2 Announcements

Recitation sessions:

- Review of proof techniques and probability
  - **Friday January 17, 3:00-4:10 PM in Skilling Auditorium**
- Review of linear algebra
  - **Friday January 17, 4:20-5:20 PM in Skilling Auditorium**

Deadlines tonight, 11:59 PM:

- Colab 0 (Spark Tutorial), Colab 1

Note to other teachers and users of these slides: We would be delighted if you found our material useful for giving your own lectures. Feel free to use these slides verbatim, or to modify them to fit your own needs. If you make use of a significant portion of these slides in your own lecture, please include this message, or a link to our web site: http://www.mmds.org

Theory of Locality Sensitive Hashing

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

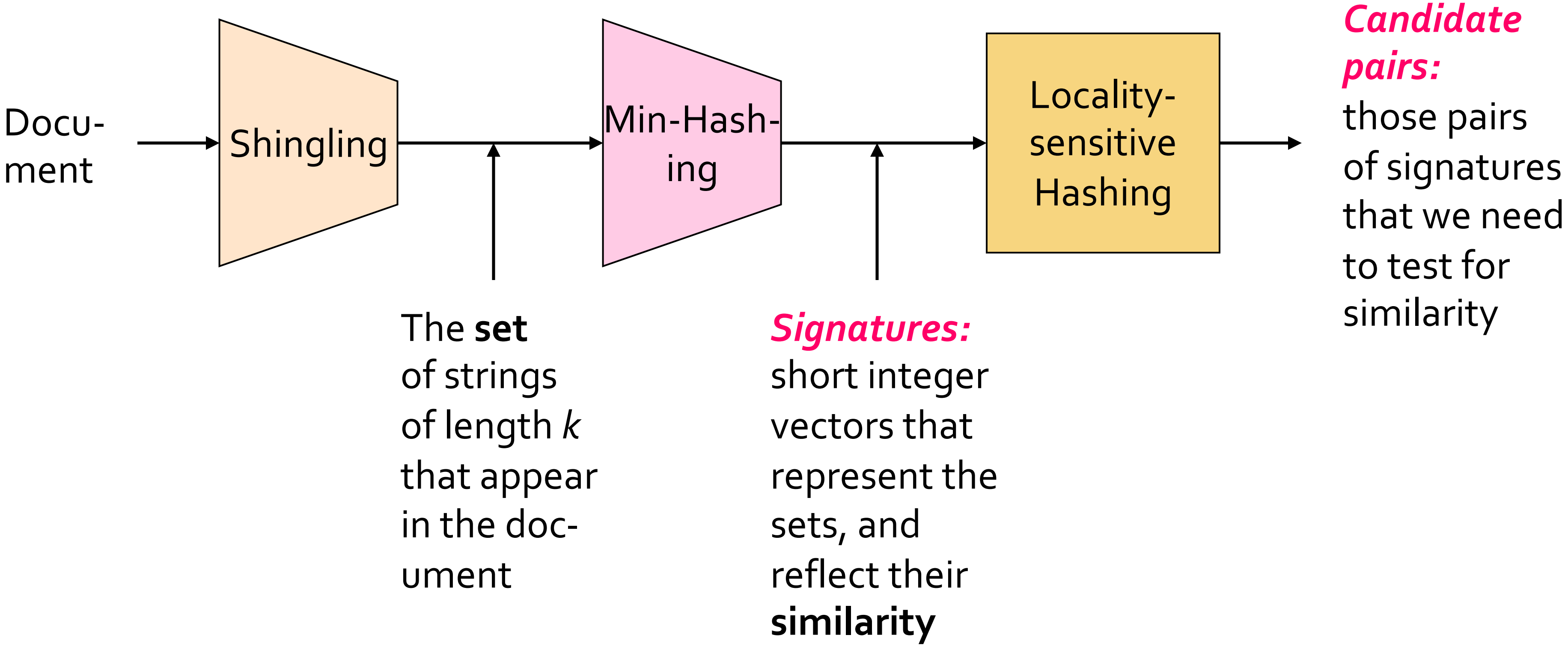
Recap: Finding similar documents

- **Task:** Given a large number (***N*** in the millions or billions) of documents, find "near duplicates"

- **Problem:**
  - Too many documents to compare all pairs

- **Solution:** Hash documents so that similar documents hash into the same bucket
  - Documents in the same bucket are then **candidate pairs** whose similarity is then evaluated

Recap: The Big Picture



Docu-ment

Shingling

Min-Hash-ing

Locality-sensitive Hashing

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

Recap 1: Shingles

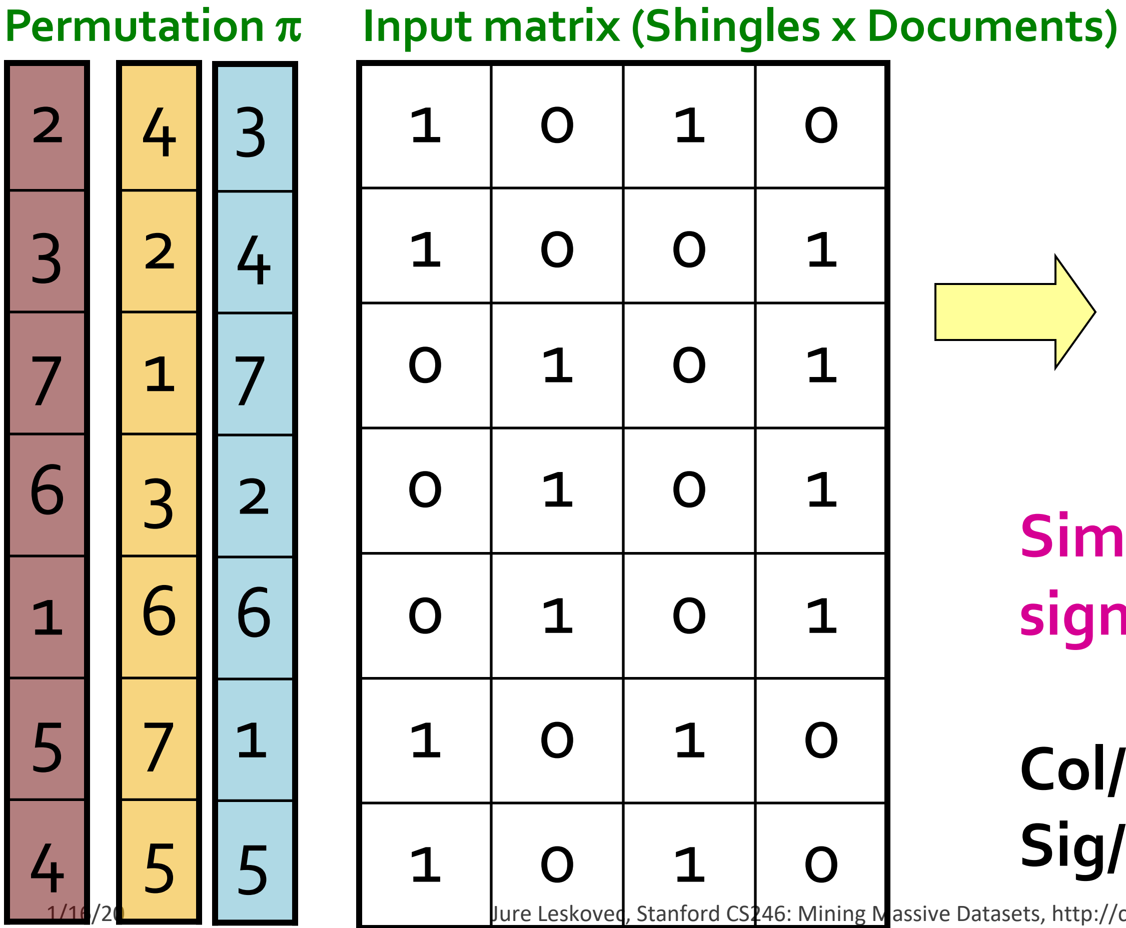
- A *k*-shingle (or *k*-gram) is a sequence of *k* tokens that appears in the document
  - Example: **k=2**; $\mathbf{D_1}$ = abcab
    Set of 2-shingles: $\mathbf{C_1}$ = $S(D_1)$ = {ab, bc, ca}
- Represent a doc by a set of hash values of its *k*-shingles
- A natural **similarity measure** is then the **Jaccard similarity:**

