Machine Learning for Data Mining

Finding Similar Items in High Dimensional Spaces

Andres Mendez-Vazquez

August 17, 2018

Outline

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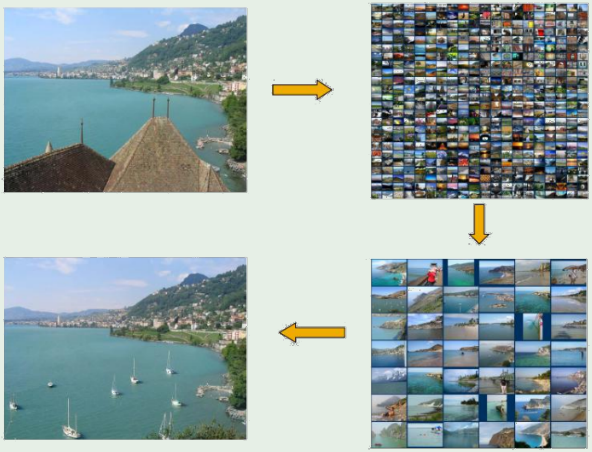
Scene Completion Problem

Example



Scene Completion Problem

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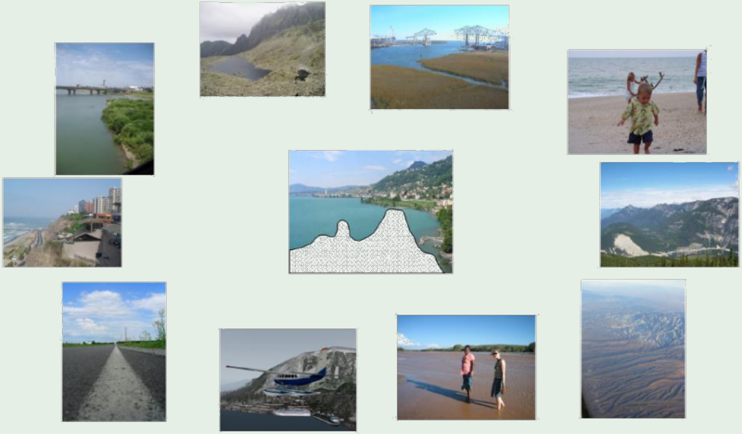
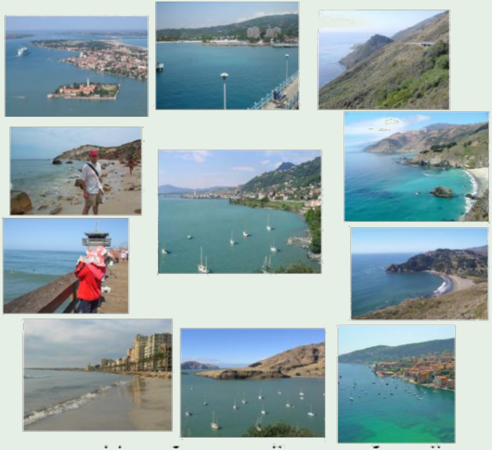
10 nearest neighbors from a collection of 20,000 images



Scene Completion Problem

10 nearest neighbors from a collection of 2 million images



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A Common Idea

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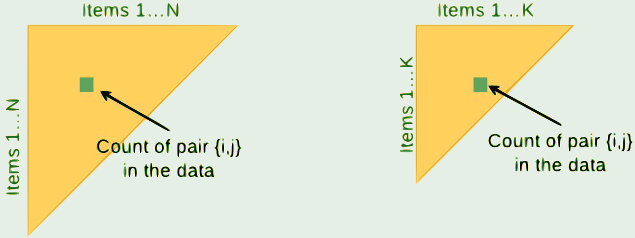
Relation to Previous Lecture

Last time: Finding frequent pairs



We had the Naïve solution

Single pass but requires space quadratic in the number of items:

