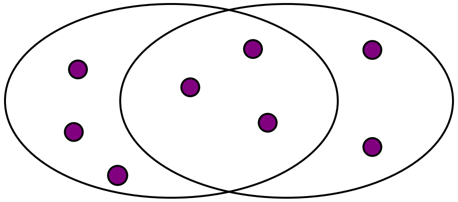
- **And some distance function $d(x_1, x_2)$**
  - Which quantifies the "distance" between x_1 and x_2
- **Goal:** Find **all pairs of data points (x_i, x_j)** that are within some distance threshold $d(x_i, x_j) \le s$
- **Note:** Naïve solution would take $O(N^2)$ ☹
  where N is the number of data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

Outline

- ☑ Motivation
- ☐ **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:** $d(C_1, C_2) = 1 - |C_1 \cap C_2| / |C_1 \cup C_2|$

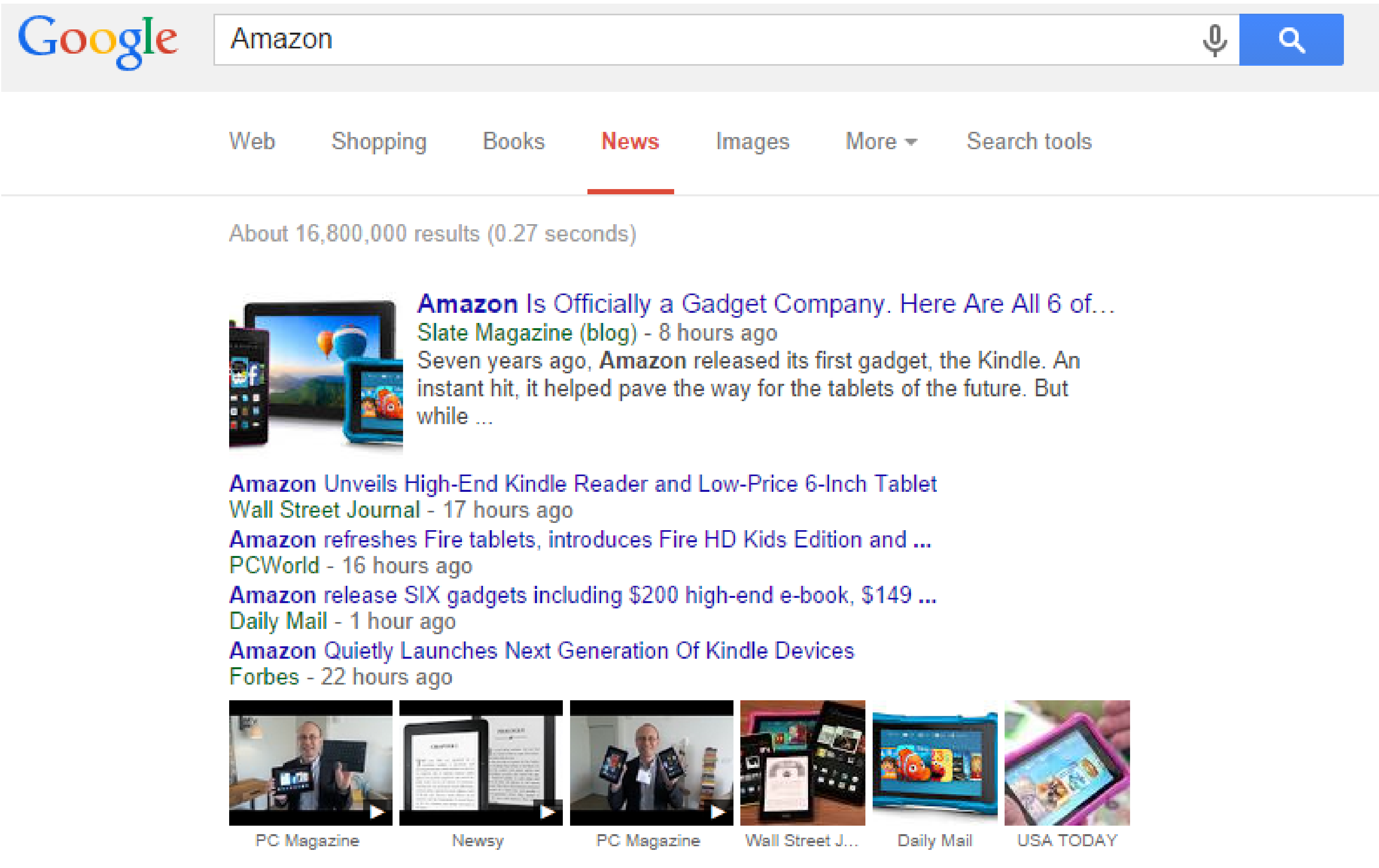


3 in intersection
8 in union
Jaccard similarity= 3/8
Jaccard distance = 5/8

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"

