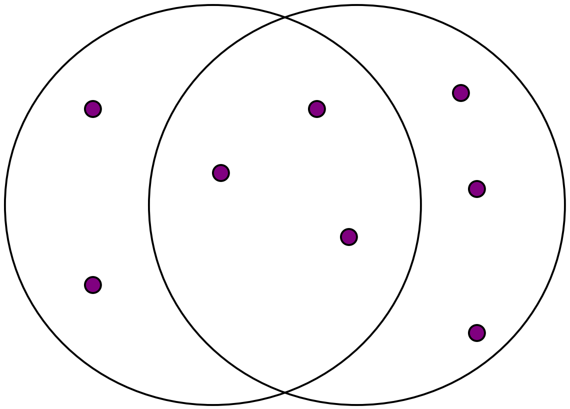
DATA MINING
LECTURE 6

Sketching, Locality Sensitive Hashing

Jaccard Similarity

- The Jaccard similarity (Jaccard coefficient) of two sets S_1, S_2 is the size of their intersection divided by the size of their union.
  - JSim $(S_1, S_2) = |S_1 \cap S_2| / |S_1 \cup S_2|$.



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

  - Extreme behavior:
    - Jsim(X,Y) = 1, iff X = Y
    - Jsim(X,Y) = 0 iff X,Y have no elements in common
  - JSim is symmetric

Cosine Similarity

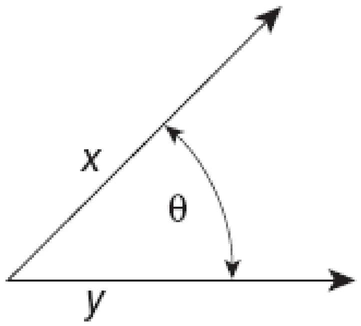


Figure 2.16. Geometric illustration of the cosine measure.

- Sim(X,Y) = cos(X,Y)
  - The cosine of the angle between X and Y

- If the vectors are aligned (correlated) angle is zero degrees and cos(X,Y)=1
- If the vectors are orthogonal (no common coordinates) angle is 90 degrees and cos(X,Y) = 0

- Cosine is commonly used for comparing documents, where we assume that the vectors are normalized by the document length.

Application: Recommendations

- Recommendation systems
  - When a user buys or rates an item we want to recommend other items that the user may like
    - Initially applied to books, but now recommendations are everywhere: songs, movies, products, restaurants, hotels, etc.

- Commonly used algorithms:
  - Find the k users most similar to the user at hand and recommend items that they like.
  - Find the items most similar to the items that the user has previously liked, and recommend these items.

Application: Finding near duplicates

- Find duplicate and near-duplicate documents from a web crawl.
- Why is it important:
  - Identify mirrored web pages, and avoid indexing them, or serving them multiple times
  - Find replicated news stories and cluster them under a single story.
  - Identify plagiarism
- Near duplicate documents differ in a few characters, words or sentences

Finding similar items

- The problems we have seen so far have a common component
  - We need a quick way to find highly similar items to a query item
  - OR, we need a method for finding all pairs of items that are highly similar.
- Also known as the Nearest Neighbor problem, or the All Nearest Neighbors problem

SKETCHING AND LOCALITY SENSITIVE HASHING

Thanks to:

Rajaraman and Ullman, “Mining Massive Datasets”

Evimaria Terzi, slides for Data Mining Course.

Problem

- Given a (large) collection of documents find all pairs of documents which are near duplicates
  - Their similarity is very high

- What if we want to find identical documents?

Main issues

- What is the right representation of the document when we check for similarity?
  - E.g., representing a document as a set of characters will not do (why?)
- When we have billions of documents, keeping the full text in memory is not an option.
  - We need to find a shorter representation
- How do we do pairwise comparisons of billions of documents?
  - If we wanted exact match it would be ok, can we replicate this idea?

Three Essential Techniques for Similar Documents

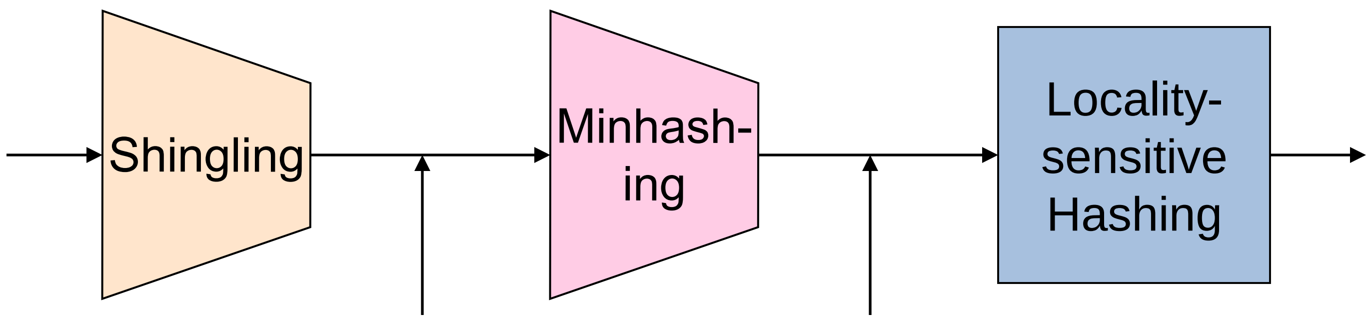
1. Shingling : convert documents, emails, etc., to sets.

2. Minhashing : convert large sets to short signatures, while preserving similarity.

3. Locality-Sensitive Hashing (LSH): focus on pairs of signatures likely to be similar.

The Big Picture

Docu-
ment



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

Shingles

- A k -shingle (or k -gram) for a document is a sequence of k characters that appears in the document.
- Example: document = abcab. k=2
  - Set of 2-shingles = {ab, bc, ca}.
  - Option: regard shingles as a bag, and count ab twice.

- Represent a document by its set of k-shingles.