- N = number of distinct items
- K =number of items with support $\geq s$

However the A-priori Algorithm

- First pass: Find frequent singletons
  - For a pair to be a candidate for a frequent pair, its singletons have to be frequent!
- Second pass:
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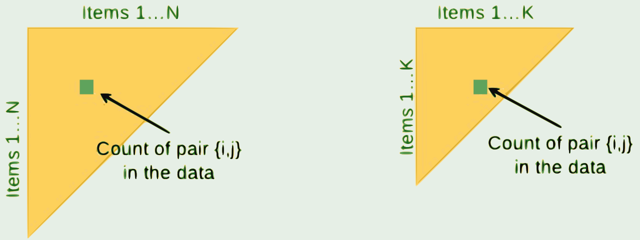

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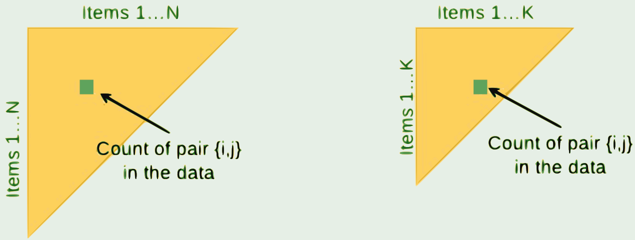

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- Pass 1:
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  - Take pairs of items $\{i, j\}$, hash them into B buckets and count of the number of pairs that hashed to each bucket:

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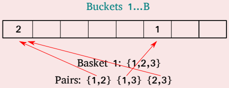

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Pass 2:

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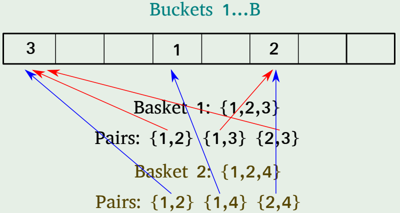

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Previous Lecture: A-Priori

- Main Idea: Candidates
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Today's Lecture

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  - Pass 1: Take documents and has them to buckets such that **documents that are similar hash to the same bucket.**
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- Find near-neighbors in high-dim. space
  - We formally define "near neighbors" as points that are a "small distance" apart.

Application

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Today: Jaccard distance (/similarity)

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  - $sim(C_1, C_2) = |C_1 \bigcap C_2| / |C_1 \bigcup C_2|$
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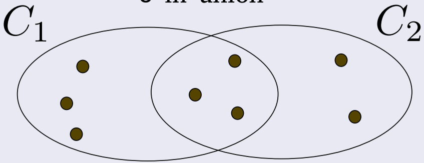
3 in intersection

8 in union



$$sim(C_1, C_2) = \frac{3}{8}$$

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Convert documents to sets

Step 2: Minhashing

Convert large sets to short signatures, while preserving similarity

Locality-sensitive hashing

Focus on pairs of signatures likely to be from similar documents

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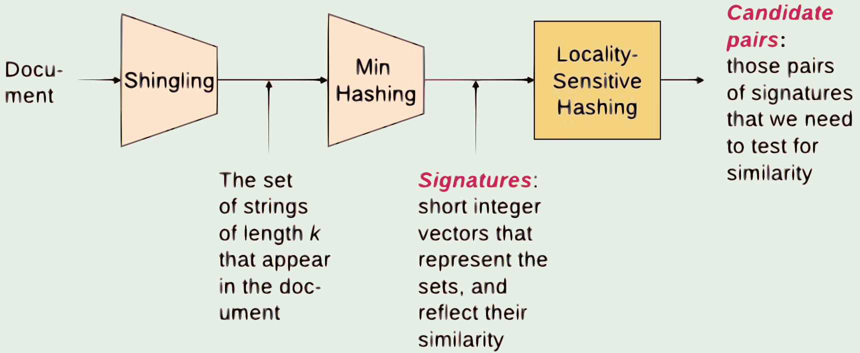
The Big Picture

The Process of Identification



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Idea

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Code - SWAR-Popcount - Divide and Conquer