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

  - Similarity of two documents is the Jaccard similarity of their shingles

Recap 2: Minhashing

- ***Min-Hashing***: Convert large sets into short signatures, while preserving similarity: **$\Pr[h(C_1) = h(C_2)] = sim(D_1, D_2)$**



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*

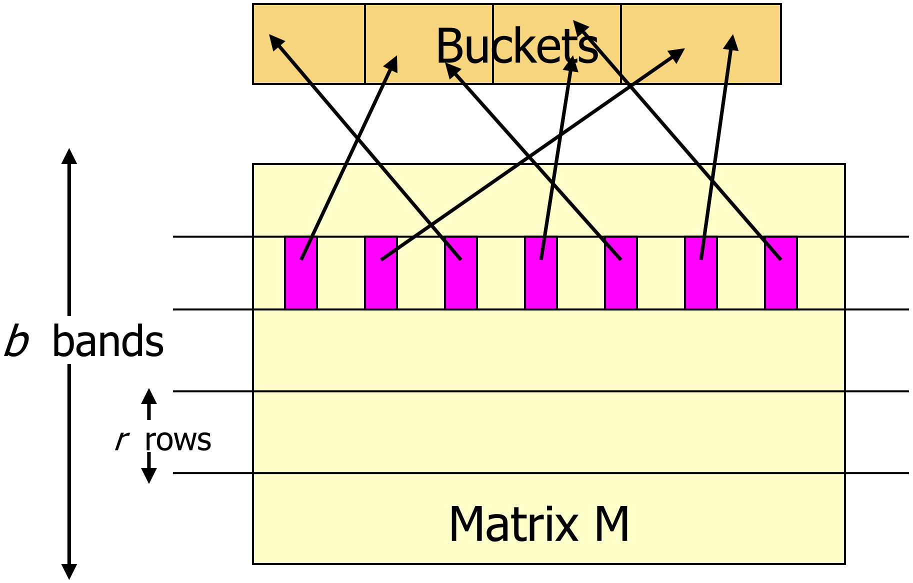
2	1	2	1
2	1	4	1
1	2	1	2

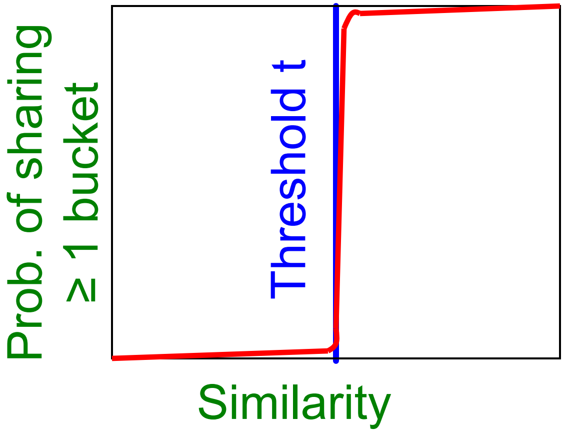
Similarities of columns and signatures (approx.) match!

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

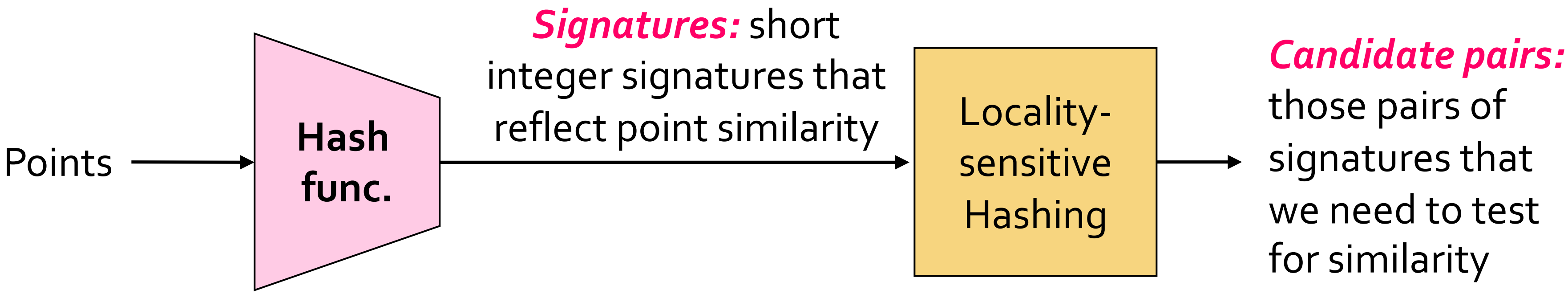
Recap 3: LSH

- **Hash columns of the signature matrix *M*:** **Similar columns likely hash to same bucket**
  - Divide matrix *M* into ***b*** bands of ***r*** rows (M=b·r)
  - ***Candidate*** column pairs are those that hash to the same bucket for ≥ **1** band





Today: Generalizing Min-hash

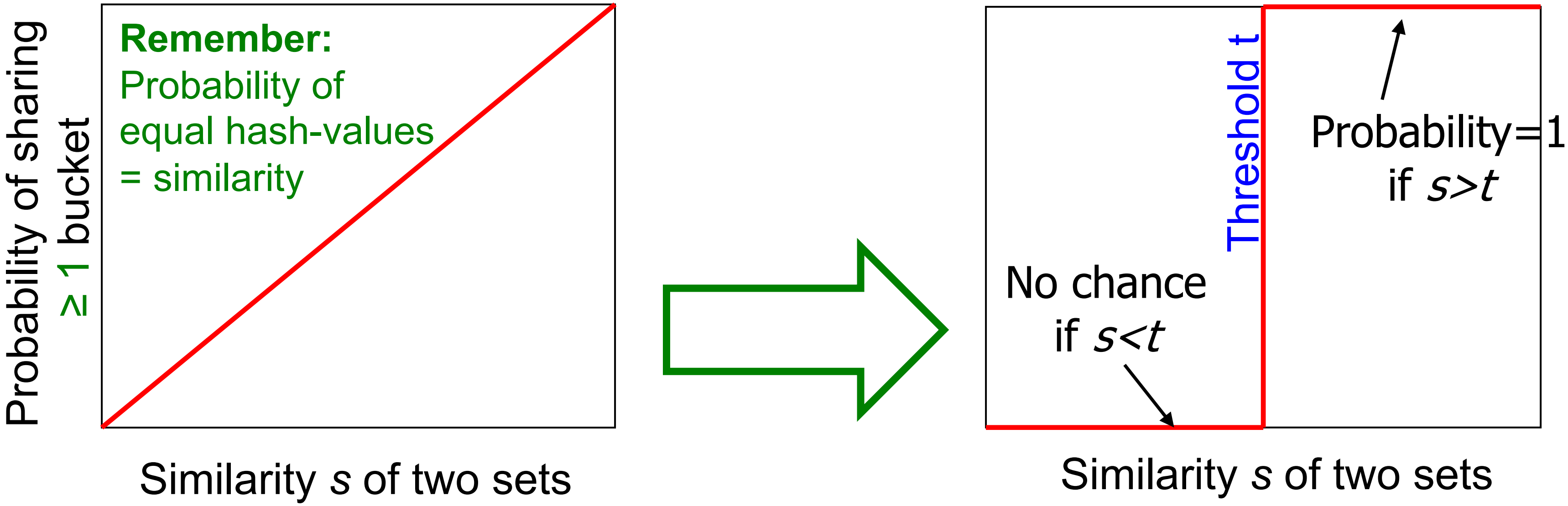

Points
Hash func.
Signatures: short integer signatures that reflect point similarity
Locality-sensitive Hashing
Candidate pairs: those pairs of signatures that we need to test for similarity