Task: Finding Similar Documents



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

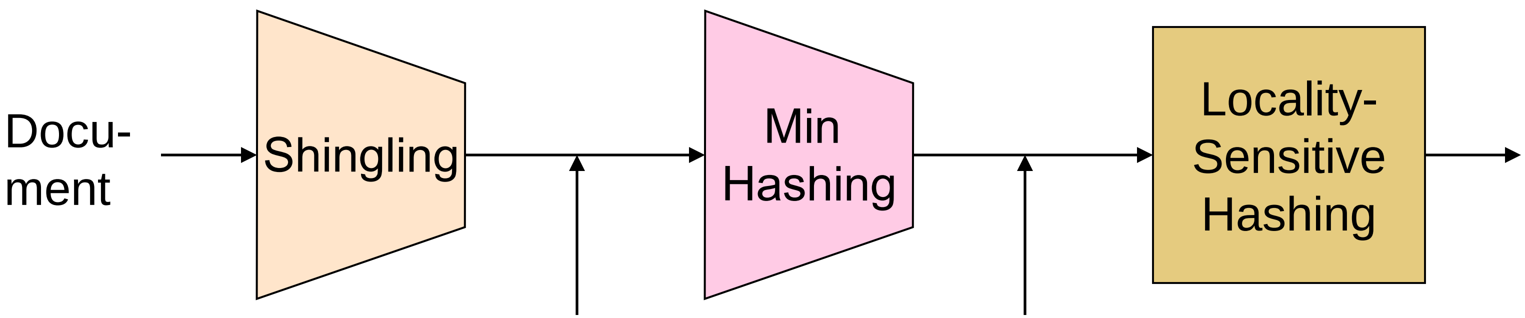
3 Essential Steps for Similar Docs

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!**

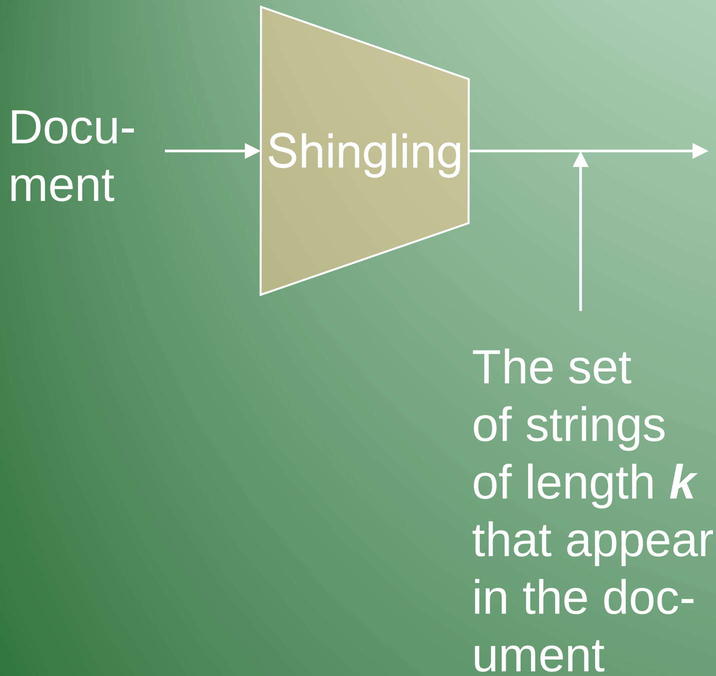
The Big Picture



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

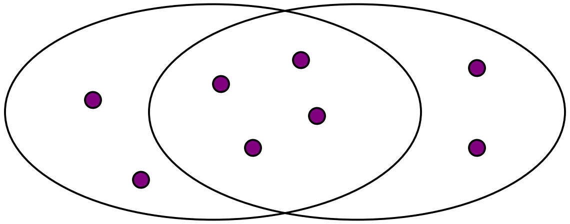
- **Represent a document by the set of hash values of its *k*-shingles**

- **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**

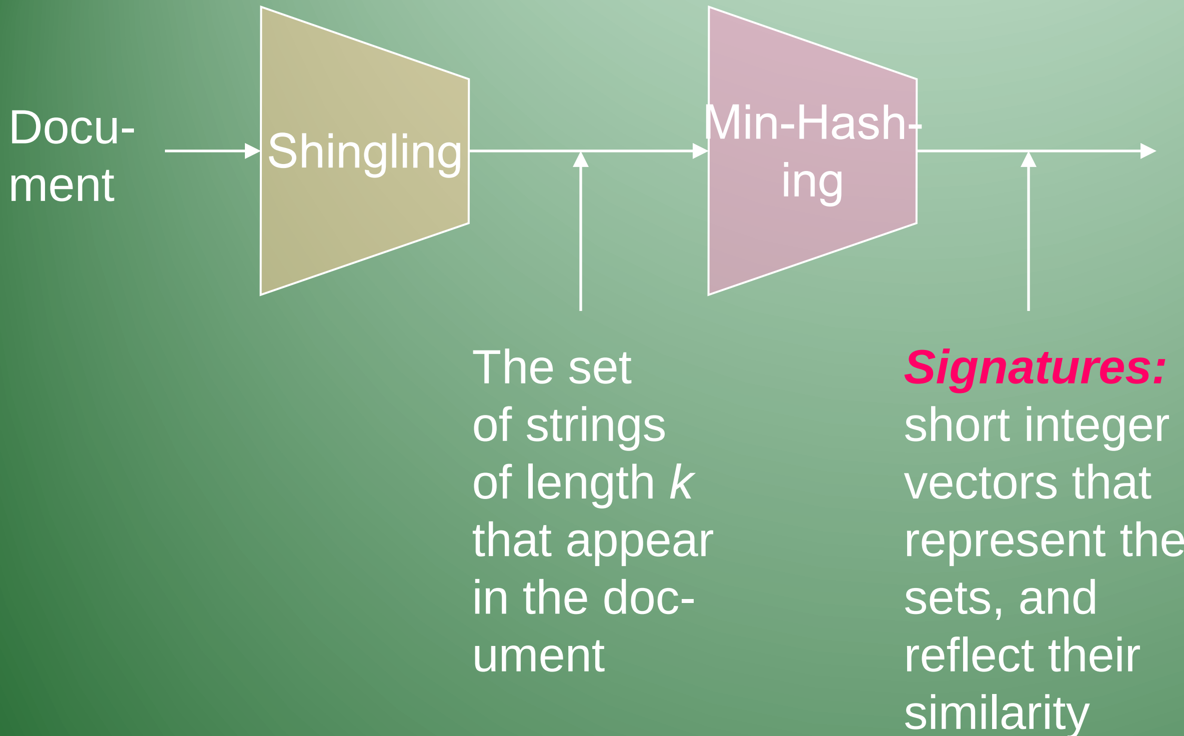
- **Caveat:** You must pick ***k*** large enough, or most documents will have most shingles
  - ***k*** = 5 is OK for short documents
  - ***k*** = 10 is better for long documents