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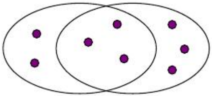
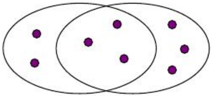


Encoding Sets as Bit Vectors



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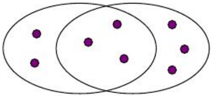

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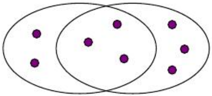

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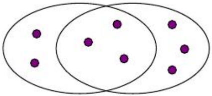

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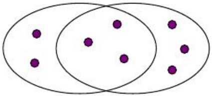

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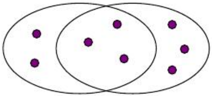

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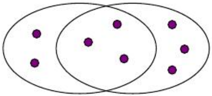

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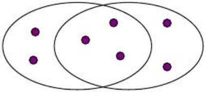

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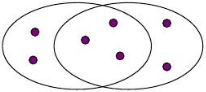

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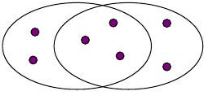

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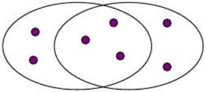

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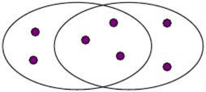

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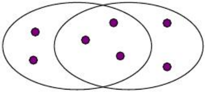

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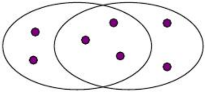

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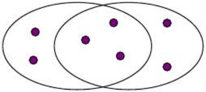

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  - Not all similarity metrics have a suitable hash function.

Hash function

- There is a suitable hash function for Jaccard similarity: **Min-hashing.**

Min-Hashing

Goal

- Find a hash function $h(\cdot)$ such that:
  - if $sim(C_1, C_2)$ is high, then with high prob. $h(C1) = h(C2)$
  - if $sim(C_1, C_2)$ is low, then with high prob. $h(C_1) \neq h(C_2)$

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Random permutation

Imagine the rows of the boolean matrix permuted under random permutation π .

"Hash" function $h_\pi(C)$

- Define a "hash" function $h_\pi(C)$ = the number of the first (in the permuted order π) row in which column C has value 1:

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

What can we do?

- Use several (e.g., 100) independent hash functions to create a signature of a column

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

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

Something Notable

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

Surprising Property

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?

Surprising Property

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1	1
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Why?

- Let X be a document (set of shingles)
- Then: $Pr[\pi(x) = min(\pi(X))] = 1/|X|$
- It is equally likely that any $x \in X$ is mapped to the min element
- Let x be s.t. $\pi(x) = min(\pi(C_1 \bigcup C_2))$
- Then either: $\pi(x) = min(\pi(C_1))$ if $x \in C_1$, or $\pi(x) = min(\pi(C_2))$ if $x \in C2$
  - One of the two cols had to have 1 at position x
- So the prob. that both are true is the prob. $x \in C_1 \bigcap C_2$

$$Pr[min(\pi(C_1)) = min(\pi(C_2))] = \frac{|C_1 \bigcap C_2|}{|C_1 \cup C_2|} = sim(C_1, C_2) \qquad (2)$$

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Four Types of Rows between two Documents

Given cols C_1 and C_2, rows may be classified as

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

$a = \#$rows of type A, etc.

Note

$$sim(C_1, C_2) = \frac{a}{a+b+c} \quad (3)$$

Then

- Then: $Pr[h(C_1) = h(C_2)] = sim(C_1, C_2)$

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- $Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
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Min-Hashing Example

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

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

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

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- Note: The sketch (signature) of document C is small – ~ 100 bytes!

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Outline

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Row hashing!

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- Ordering under k_i gives a random row permutation!

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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
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- 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-function k_i keep a "slot" for the min-hash value

- Initialize all $sig(C)[i] = \infty$
- Scan rows looking for 1s
  - Suppose row j has 1 in column C
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If $k_i(j) < sig(C)[i]$, then $sig(C)[i] \leftarrow k_i(j)$

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Outline

Trying to define LSH

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Goal

- Find documents with Jaccard similarity at least s (for some similarity threshold, e.g., $s = 0.8$)

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- 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.

