Finding Similar Items: Locality Sensitive Hashing

Adapted from slides of:
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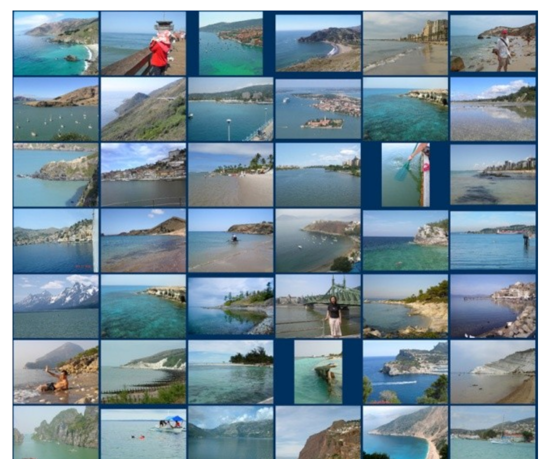
[Hays and Efros, SIGGRAPH 2007]

Scene Completion Problem



[Hays and Efros, SIGGRAPH 2007]

Scene Completion Problem

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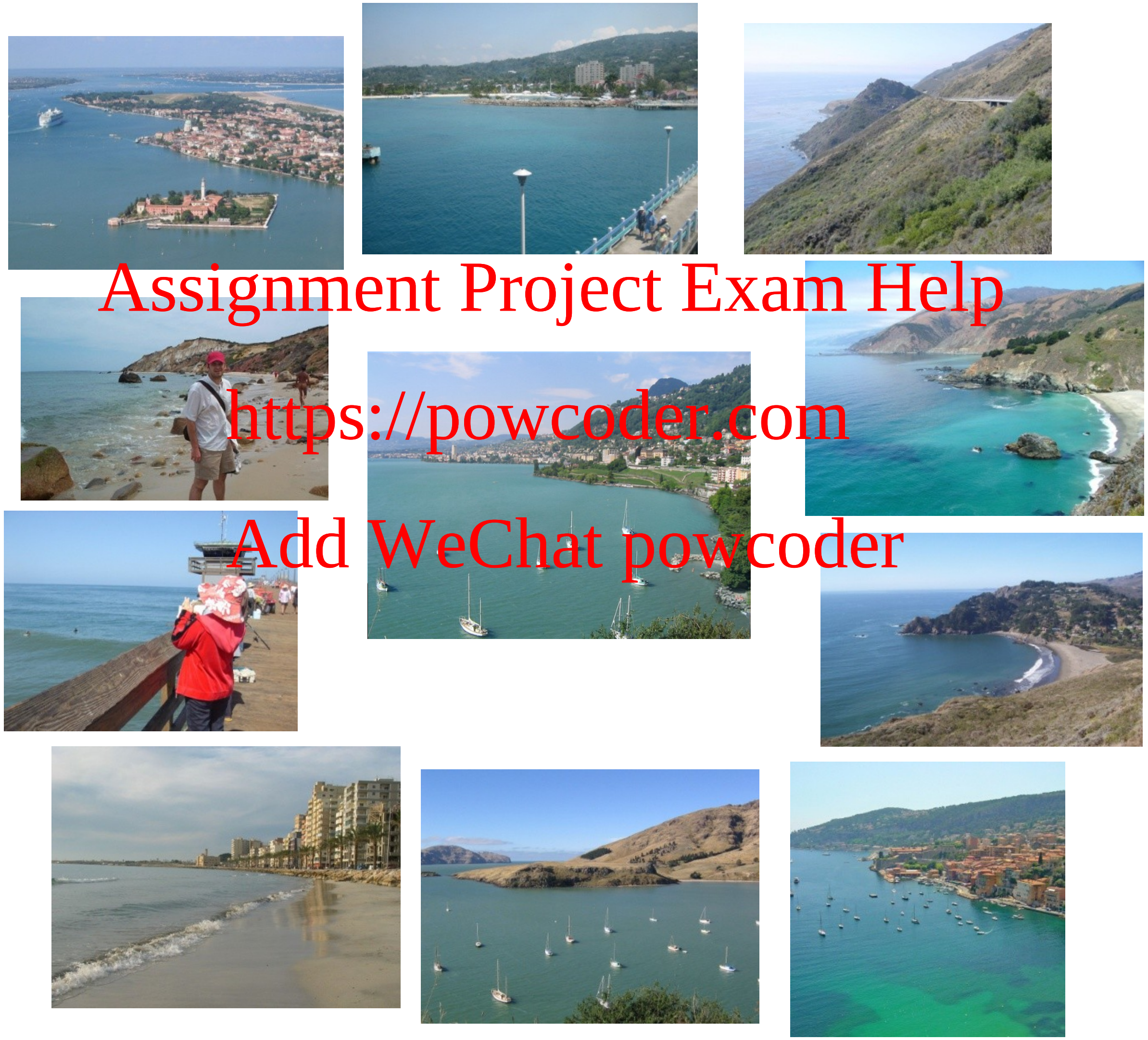
Scene Completion Problem

10 nearest neighbors from a collection of 20,000 images

[Hays and Efros, SIGGRAPH 2007]

Scene Completion Problem



10 nearest neighbors from a collection of 2 million

A Common Metaphor

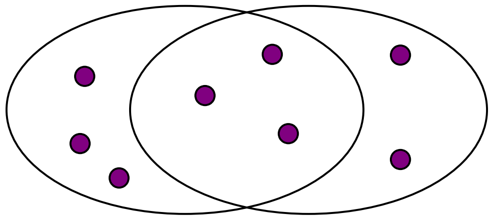
- Many problems can be expressed as finding "similar" sets:
  - Find near-neighbors in high-dimensional space
- Examples:
  - Pages with similar words
    - For duplicate detection, classification by topic
  - Customers who purchased similar products
    - Products with similar customer sets
  - Images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

