Finding Similar Items: Locality Sensitive Hashing

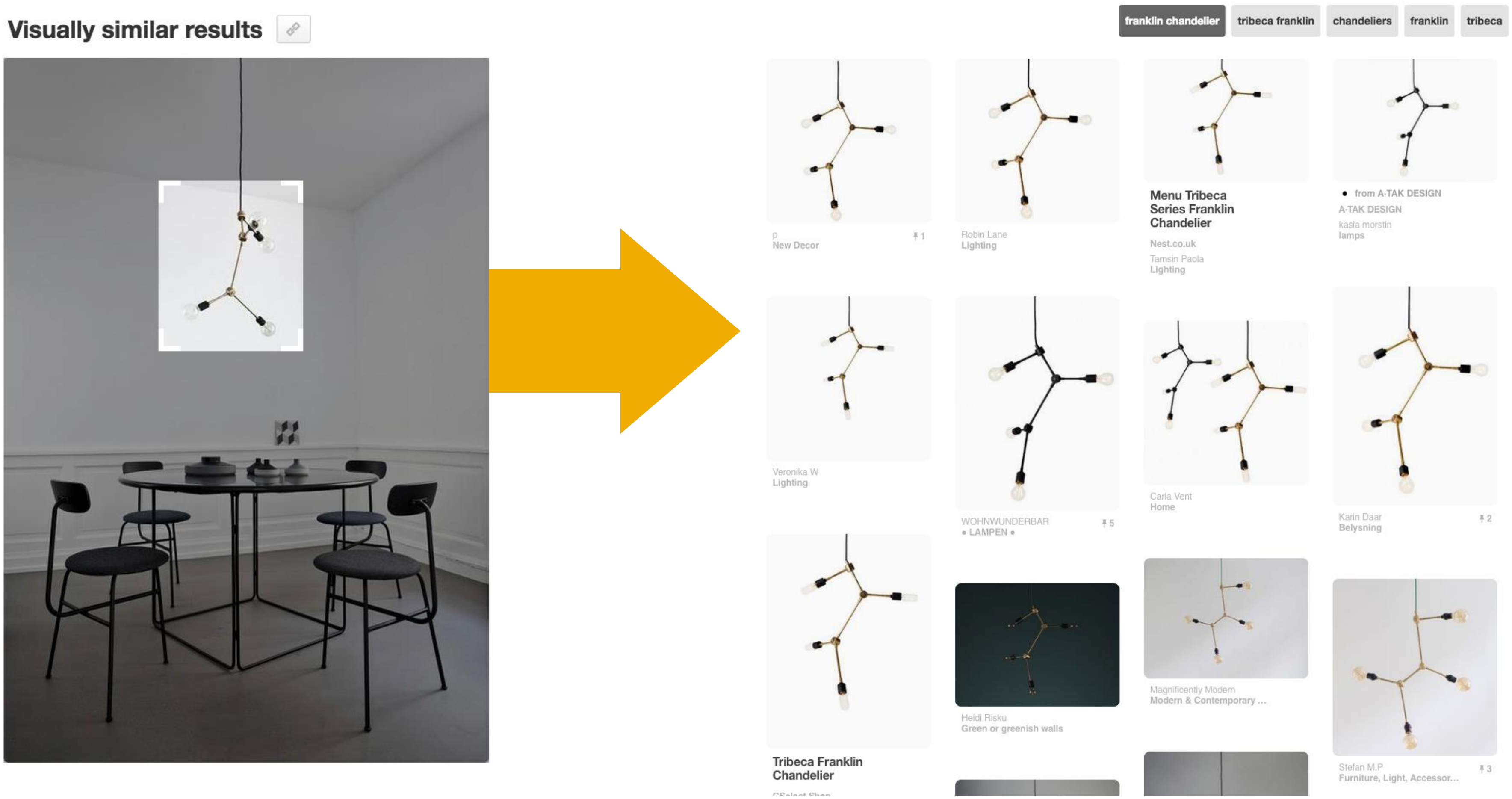
CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
http://cs246.stanford.edu

New thread: High dim. data

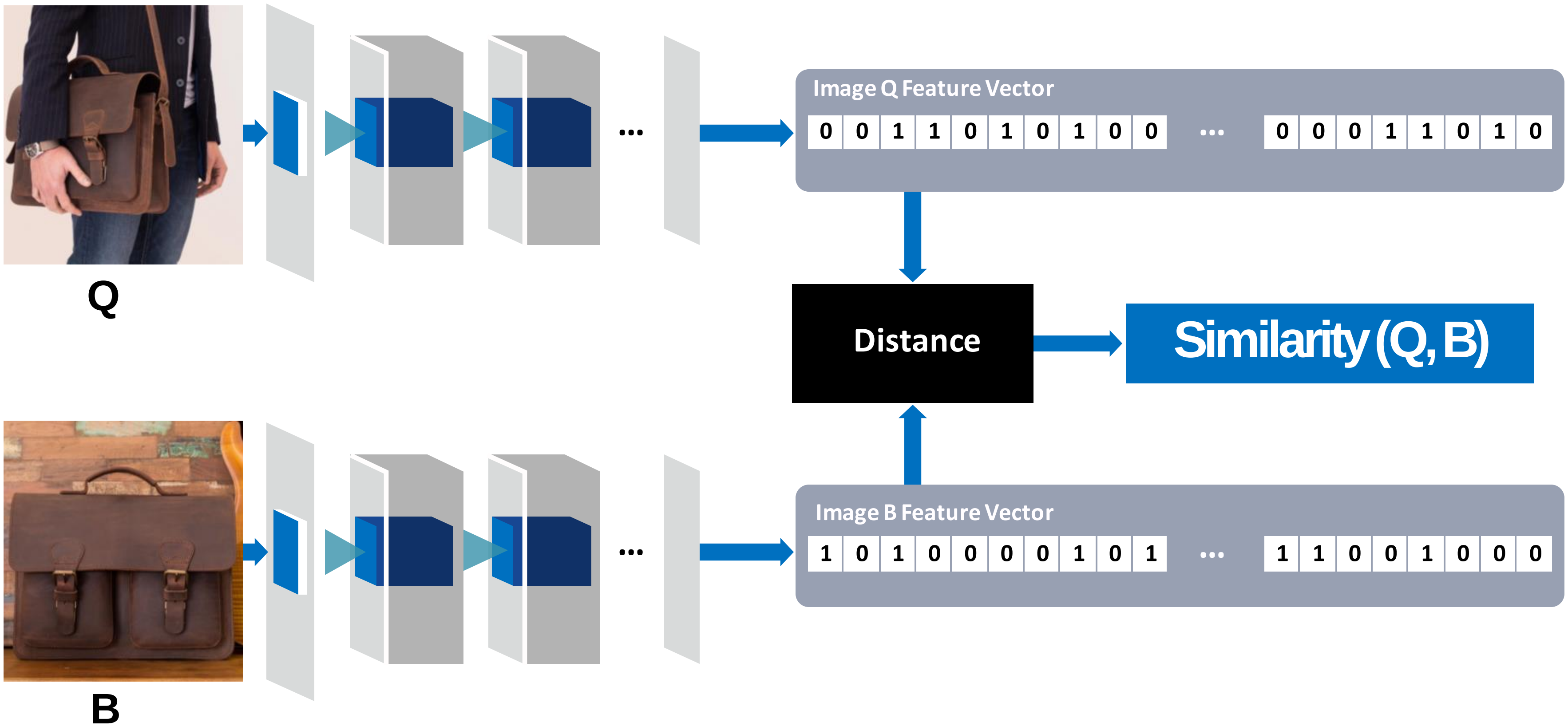
High dim. data	Graph data	Infinite data	Machine learning	Apps
Locality sensitive hashing	PageRank, SimRank	Filtering data streams	SVM	Recommender systems
Clustering	Network Analysis	Web advertising	Decision Trees	Association Rules
Dimensionality reduction	Spam Detection	Queries on streams	Perceptron, kNN	Duplicate document detection

Pinterest Visual Search

Given a **query image patch**, find similar images



How does it work?