Shingling

- Shingle: a sequence of k contiguous characters

```
a rose is a rose is a rose
a rose is
 rose is a
  rose is a
   ose is a r
    se is a ro
     e is a ros
       is a rose
        is a rose
         s a rose i
           a rose is
            a rose is
```

Shingling

- Shingle: a sequence of k contiguous characters

```
a rose is a rose is a rose
a rose is
 rose is a
rose is a
ose is a r
se is a ro
e is a ros
 is a rose
is a rose
s a rose i
 a rose is
a rose is
```

```
a rose is
 rose is a
rose is a
ose is a r
se is a ro
e is a ros
 is a rose
is a rose
s a rose i
 a rose is
```

Working Assumption

- Documents that have lots of shingles in common have similar text, even if the text appears in different order.
- Careful: you must pick k large enough, or most documents will have most shingles.
  - Extreme case $k = 1$: all documents are the same
  - $k = 5$ is OK for short documents; $k = 10$ is better for long documents.
- Alternative ways to define shingles:
  - Use words instead of characters
  - Anchor on stop words (to avoid templates)

Shingles: Compression Option

- To compress long shingles, we can hash them to (say) 4 bytes.

$$h: V^k \to \{0,1\}^{64}$$

- Represent a doc by the set of hash values of its *k*-shingles.
  - Shingle s will be represented by the 64-bit integer $h(s)$
- From now on we will assume that shingles are integers
  - Collisions are possible, but very rare

Fingerprinting

- Hash shingles to 64-bit integers

Set of Shingles	Hash function (Rabin's fingerprints)	Set of 64-bit integers
a rose is	→	1111
rose is a	→	2222
rose is a	→	3333
ose is a r	→	4444
se is a ro	→	5555
e is a ros	→	6666
is a rose	→	7777
is a rose	→	8888
s a rose i	→	9999
a rose is	→	0000

Basic Data Model: Sets

- Document: A document is represented as a set shingles (more accurately, hashes of shingles)

- Document similarity: Jaccard similarity of the sets of shingles.
  - Common shingles over the union of shingles
  - $Sim\ (C_1, C_2) = |C_1 \cap C_2| / |C_1 \cup C_2|$.

- Although we use the documents as our driving example the techniques we will describe apply to any kind of sets.
  - E.g., similar customers or items.

Signatures

- Problem: shingle sets are still too large to be kept in memory.
- Key idea: "hash" each set S to a small signature Sig (S), such that:

  1. Sig (S) is small enough that we can fit a signature in main memory for each set.
  2. Sim (S_1, S_2) is (almost) the same as the "similarity" of Sig (S_1) and Sig (S_2). (signature preserves similarity).

- Warning: This method can produce false negatives, and false positives (if an additional check is not made).
  - False negatives: Similar items deemed as non-similar
  - False positives: Non-similar items deemed as similar

From Sets to Boolean Matrices

- Represent the data as a boolean matrix M
  - Rows = the universe of all possible set elements
    - In our case, shingle fingerprints take values in $[0\ldots2^{64}-1]$
  - Columns = the sets
    - In our case, documents, sets of shingle fingerprints
  - M(r,S) = 1 in row r and column S if and only if r is a member of S.
- Typical matrix is sparse.
  - We do not really materialize the matrix

Example

- Universe: **U = {A,B,C,D,E,F,G}**

- X = {A,B,F,G}
- Y = {A,E,F,G}

- Sim(X,Y) = $\frac{3}{5}$

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

Example

- Universe: **U = {A,B,C,D,E,F,G}**

- X = {A,B,F,G}
- Y = {A,E,F,G}

- Sim(X,Y) = $\frac{3}{5}$

At least one of the columns has value 1

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

Example

- Universe: **U = {A,B,C,D,E,F,G}**

- X = {A,B,F,G}
- Y = {A,E,F,G}

- Sim(X,Y) = $\frac{3}{5}$

Both columns have value 1

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

Minhashing

- Pick a random permutation of the rows (the universe U).
- Define "hash" function for set S
  - h(S) = the index of the first row (in the permuted order) in which column S has 1.

  same as:
  - h(S) = the index of the first element of S in the permuted order.
- Use k (e.g., k = 100) independent random permutations to create a signature.

Example of minhash signatures

- Input matrix

elem ent	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	1	1
F	1	0	1	0
G	1	0	1	0

Random Permutation

A
C
G
F
B
E
D

index	elem ent	S_1	S_2	S_3	S_4
1	**A**	1	0	1	0
2	**C**	0	1	0	1
3	**G**	1	0	1	0
4	**F**	1	0	1	0
5	**B**	1	0	0	1
6	**E**	0	1	1	1
7	**D**	0	1	0	1
		1	**2**	**1**	**2**

Example of minhash signatures

- Input matrix

element	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	1	1
F	1	0	1	0
G	1	0	1	0

Random Permutation

D
B
A
C
F
G
E

index	element	S_1	S_2	S_3	S_4
1	**D**	0	1	0	1
2	**B**	1	0	0	1
3	**A**	1	0	1	0
4	**C**	0	1	0	1
5	**F**	1	0	1	0
6	**G**	1	0	1	0
7	**E**	0	1	1	1
		2	**1**	**3**	**1**

Example of minhash signatures

- Input matrix

element	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	1	1
F	1	0	1	0
G	1	0	1	0

Random Permutation

C
D
G
F
A
B
E

index	element	S_1	S_2	S_3	S_4
1	**C**	0	1	0	1
2	**D**	0	1	0	1
3	**G**	1	0	1	0
4	**F**	1	0	1	0
5	**A**	1	0	1	0
6	**B**	1	0	0	1
7	**E**	0	1	1	1