Problem formuation

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

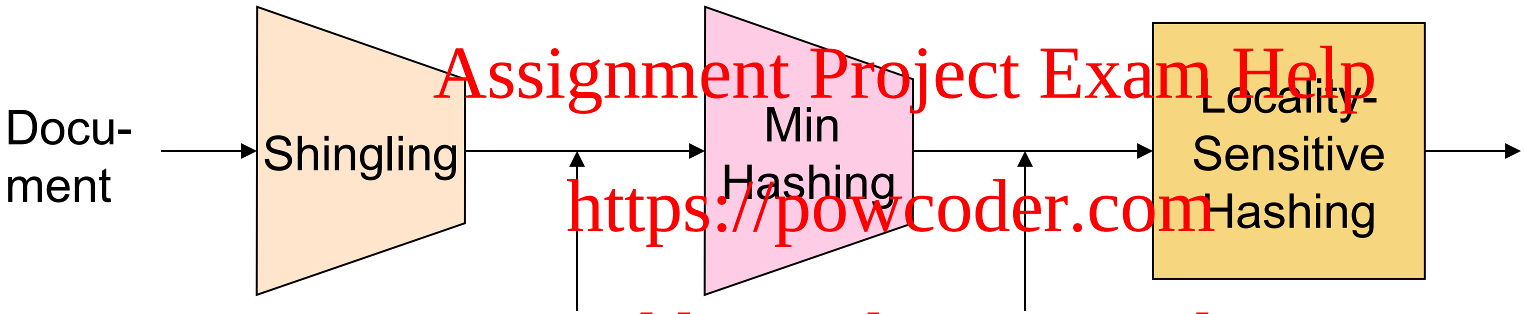
3 Essential Steps for Similar Docs

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!**

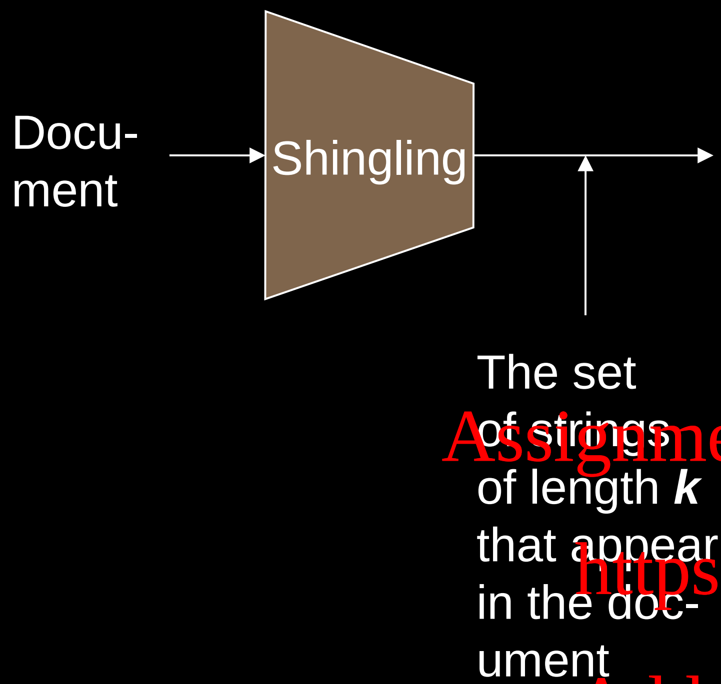
The Big Picture



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

- 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}

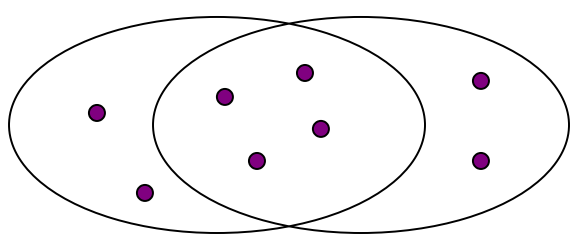
Compressing Shingles

- 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

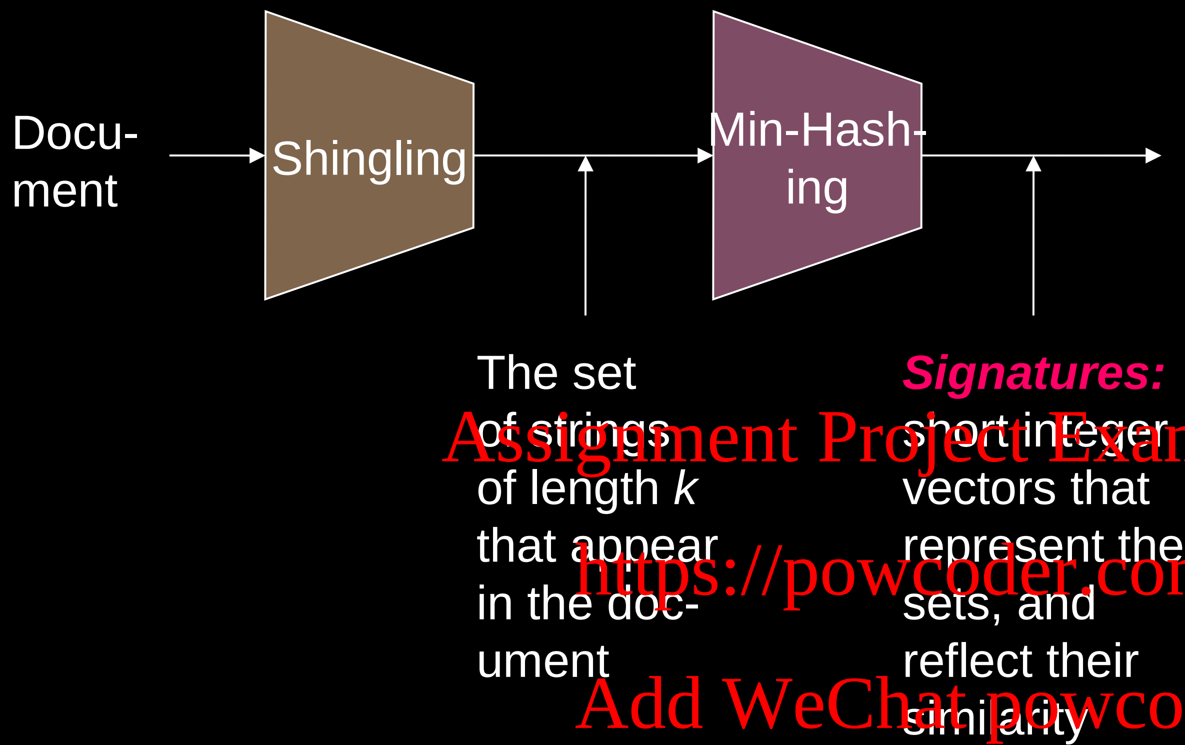
- **Suppose we need to find near-duplicate documents among $N = 1$ million documents**

- Naïvely, we would have to compute **pairwise Jaccard similarities** for **every pair of docs**

  - $N(N-1)/2 \approx 5*10^{11}$ comparisons

  - At 10^5 secs/day and 10^6 comparisons/sec, it would take **5 days**

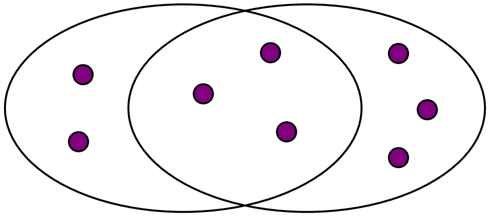
- For $N = 10$ million, it takes more than a year…



MinHashing

Step 2: ***Minhashing:*** Convert **large sets** to **short signatures**, while **<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**

An example of the matrix

Element	S_1	S_2	S_3	S_4
a	1	0	0	1
b	0	0	1	0
c	0	1	0	1
d	1	0	1	1
e	0	0	1	0

$S_1 = \{a, d\}$, $S_2 = \{c\}$, $S_3 = \{b, d, e\}$, and $S_4 = \{a, c, d\}$.

It saves space to represent a sparse matrix of 0's and 1's by the positions in which the 1's appear

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 $h(\cdot)$ 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

- 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

Example

Element	S_1	S_2	S_3	S_4
a	1	0	0	1
b	0	0	1	0
c	0	1	0	1
d	1	0	1	1
e	0	0	1	0

Element	S_1	S_2	S_3	S_4
b	0	0	1	0
e	0	0	1	0
a	1	0	0	1
d	1	0	1	1
c	0	1	0	1

Apply one permutation.
h(S1) = a; h(S2)=c; h(S3)=b; h(S4)=a)

Element	S1	S2	S3	S4
h	a	c	b	a

permutate

Another example