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**
  - $N(N-1)/2$ **≈ 5*10^{11}** comparisons
  - At 10^5 secs/day and 10^6 comparisons/sec, it would take **5 days**

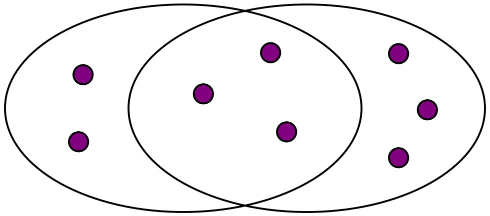
- For $N = 10$ million, it takes more than a year…



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**

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

- **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

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

- 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

- Original Sets
  - S1 = {1, 4} min(S1) = 1
  - S2 = {2, 3, 4} min(S2) = 2
  - S3 = {3, 5} min(S3) = 3

- Permutation π: $(1\ 2\ 3\ 4\ 5) \Rightarrow\ (4\ 1\ 5\ 3\ 2)$
  - This means row 1 is mapped to row 4, row 2 is mapped to row 1, …
  - Min-hash(S1) = 3
  - Min-hash(S2) = 1
  - Min-hash(S3) = 2

- Intuition: if two sets are similar, there min-hashes are likely to be the same

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)

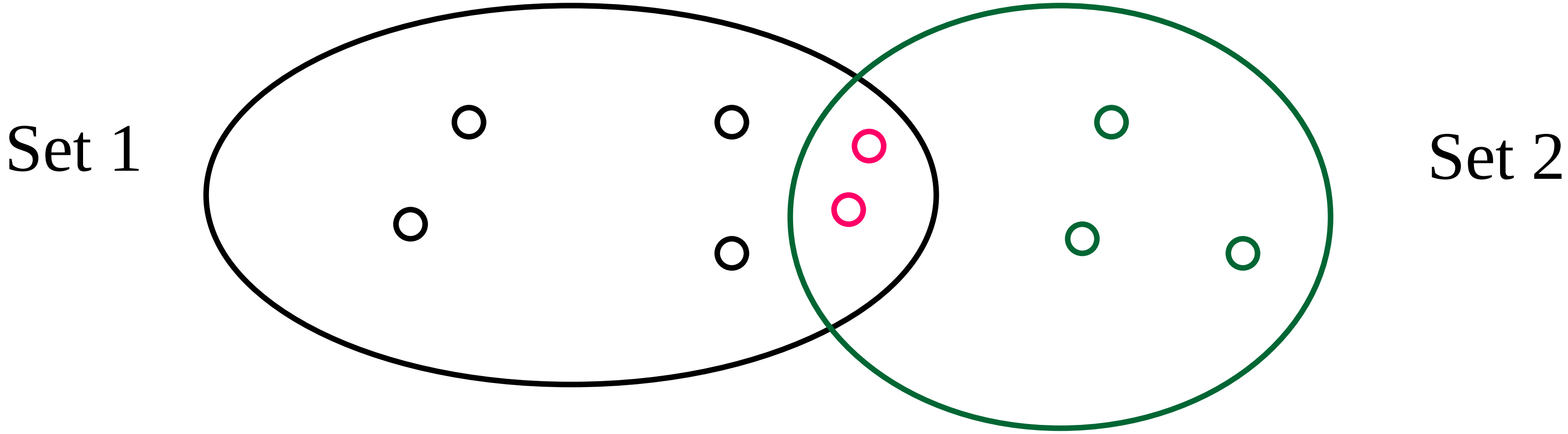
1	0	1	0
1	0	0	1
0	1	0	1
0	1	0	1
0	1	0	1
1	0	1	0
1	0	1	0

Signature matrix *M*

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

The Min-Hash Property

- **Choose a random permutation π**
- **<u>Claim:</u>** $\Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
- **Why? (intuition)**



Let w be an item which has the smallest hash value among all items in set1 and set2.

When do the min-hashes of the two sets agree?

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

- **[Aside]**
  - Assume we have a biased coin with P(head) = c ($\neq 0.5$)
  - How can we find out c?
  - We toss coin n times, and find out the number h for the 'head'.
  - A good estimator of c is h/n
  - (expected number of 'head' : n * c = h)

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*

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

- **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 ***sig(C)[i] = ∞***
  - **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 … integers
p … prime number (p > N)

Implementation Trick

- Raw Data and Hash Functions

Row	S_1	S_2	S_3	S_4	$x+1 \mod 5$	$3x+1 \mod 5$
0	1	0	0	1	1	1
1	0	0	1	0	2	4
2	0	1	0	1	3	2
3	1	0	1	1	4	0
4	0	0	1	0	0	3

