DS 503: Advanced Data Analytics

Lecture 5: Locality Sensitive Hashing

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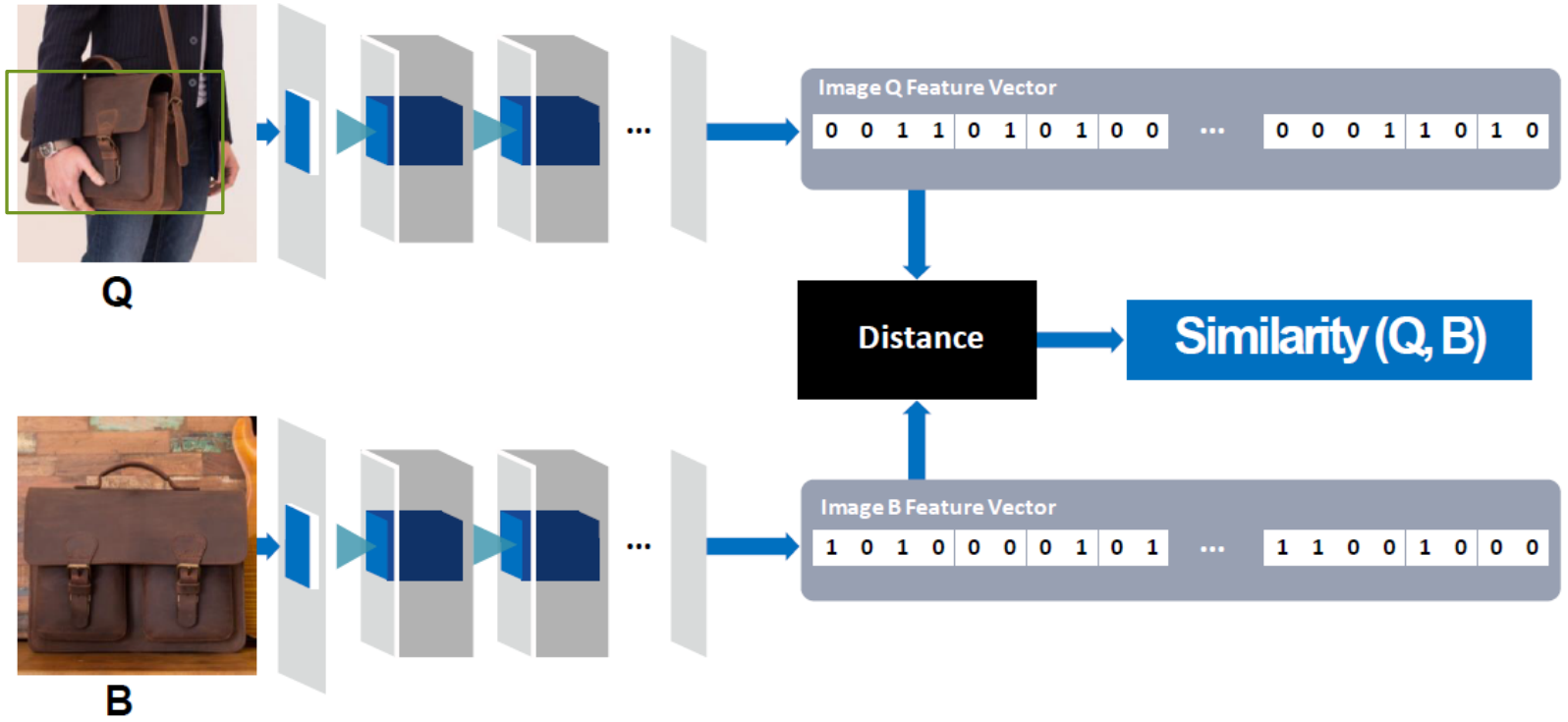
Finding similar sets

- Find near-neighbors in high-dimensional space
- **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**

Image Completion Problem

Finding similar objects/items

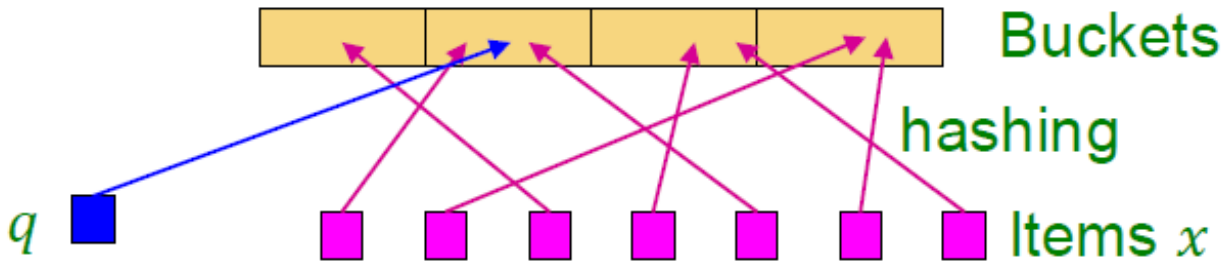


- Pinterest Visual Search
  - Given a query image patch (Q) , find similar images among the collection
  - Determine a feature vector and find nearest neighbors

Problem Statement

- Given, high dimensional points $x_1, x_2 \ldots x_n$
  - Example, images are long vectors of pixels
- And some distance function $d(x_1, x_2)$
  - Which quantifies distance between x_1 and x_2
- Goal 1: Given a query point q, find all x_j that are within a distance threshold $d(q, x_j) \leq s$
  - Can it be done in O(1)?
- Goal 2: Find all pairs of data points x_i, x_j that are within a distance threshold $d(x_i, x_j) \leq s$
  - Can it be done in O(n)?

LSH Algorithm (High Level Idea)

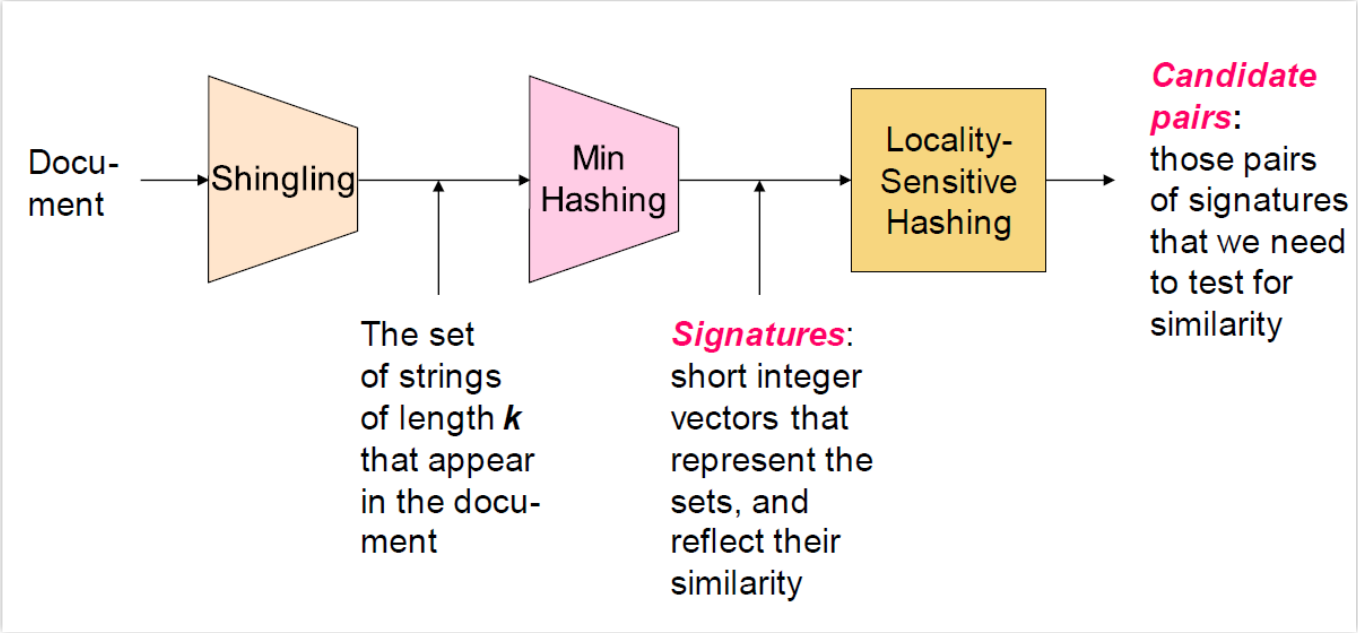


- LSH is a family of related techniques
- In general, one uses several hash functions to throw items into buckets
- Examine only those items that share a bucket for at least one hash function
- **Advantage:** With good design, only a small fraction of points are examined
- **Downside:** Some similar items may get missed (false negatives)

Motivating Example

- Near Duplicate Document in a Large Set
  - Suppose N=1 million
  - Pair-wise similarity = $5 * 10^{11}$ comparisons
  - At 10^5 seconds a day, 10^6 comparisons a sec
    - It would take 5 days
  - For N=10 million
    - It would take a year!
- Similarly, if we have a dataset of 1 B documents, finding the document which is most similar to query document q

Document Similarity (3-step process)



- Shingling produces a set representation of the document (Boolean vector)
- Min-hashing converts large sets to short signatures while preserving similarity
- LSH focuses on the pair of signatures that are most likely from similar documents

Step 1: Shingling

- Converts a document into a set
- A k-shingle (or k-gram) is a sequence of k tokens that appear in the document
  - Tokens: characters, words, or something else
- To compress shingles, we can hash them (4 bytes)
- Represent the document by the set of hash values of its shingles

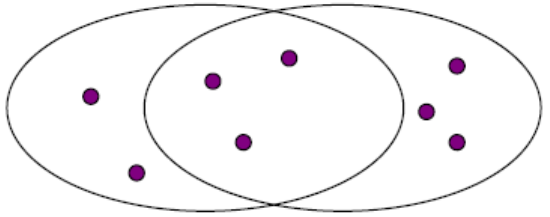
- **Example:** k=3; Document $D_1 = abdgabdga$
- Set of 3-shingles: $\{abd, bdg, dga, gab\}$
- Hash the shingles: $h(D_1)$ = {1,3,9,11}
- K= 8, 9, 10 is often used in practice