Design a **locality sensitive hash function (for a given distance metric)**

Apply the “Bands” technique

The S-Curve

- **The S-curve is where the "magic" happens**



Remember: Probability of equal hash-values = similarity

This is what 1 hash-code gives you

$\Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(D_1, D_2)$

This is what we want!

How to get a step-function?

By choosing *r* and *b*!

How Do We Make the S-curve?

- **Remember:** ***b*** bands, ***r*** rows/band
- Let $sim(C_1, C_2) = s$

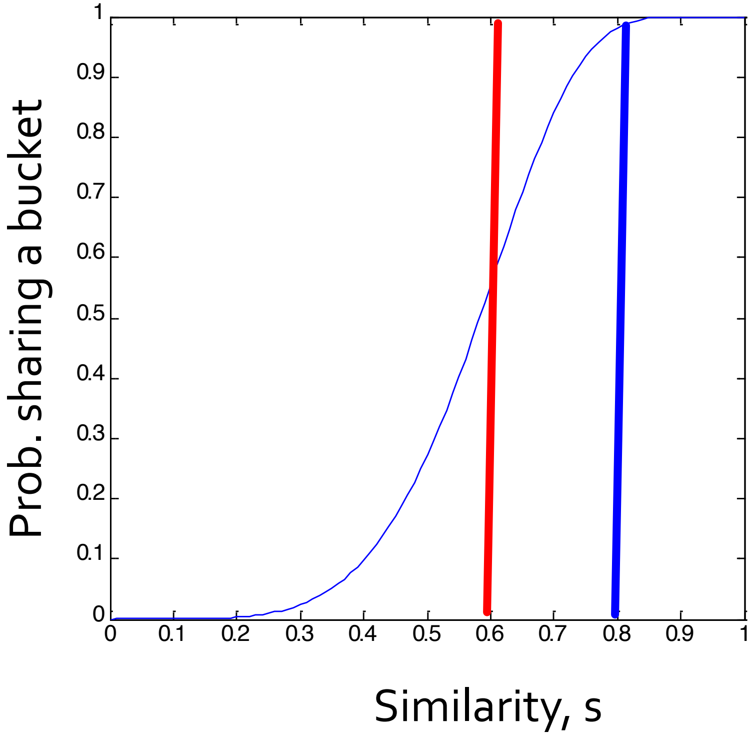
What's the prob. that at least 1 band is equal?

- Pick some band (r rows)
  - Prob. that elements in a single row of columns **C**$_1$ and **C**$_2$ are equal $= s$
  - Prob. that all rows in a band are equal $= s^r$
  - Prob. that some row in a band is not equal $= 1 - s^r$
- Prob. that all bands are not equal $= (1 - s^r)^b$
- Prob. that at least 1 band is equal $= 1 - (1 - s^r)^b$

$P(C_1, C_2 \text{ is a candidate pair}) = 1 - (1 - s^r)^b$

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

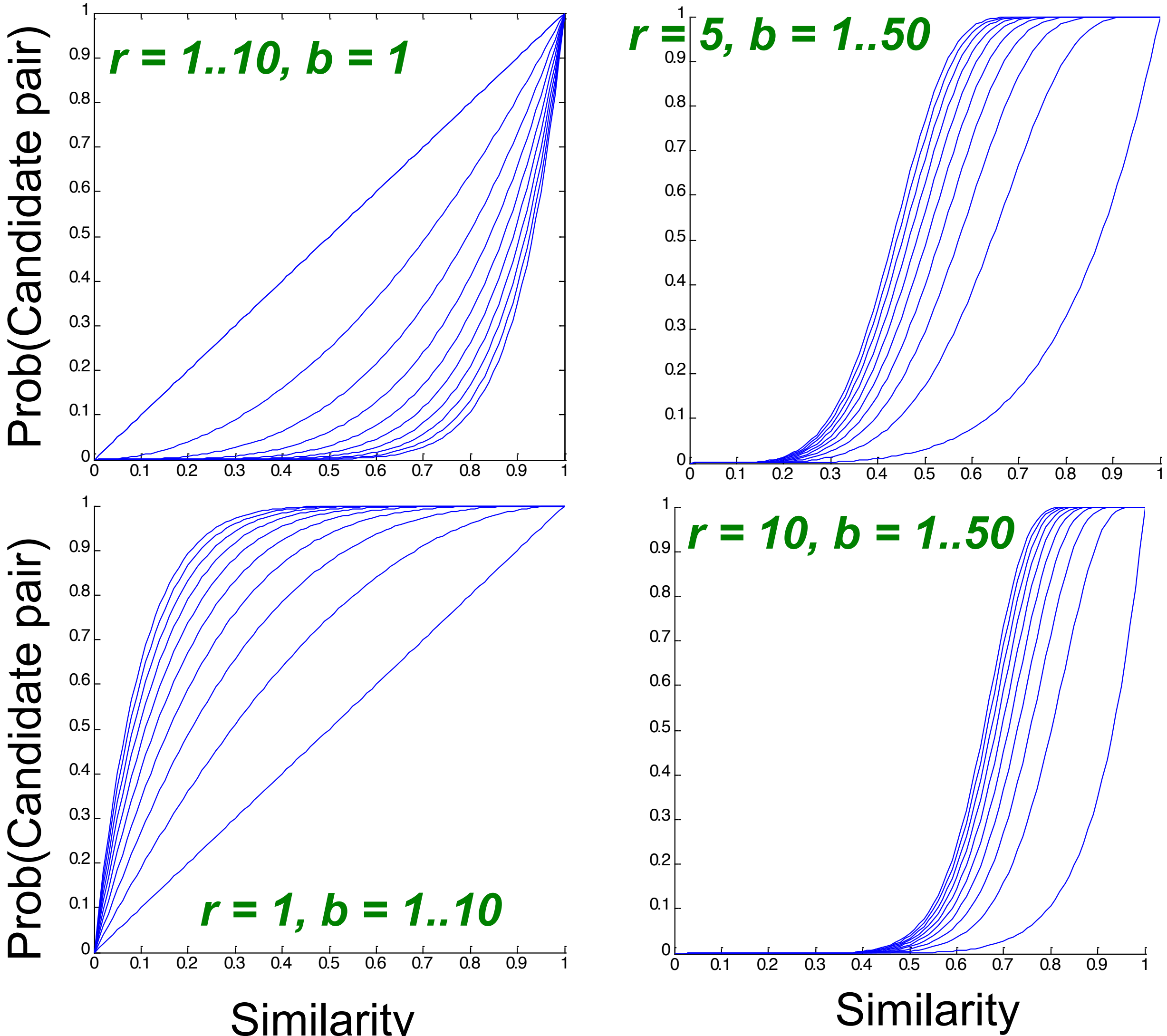
- **Picking *r* and *b* to get the best S-curve**
  - 50 hash-functions (r=5, b=10)



S-curves as a func. of *b* and *r*

Given a fixed threshold ***t***.