Element	S_1	S_2	S_3	S_4
1	1	0	0	1
2	1	0	1	0
3	0	1	1	0
4	0	0	1	1
5	1	0	0	0
6	0	0	1	1

Element	S_1	S_2	S_3	S_4
2	1	0	1	0
5	1	0	0	0
6	0	0	1	1
1	1	0	0	1
4	0	0	1	1
3	0	1	1	0

$$m(S_1) = 2$$
$$m(S_2) = 3$$
$$m(S_3) = 2$$
$$m(S_4) = 6$$

Min-Hashing Exampl

Note: Another (equivalent) way is to
store row indexes: soft permutation

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**
- **<u>Claim:</u>** $\Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
- **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. $y \in C_1 \cap C_2$
  - $\Pr[\min(\pi(C_1))=\min(\pi(C_2))]=|C_1 \cap C_2|/|C_1 \cup C_2| = sim(C_1, C_2)$

Four Types of Rows

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

	$\underline{C_1}$	$\underline{C_2}$
A	1	1
B	1	0
C	0	1
D	0	0

  - **a** = # rows of type A, etc.
- **Note:** $\text{sim}(C_1, C_2) = a/(a + b + c)$
- **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 **Input matrix (Shingles x Documents)**

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

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 **~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]* = ∞**
  - **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)

Implementation

The hash function takes the row index as input, and outputs another "row index" (simulating row permutation). There are n hash functions

For each row r, do the following:

1. Compute $h_1(r), h_2(r), \ldots, h_n(r)$.

2. For each column c do the following:

   (a) If c has 0 in row r, do nothing.

   (b) However, if c has 1 in row r, then for each $i = 1, 2, \ldots, n$ set $\text{SIG}(i, c)$ to the smaller of the current value of $\text{SIG}(i, c)$ and $h_i(r)$.

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

1. Compute $h_1(r), h_2(r), \ldots, h_n(r)$.

2. For each column c do the following:

   (a) If c has 0 in row r, do nothing.