Benefits

- 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

- **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:**
  - $Sim(D_1, D_2) = \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|}$
- **Jaccard distance:**
  - $d(C_1, C_2) = 1 - \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|}$
- **Boolean Matrix Representation**
  - 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 = Jaccard similarity of sets
  - Each document is a column



3 in intersection.
8 in union.
Jaccard similarity
= 3/8

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

Min-hashing: Convert large sets to small signatures

- Important: While converting sets to small signatures, we need to preserve similarity
- Key idea: "hash" each column C to a small signature h(C) such that:
  - Sim(C1,C2) = "similarity" of signatures h(C1) and h(C2)
- **Goal:** Find a hash function $h(\cdot)$ such that:
  - If ***sim(C1,C2)*** is high, then with high prob. ***h(C1) = h(C2)***
  - If ***sim(C1,C2)*** is low, then with high prob. ***h(C1) ≠ h(C2)***
- **Idea: Hash docs into buckets. Expect that "most" pairs of near duplicate docs hash into the same bucket!**
  - Clearly, the hash function depends on the similarity metric
  - For Jaccard similarity, the hash function is called **Min-Hashing**

Min-hashing overview

- Imagine the rows of the boolean matrix permuted under **random permutation π**
- Define a **"minhash" function for this permutation,**
- $h_\pi(C)$ = the index of the **first** (in the permuted order π) row in which column ***C*** has value **1**:

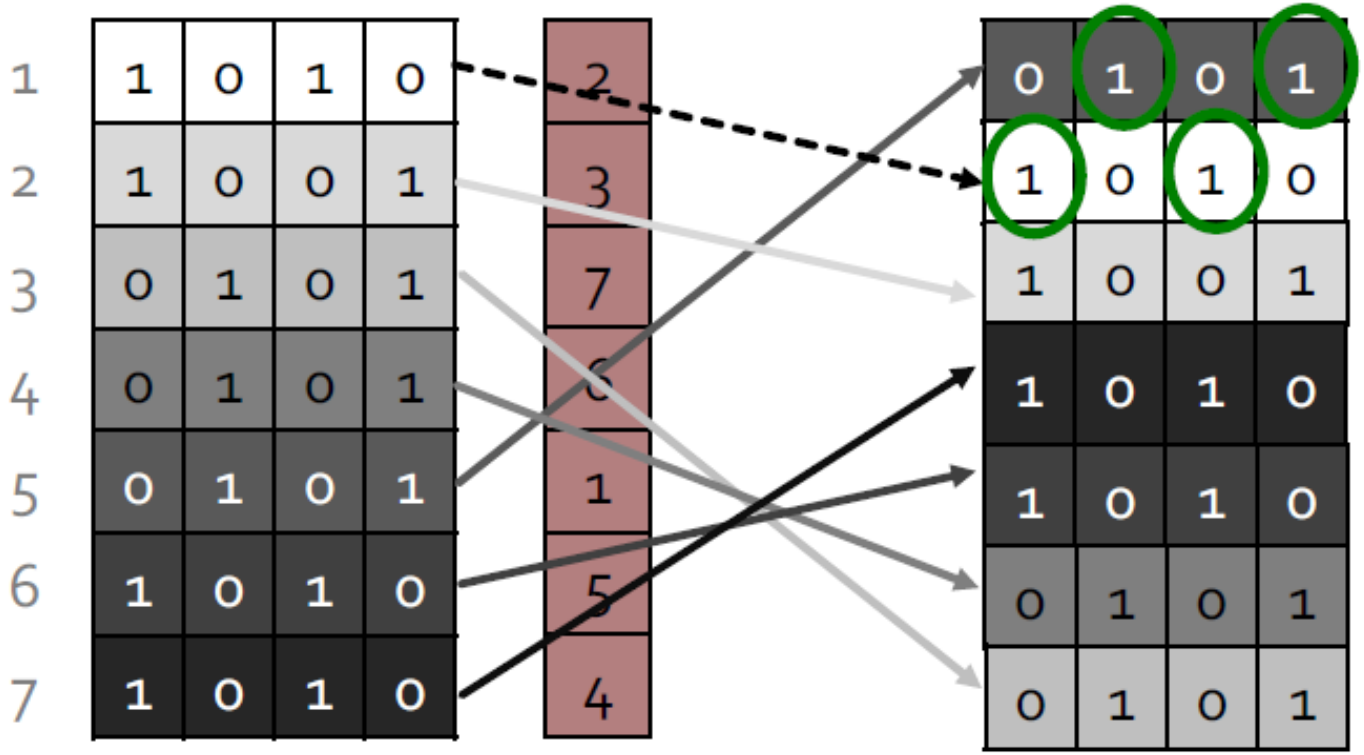
$$h_\pi(C) = min_\pi\, \pi(C)$$

- Apply, to all columns, several randomly chosen permutations π (e.g. 100) to create a signature for each column
- **Result is a signature matrix:** Columns = sets, Rows = minhash values for each permutation π

Min-hashing example

Input matrix
(Shingles x Documents)

Permutation π



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

Signature matrix *M*

2	1	2	1

new

OR

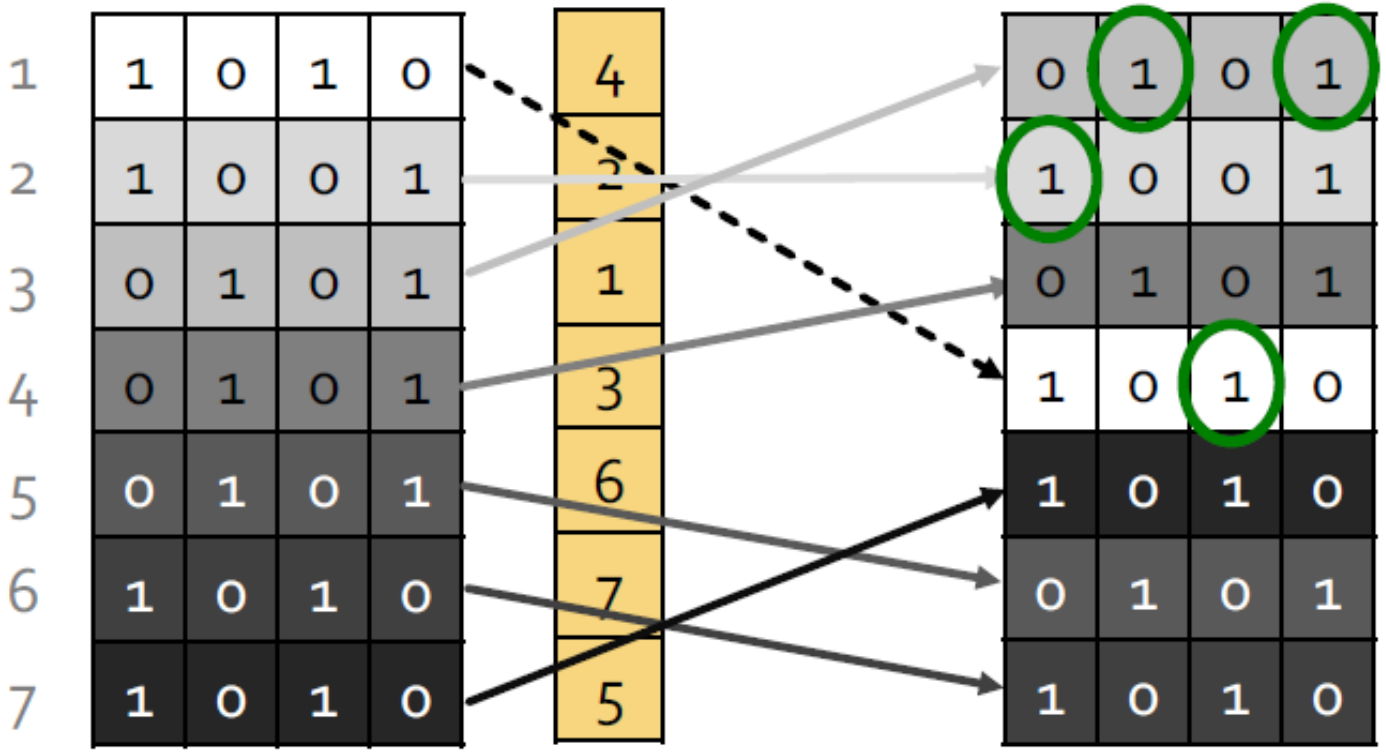
1	5	1	5

old

Min-hashing example

Input matrix
(Shingles x Documents)