We want choose ***r*** and ***b*** such that the ***P(Candidate pair)*** has a "step" right around ***t***.



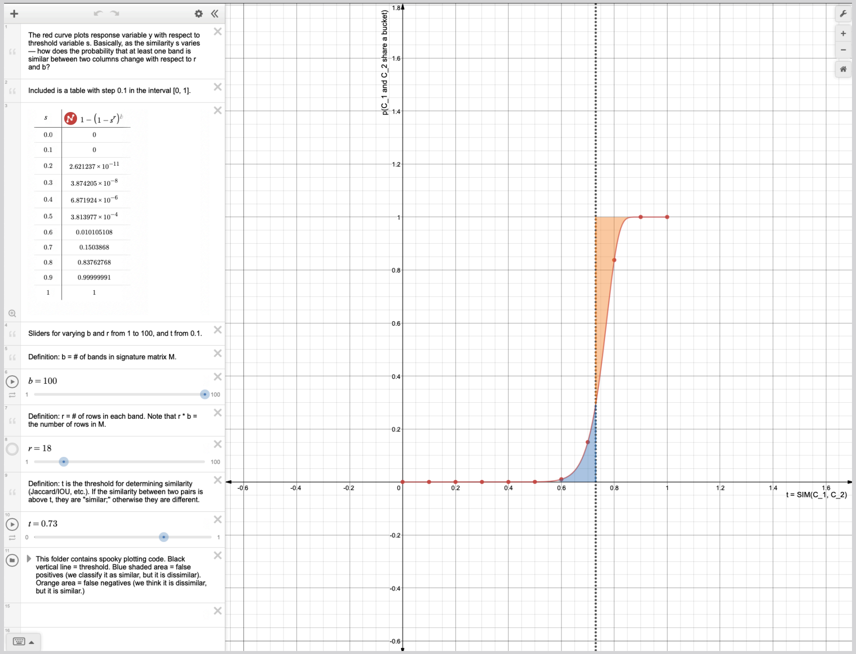
***prob* = 1 - (1 - *s* ^{r})^{b}**

Visualizing S-Curves

Visualization of the effect of threshold, band size, and # of rows in LSH

by Trenton Chang (Thank you!!)

https://www.desmos.com/calculator/lzzvfjiujn



The red curve plots response variable y with respect to threshold variable s. Basically, as the similarity s varies — how does the probability that at least one band is similar between two columns change with respect to r and b?

Included is a table with step 0.1 in the interval [0, 1].

s	$1-(1-s^r)^b$
0.0	0
0.1	0
0.2	2.621237×10^{-11}
0.3	3.874205×10^{-8}
0.4	6.871924×10^{-6}
0.5	3.813977×10^{-4}
0.6	0.010105108
0.7	0.1503868
0.8	0.83762768
0.9	0.99999991
1	1

Sliders for varying b and r from 1 to 100, and t from 0.1.

Definition: b = # of bands in signature matrix M.

$b = 100$

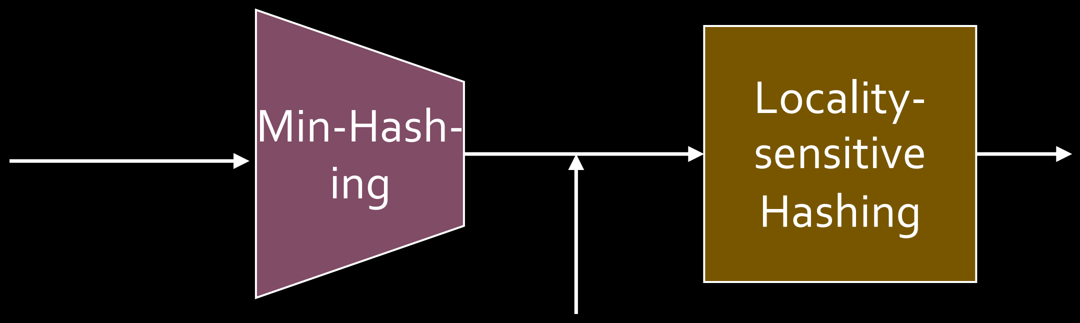
Definition: r = # of rows in each band. Note that r * b = the number of rows in M.

$r = 18$

Definition: t is the threshold for determining similarity (Jaccard/IOU, etc.). If the similarity between two pairs is above t, they are "similar;" otherwise they are different.

$t = 0.73$

This folder contains spooky plotting code. Black vertical line = threshold. Blue shaded area = false positives (we classify it as similar, but it is dissimilar). Orange area = false negatives (we think it is dissimilar, but it is similar.)



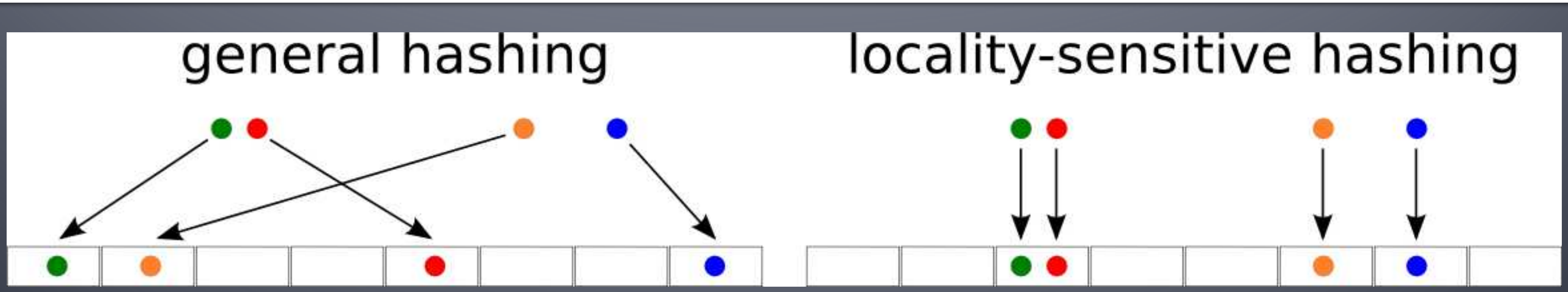
Min-Hash-ing

Locality-sensitive Hashing

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

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

Theory of LSH



Theory of LSH

- **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

- $\boldsymbol{d}(\cdot)$ is a **distance measure** if it is a function from pairs of points **x,y** to real numbers such that:
  - $d(x,y) \geq 0$
  - $d(x,y) = 0 \; iff \; x = y$
  - $d(x,y) = d(y,x)$
  - $d(x,y) \leq d(x,z) + d(z,y)$ (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 dimension
    - 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

Families of Hash Functions

- **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***”
- 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