3	**1**	**3**	**1**

Example of minhash signatures

- Input matrix

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	1	1
F	1	0	1	0
G	1	0	1	0

$\approx$

Signature matrix

	S_1	S_2	S_3	S_4
h_1	1	2	1	2
h_2	2	1	3	1
h_3	3	1	3	1

- Sig(S) = vector of hash values
  - e.g., $Sig(S_2) = [2,1,1]$
- Sig(S,i) = value of the i-th hash function for set S
  - E.g., $Sig(S_2,3) = 1$

Hash function Property

$$Pr(h(S_1) = h(S_2)) = Sim(S_1,S_2)$$

- where the probability is over all choices of permutations.
- Why?
  - The first row where one of the two sets has value 1 belongs to the union.
    - Recall that union contains rows with at least one 1.
  - We have equality if both sets have value 1, and this row belongs to the intersection

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

Rows C,D could be anywhere they do not affect the probability

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

The * rows belong to the union

- Union =
  {A,B,E,F,G}
- Intersection =
  {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universise: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

The question is what is the value of the **first *** element

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

If it belongs to the intersection then h(X) = h(Y)

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

Every element of the union is equally likely to be the * element

$$\Pr(h(X) = h(Y)) = \frac{|\{A,F,G\}|}{|\{A,B,E,F,G\}|} = \frac{3}{5} = \mathrm{Sim}(X,Y)$$

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Similarity for Signatures

- The similarity of signatures is the fraction of the hash functions in which they agree.

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	1	1
F	1	0	1	0
G	1	0	1	0

$\approx$

Signature matrix

S_1	S_2	S_3	S_4
1	2	1	2
2	1	3	1
3	1	3	1

	Actual	Sig
(S_1, S_2)	0	0
(S_1, S_3)	3/5	2/3
(S_1, S_4)	1/7	0
(S_2, S_3)	0	0
(S_2, S_4)	3/4	1
(S_3, S_4)	0	0

Zero similarity is preserved
High similarity is well approximated

- With multiple signatures we get a good approximation

Is it now feasible?

- Assume a billion rows
- Hard to pick a random permutation of 1…billion
- **Even representing a random permutation requires 1 billion entries!!!**
- How about accessing rows in permuted order?
- ☹

Being more practical

Approximating row permutations: pick $k=100$ hash functions $(h_1,\ldots,h_k)$

In practice this means selecting the function parameters

for each row r

In practice only the rows (shingles) that appear in the data

for each hash function h_i

compute $h_i(r)$

$h_i(r)$ = index of shingle r in permutation

for each column S that has **1** in row r

S contains shingle r

if $h_i(r)$ is a smaller value than $Sig(S,i)$ **then**

$Sig(S,i) = h_i(r)$;

Find the shingle r with minimum index

$Sig(S,i)$ will become the smallest value of $h_i(r)$ among all rows (shingles) for which column S has value **1** (shingle belongs in S); *i*.e., $h_i(r)$ gives the min index for the i-th permutation

Example

x	Row	S1	S2	h(x)	g(x)
0	A	1	0	1	3
1	B	0	1	2	0
2	C	1	1	3	2
3	D	1	0	4	4
4	E	0	1	0	1

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

Row	S1	S2
E	0	1
A	1	0
B	0	1
C	1	1
D	1	0

Row	S1	S2
B	0	1
E	0	1
C	1	0
A	1	1
D	1	0

	Sig1	Sig2
$h(0) = 1$	1	-
$g(0) = 3$	3	-
$h(1) = 2$	1	2
$g(1) = 0$	3	0
$h(2) = 3$	1	2
$g(2) = 2$	2	0
$h(3) = 4$	1	2
$g(3) = 4$	2	0
$h(4) = 0$	1	0
$g(4) = 1$	2	0

Implementation – (4)

- Often, data is given by column, not row.
  - E.g., columns = documents, rows = shingles.
- If so, sort matrix once so it is by row.
- And always compute $h_i(r)$ only once for each row.

Finding similar pairs

- Problem: Find all pairs of documents with similarity at least $t = 0.8$
- While the signatures of all columns may fit in main memory, comparing the signatures of all pairs of columns is quadratic in the number of columns.
- Example: 10^6 columns implies $5*10^{11}$ column-comparisons.
- At 1 microsecond/comparison: 6 days.

Locality-Sensitive Hashing

- What we want: a function f(X,Y) that tells whether or not X and Y is a candidate pair: a pair of elements whose similarity must be evaluated.