- In the beginning

	S_1	S_2	S_3	S_4
h_1	∞	∞	∞	∞
h_2	∞	∞	∞	∞

Implementation Trick

- Row 0

	S_1	S_2	S_3	S_4
h_1	1	∞	∞	1
h_2	1	∞	∞	1

Row 1

	S_1	S_2	S_3	S_4
h_1	1	∞	2	1
h_2	1	∞	4	1

- Row 2

	S_1	S_2	S_3	S_4
h_1	1	3	2	1
h_2	1	2	4	1

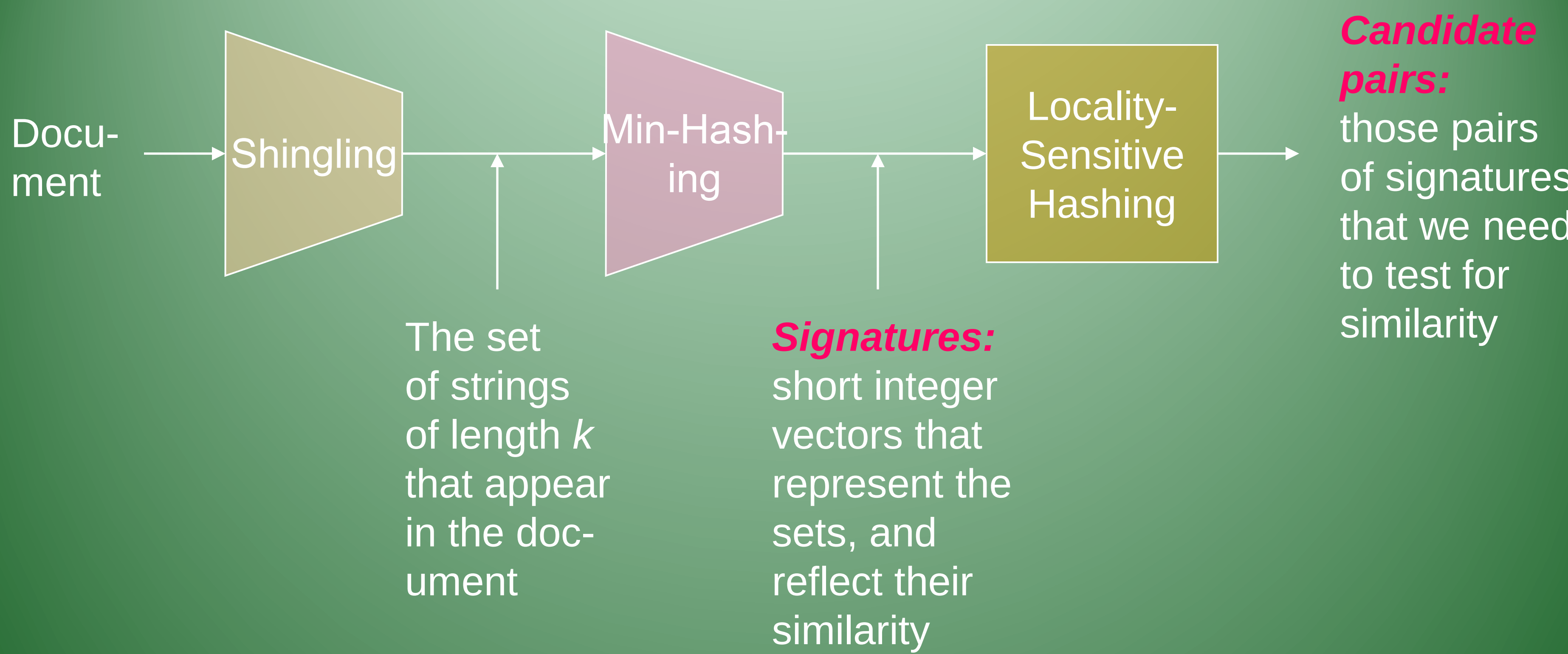
Row 3

	S_1	S_2	S_3	S_4
h_1	1	3	2	1
h_2	0	2	0	0

- … Finally

	S_1	S_2	S_3	S_4
h_1	1	3	0	1
h_2	0	2	0	0

Row	S_1	S_2	S_3	S_4	$x+1 \mod 5$	$3x+1 \mod 5$
0	1	0	0	1	1	1
1	0	0	1	0	2	4
2	0	1	0	1	3	2
3	1	0	1	1	4	0
4	0	0	1	0	0	3



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

- **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

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

Problem: we have to compare all pairs of columns!