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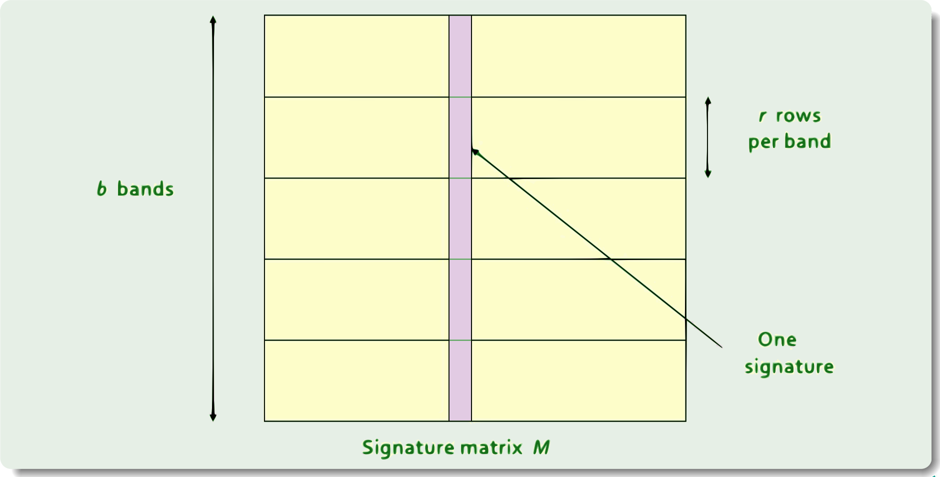

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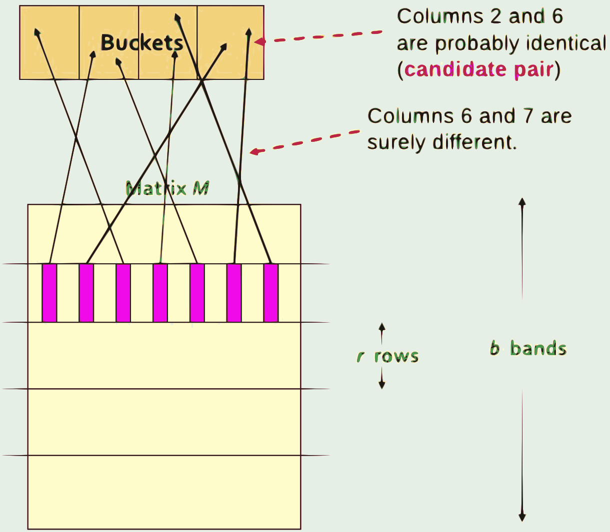

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Identical

- There are enough buckets that columns are unlikely to hash to the same bucket unless they are identical in a particular band

Same bucket

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Assume the following case

- Suppose $100,000$ columns of M $(100k$ docs)
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- Probability C_1, C_2 identical in one particular band: $(0.8)^5 = 0.328$

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- 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.
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- The number of minhashes (rows of M).
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cinvestav