   (b) However, if c has 1 in row r, then for each $i = 1, 2, \ldots, n$ set $\mathrm{SIG}(i, c)$ to the smaller of the current value of $\mathrm{SIG}(i, c)$ and $h_i(r)$.

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

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

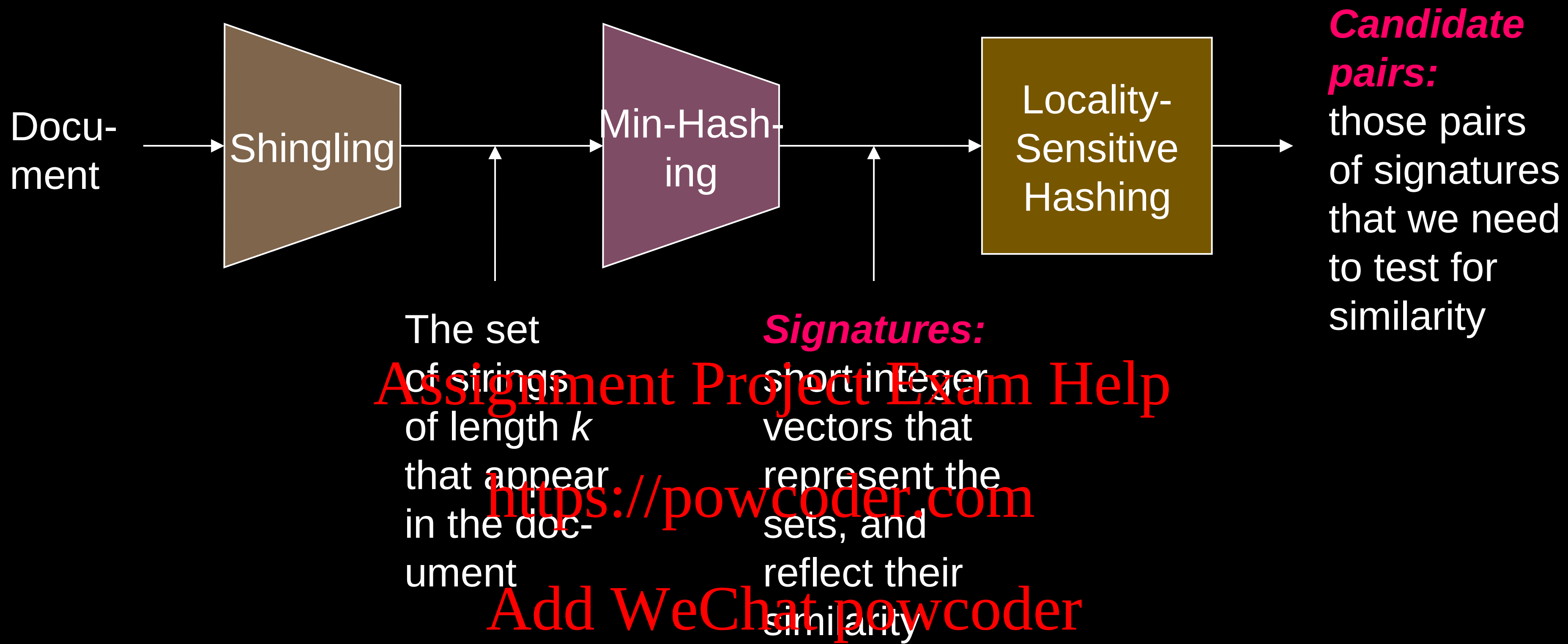
	S_1	S_2	S_3	S_4
h_1	1	∞	∞	1
h_2	1	∞	∞	1

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

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

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

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



Locality Sensitive Hashing

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

Original references

- LSH was developed by Indyk and Motwani (Indyk and Motwani, 1998) and later refined by Gionis and coworkers (Gionis et. al., 1999) for solving high-dimensional computational geometry problems such as finding nearest neighbors