- Collect billions of images
- Determine feature vector for each image (4k dim)
- **Given a query Q, find nearest neighbors FAST**

How does it work?

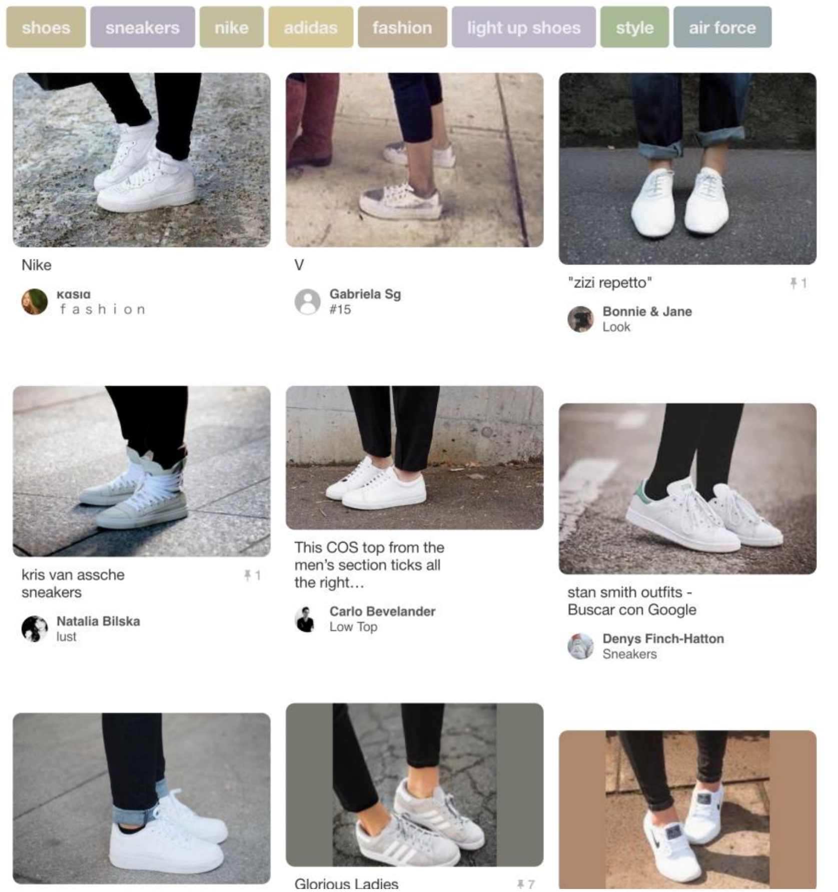
Q

Nearest neighbor query
in the embedding space

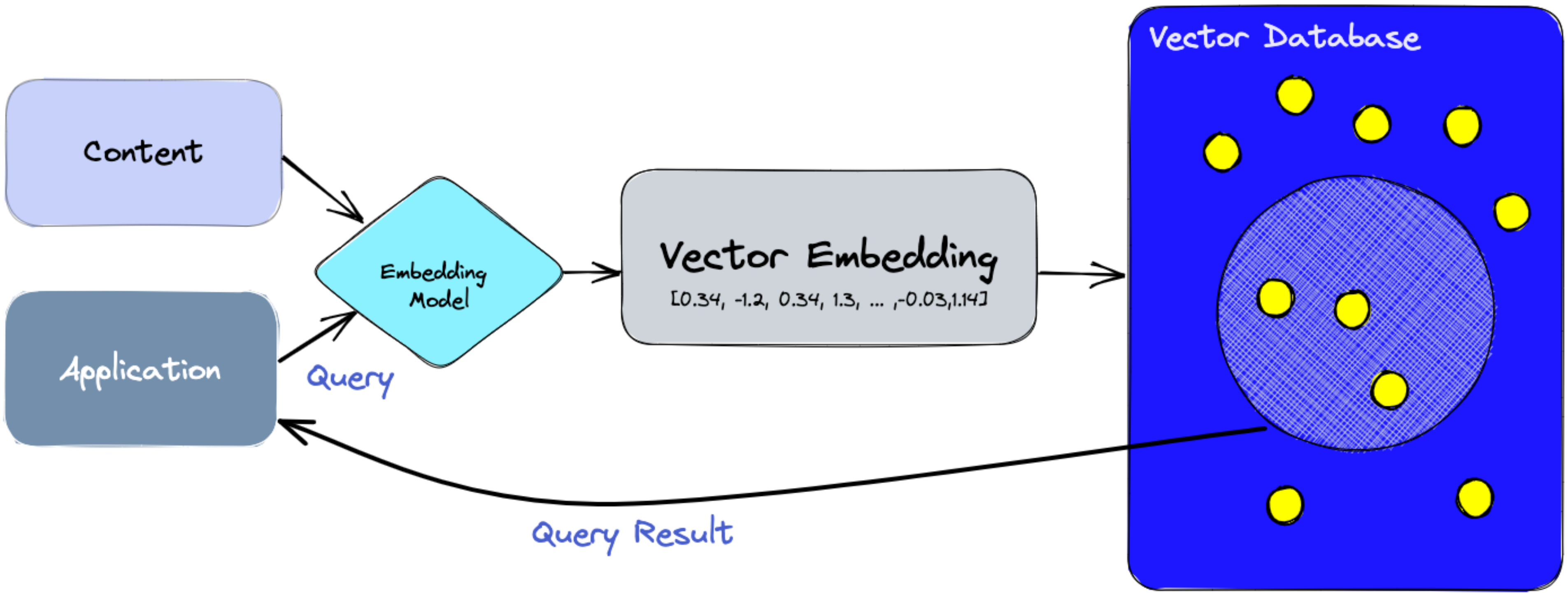
Application: Visual Search

Visually similar results

Q



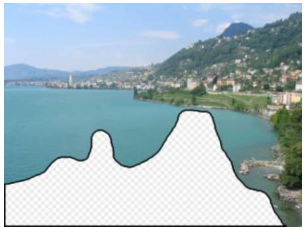
Technology Behind Vector DBs



https://www.pinecone.io/learn/vector-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**
    - Image completion
  - **Recommendations and search**



Problem for today's lecture (1)