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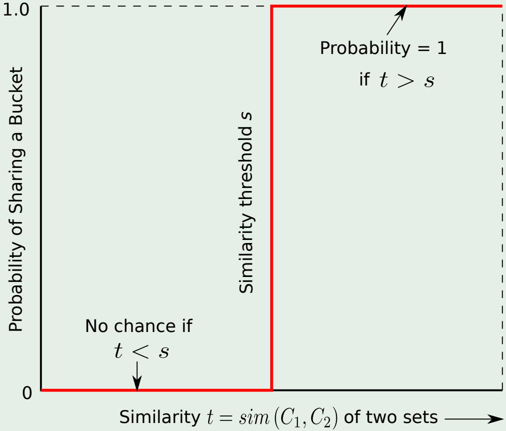
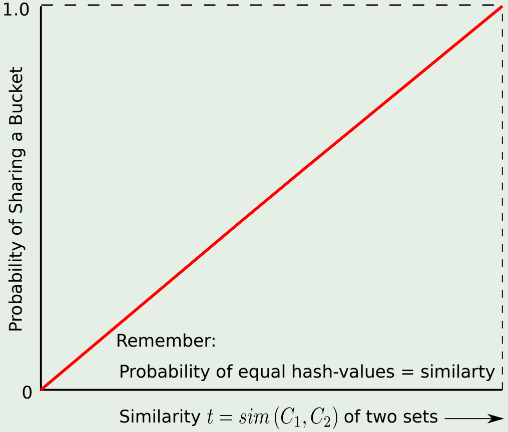
Analysis of LSH - What We Want

The Ideal detection of similar objects



What 1 Band of 1 Row Gives You

Not so great



Given that probability of two documents aggree in a row is s

We can calculate the probability that these documents become a candidate pair as follows

1. The probability that the signatures agree in all rows of one particular band is s^r.
2. The probability that the signatures disagree in at least one row of a particular band is $1 - s^r$.
3. The probability that the signatures disagree in at least one row of each of the bands is $(1 - s^r)^b$.
4. The probability that the signatures agree in all the rows of at least one band, and therefore become a candidate pair, is $1 - (1 - s^r)^b$.

Given that probability of two documents aggree in a row is s

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1. The probability that the signatures agree in all rows of one particular band is s^r.
2. The probability that the signatures disagree in at least one row of a particular band is $1 - s^r$.
3. The probability that the signatures disagree in at least one row of each of the bands is $(1 - s^r)^b$.
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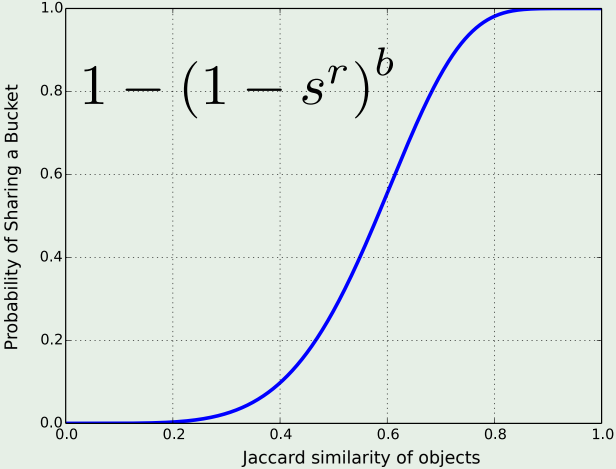
If you fix r and b

Something Notable



Example: $b = 20; r = 5$

Given

- Similarity threshold s

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

s	$1-(1-s^r)^b$
.2	0.006
.3	0.047
.4	0.186
.5	0.470
.6	0.802
.7	0.975
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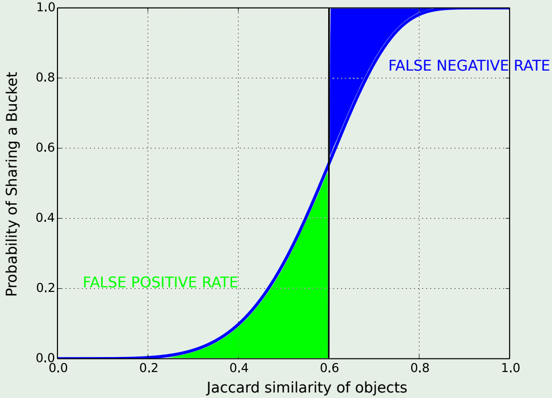
Picking r and b: The S-curve

Picking r and b to get the best S-curve

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



LSH Summary

Tune M, b, r

- 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

- 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

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  - We used hashing to assign each shingle an ID Min-hashing: Convert large sets to short

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