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-Has

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

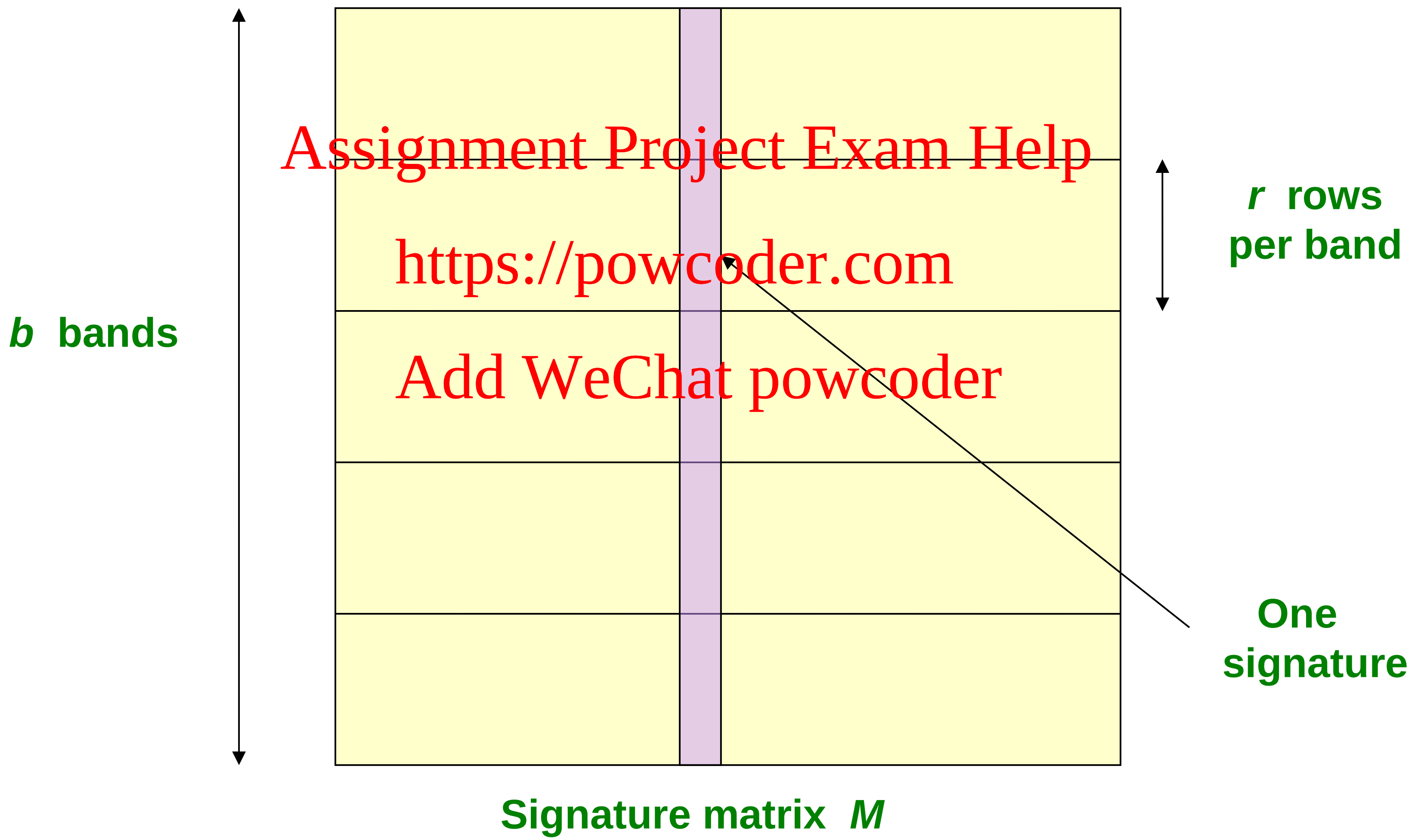
- **Big idea: Hash columns of signature matrix *M* several times**

- 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* Band

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



Partition M into Bands

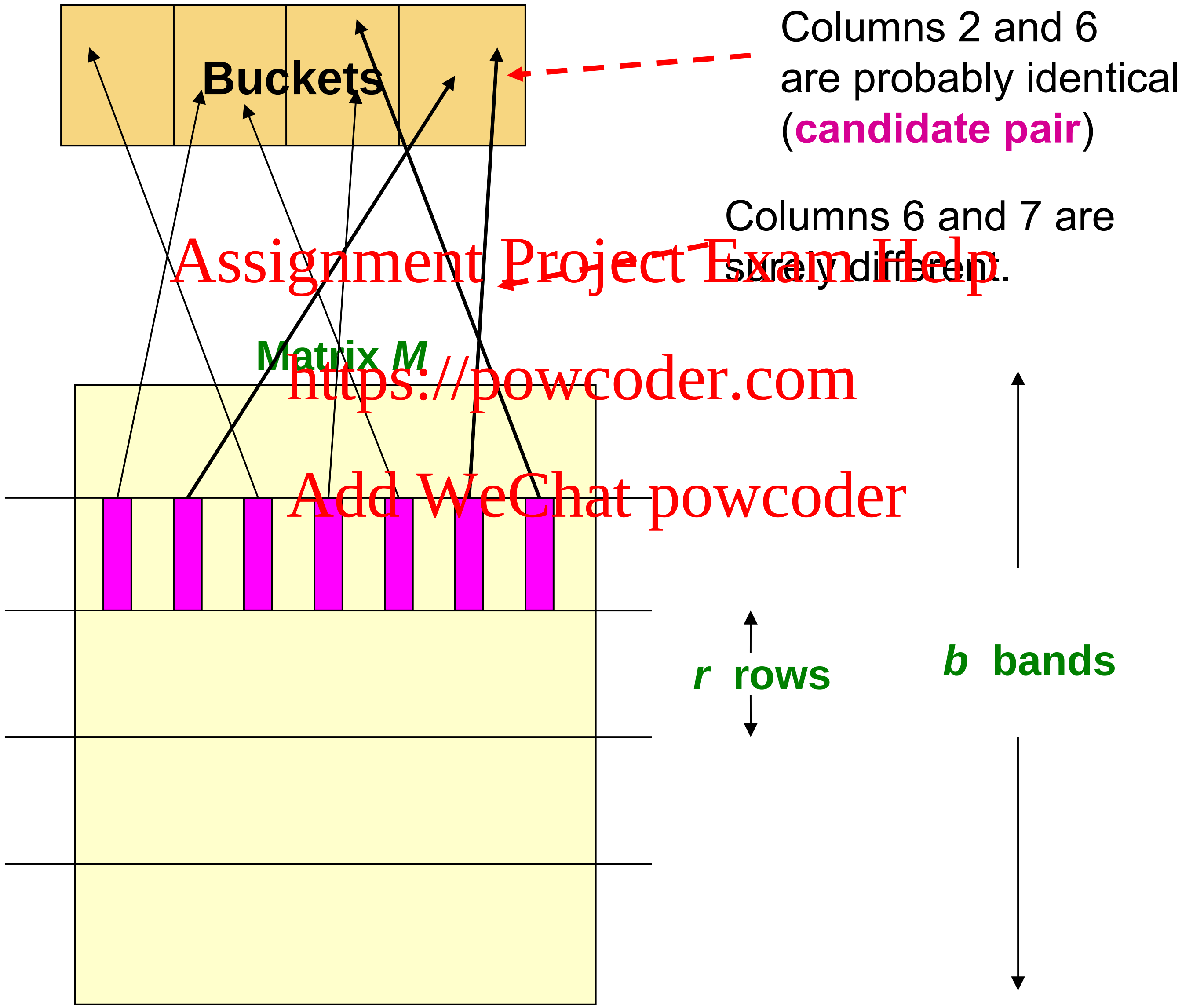
- Divide matrix ***M*** into ***b*** bands of ***r*** rows