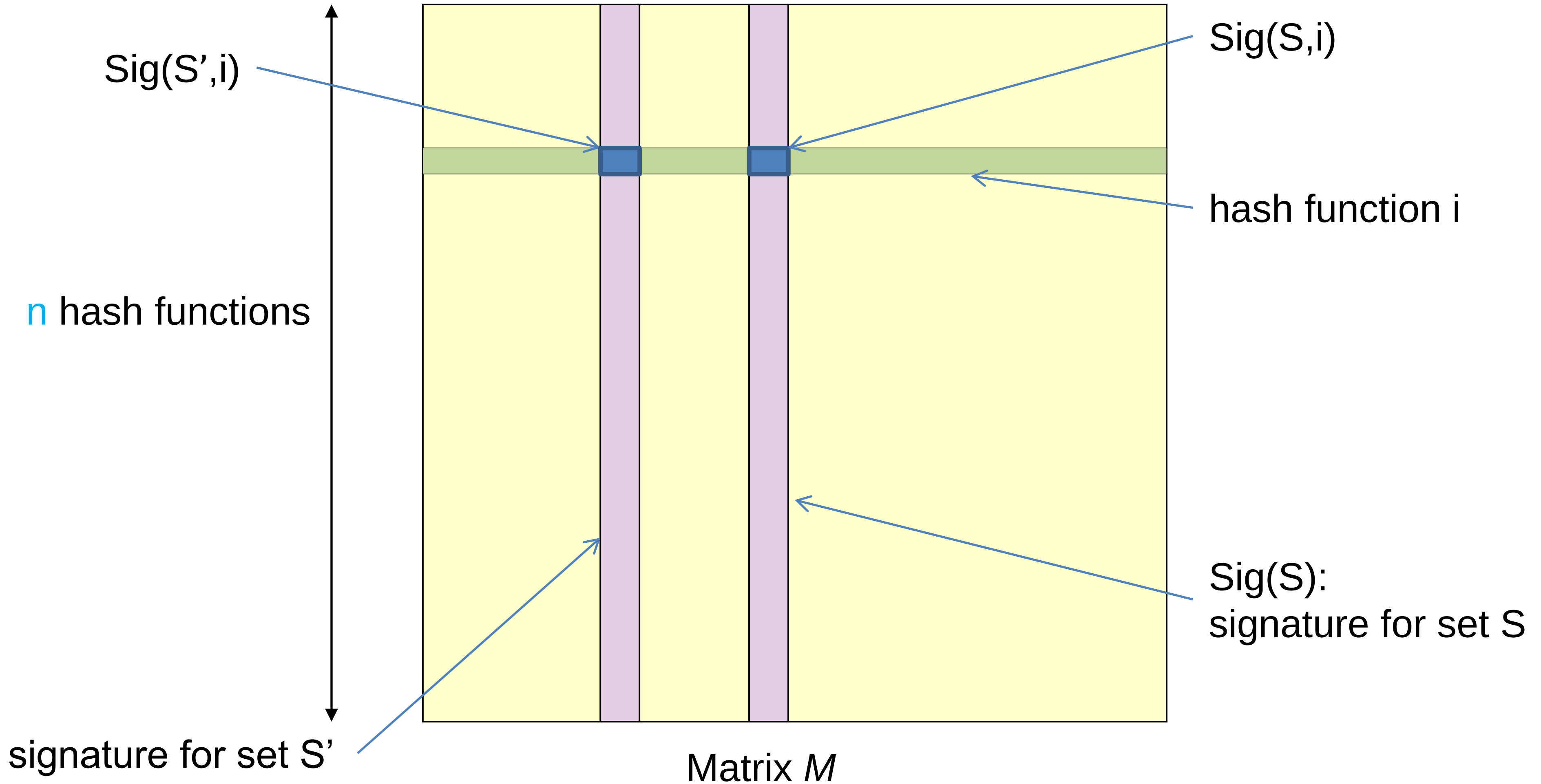
- A simple idea: X and Y are a candidate pair if they have the same min-hash signature.
  - Easy to test by hashing the signatures.
  - Similar sets are more likely to have the same signature.
  - Likely to produce many false negatives.
    - Requiring full match of signature is strict, some similar sets will be lost.

! Multiple levels of Hashing!

- Improvement: Compute multiple signatures; candidate pairs should have at least one common signature.
  - Reduce the probability for false negatives.

Signature matrix reminder

Prob(Sig(S,i) == Sig(S',i)) = sim(S,S')

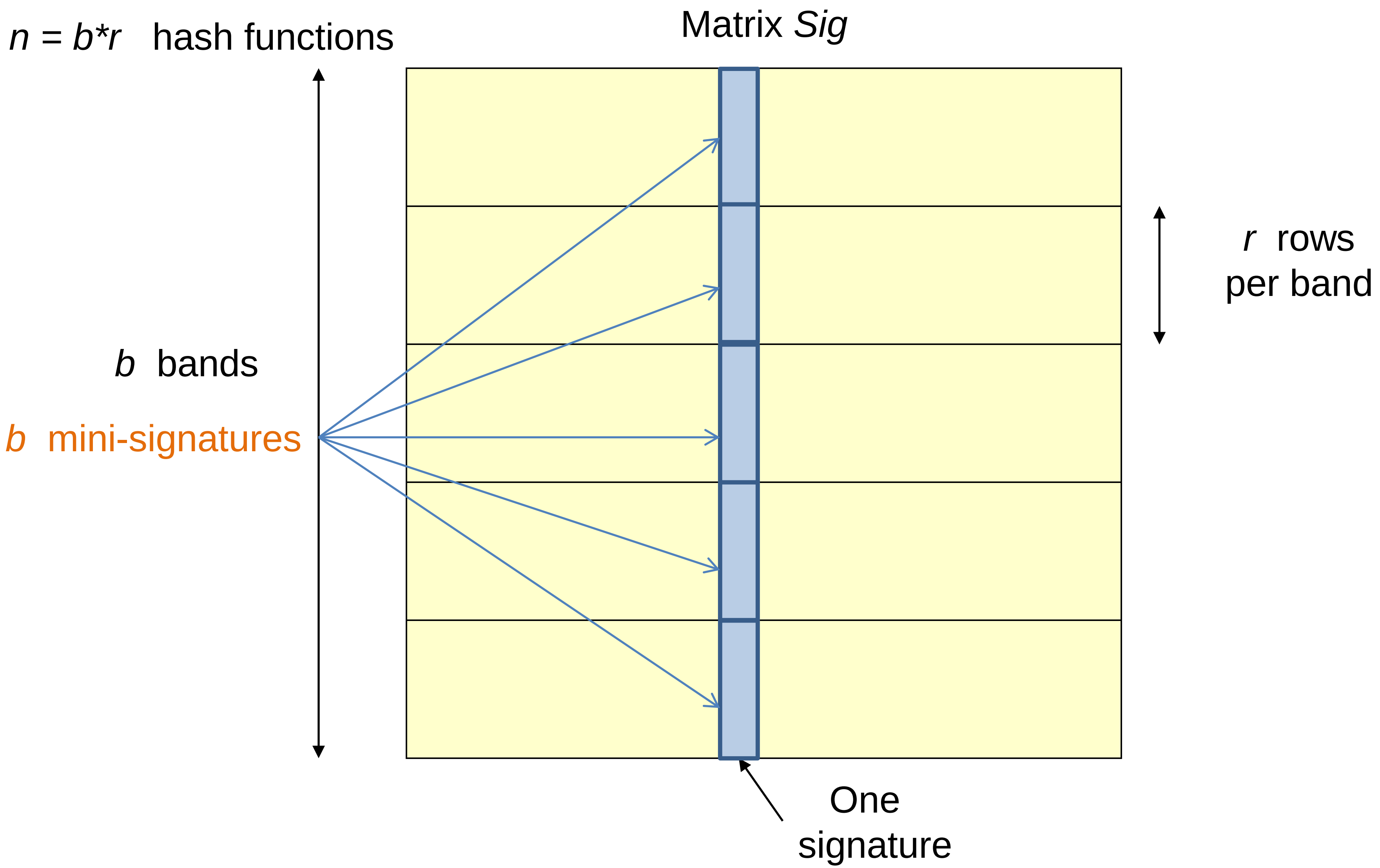


Matrix *M*

Partition into Bands – (1)