Locality-Sensitive (LS) Families

- **Suppose we have a space *S* of points with a distance measure *d(x,y)***

Critical assumption

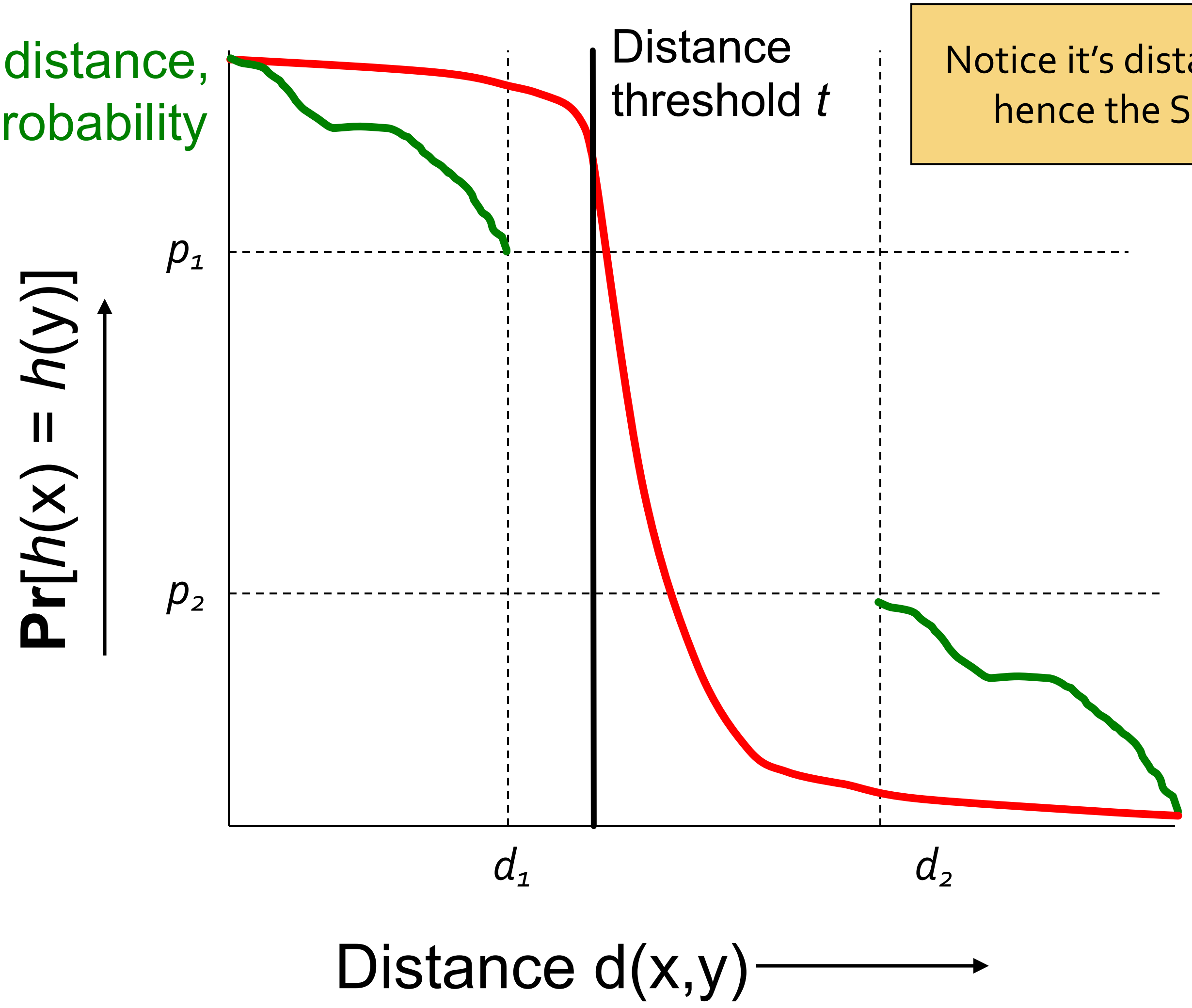
- A family ***H*** of hash functions is said to be ***(d_1, d_2, p_1, p_2)-sensitive*** if for any ***x*** and ***y*** in ***S***:

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

With a LS Family we can do LSH!

A (d_1,d_2,p_1,p_2)-sensitive function

Small distance, high probability



Notice it's distance, not similarity, hence the S-curve is flipped!

Large distance, low probability of hashing to the same value

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 $\boldsymbol{h} \in \boldsymbol{H}$:

$$Pr[h(x) = h(y)] = 1 - d(x, y)$$

  - Simply restates theorem about Min-Hashing in terms of distances rather than similarities

Example: LS Family – (2)

- **Claim: Min-hash *H*** is a $(\boxed{1/3}, 2/3, \boxed{2/3}, 1/3)$-sensitive family for ***S*** and ***d***.

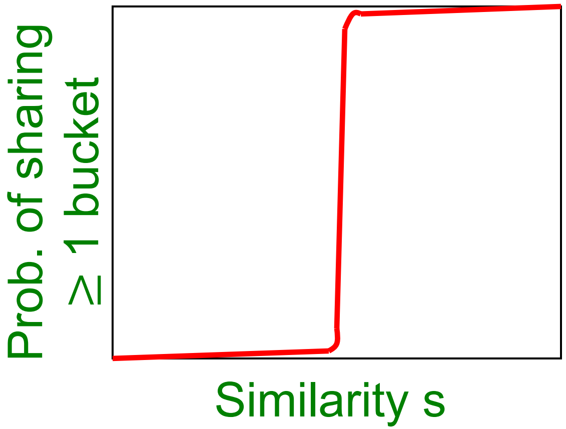
If distance ≤ 1/3
(so similarity ≥ 2/3)

Then probability
that Min-Hash values
agree is ≥ 2/3

- **For Jaccard similarity, Min-Hashing gives a $(d_1,d_2,(1-d_1),(1-d_2))$-sensitive family for any $d_1<d_2$**

Amplifying a LS-Family

- Can we reproduce the "S-curve" effect we saw before for any LS family?



- The "**bands**" technique we learned for signature matrices carries over to this more general setting
- **Can do LSH with any *(d_1, d_2, p_1, p_2)-sensitive* family!**

- **Two constructions:**
  - **AND** construction like "rows in a band"
  - **OR** construction like "many bands"

Amplifying Hash Functions: AND and OR

AND of Hash Functions

- Given family ***H***, construct family ***H'*** consisting of ***r*** functions from ***H***
- For $h = [h_1,\dots,h_r]$ in **H'**, we say **h(x) = h(y)** if and only if $\mathbf{h_i(x) = h_i(y)}$ for **all *i*** $1 \le i \le r$
  - Note this corresponds to creating a band of size **r**

- **Theorem:** If ***H*** is (d_1, d_2, p_1, p_2)-sensitive, then **H'** is $(d_1, d_2, (p_1)^r, (p_2)^r)$-sensitive
- **Proof:** Use the fact that h_i's are **independent**

Also lowers probability for small distances (Bad)

Lowers probability for large distances (Good)

Subtlety Regarding Independence

- **Independence of hash functions (HFs) really means that the prob. of two HFs saying "yes" is the product of each saying "yes"**
  - **But** two particular hash functions could be highly correlated
    - For example, in Min-Hash if their permutations agree in the first one million entries
  - **However**, the probabilities in definition of a LSH-family are over all possible members of ***H, H'*** (i.e., average case and not the worst case)

OR of Hash Functions

- Given family H, construct family H' consisting of b functions from H

- For $h = [h_1,\dots,h_b]$ in H',
  h(x) = h(y) if and only if $\mathbf{h_i(x) = h_i(y)}$ for **at least 1** i

- **Theorem:** If H is (d_1, d_2, p_1, p_2)-sensitive, then H' is $(d_1, d_2, 1\text{-}(1\text{-}p_1)^b, 1\text{-}(1\text{-}p_2)^b)$-sensitive
- **Proof:** Use the fact that h_i's are **independent**