Permutation π



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

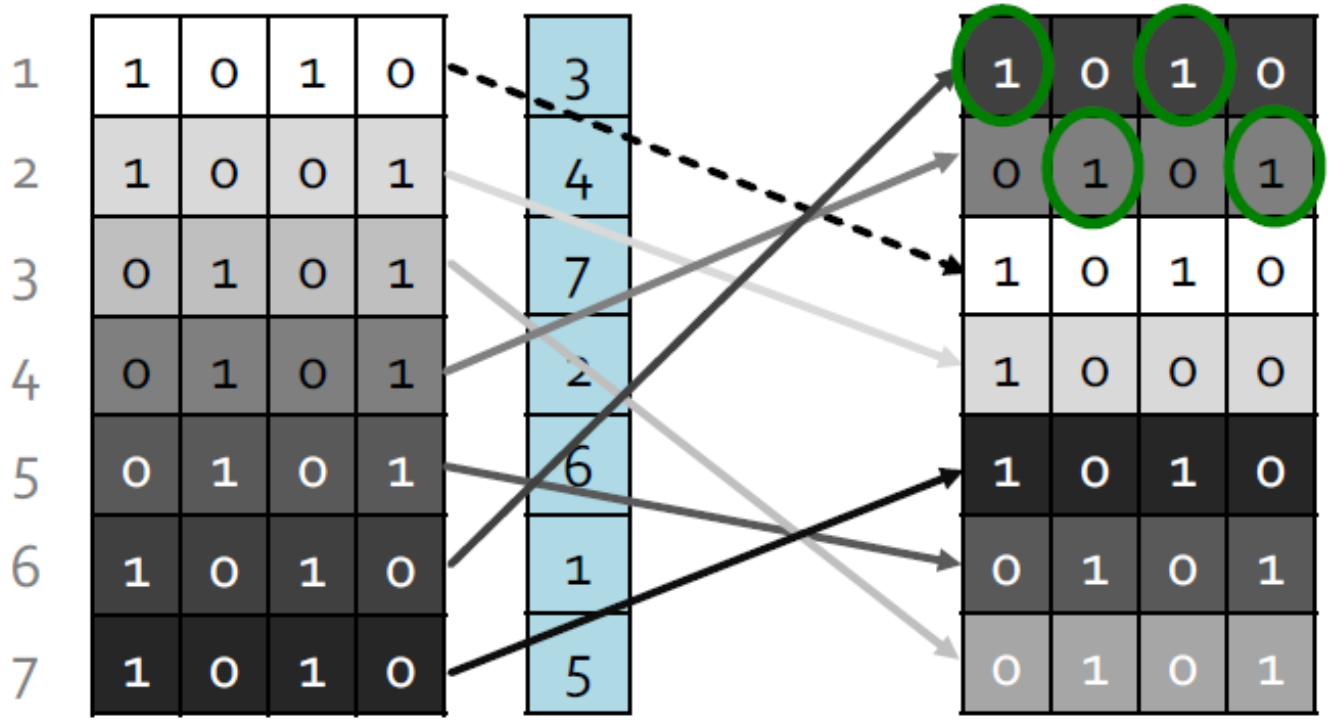
Signature matrix *M*

2	1	2	1
2	1	4	1

Min-hashing example

Input matrix
(Shingles x Documents)

Permutation π



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

Signature matrix *M*

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

Min-Hash Property

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

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

Similarity of Signatures

- We know: $\mathbf{Pr[}h_\pi(C_1) = h_\pi(C_2)\mathbf{]} = sim(C_1, C_2)$
- 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
- To get good estimates, we must use a lot of Min-Hash functions

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

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)

Example Code

```
for each row r do begin
    for each hash function h_i do
        compute h_i(r);
    for each column c
        if c has 1 in row r
            for each hash function h_i do
                if h_i(r) < M(i, c) then
                    M(i, c) := h_i(r);
end;
```

Important: so you hash r only once per hash function, not once per 1 in row r.

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)

Example run

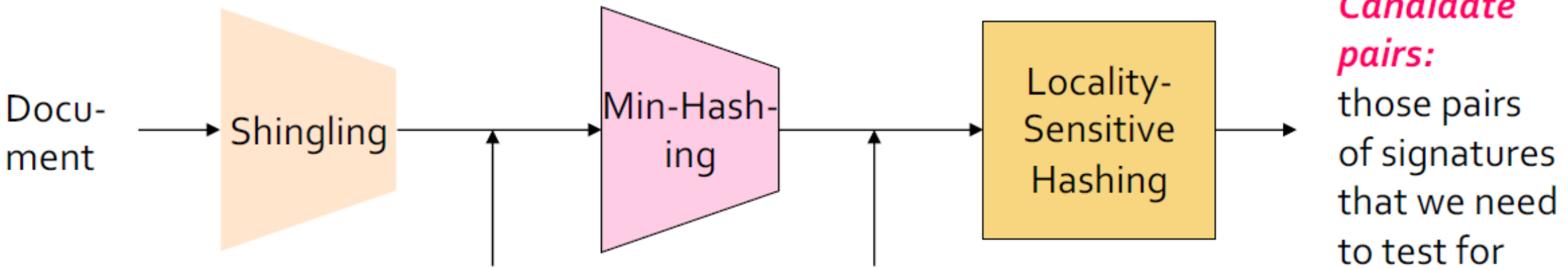
permutation h(x)	g(x)	Row	C_1	C_2
1	3	1	1	0
2	0	2	0	1
3	2	3	1	1
4	4	4	1	0
0	1	5	0	1

$h(x) = x \bmod 5$
$g(x) = (2x+1) \bmod 5$

	$M(i, C_1)$	$M(i, C_2)$
$h(1) = 1$	1	∞
$g(1) = 3$	3	∞
$h(2) = 2$	1	2
$g(2) = 0$	3	0
$h(3) = 3$	1	2
$g(3) = 2$	2	0
$h(4) = 4$	1	2
$g(4) = 4$	2	0
$h(5) = 0$	1	0
$g(5) = 1$	2	0

Signature matrix *M*

Locality Sensitive Hashing



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

The set of strings of length *k* that appear in the doc-ument

Signatures:
short integer vectors that represent the sets, and reflect their similarity

Key Idea of LSH

- **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**

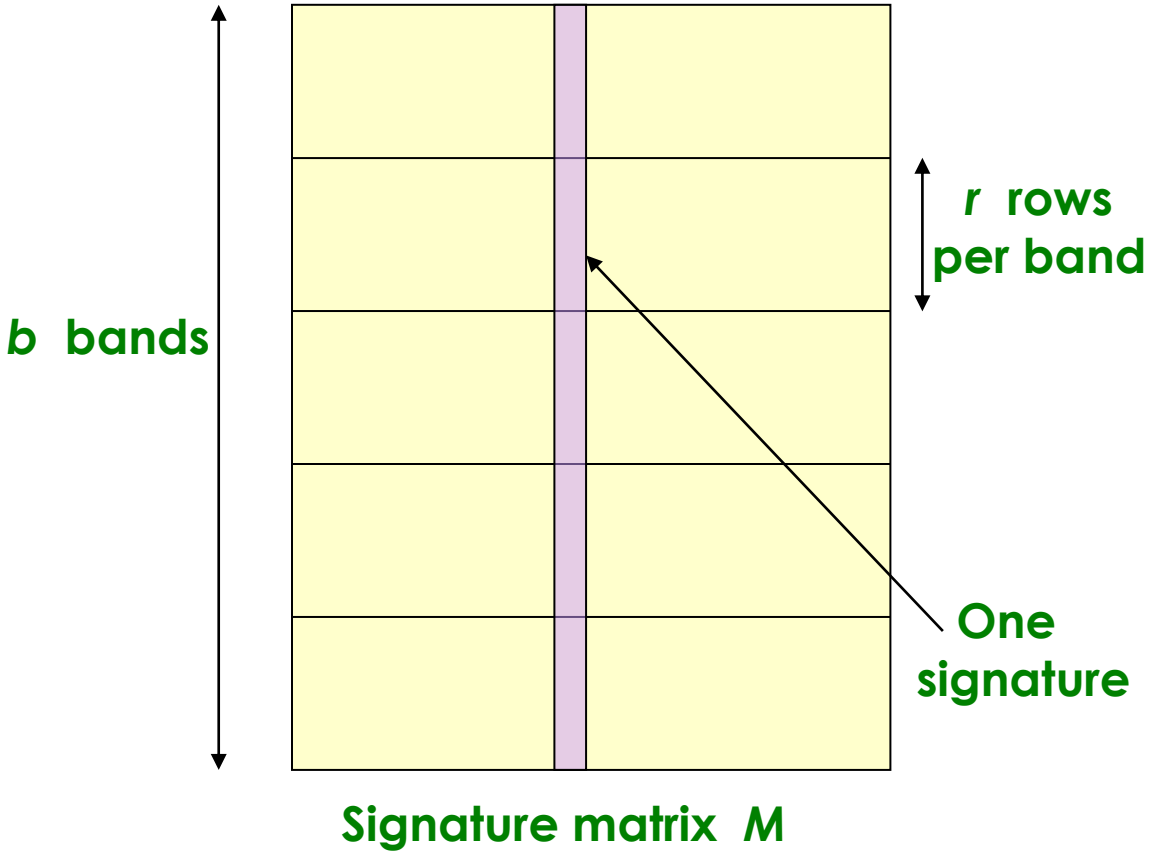
2	1	4	1
1	2	1	2
2	1	2	1

Picking Good Candidates

- **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
- **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**