- **Given: High dimensional data points $x_1, x_2, \ldots$**
  - **For example:** Image is a long vector of pixel colors
- **And some distance function $d(x_1, x_2)$**
  - which quantifies the "distance" between x_1 and x_2

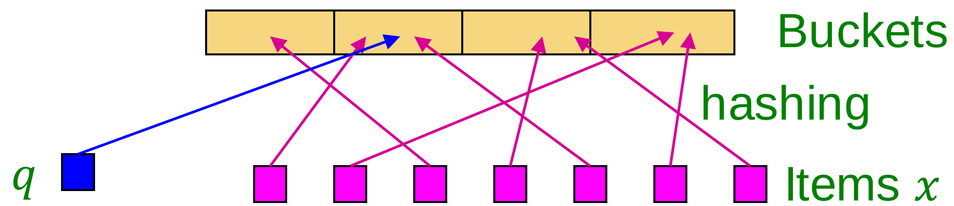
- **Goal:** Given q, find **data points x_j** that are within distance threshold $d(q, x_j) \leq s$
- **Note:** Naïve solution would take $O(N)$ where N is the number of data points
- **MAGIC: This can be done in $O(1)$!! How??**

Problem for today's lecture (2)

- **Given: High dimensional data points $x_1, x_2, \ldots$**
  - **For example:** Image is a long vector of pixel colors
- **And some distance function $d(x_1, x_2)$:**
  - To be a distance func. d needs to satisfy 4 rules: d(x,x)=0; d(x,y)≥0; d(x,y)=d(y,x); d(x,z)≤d(x,y)+d(y,z)
- **Goal:** Find **all pairs of data points** (x_i, x_j) that are within 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??**

Overview of LSH: The Bigfoot of CS

- LSH is really a family of related techniques
- In general, one throws items into buckets using several different "hash functions".
- You examine only those pairs of items that share a bucket for at least one of these hashings.



- **Upside:** Designed correctly, only a small fraction of points are ever examined
- **Downside:** There are *false negatives* – there might be similar items that get missed

Motivating Application: Finding Similar Documents

Motivation for Min-Hash/LSH

- **Suppose we need to find near-duplicate documents among $N = 1$ million documents**
  - Naïvely, we would have to compute **pairwise 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…

- Similarly, we have a dataset of 10B documents, quickly find the document that is most similar to query document q.

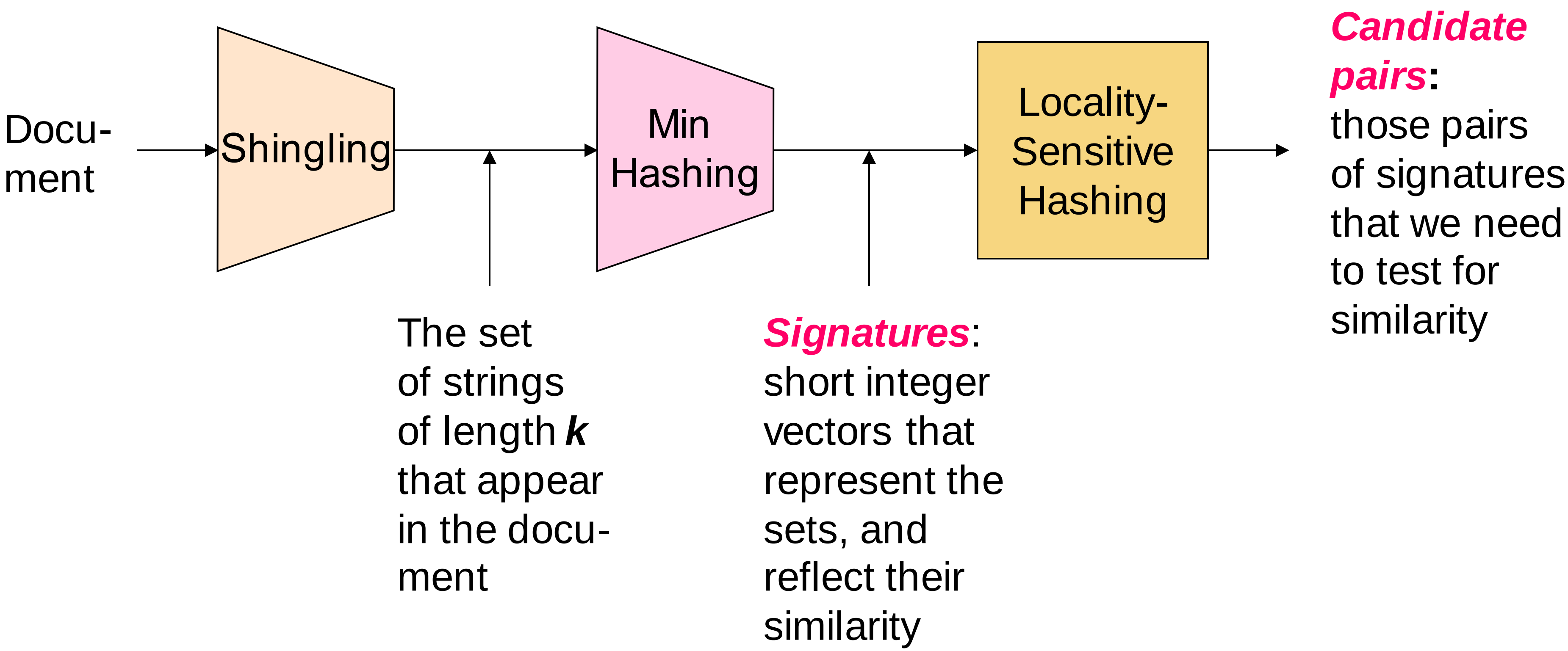
3 Essential Steps for Similar Docs

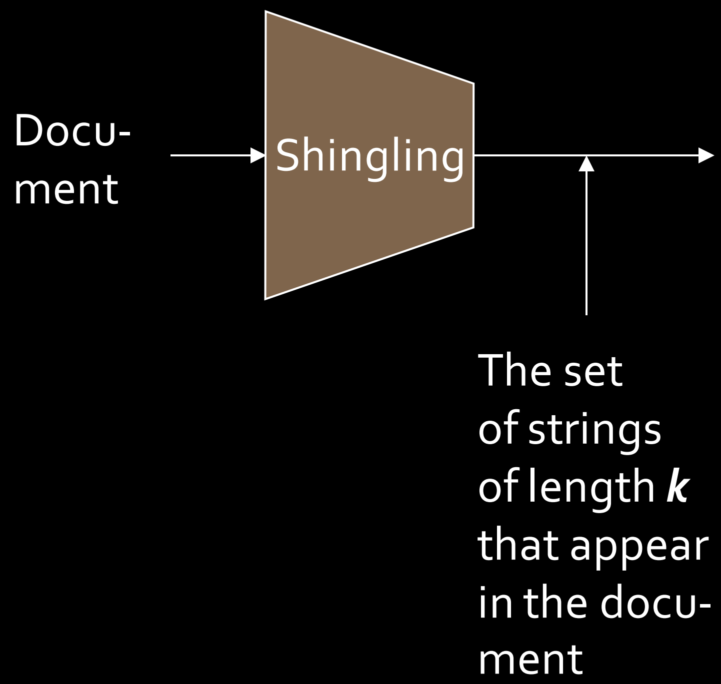
1. ***Shingling:*** Converts a document into a set representation (Boolean vector)