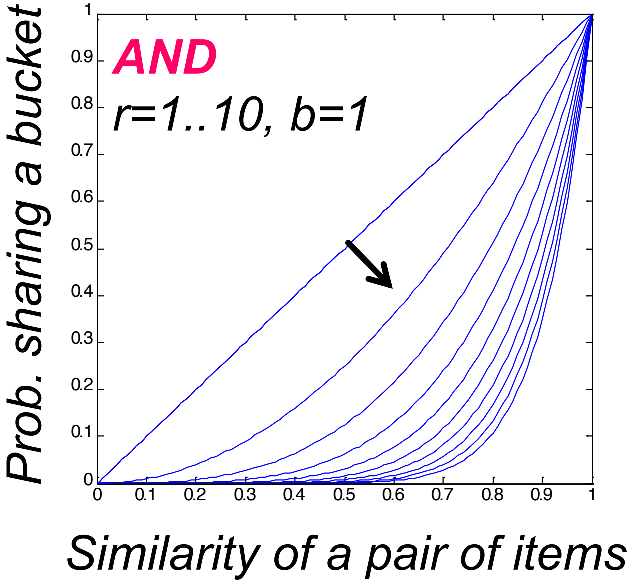
Raises probability for small distances (Good)

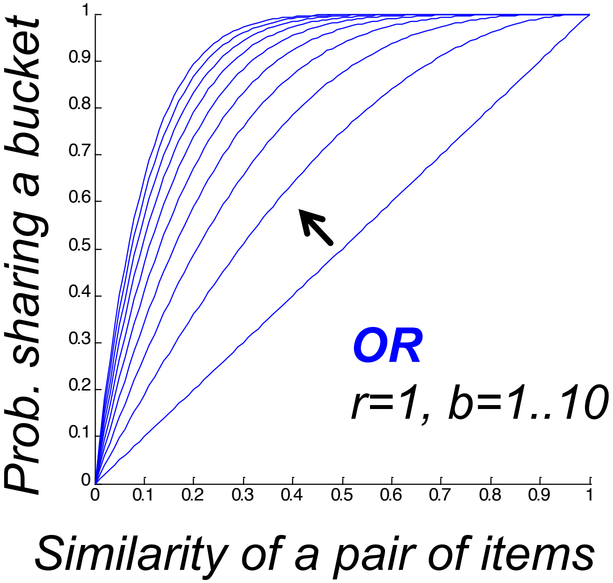
Raises probability for large distances (Bad)

Effect of AND and OR Constructions

- **AND** makes all probs. **shrink**, but by choosing ***r*** correctly, we can make the lower prob. approach 0 while the higher does not

- **OR** makes all probs. **grow**, but by choosing ***b*** correctly, we can make the higher prob. approach 1 while the lower does not





Combine AND and OR Constructions

- By choosing ***b*** and ***r*** correctly, we can make the lower probability approach 0 while the higher approaches 1

- As for the signature matrix, we can use the AND construction followed by the OR construction
  - Or vice-versa
  - Or any sequence of AND's and OR's alternating

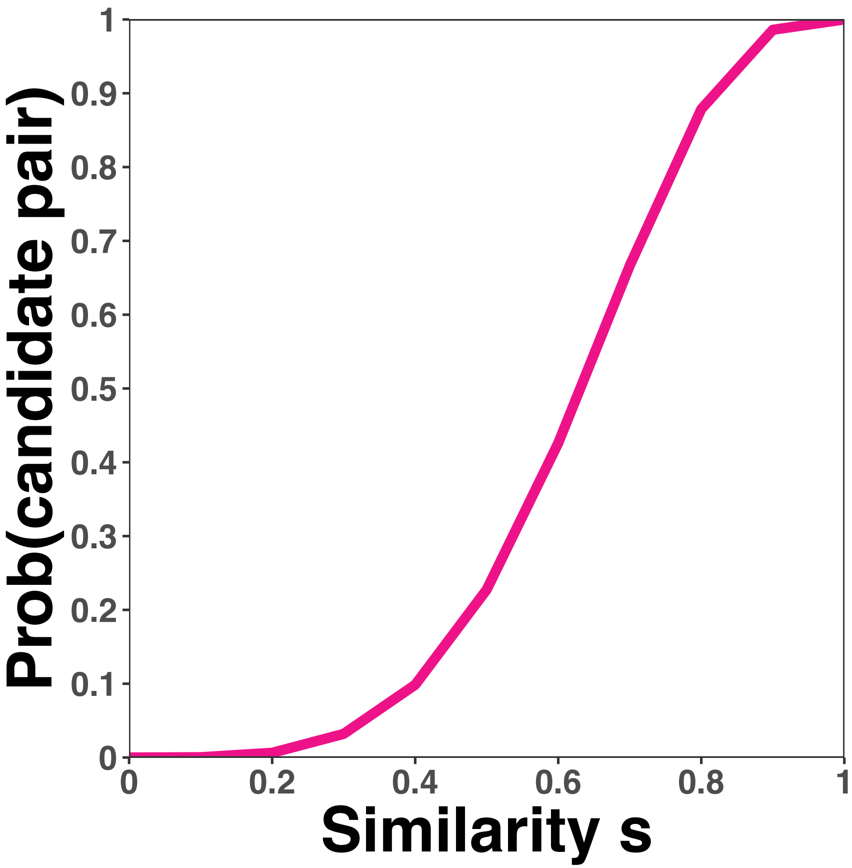
Composing Constructions

- *r*-way **AND** followed by ***b***-way **OR** construction
  - **Exactly what we did with Min-Hashing**
    - **AND:** If bands match in **all** ***r*** values hash to same bucket
    - **OR:** Cols that have ≥ 1 common bucket → **Candidate**

- Take points ***x*** and ***y*** s.t. ***Pr[h(x) = h(y)] = s***
  - ***H*** will make **(x,y)** a candidate pair with prob. **s**
- Construction makes **(x,y)** a candidate pair with probability $1\text{-}(1\text{-}s^r)^b$ **The S-Curve!**
  - **Example:** Take **H** and construct **H'** by the **AND** construction with ***r* = 4**. Then, from **H'**, construct **H''** by the **OR** construction with ***b* = 4**

Table for Function 1-(1-s⁴)⁴

s	$p=1-(1-s^4)^4$
.2	**.0064**
.3	.0320
.4	.0985
.5	.2275
.6	.4260
.7	.6666
.8	**.8785**
.9	.9860