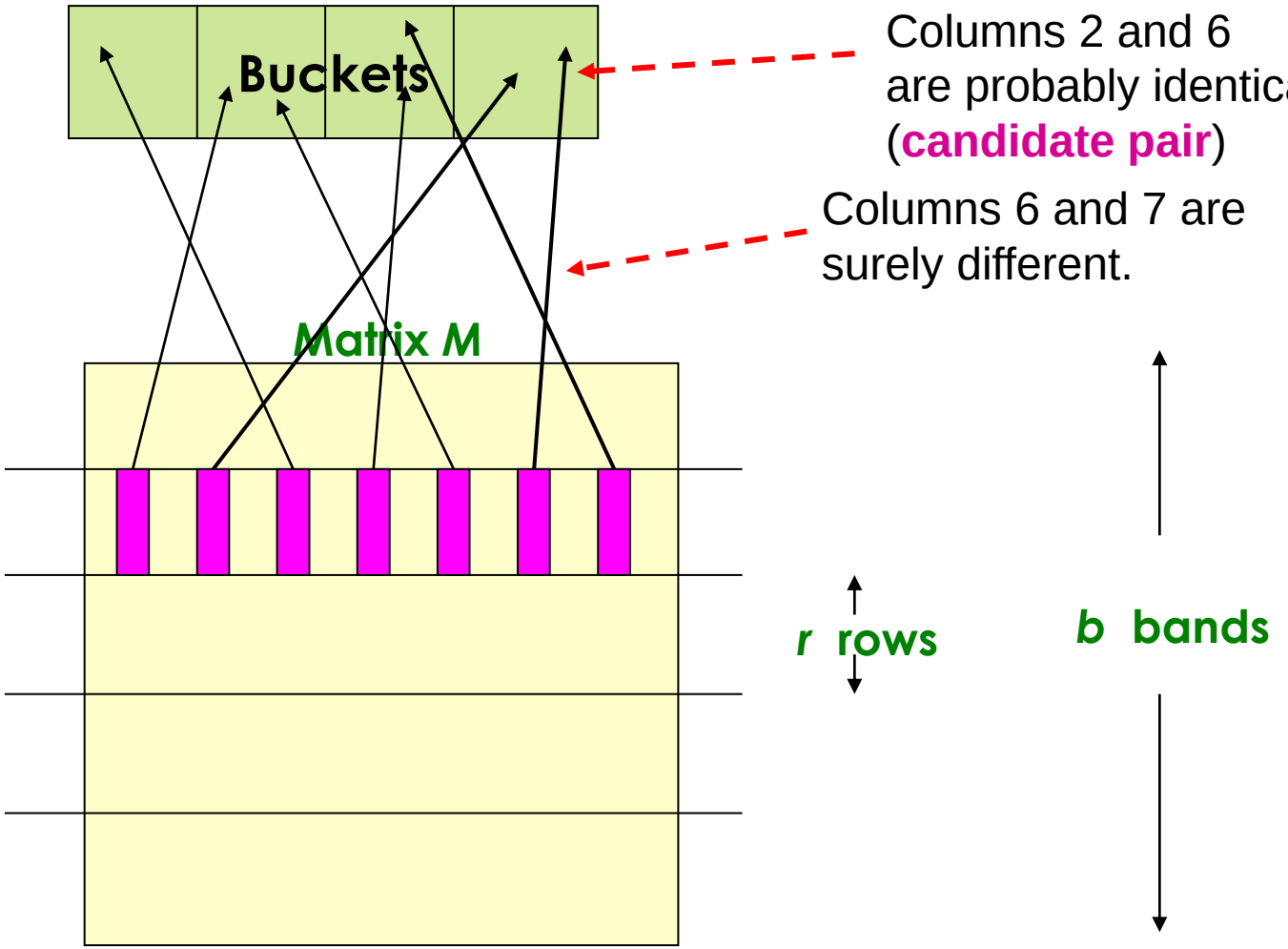
Partition Signature Matrix Into Bands

- 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 into Buckets

- 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



Analysis for a simple example

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

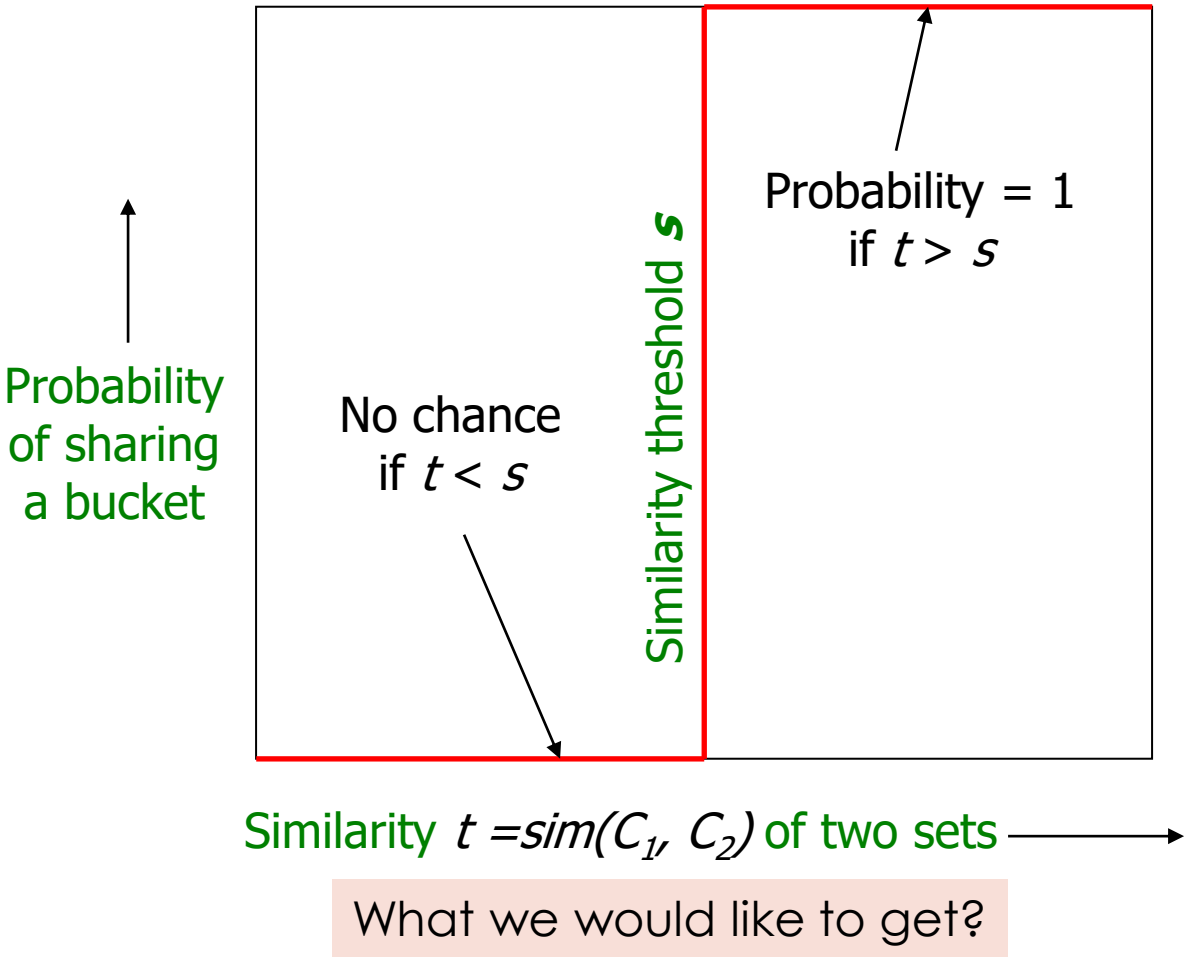
- **Goal:** Find pairs of documents that are at least ***s*** = *0.8* similar
  - **Find pairs of ≥ *s*=0.8 similarity, set b=20, r=5**
- **Assume:** $\text{sim}(C_1, C_2) = 0.8$
  - Since $\text{sim}(C_1, C_2) \geq \mathbf{s}$, we want C_1, C_2 to be a **candidate pair**: We want them to hash to at **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**

Eliminating False Positives

- **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**

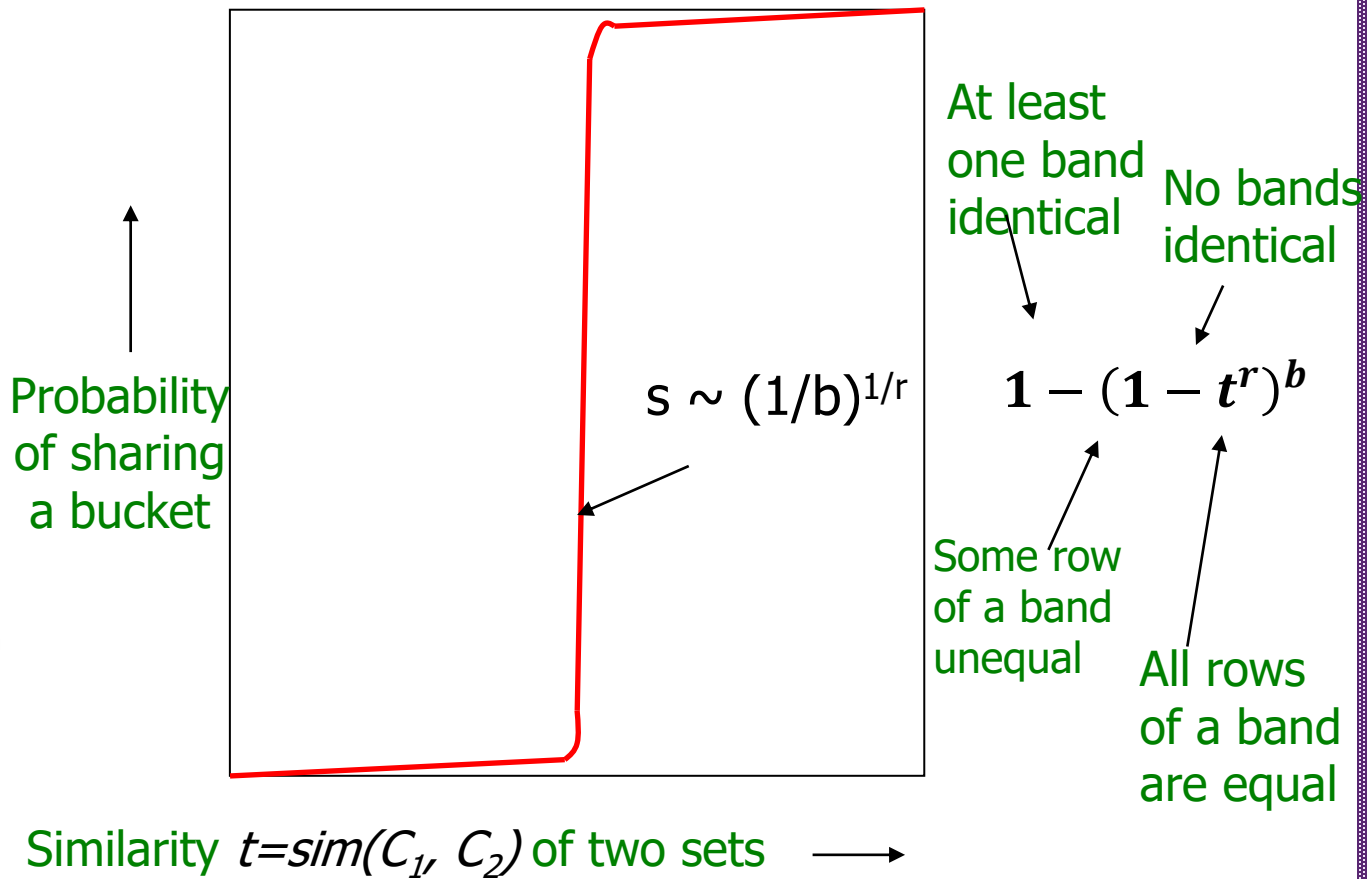
LSH Trade-off

- **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 (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 (it's harder to become a candidate pair in the bucket now)