- 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

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) = 0.8
  - 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** 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

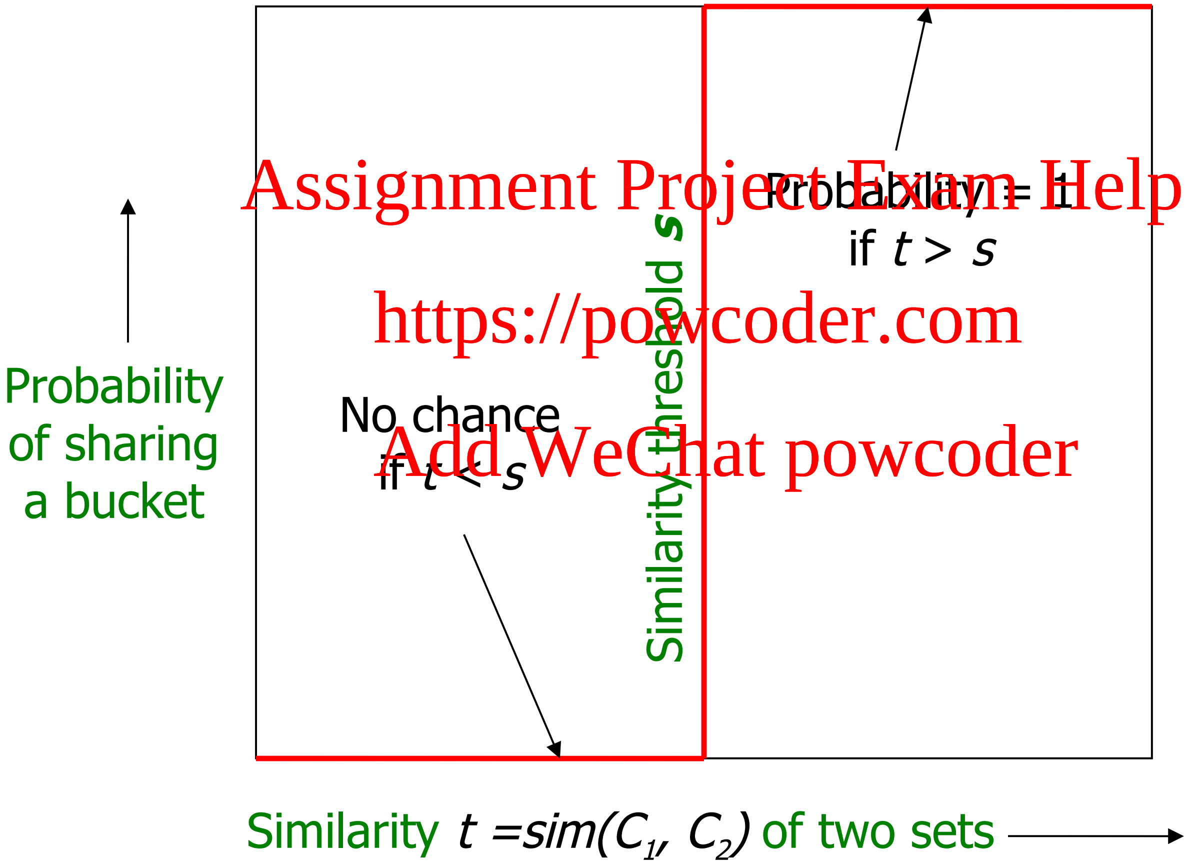
2	1	4	1
1	2	1	2
2	1	2	1

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

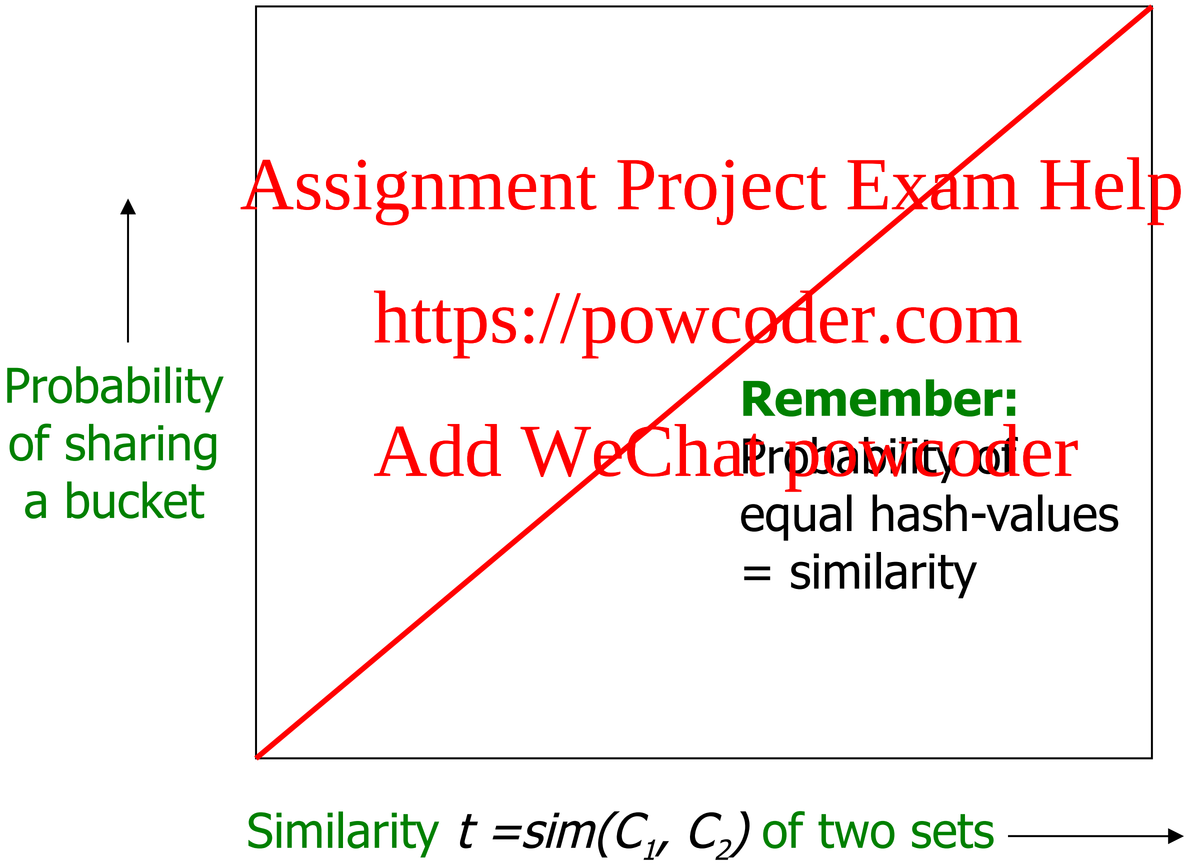
  to balance false positives/negatives

- **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

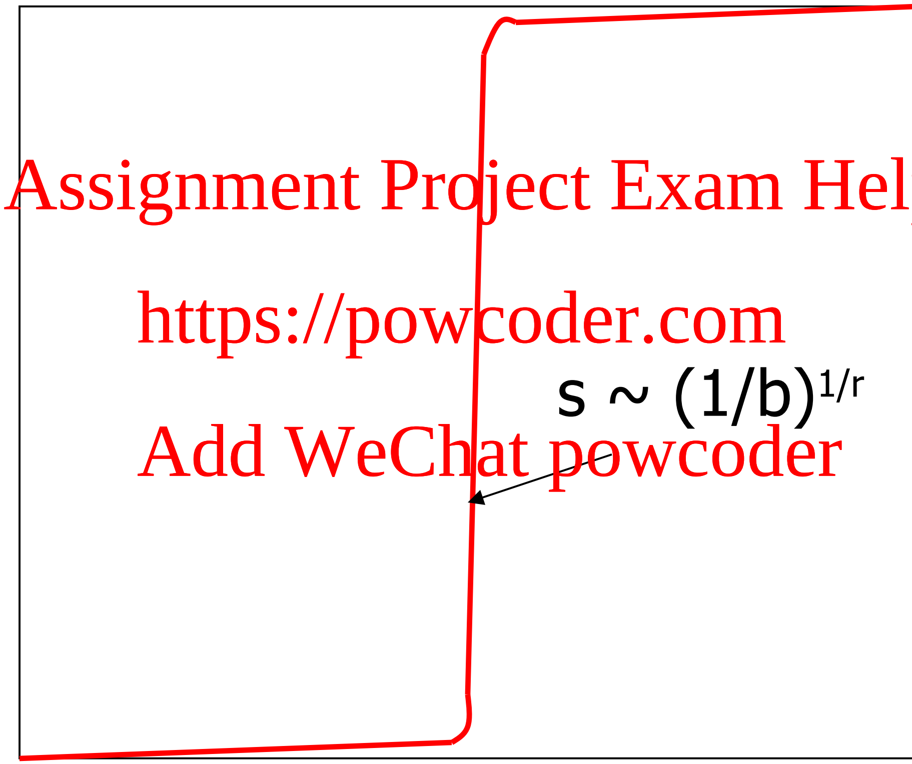