LSH for Min-Hash

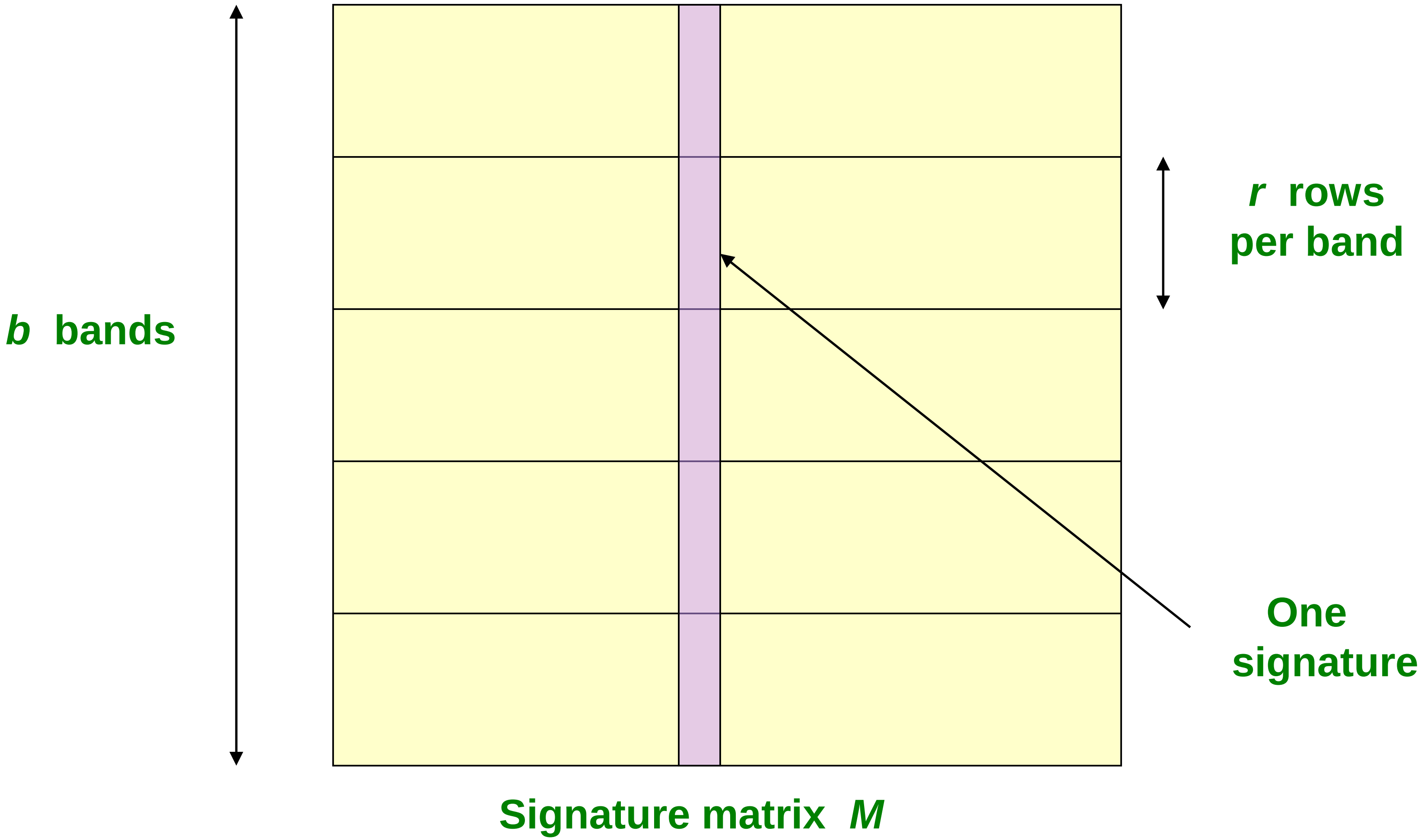
2	1	4	1
1	2	1	2
2	1	2	1

- **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**

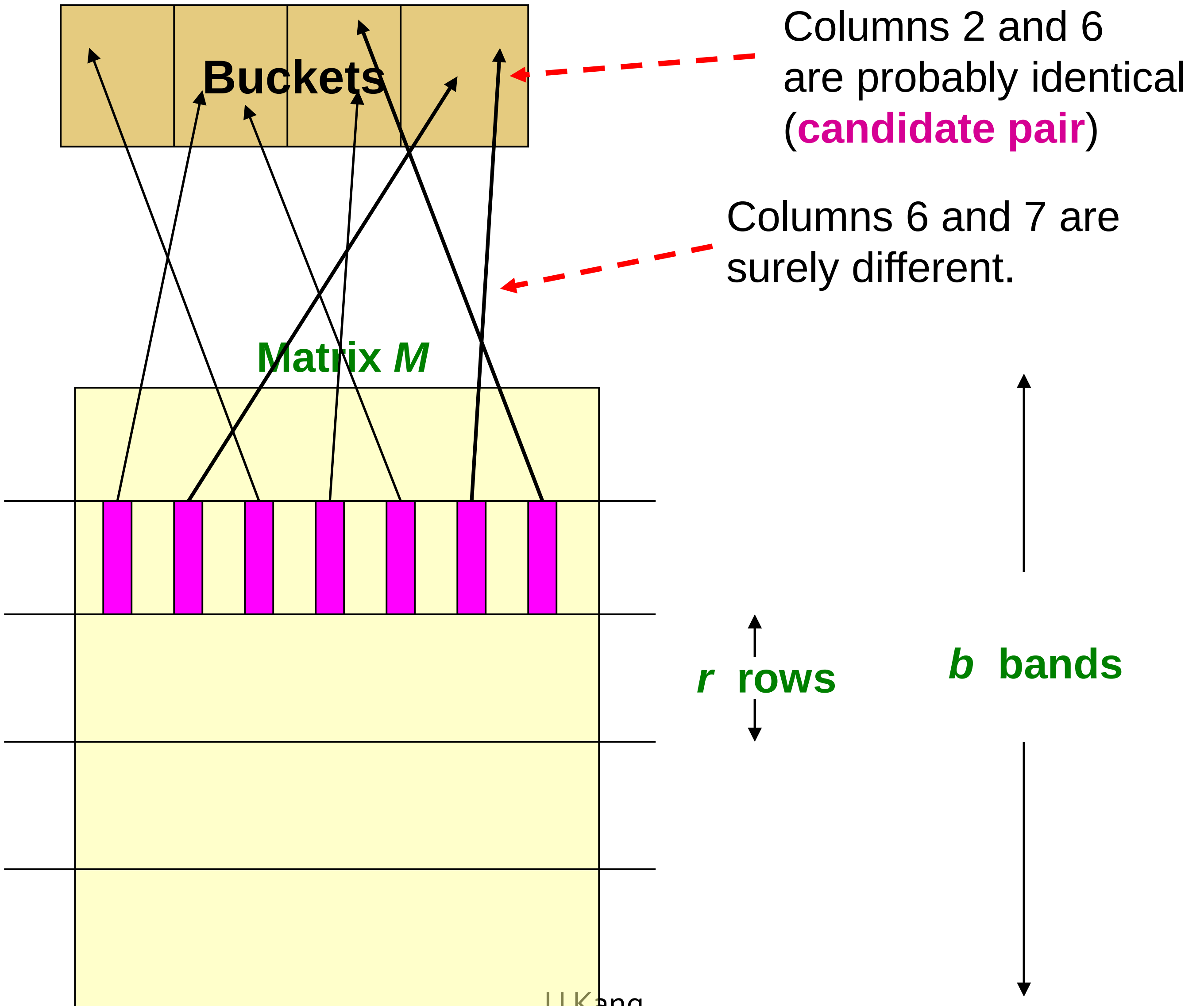
Partition *M* into *b* Bands



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

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

- **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**

False Positive and Negative

		(Truth)	
		Similar	Not similar
Our Algorithm says	Similar	True Positive	**False Positive**
	Not Similar	**False Negative**	True Negative