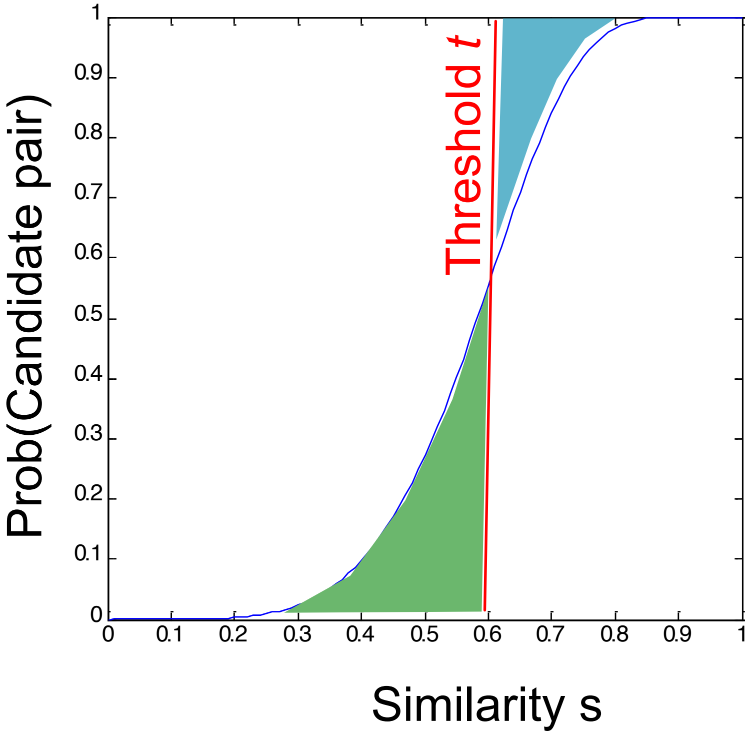


***r* = 4, *b* = 4** transforms a (.2,.8,.8,.2)-sensitive family into a (.2,.8,.8785,.0064)-sensitive family.

How to choose *r* and *b*

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

- **Picking *r* and *b* to get desired performance**
  - **50 hash-functions (*r* = 5, *b* = 10)**

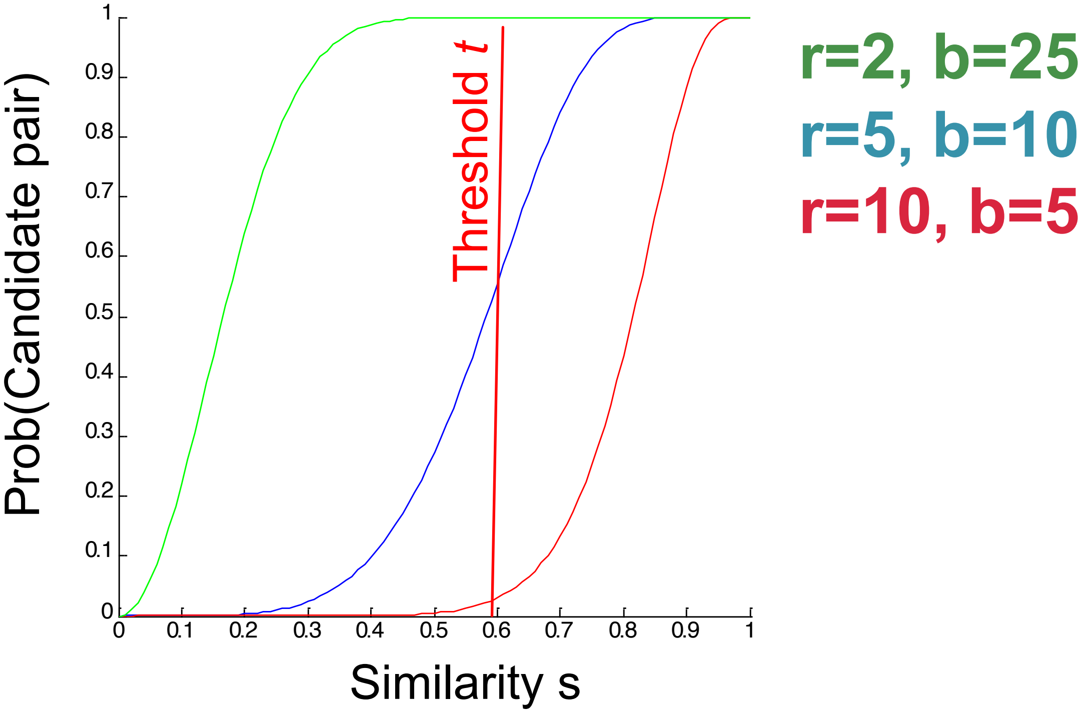


Blue area *X*: False Negative rate
These are pairs with ***sim* > *t*** but the ***X*** fraction won't share a band and then will **never become candidates.** This means we will never consider these pairs for (slow/exact) similarity calculation!

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

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

- **Picking *r* and *b* to get desired performance**
    - **50 hash-functions (*r* * *b* = *50*)**



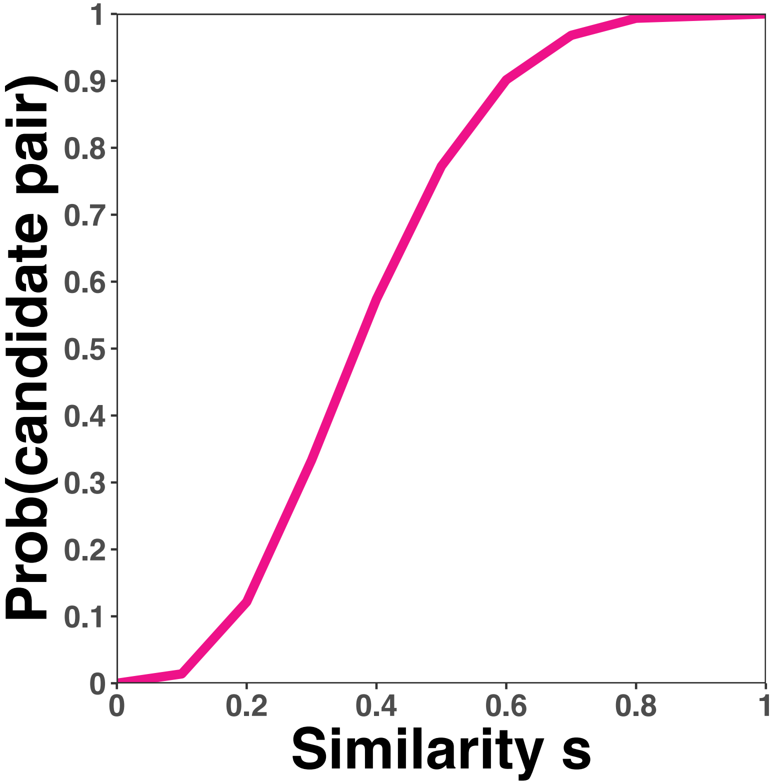
OR-AND Composition

- Apply a ***b***-way **OR** construction followed by an ***r***-way **AND** construction
- Transforms similarity ***s*** (probability p) into $\boldsymbol{(1-(1-s)^b)^r}$
  - **The same S-curve, mirrored horizontally and vertically**

- **Example:** Take **H** and construct **H'** by the **OR** construction with ***b*** = 4. Then, from **H'**, construct **H''** by the **AND** construction with ***r*** = 4

Table for Function $(1-(1-s)^4)^4$

s	$p=(1-(1-s)^4)^4$
.1	.0140
.2	**.1215**
.3	.3334
.4	.5740
.5	.7725
.6	.9015
.7	.9680
.8	**.9936**



The example transforms a (.2,.8,.8,.2)-sensitive family into a (.2,.8,.9936,.1215)-sensitive family