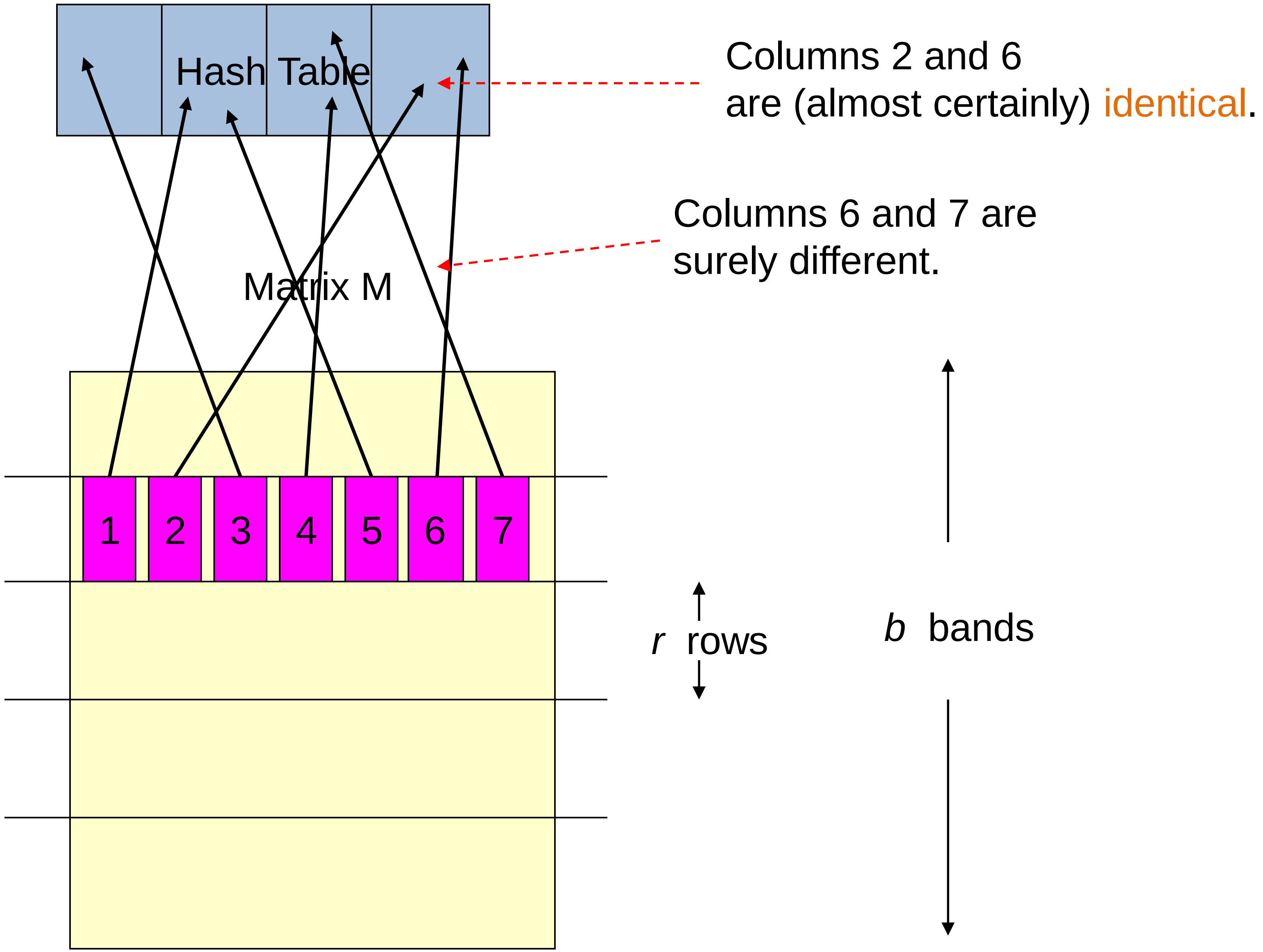
- Divide the signature matrix Sig into *b* bands of *r* rows.
  - Each band is a mini-signature with r hash functions.

Partitioning into bands



Partition into Bands – (2)

- Divide the signature matrix Sig into *b* bands of *r* rows.
  - Each band is a mini-signature with r hash functions.
- For each band, hash the mini-signature to a hash table with *k* buckets.
  - Make *k* as large as possible so that mini-signatures that hash to the same bucket are almost certainly identical.