- **False Positive is called Type 1 Error**
- **False Negative is called Type 2 error**

Talk

You got a cold
You didn’t get a cold

C_1, C_2 are 30% Similar

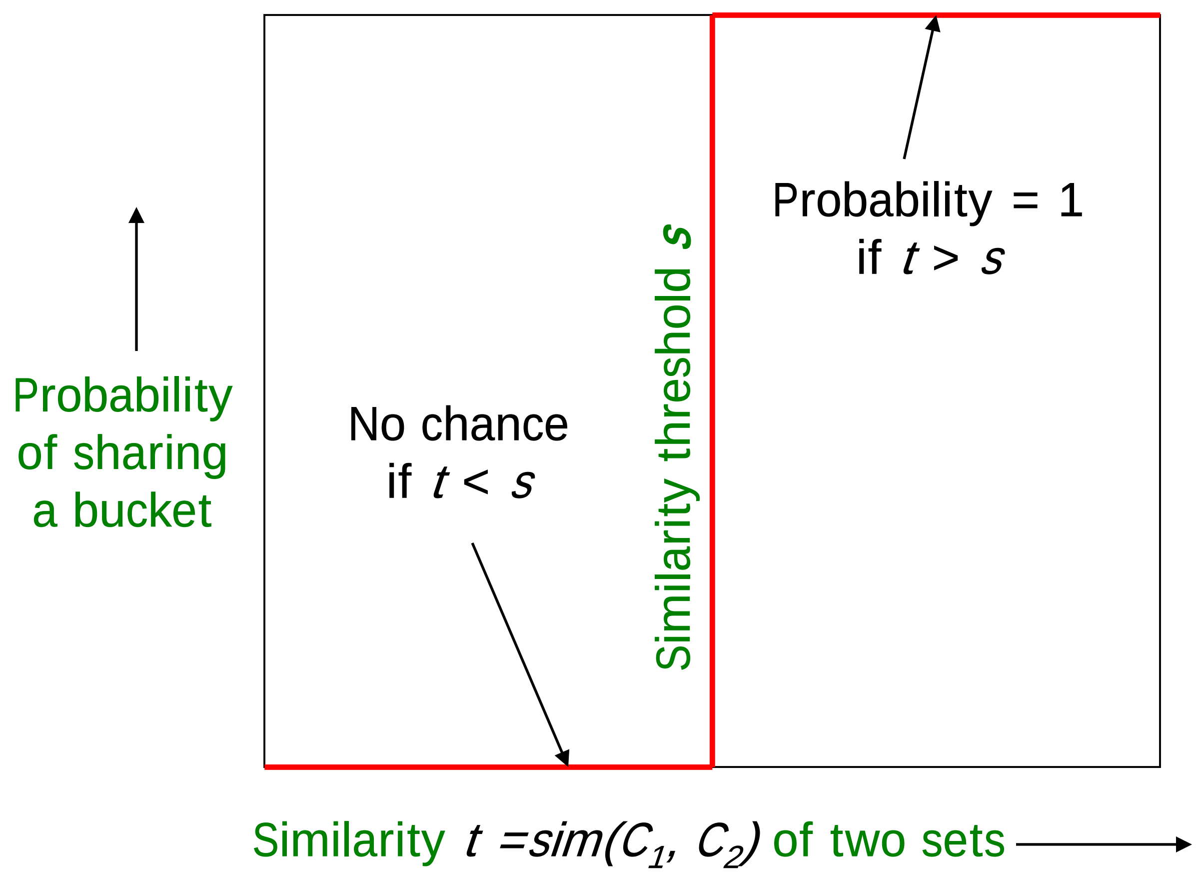
- **Find pairs of ≥ *s*=0.8 similarity, set b=20, r=5**
- **Assume:** $\text{sim}(C_1, C_2) = 0.3$
  - Since $\text{sim}(C_1, C_2) <$ **s** we want C_1, C_2 to hash to **NO common buckets** (all bands should be different)
- **Probability C_1, C_2 identical in one particular band:** $(0.3)^5 = 0.00243$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