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 a document into a set

Documents as High-Dim Data

Step 1: *Shingling:* Converts a document into a set

- 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
  - For example, let's assume: tokens = characters
- 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**

Compressing Shingles

- **Example: k=2**; document $\mathbf{D_1}$= abcab
  Set of 2-shingles: $\mathbf{S(D_1)}$ = {ab, bc, ca}
  Hash the shingles: $\mathbf{h(D_1)}$ = {1, 5, 7}
- ***k*** = 8, 9, or 10 is often used in practice

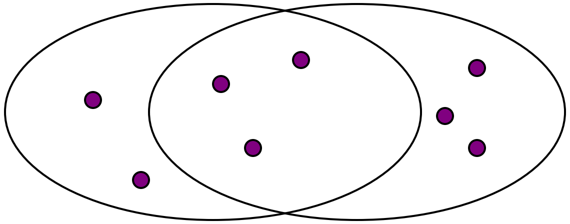
- **Benefits of shingles:**
  - Documents that are intuitively similar will have many shingles in common
  - Changing a word only affects k-shingles within distance k-1 from the word

Similarity Metric for Shingles

- **Document D_i is represented by a set of its k-shingles $C_i = S(D_i)$**
- **A natural similarity measure is the Jaccard similarity:**

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

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

From Sets to Boolean Matrices

Encode sets using 0/1 (bit, Boolean) vectors

- **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

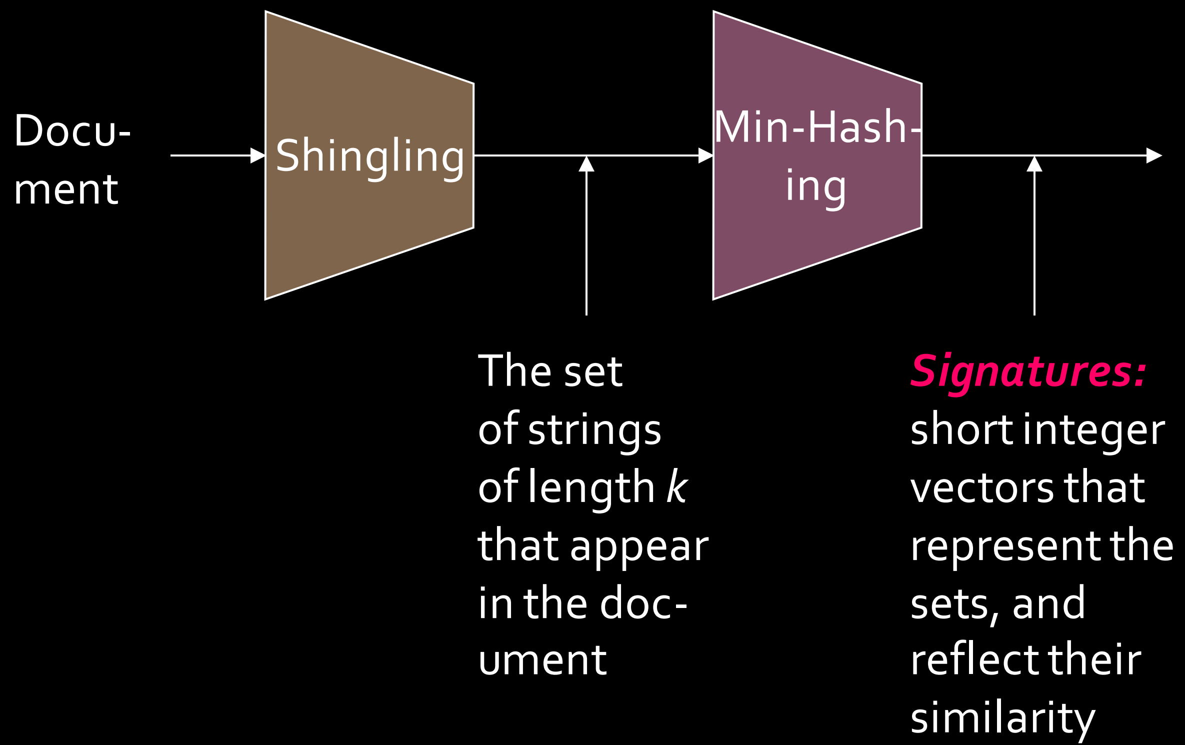
Shingles

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

We don't really construct the matrix; just imagine it exists

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**
- **Warnings:**
  - Comparing all pairs takes too much time: **Job for LSH**
    - These methods can produce false negatives, and even false positives (if the optional check is not made)



Min-Hashing

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

Hashing Columns (Signatures)

- **Key idea:** "hash" each column C to a small ***signature*** $h(C)$, such that:
  - $sim(C_1, C_2)$ 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. $h(C_1) \neq h(C_2)$

- **Idea: Hash docs into buckets. Expect that "most" pairs of near duplicate docs hash into the same bucket!**

Min-Hashing: Goal

- **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**
  - Next lecture we'll cover what other similarity functions can be used with LSH

Min-Hashing: Overview

- Permute the rows of the Boolean matrix using some permutation π
  - Thought experiment – not real
- Define minhash function for this permutation π, $\mathbf{h}_{\pi}\mathbf{(C)}$ **=** the number of the first (in the permuted order) row in which column C has value 1.
  - Denoted this as: $\boldsymbol{h_{\pi}(C) = min_{\pi}\, \pi(C)}$
- Apply, to all columns, several randomly chosen permutations π to create a signature for each column
- **Result is a signature matrix:** Columns = sets, Rows = minhash values for each permutation π

Min-Hashing Example

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

$h_\pi(C) = min_\pi \, \pi(C)$

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

$h_2(3)=4$ (permutation 2, column 3)

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

A Subtle Point

- Students sometimes ask whether the minhash value should be the original number of the row, or the number in the permuted order (as we did in our example).

- **Answer: It doesn't matter.**
  - We only need to be consistent and assure that two columns get the same value if and only if their first 1's in the permuted order are in the same row.