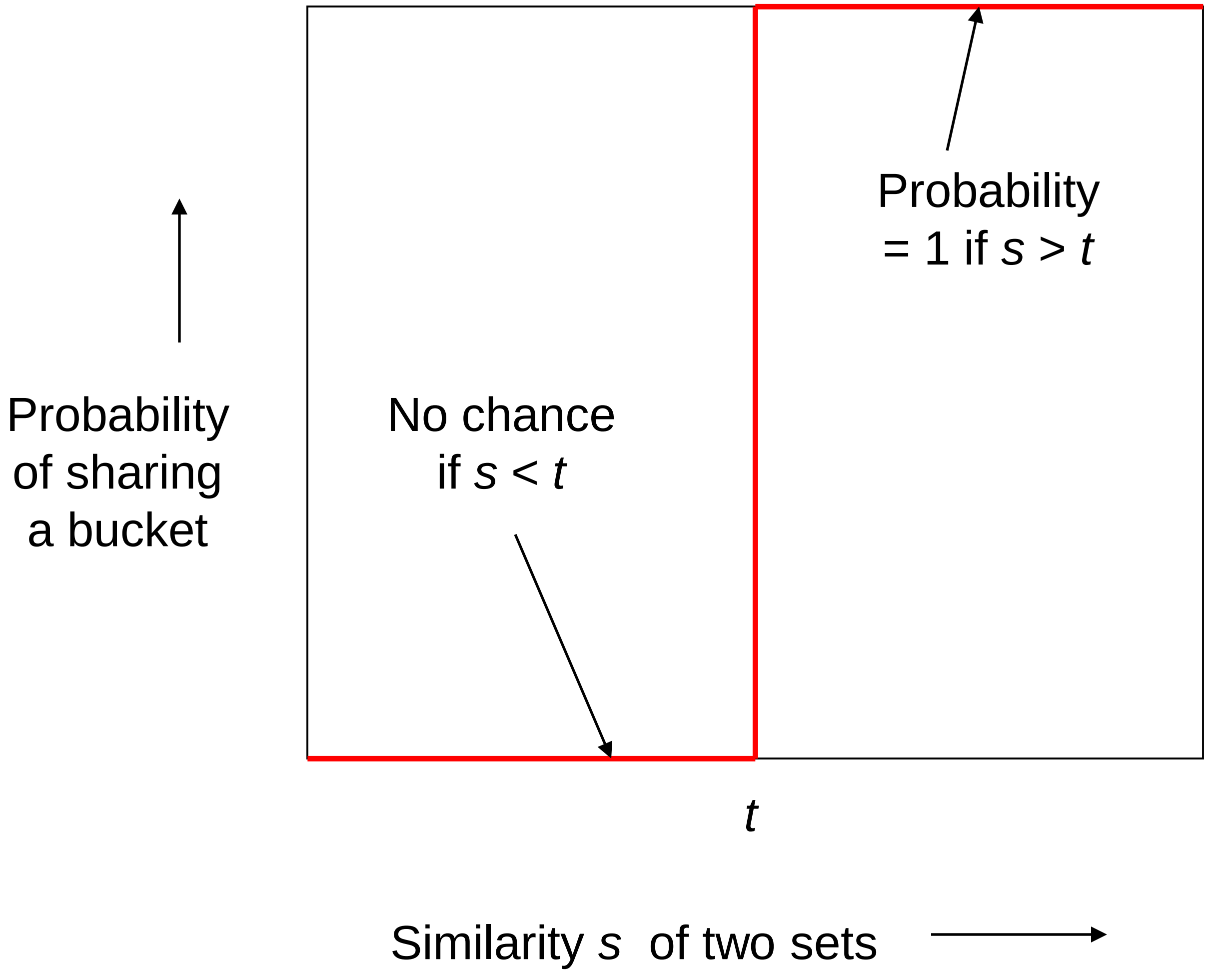


Hash Table
Columns 2 and 6
are (almost certainly) identical.
Columns 6 and 7 are
surely different.
Matrix M
1
2
3
4
5
6
7
r rows
b bands

Partition into Bands – (2)

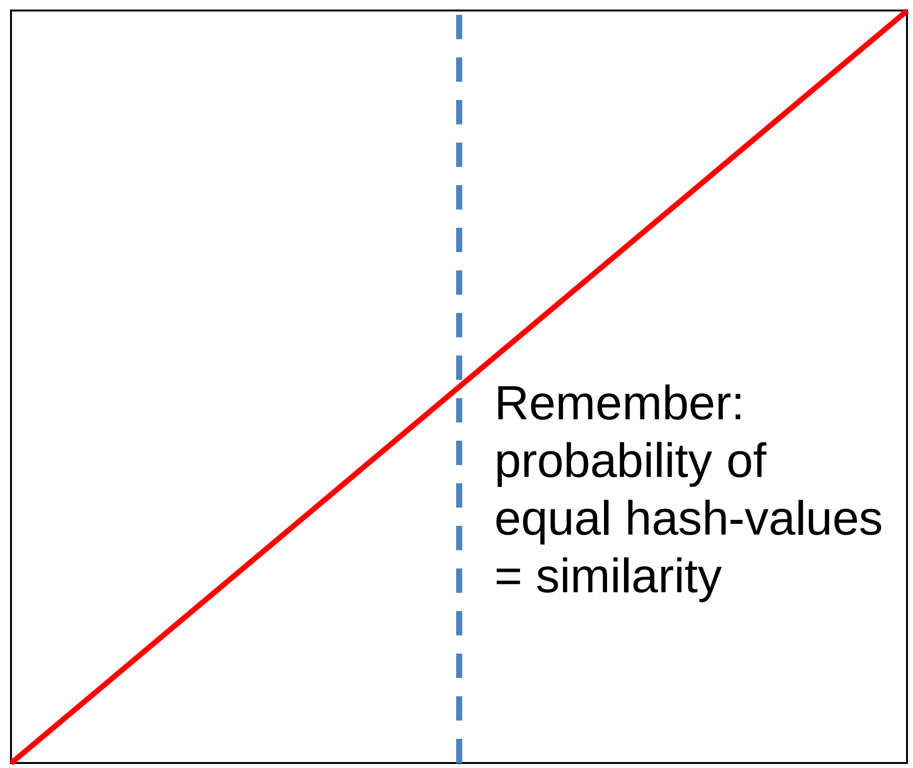
- Divide the signature matrix Sig into *b* bands of *r* rows.
  - Each band is a mini-signature with r hash functions.
- For each band, hash the mini-signature to a hash table with *k* buckets.
  - Make *k* as large as possible so that mini-signatures that hash to the same bucket are almost certainly identical.
- Candidate column pairs are those that hash to the same bucket for at least 1 band.
  - I.e., they have at least one mini-signature in common.
- Tune *b* and *r* to catch most similar pairs, but few non-similar pairs.