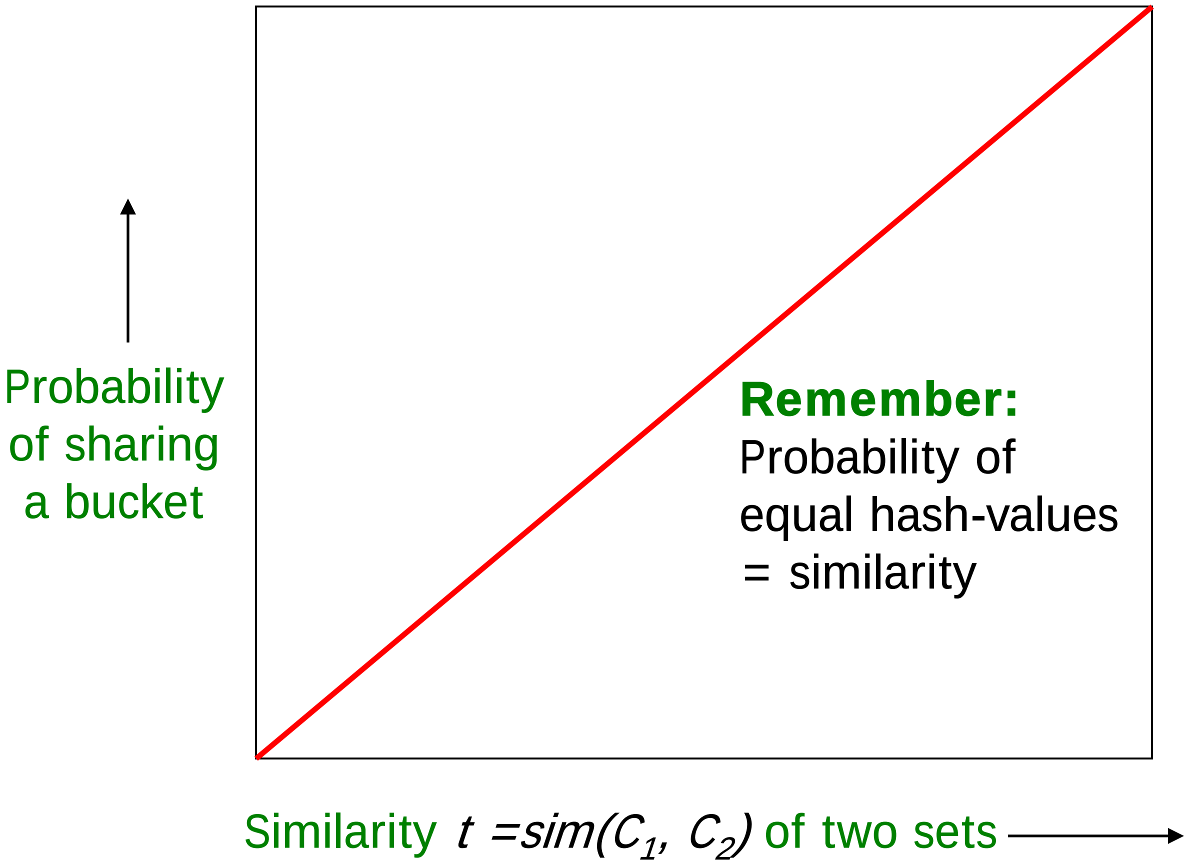
- **Pick:**
  - The number of Min-Hashes (rows of ***M***)
  - The number of bands ***b***, and
  - The number of rows ***r*** per band