The Min-Hash Property (1)

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), $z \in X$ is a shingle
  - **Then:** $\Pr[\pi(z) = \min(\pi(X))] = 1/|X|$
    - It is equally likely that any $z \in X$ is mapped to the ***min*** element
  - **Now,** 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 should have 1 at position ***y***

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

Another Way to See This

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

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

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

  - **Define: 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 permuted 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**

- Thus, the expected similarity of two signatures equals the Jaccard similarity of the columns or sets that the signatures represent
  - And the longer the signatures, the smaller will be the expected error

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

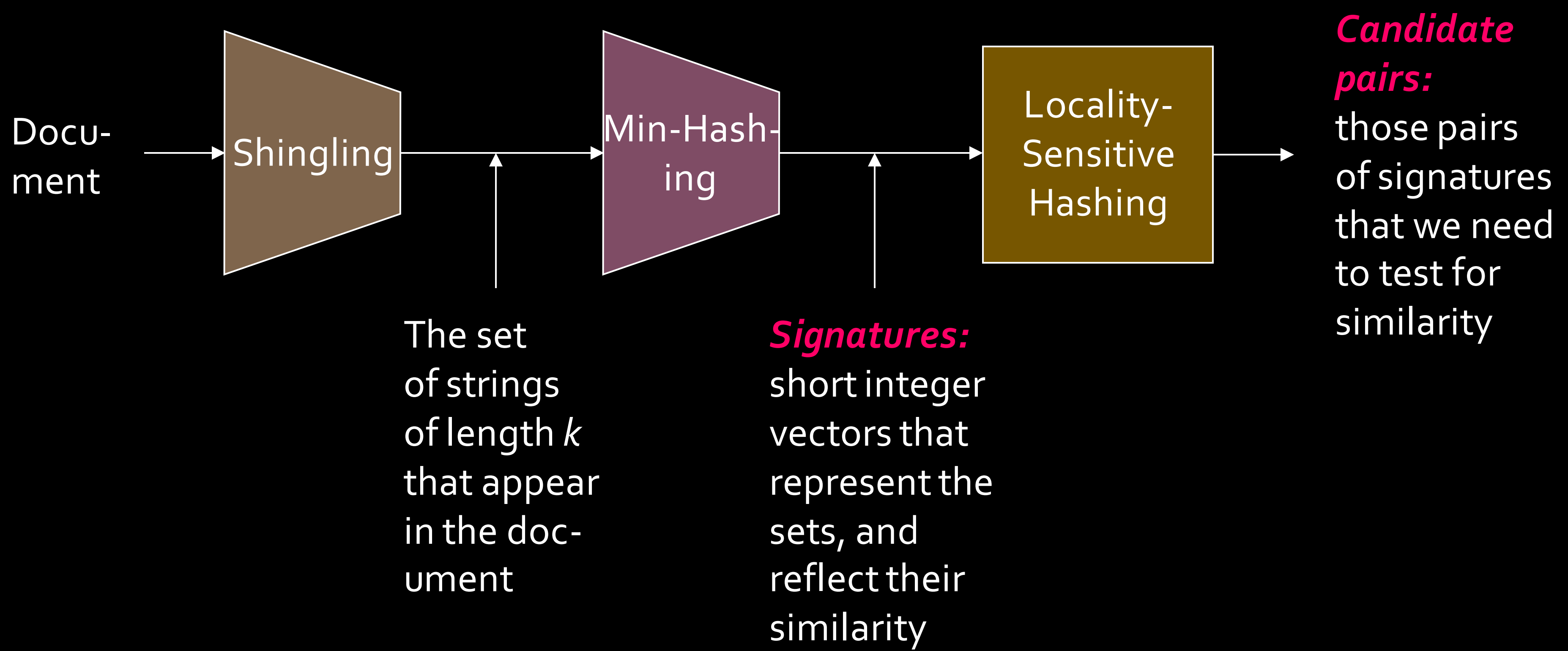
Similarities:

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

Implementation Trick

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

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: Overview

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 hash function 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**

LSH: Overview

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

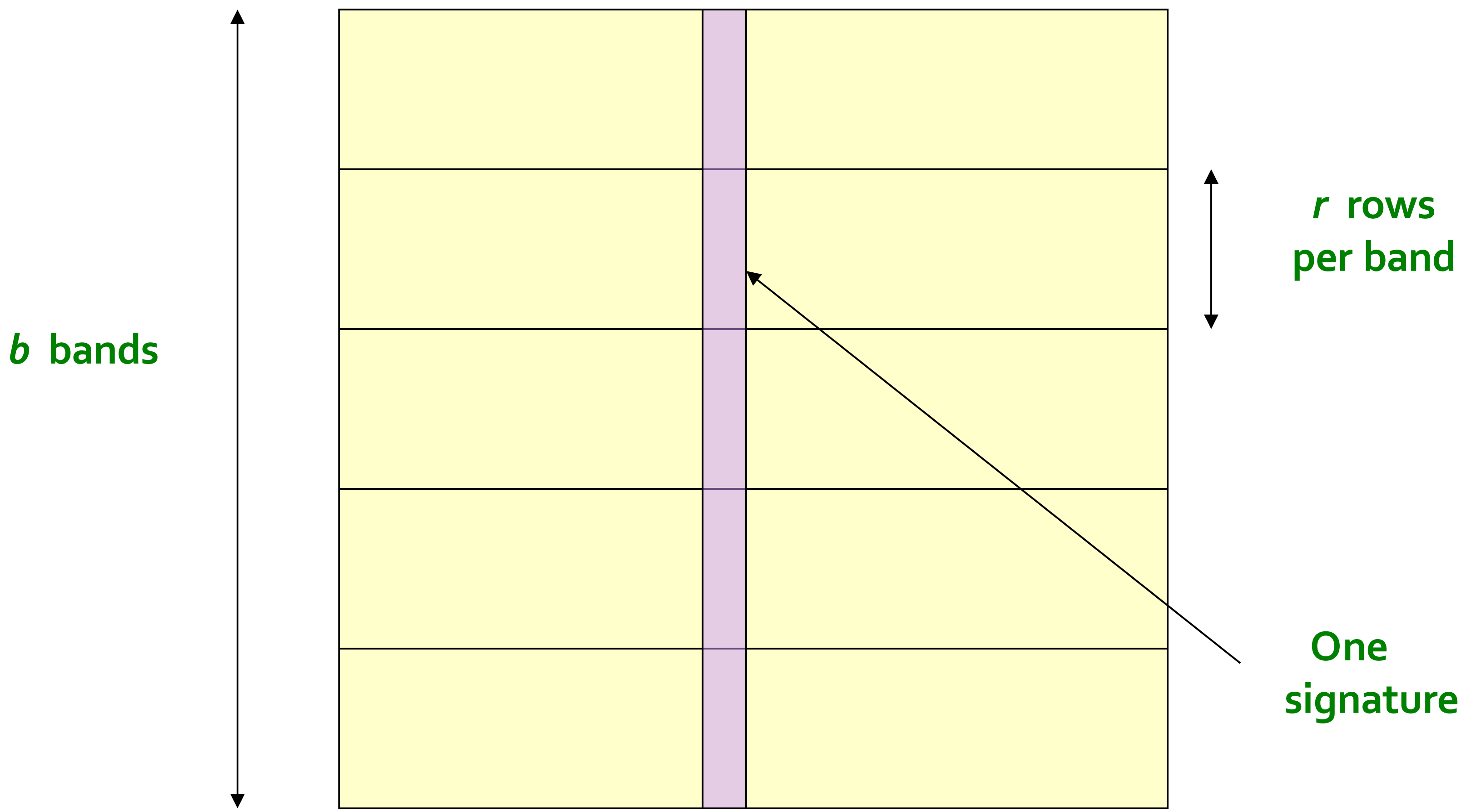
- **Big idea: Hash columns of signature matrix *M* several times**