b bands, *r* rows/band

- 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 =

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

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

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

Some row of a band unequal

All rows of a band are equal

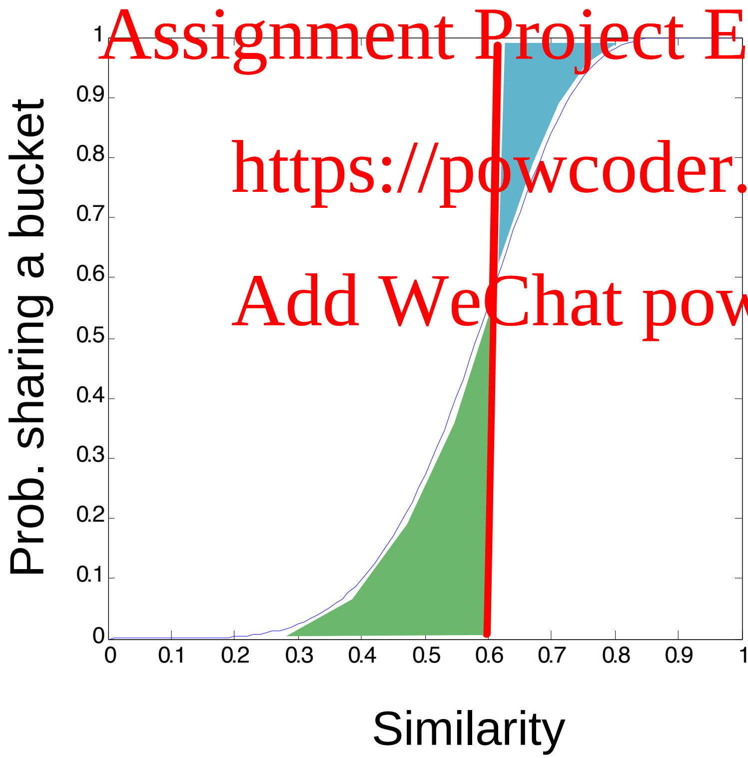
Example: $b = 20$; $r = 5$

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

NATURE BIOTECHNOLOGY | RESEARCH | ARTICLE

日本語要約

Assembling large genomes with single-molecule sequencing and locality-sensitive hashing