LSH Design Parameters (b bands and 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 = $1 - (1 - t^r)^b$
-



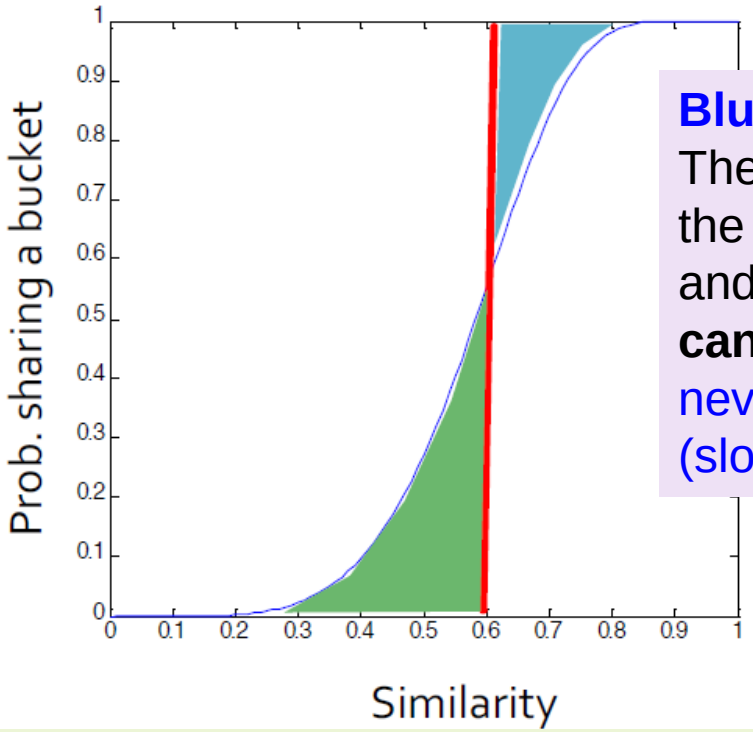
Example Calculation (r=5, b=10)

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

s	$1-(1-s^r)^b$
.2	0.003
.3	0.024
.4	0.098
.5	0.272
.6	0.555
.7	0.841
.8	0.981

Picking *r* and *b* to get the best S-curve

50 hash-functions (r=5, b=10)

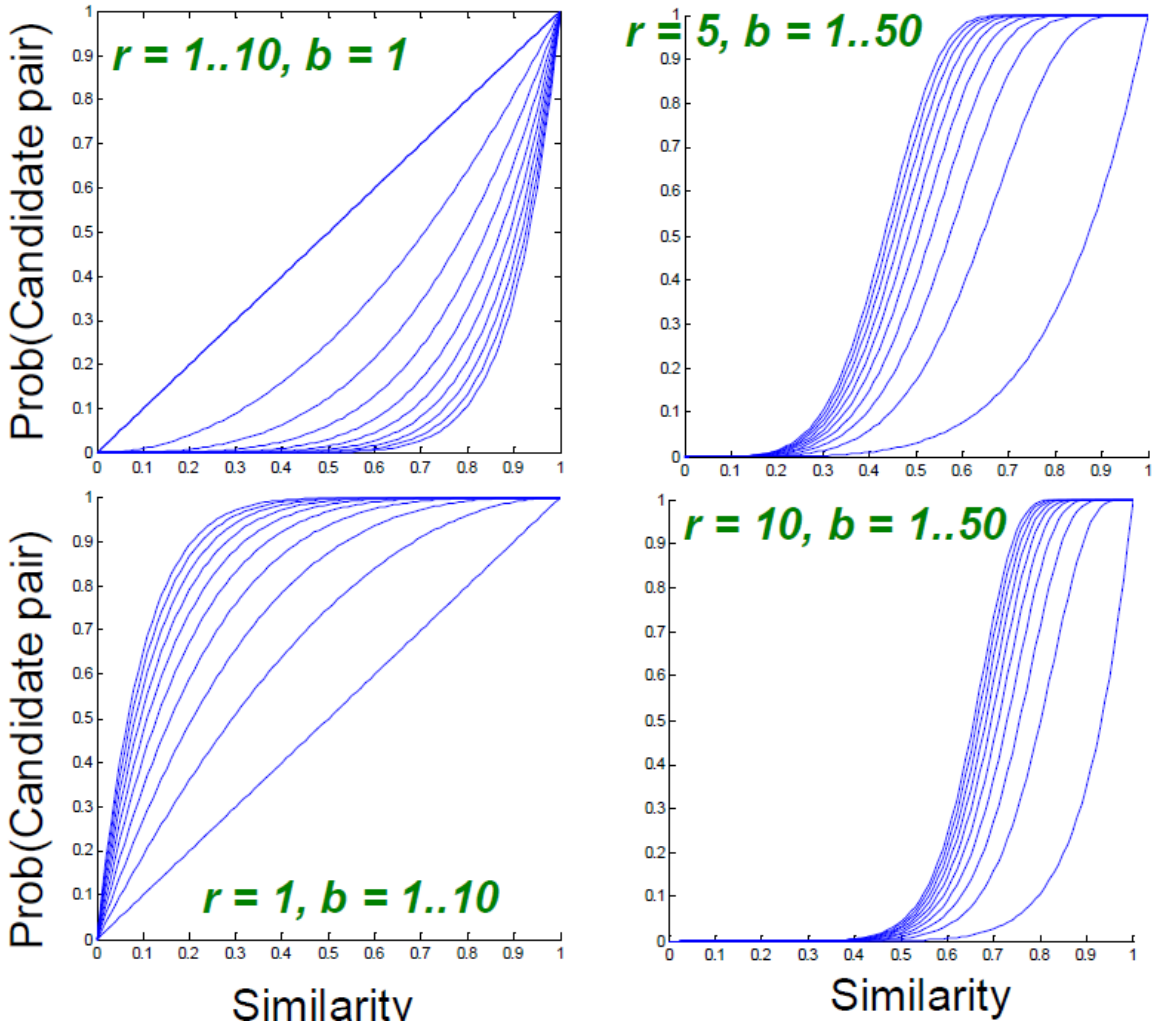


Blue area *X*: False Negative rate
These are pairs with ***sim* > *s*** but the ***X*** fraction won't share a band and then will **never become candidates.** This means we will never consider these pairs for (slow/exact) similarity calculation!

Green area Y: False Positive rate
These are pairs with ***sim* < *s*** but we will consider them as candidates. This is not too bad, we will consider them for (slow/exact) similarity computation and discard them.

S curves as a function of b and r

- Given a fixed threshold ***t*** in the query
- We want choose ***r*** and ***b*** such that the ***P(Candidate pair)*** has a “step” right around ***t***.
- **Visualization of the effect of threshold, band size, and # of rows in LSH**
- https://www.desmos.com/calculator/lzzvfjiujn



Conclusion

- 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
- 3 Step Process:
- **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**

Generalization of distance functions

- **We have used LSH to find similar documents**
- More generally, we found similar columns in large sparse matrices with high Jaccard similarity
- **Can we use LSH for other distance measures?**
- e.g., Euclidean distances, Cosine distance
- **Let's generalize what we've learned!**

Distance Measures

- $d(\cdot)$is a **distance measure** if it is a function from pairs of points **x,y** to real numbers s.t.:
  - $d(x,y) \geq 0$
  - $d(x,y) = 0 \; iff \; x = y$
  - $d(x,y) = d(y,x)$
  - $dx,y \leq d(x,z) + d(z,y)$ (triangle inequality)
- Jaccard distance for sets = 1 -Jaccard similarity
- Cosine distance for vectors = angle between the vectors
- Euclidean distances:
  - *L*2 *norm*: d(x, y) = square root of the sum of the squares of the differences between *x* and *y* in each dim
  - The most common notion of “distance”
  - *L*1 *norm*: sum of absolute value of the differences in each dimension
  - *Manhattan distance*= distance if you travel along axes only

Locally Sensitive (LS) Families of Hash Function

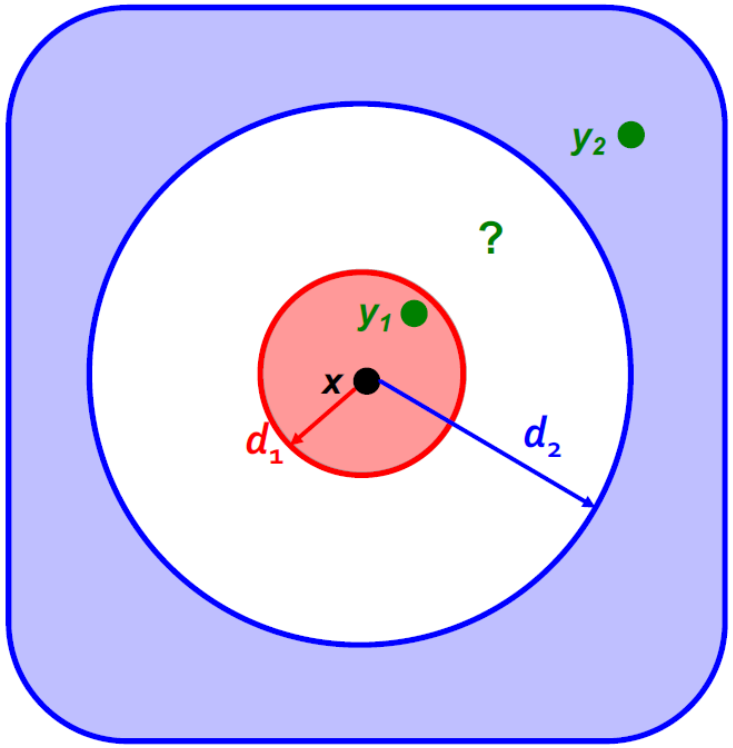
- **For Min-Hashing signatures, we got a Min-Hash function for each permutation of rows**
- A "hash function" is any function that allows us to say whether two elements are **"equal"**
- **Shorthand: *h(x) = h(y)*** means "***h says x and y are equal w.h.p.***"
- A ***family*** of hash functions is any set of hash functions from which we can ***efficiently pick one at random***
- **Example:** The set of Min-Hash functions generated from permutations of rows