to balance false positives/negatives

Analysis of LSH – What We Want



What 1 Band of 1 Row Gives You

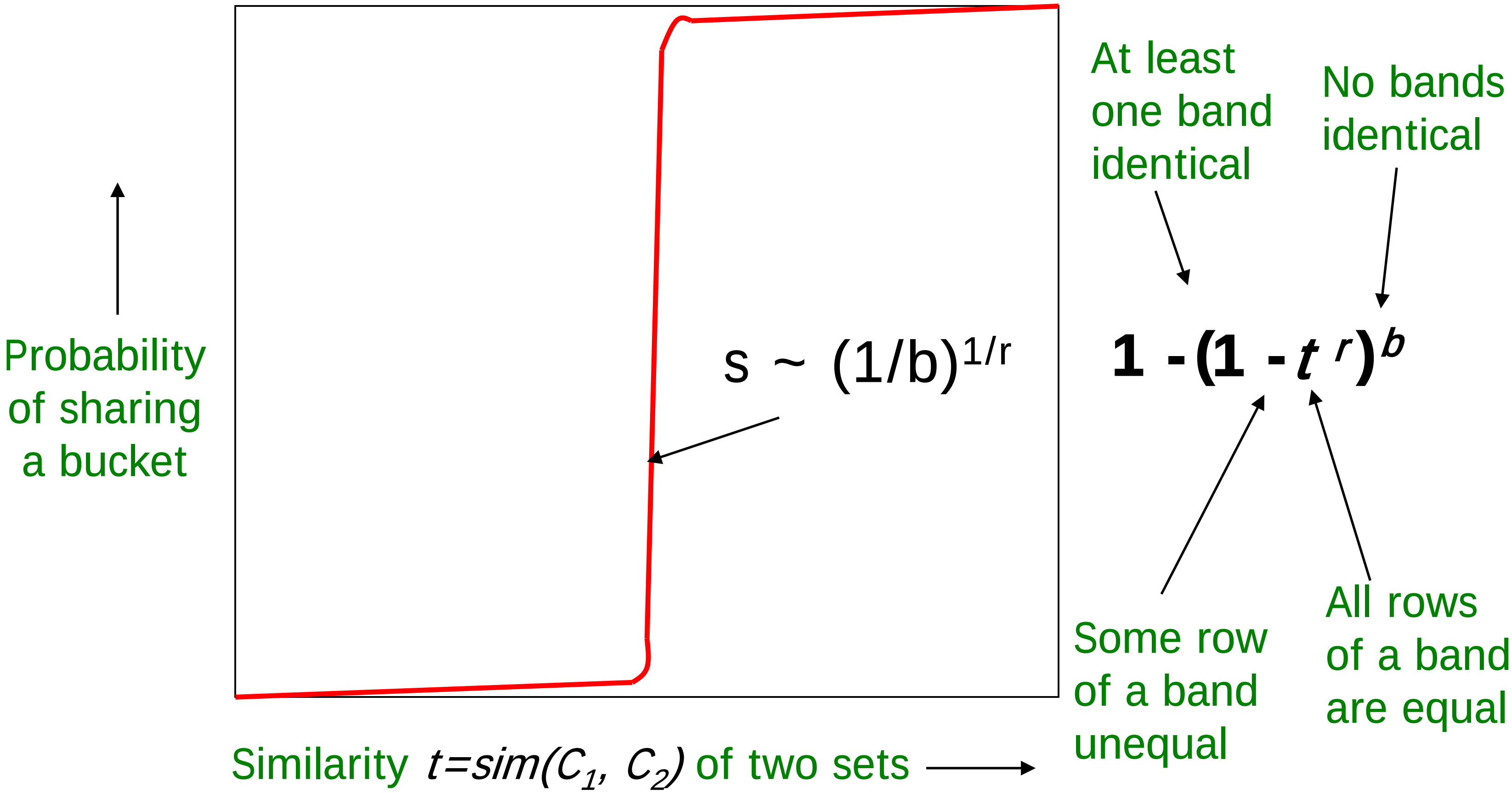


b bands, *r* rows/band

- 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



By controlling s, you can determine the shape of the function

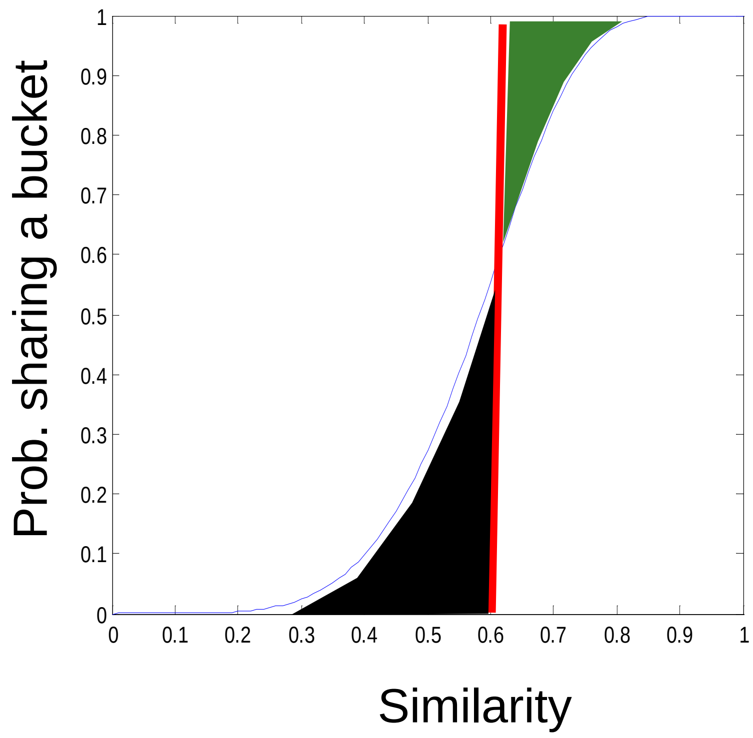
Example: $b = 20$; $r = 5$

- Similarity of two sets = t
- Prob. that at least 1 band is identical:

t	$1-(1-t^r)^b$
.2	.006
.3	.047
.4	.186
.5	.470
.6	.802
.7	.975
.8	.9996

Picking *r* and *b*: The S-curve

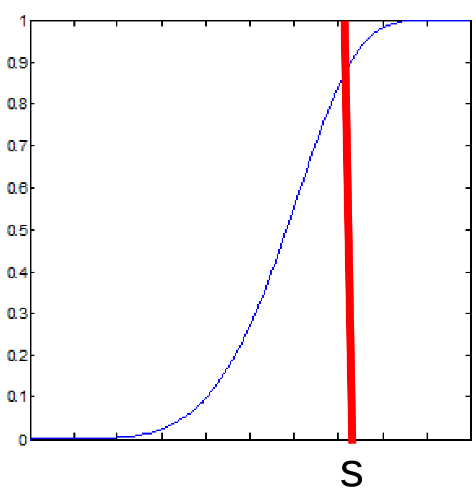
- **Picking *r* and *b* to get the best S-curve**
  - 50 hash-functions (r=5, b=10)

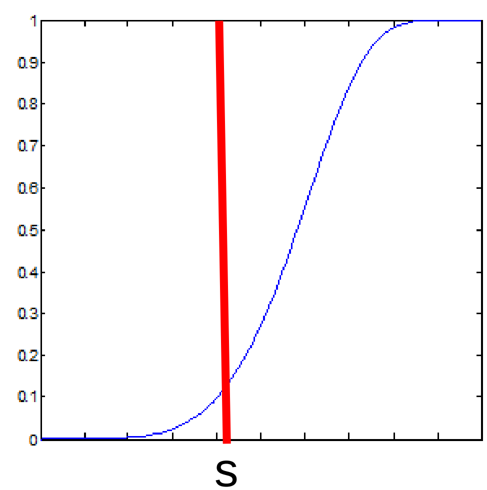


Green area: False Negative rate
Black area: False Positive rate

Picking *r* and *b*: The S-curve

- **If avoiding false negatives is important (accuracy is important)**
  - Make (1/b)^(1/r) smaller than s (desired similarity)
- **If avoiding false positives is important (speed is important)**
  - Make (1/b)^(1/r) larger than s (desired similarity)





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**

Questions?