Analysis of LSH – What We Want



What One Band of One Row Gives You

Probability of sharing a bucket



Single hash signature

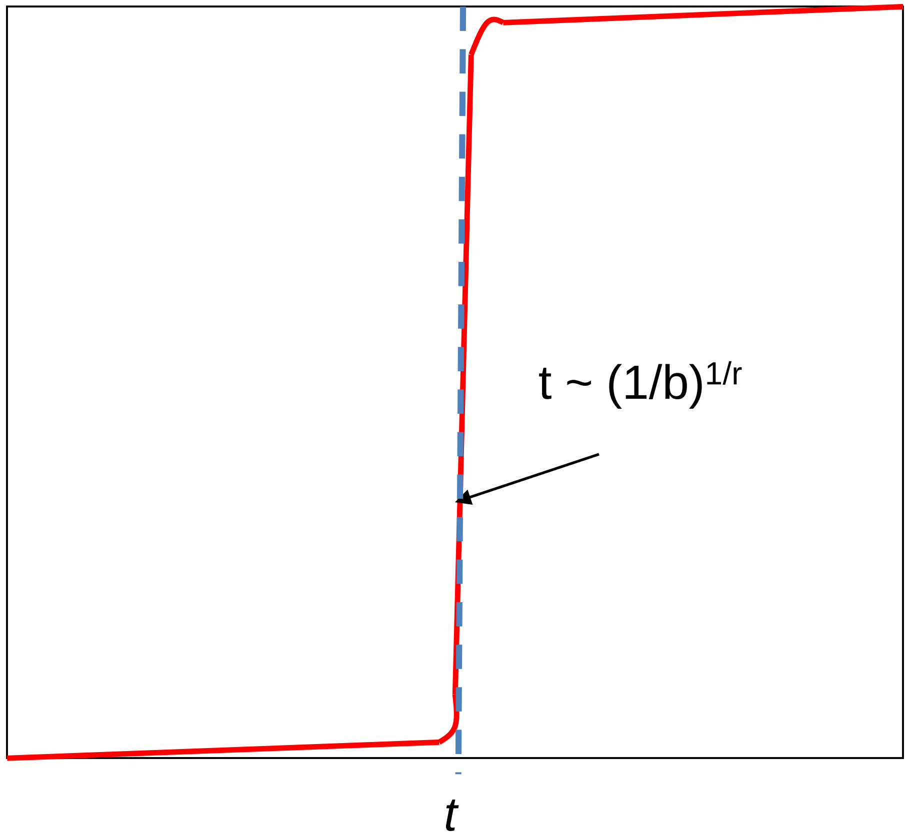
t

Prob(Sig(S,i) == Sig(S',i)) = sim(S,S')

Similarity s of two sets

What *b* Bands of *r* Rows Gives You

Probability of sharing a bucket



Similarity s of two sets

At least one band identical

No bands identical

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

Some row of a band unequal

All rows of a band are equal

Example: $b = 20; r = 5$

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

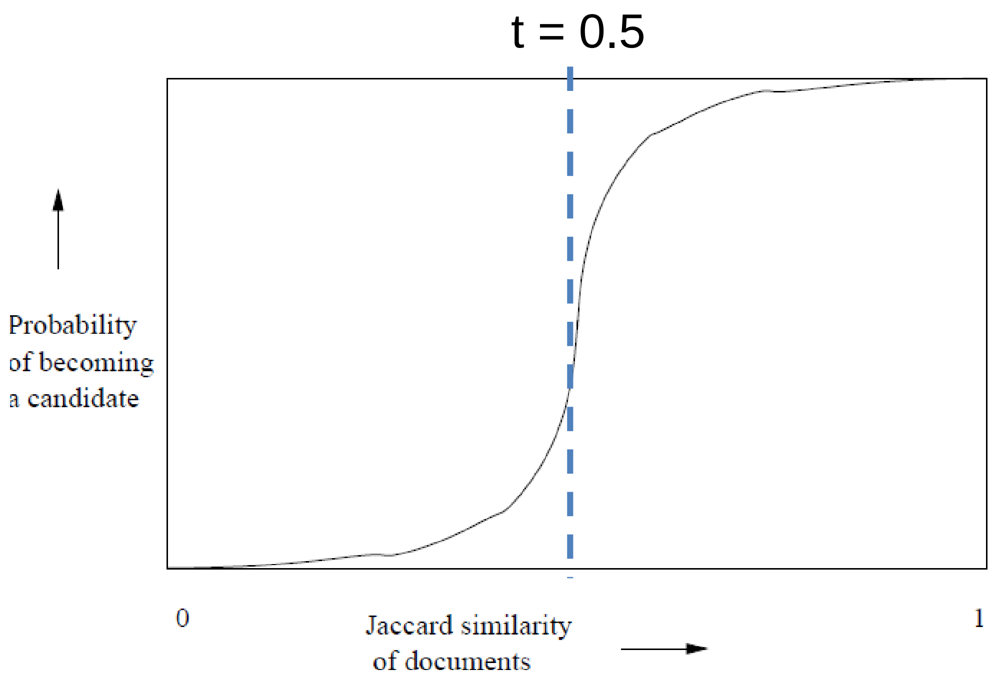


Figure 3.7: The S-curve

Suppose S_1, S_2 are 80% Similar

- We want all 80%-similar pairs. Choose 20 bands of 5 integers/band.

- Probability S_1, S_2 identical in one particular band:

  $$(0.8)^5 = 0.328.$$

- Probability S_1, S_2 are not similar in any of the 20 bands:

  $$(1-0.328)^{20} = 0.00035$$

  - i.e., about 1/3000-th of the 80%-similar column pairs are false negatives.