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Affiliations | Contributions | Corresponding author

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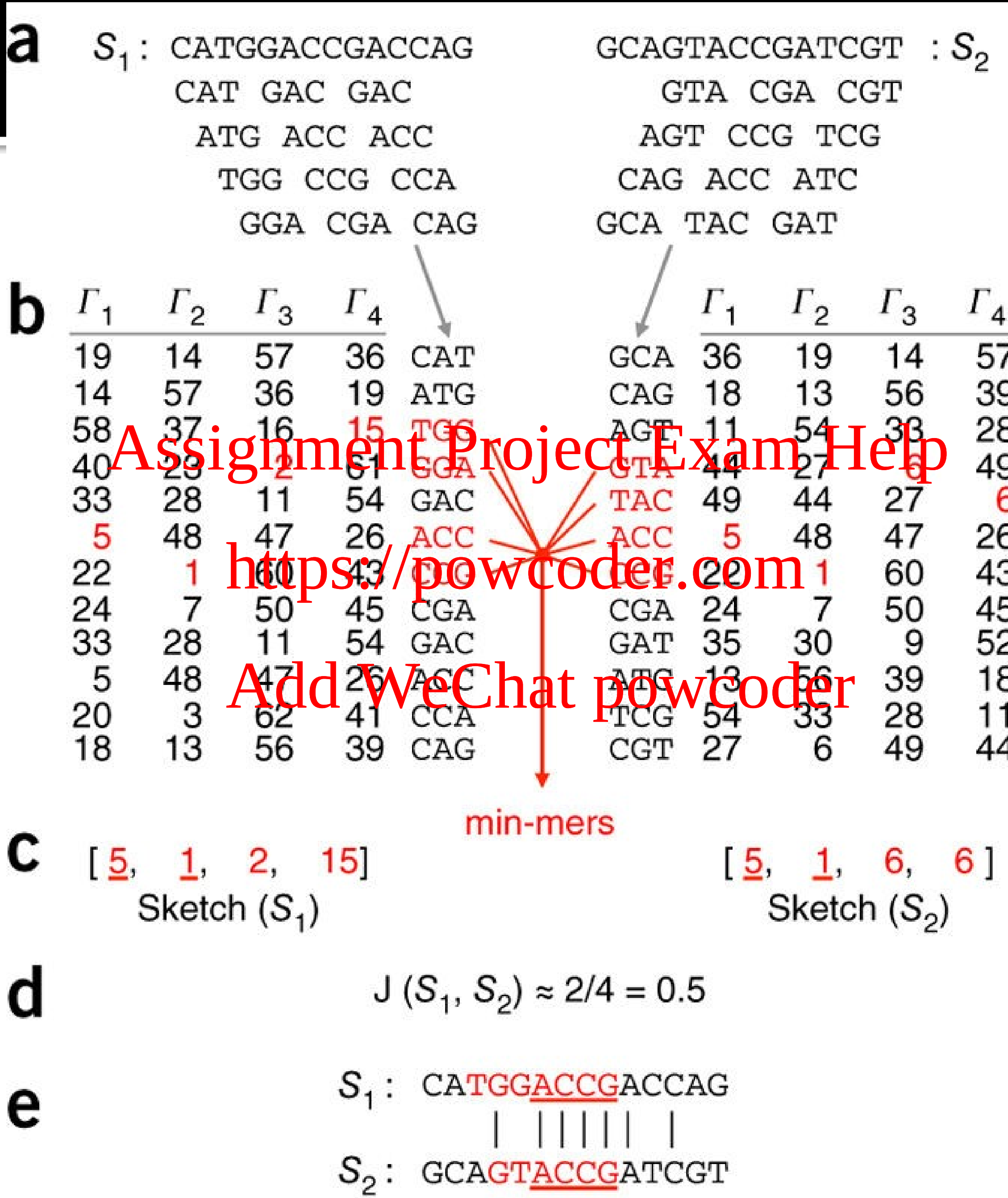
a
S_1 : CATGGACCGACCAG
CAT GAC GAC
ATG ACC ACC
TGG CCG CCA
GGA CGA CAG
GCAGTACCGATCGT : S_2
GTA CGA CGT
AGT CCG TCG
CAG ACC ATC
GCA TAC GAT
b
Γ_1 Γ_2 Γ_3 Γ_4
min-mers
c
[5, 1, 2, 15]
Sketch (S_1)
[5, 1, 6, 6]
Sketch (S_2)
d
J (S_1, S_2) ≈ 2/4 = 0.5
e
S_1 : CATGGACCGACCAG
S_2 : GCAGTACCGATCGT