Suppose we have a space *S* of points with a distance measure *d(x,y)*
A family ***H*** of hash functions is said to be **(d_1, d_2, p_1, p_2)-*sensitive*** if for any ***x*** and ***y*** in ***S***:

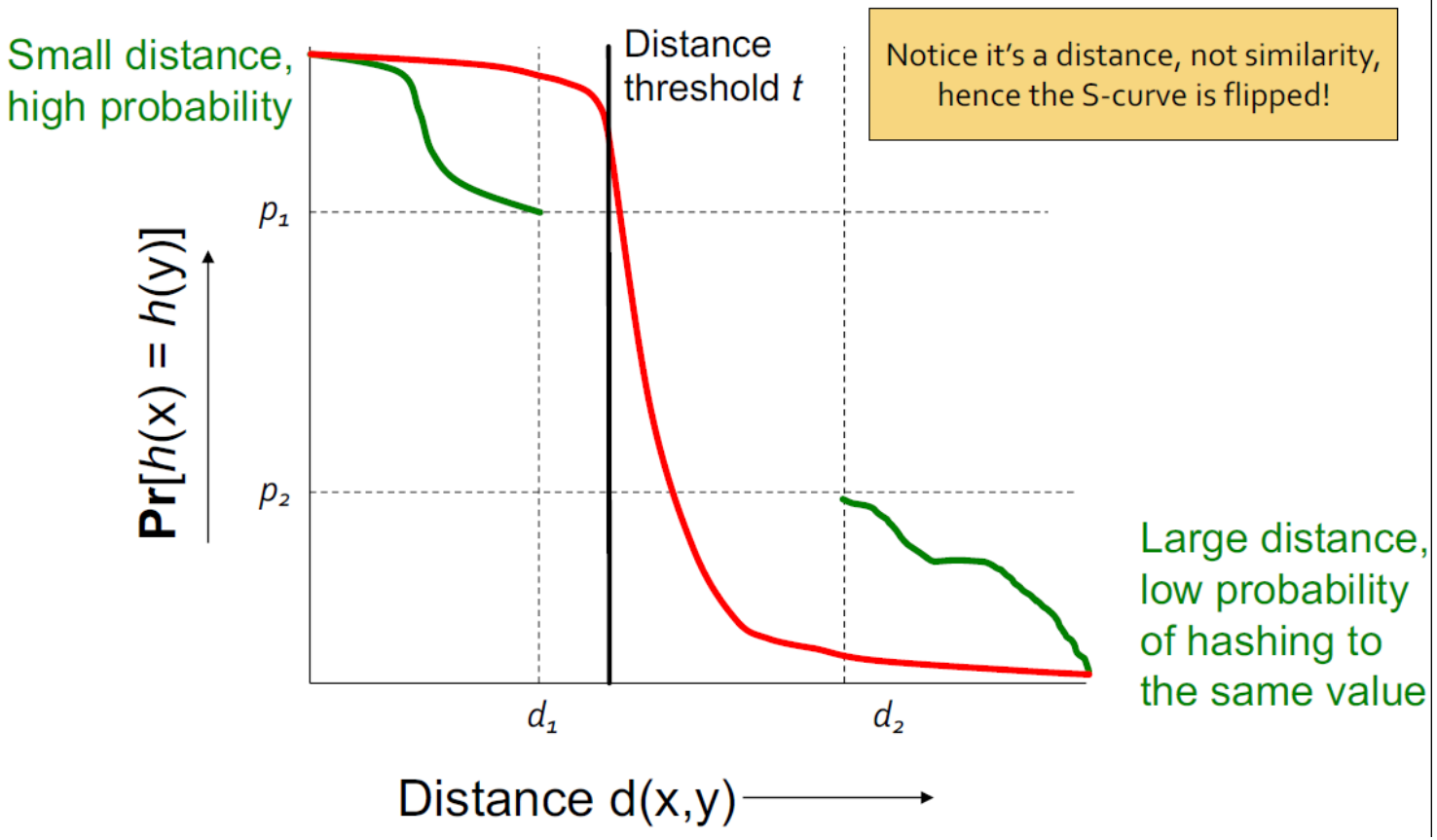
1. If $d(x, y) < d_1$, then the probability over all $h \in H$, that $h(x) = h(y)$ is at least p_1
2. If $d(x, y) > d_2$, then the probability over all $h \in H$, that $h(x) = h(y)$ is at most p_2

We can do LSH with Such Locally Sensitive (LS) Families of Hash Functions

Examples



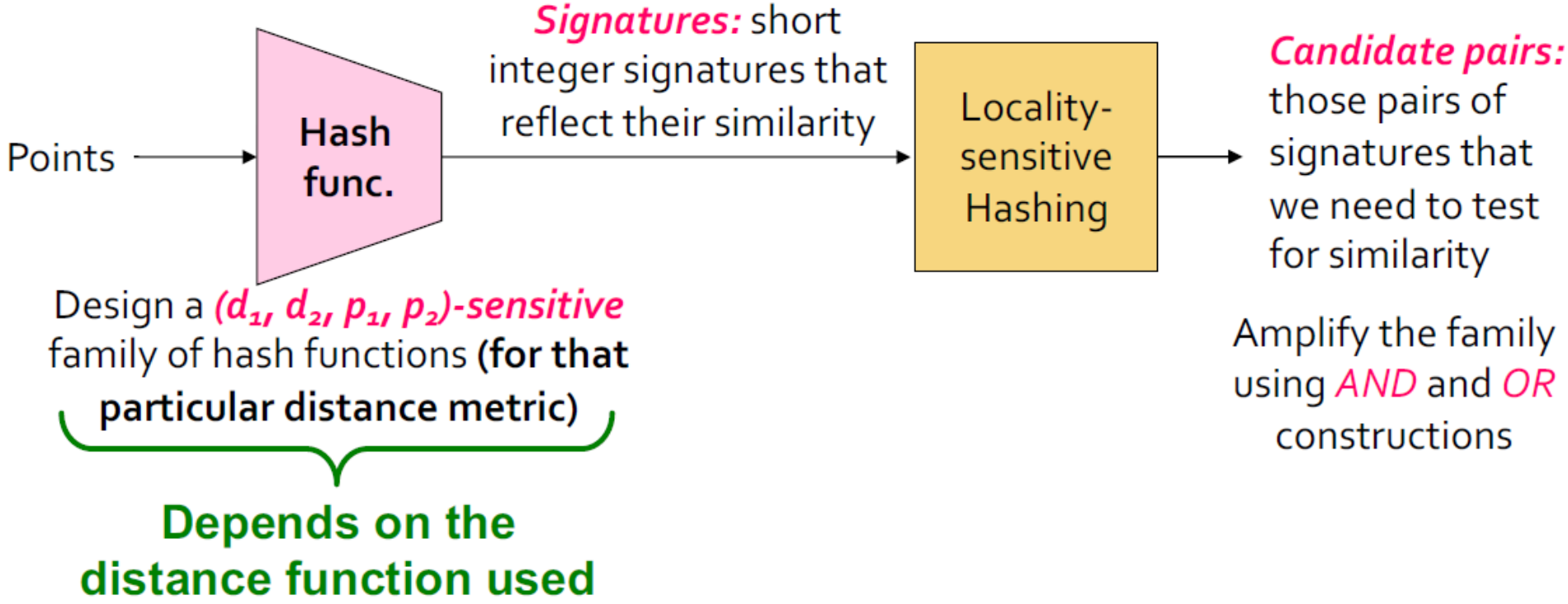
For all $h \in H$,
$P[h(x) = h(y_1)] \geq p_1$
$P[h(x) = h(y_2)] \leq p_2$



Example of LS Family: Min-Hash

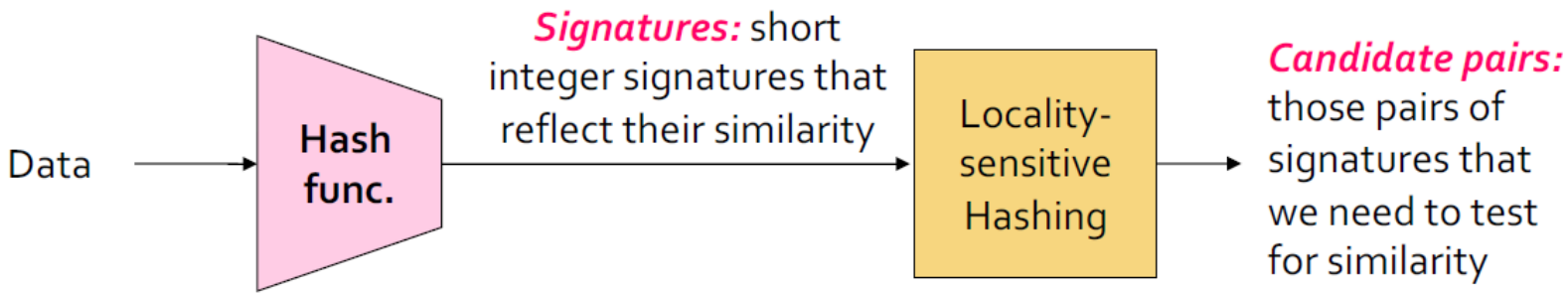
- **Let:**
  - ***S*** = space of all sets,
  - ***d*** = Jaccard distance,
  - ***H*** is family of Min-Hash functions for all permutations of rows
- Then for any hash function ***h*** ∈ ***H***:
  - ***Pr[h(x) = h(y)] = 1 - d(x, y)***
- Restate theorem about Min-Hashing in terms of distances rather than similarities
  - **Claim: Min-hash *H*** is a (1/3, 2/3, 2/3, 1/3)-sensitive family for ***S*** and ***d***.
  - If $distance \leq \frac{1}{3}$ $then$ $similarity \geq \frac{2}{3}$ Then probability that Min-Hash values agree is $\geq \frac{2}{3}$
- **For Jaccard similarity, Min-Hashing gives a *(d1,d2,(1-d1),(1-d2))*-sensitive family for any *d1<d2.***