- 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

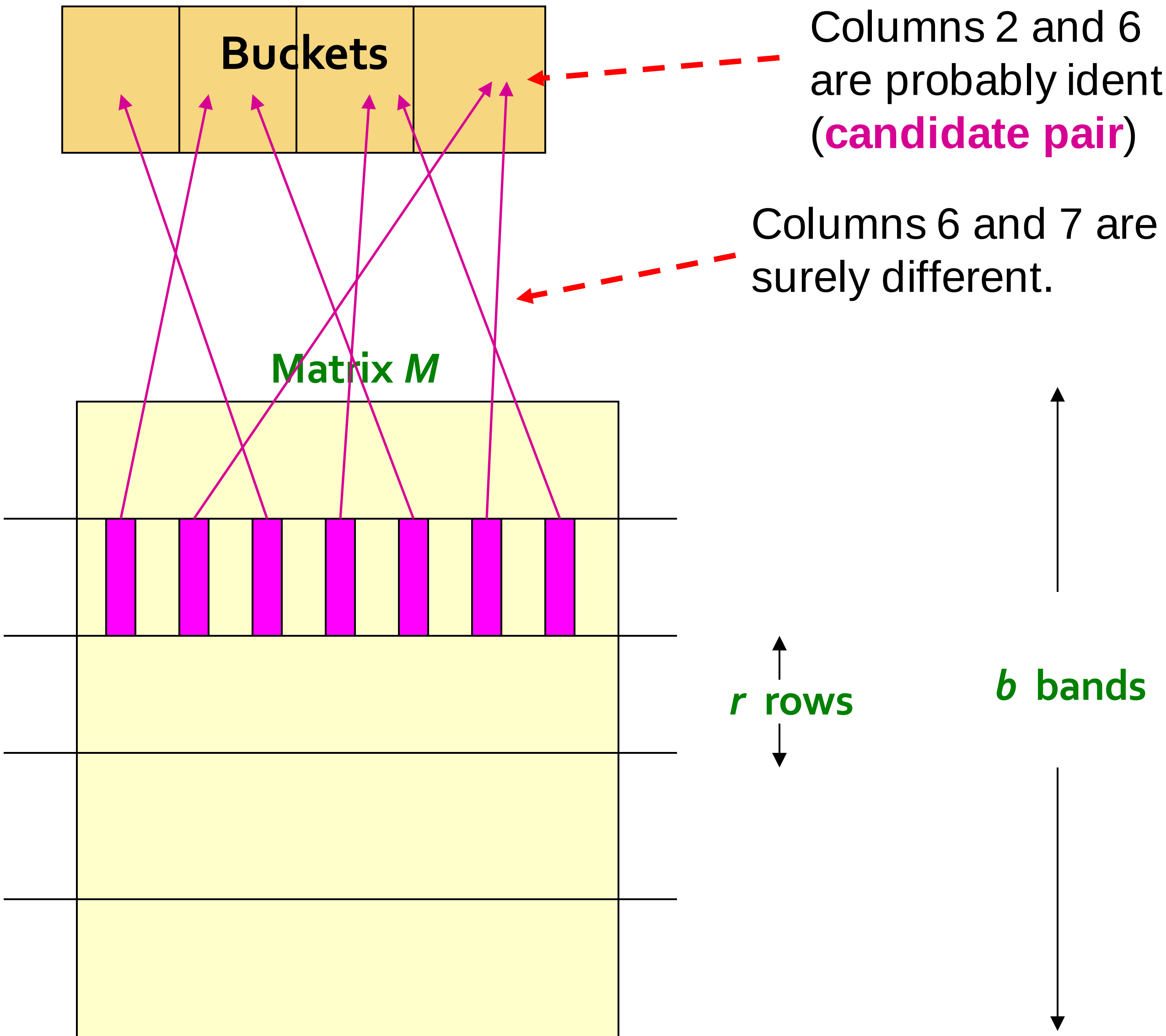


Signature matrix *M*

Partition *M* into Bands

- Divide matrix $\boldsymbol{M}$ 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 $\geq \mathbf{1}$ bands
- Tune $\boldsymbol{b}$ and $\boldsymbol{r}$ to catch most similar pairs, but few non-similar pairs

Hashing Bands



Columns 2 and 6 are probably identical (**candidate pair**)

Columns 6 and 7 are surely different.

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 length 100, stored as integers (rows)
- Therefore, signatures take 40MB
- **Goal:** Find pairs of documents that are at least ***s** = 0.8* similar
- Choose ***b*** = 20 bands of ***r*** = 5 integers/band

If 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, let's 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):
    - Prob. C1, C2 identical in one particular band: $(0.8)^5 = 0.328$
    - So, prob. C_1, C_2 are ***not*** similar in all 20 bands: $(1-0.328)^{20}$ = 0.00035
  - That is, 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**