- Probability S_1, S_2 are similar in at least one of the 20 bands:

  $$1-0.00035 = 0.999$$

Suppose S_1, S_2 Only 40% Similar

- Probability S_1, S_2 identical in any one particular band:
$$(0.4)^5 = 0.01 .$$
- Probability S_1, S_2 are not identical in any of the 20 bands:
$$(1 - 0.01)^{20} = 0.81$$
- False positive probability = 0.19. But false positives much lower for similarities << 40%.

LSH Summary

- Tune 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 *sets* .

Locality-sensitive hashing (LSH)

- Big Picture: Construct hash functions **$h: R^d \rightarrow U$** such that for any pair of points **p,q**, for distance function **D** we have:
  - If **$D(p,q) \leq r$**, then **$Pr[h(p)=h(q)]$** is high
  - If **$D(p,q) \geq cr$**, then **$Pr[h(p)=h(q)]$** is small
- Then, we can find close pairs by hashing

- LSH is a general framework: for a given distance function **D** we need to find the right **h**

LSH for Cosine Distance

- For cosine distance, there is a technique analogous to minhashing for generating a $\left(d_1, d_2, (1-d_1/180), (1-d_2/180)\right)$- sensitive family for any d_1 and d_2.
- Called *random hyperplanes*.

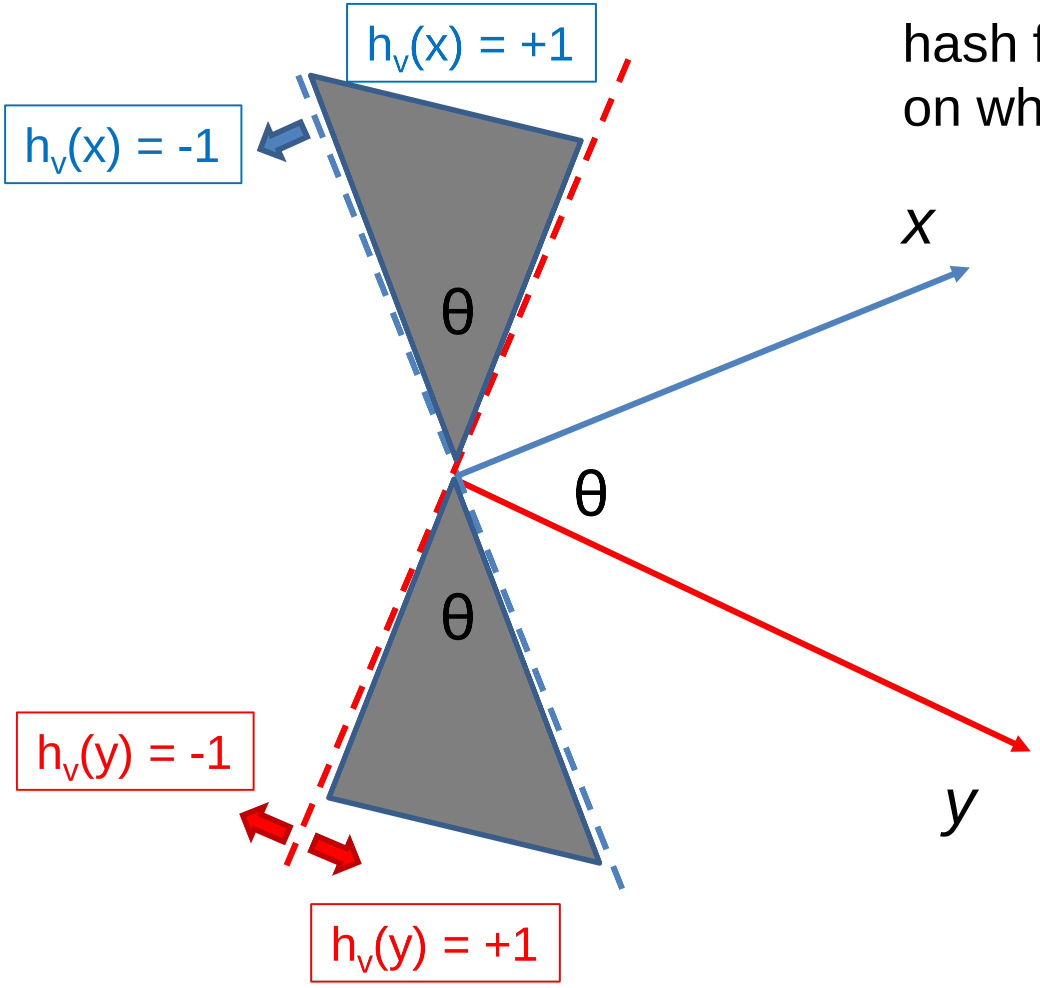
Random Hyperplanes

- Pick a random vector *v*, which determines a hash function h_v with two buckets.
  - $h_v(x) = +1$ if $v.x > 0$; $= -1$ if $v.x < 0$.
- LS-family **H** = set of all functions derived from any vector.
- Claim:
  - Prob[h(x)=h(y)] = 1 – (angle between *x* and *y*)/180

Proof of Claim

Look in the plane of x and y.

For a random vector v the values of the hash functions $h_v(x)$ and $h_v(y)$ depend on where the vector v falls



$h_v(x) \neq h_v(y)$ when v falls into the shaded area.
What is the probability of this for a randomly chosen vector v?

$P[h_v(x) \neq h_v(y)] = 2\theta/360 = \theta/180$

$P[h_v(x) = h_v(y)] = 1 - \theta/180$

Signatures for Cosine Distance

- Pick some number of vectors, and hash your data for each vector.
- The result is a signature (sketch) of +1’s and –1’s that can be used for LSH like the minhash signatures for Jaccard distance.

Simplification

- We need not pick from among all possible vectors v to form a component of a sketch.
- It suffices to consider only vectors v consisting of +1 and –1 components.