LSH for other distance functions

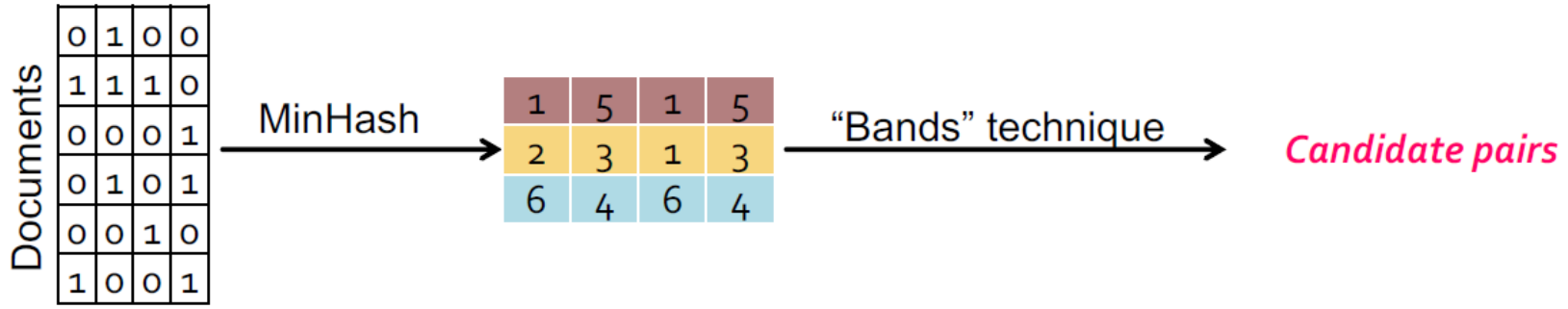


- **LSH methods for other distance metrics:**
  - **Cosine distance:** Random hyperplanes
  - **Euclidean distance:** Project on lines

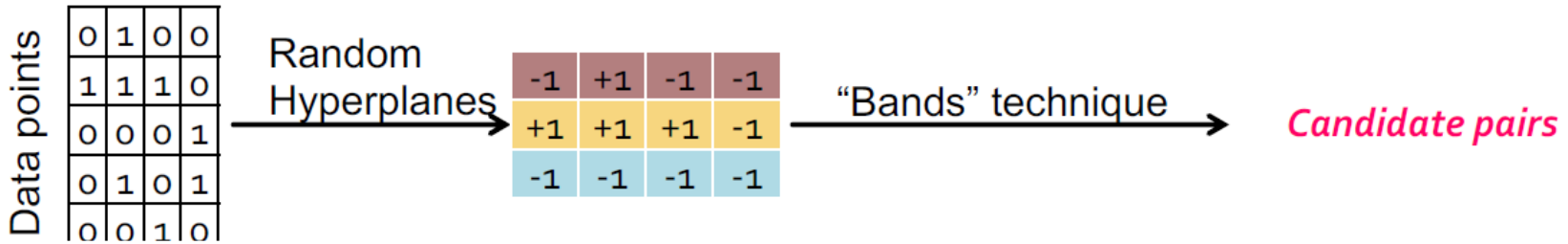
High Level Technique



Text Data



Images



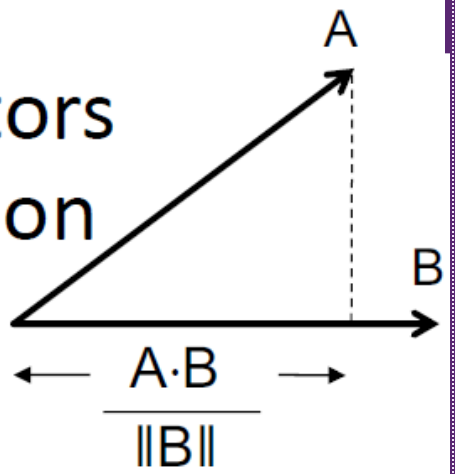
Cosine Distance

Useful metric for a variety of datasets

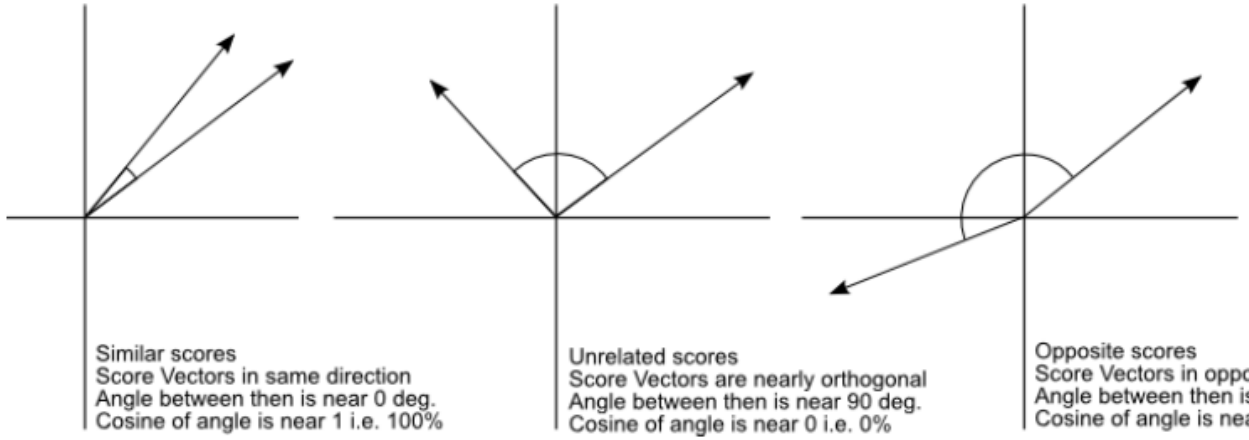
- ***Cosine distance*** = angle between vectors from the origin to the points in question

  $d(A, B) = \theta = \arccos(A \cdot B / \|A\| \cdot \|B\|)$

  - Has range $[0, \pi]$ (equivalently [0,180°])
  - Can divide θ by π to have distance in range [0,1]



- **Cosine similarity = 1-d(A,B)**
  - But often defined as **cosine sim:** $\cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$

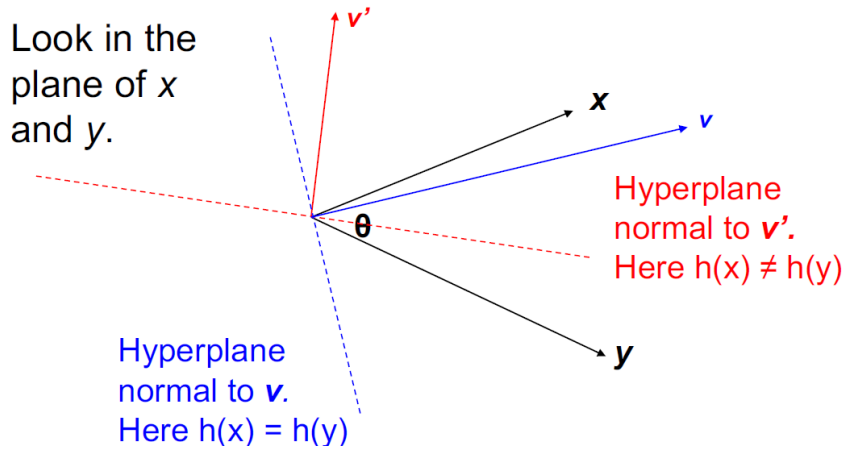


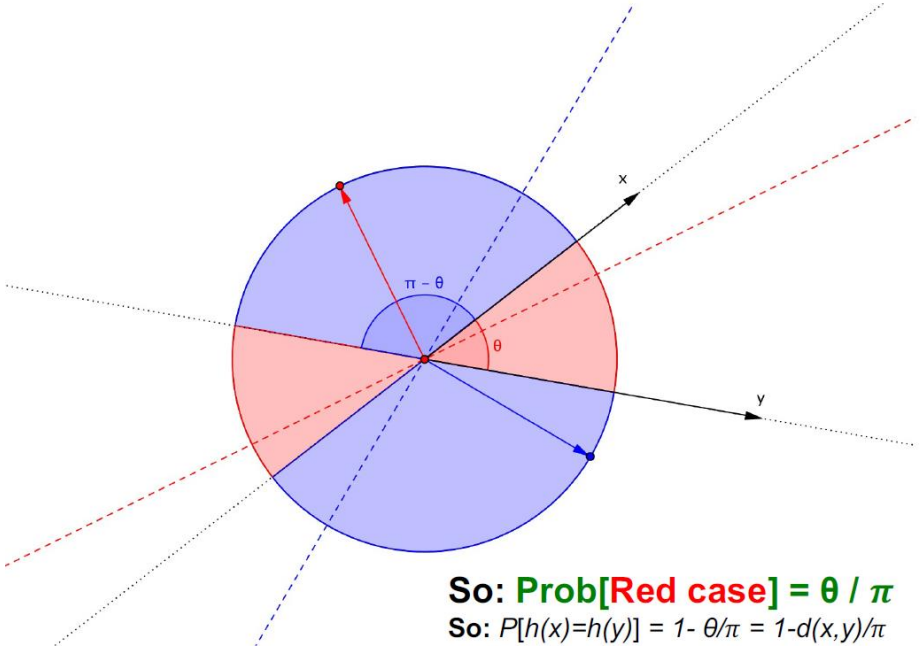
- Has range -1…1 for general vectors
- Range 0..1 for non-negative vectors (angles up to 90°)