If C_1, C_2 are 30% Similar

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

- **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**

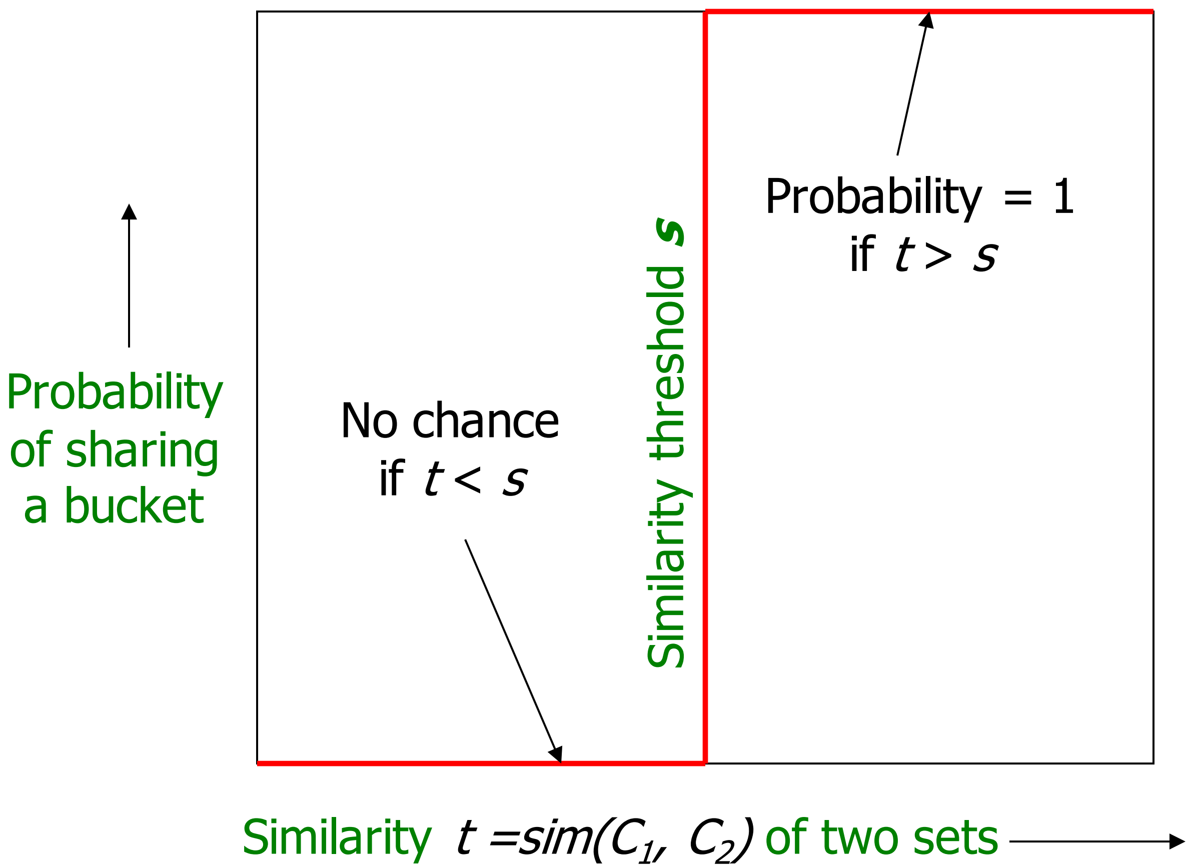
LSH Involves a Tradeoff

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
    - Note, M=b*r

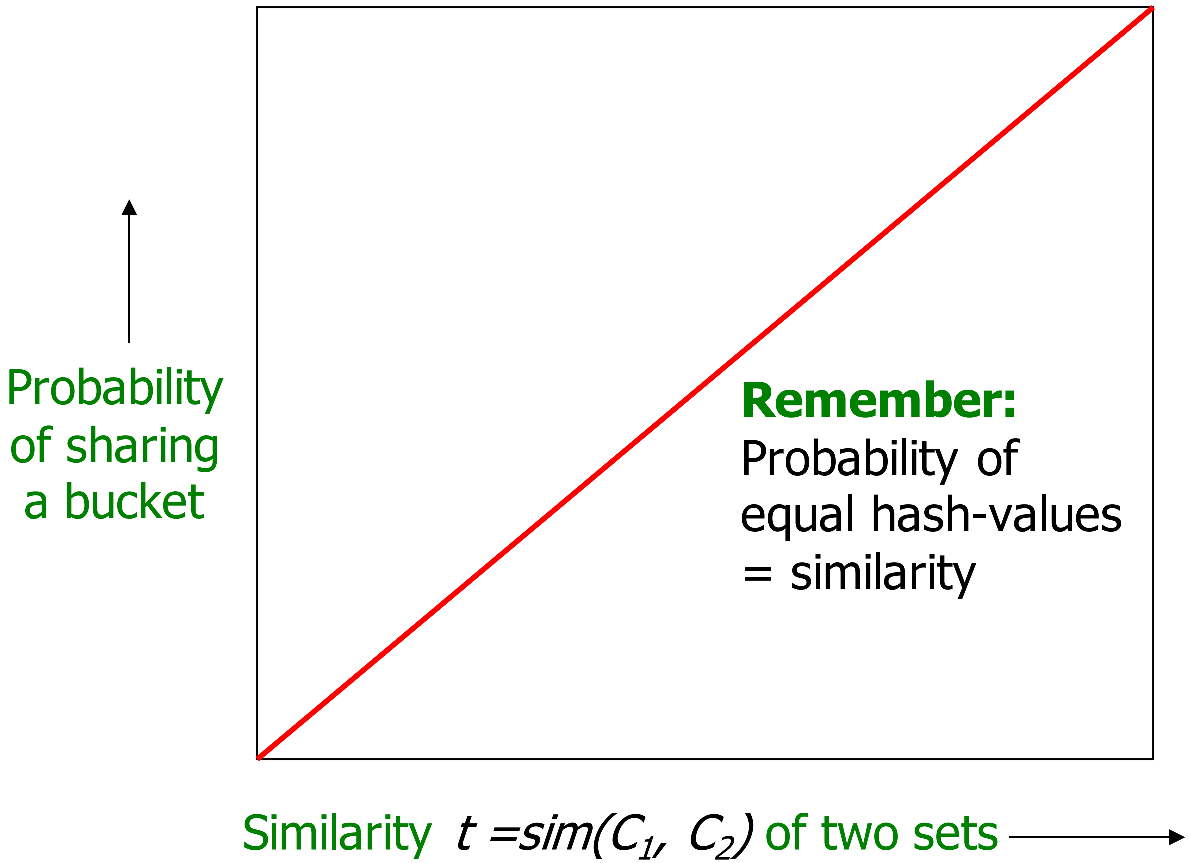
- **Example:** If we had only 10 bands of 10 rows, the number of false positives would go down, but the number of false negatives would go up

Analysis of LSH – What We Want

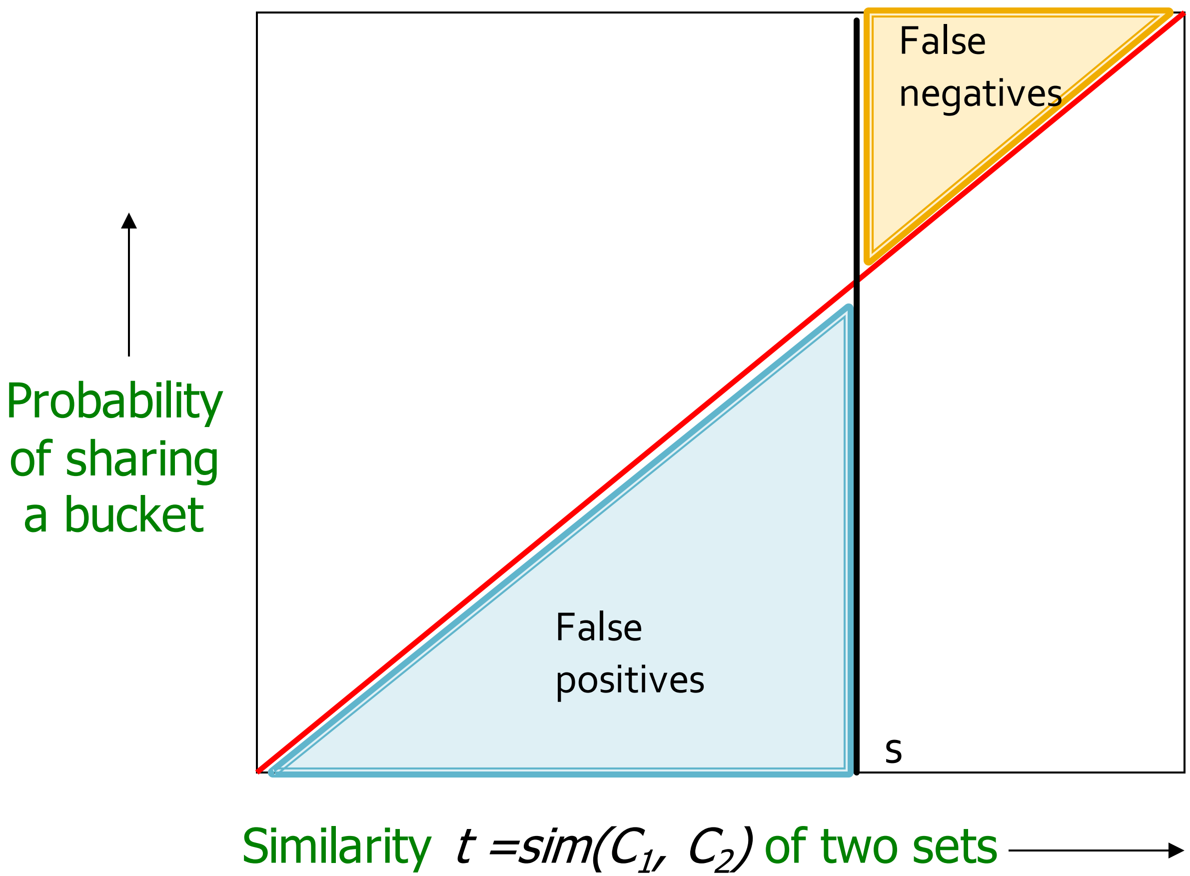


Say "yes" if you are below the line.

What 1 Band of 1 Row Gives You



What 1 Band of 1 Row Gives You



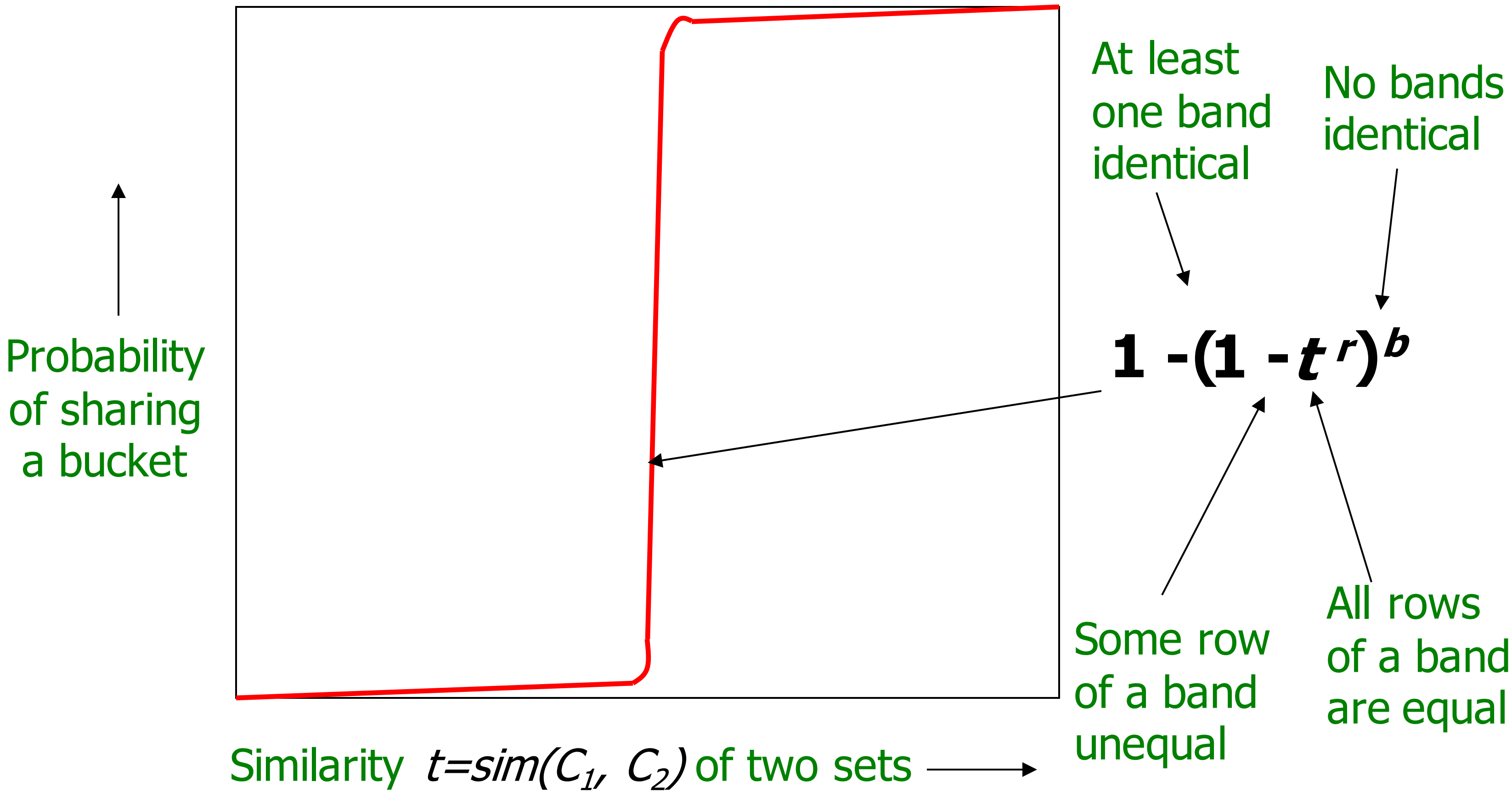
Say "yes" if you are below the line.

b bands, r rows/band

- Say 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



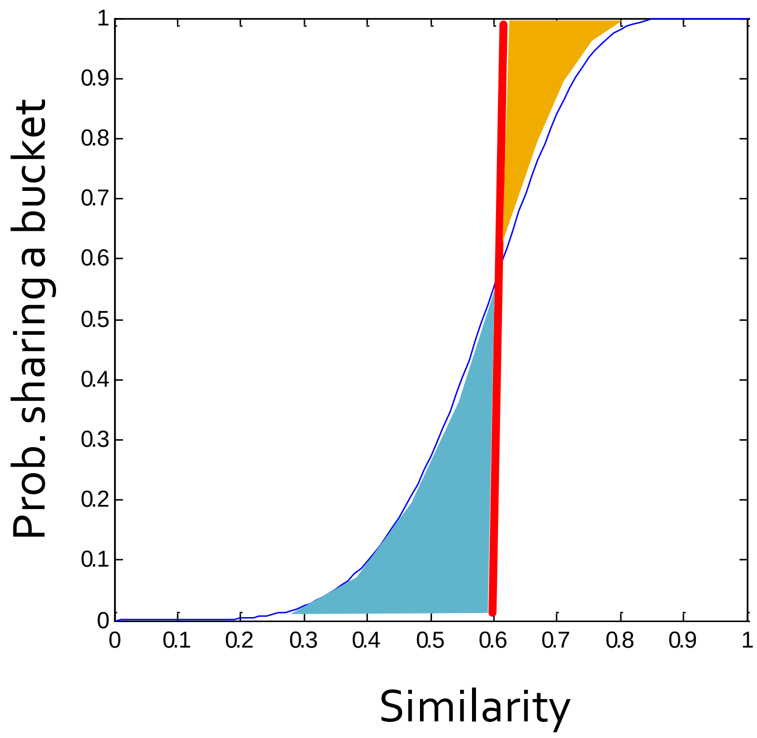
Example: $b = 20$; $r = 5$

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

s	$1-(1-s^r)^b$
0.2	0.006
0.3	0.047
0.4	0.186
0.5	0.470
0.6	0.802
0.7	0.975
0.8	0.9996

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

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



Yellow area: False Negative rate
Blue 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 the data, check that the remaining candidate pairs really represent similar documents

Summary: 3 Steps

- **Shingling:** Convert documents to set representation
  - 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**