Random Hyperplane Method

- For **cosine distance:** technique called **Random Hyperplanes**
  - Technique similar to Min-Hashing
- Each vector ***v*** determines a hash function h_v with two buckets
  - $\boldsymbol{h_v(x) = +1 \ if \ v.x \geq 0 \ ; = -1 \ if \ v.x < 0}$
  - LS-family ***H*** = set of all functions derived from any vector
- **Claim:** For points **x** and **y**,
  - **Pr[h(x) = h(y)] = 1 – d(x,y) / π**
- **Random Hyperplanes** method is a

  (d1, d2, (1-d1/π), (1-d2/π))-sensitive family for any ***d1*** and ***d2***
- **Reminder:** ***(d1, d2, p1, p2)-sensitive***
- 1. If ***d(x,y) < d1***, then prob. that ***h(x) = h(y)*** is at least ***p1***
- 2. If ***d(x,y) > d2***, then prob. that ***h(x) = h(y)*** is at most **p2**



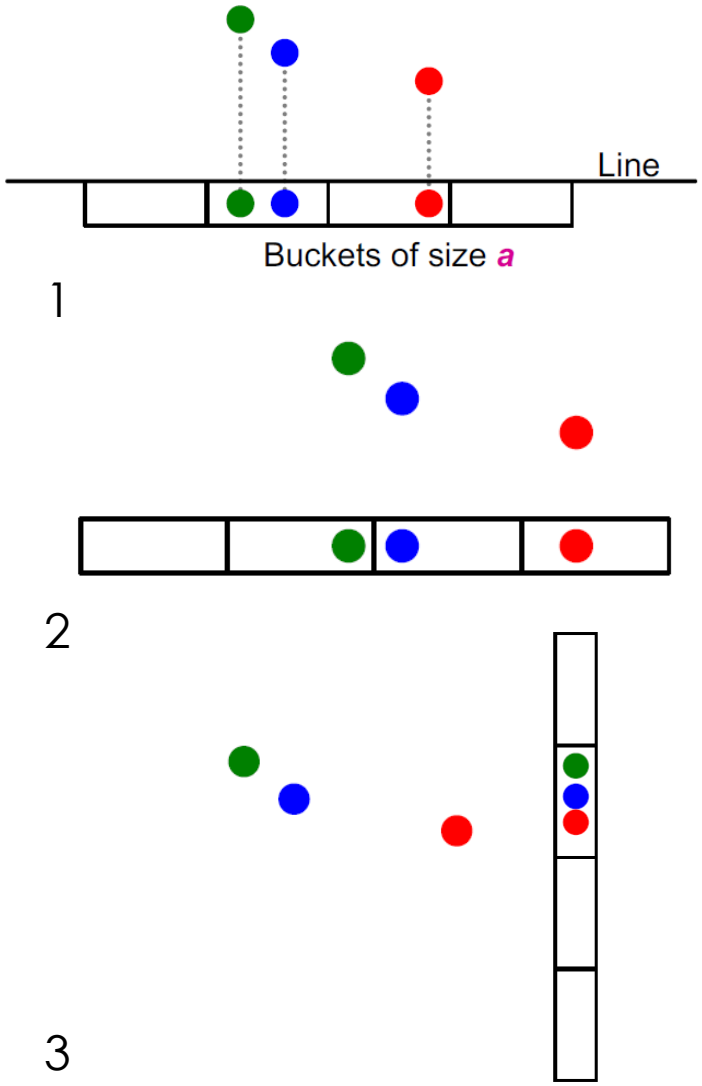


Generating Random Hyperplanes

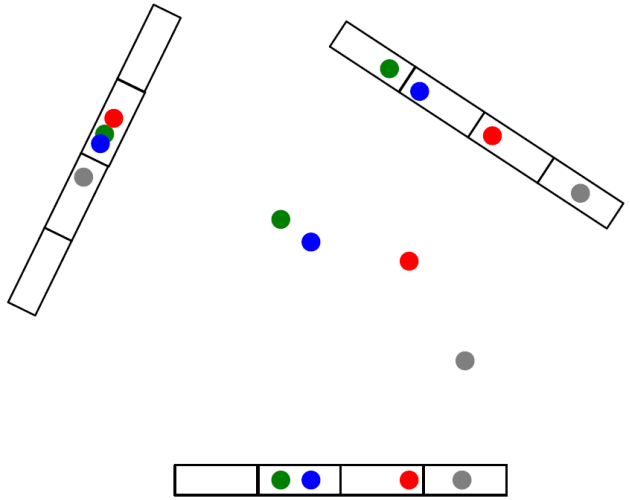
- Expensive to pick a random vector in D dimensions for large ***D***
  - Would have to generate D random numbers
- **A more efficient approach**
  - It suffices to consider only vectors ***v*** consisting of +1 and –1 components
- **Why?** Assuming data is random, then vectors of +/-1 cover the entire space evenly (and does not bias in any way)
- Pick some number of random vectors, and hash your data for each vector
  - The result is a signature (*sketch*) of **+1**'s and **–1**'s for each data point
- Can be used for LSH like we used the Min-Hash signatures for Jaccard distance
  - Amplify using **AND**/**OR** constructions (banding method)

LSH for Euclidean distance

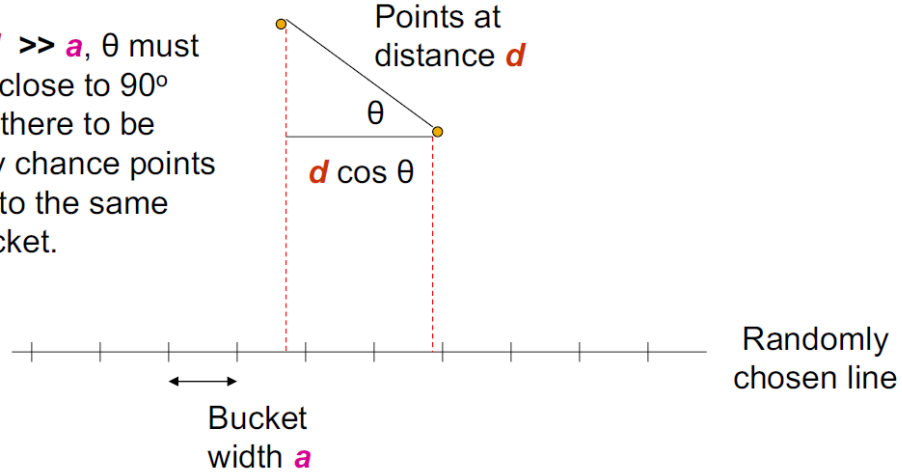
- **Idea: Hash functions correspond to lines**
  - Partition the line into buckets of size ***a***
- **Hash each point to the bucket containing its projection onto the line**
  - An element of the "Signature" is a bucket id for that given projection line
  - **Nearby points are always close**; distant points are rarely in same bucket
- **1 "Lucky" case:**
  - Points that are close hash in the same bucket
  - Distant points end up in different buckets
- **Two "unlucky" cases:**
  - **2:** unlucky quantization
  - **3:** unlucky projection



Multiple Projections

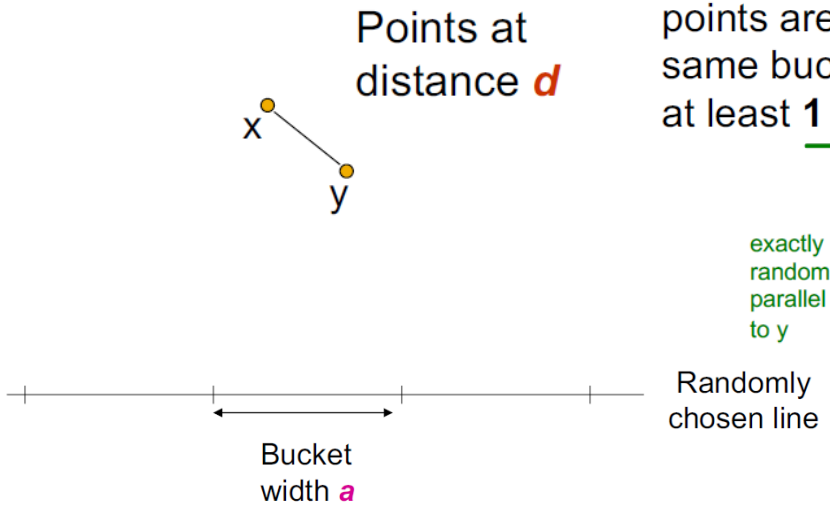


If ***d*** **>>** ***a***, θ must be close to 90° for there to be any chance points go to the same bucket.



If ***d*** **<<** ***a***, then the chance the points are in the same bucket is at least **1 – *d*/*a***.

exactly **1 – *d*/*a*** when the randomly chosen line is parallel to the line from x to y



Ls family for Euclidean distance

- If points are distance ***d < a/2***, prob. they are in same bucket ***≥ 1- d/a = 1/2***
- If points are distance ***d > 2a*** apart, then they can be in the same bucket only if ***d cos θ ≤ a***
  - cos θ ≤ 1/2
  - 60 < θ < 90, i.e., at most 1/3 probability
- Yields a ***(a/2, 2a, 1/2, 1/3)-sensitive*** family of hash functions for any ***a***
  - **Amplify using AND-OR cascades**