Cascading Constructions

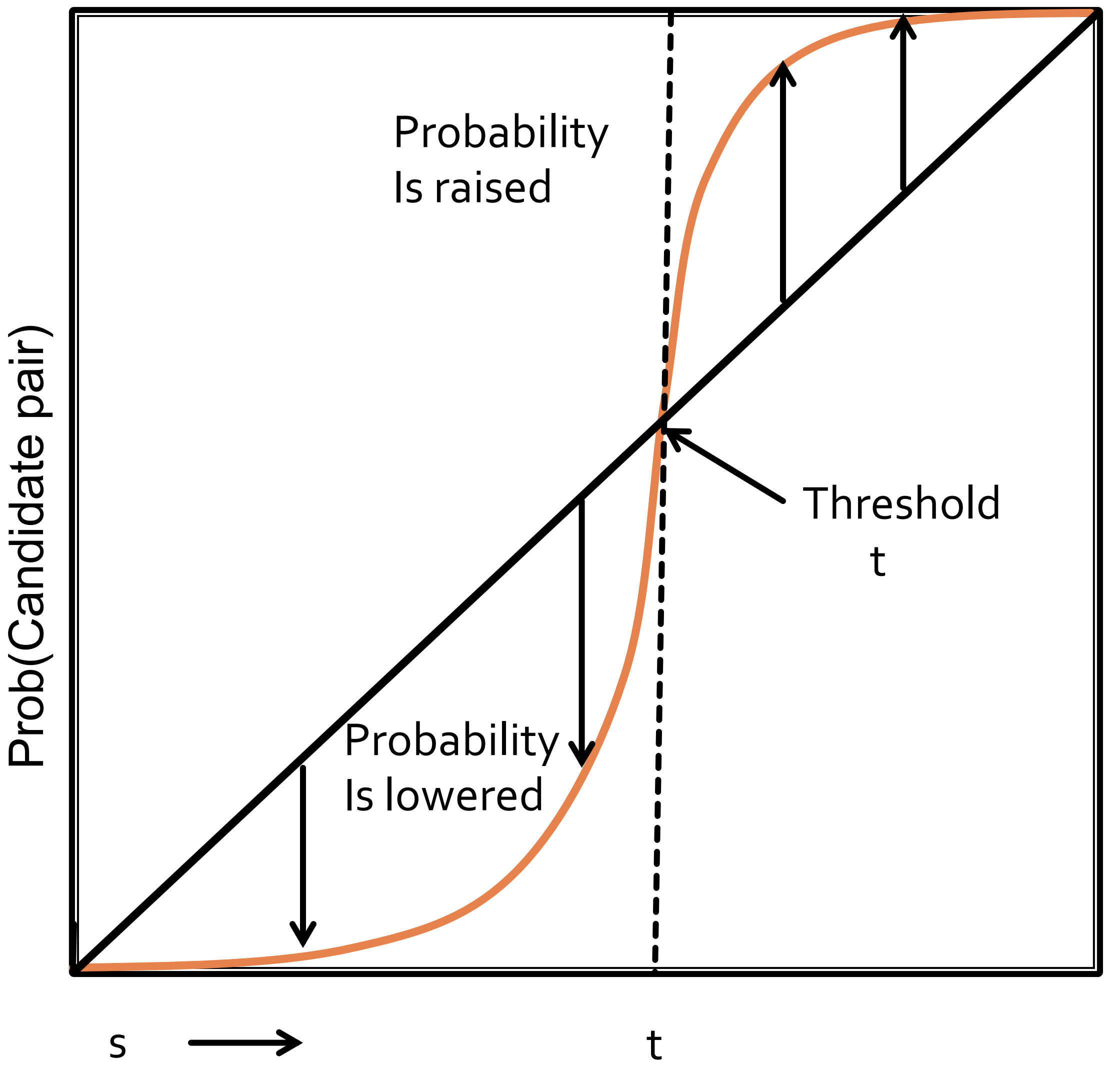
- **Example:** Apply the **(4,4) OR-AND** construction followed by the **(4,4) AND-OR** construction

- **Transforms a (.2, .8, .8, .2)-sensitive family into a (.2, .8, .9999996, .0008715)-sensitive family**
  - **Note this family uses 256 (=4*4*4*4) of the original hash functions**

General Use of S-Curves

- For each AND-OR S-curve $1-(1-s^r)^b$, there is a *threshold* *t*, for which $1-(1-t^r)^b = t$
- Above *t*, high probabilities are increased; below *t*, low probabilities are decreased
- You improve the sensitivity as long as the low probability is less than *t*, and the high probability is greater than *t*
  - Iterate as you like
- Similar observation for the OR-AND type of S-curve: $(1-(1-s)^b)^r$

Visualization of Threshold



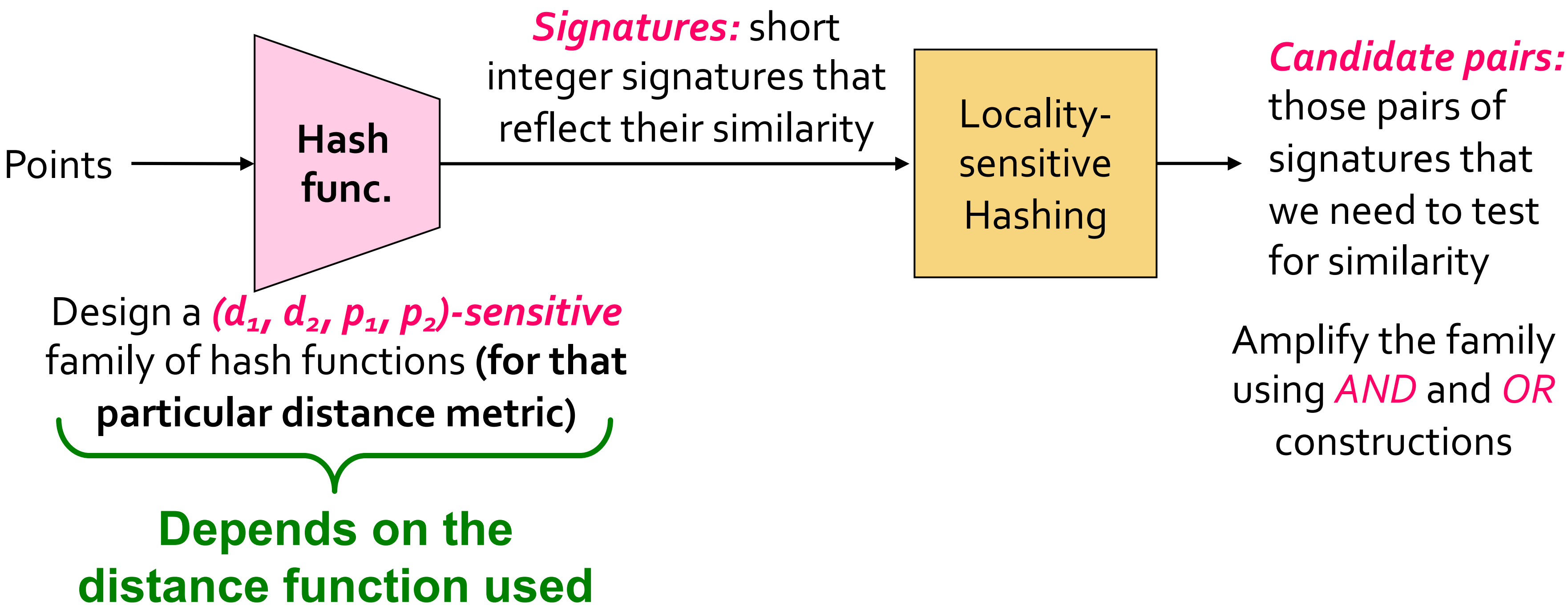
Summary

- Pick any two distances $\boldsymbol{d_1 < d_2}$
- Start with a $\boldsymbol{(d_1, d_2, (1- d_1), (1- d_2))}$-sensitive family
- Apply constructions to **amplify** $\boldsymbol{(d_1, d_2, p_1, p_2)}$-sensitive family, where $\boldsymbol{p_1}$ is almost 1 and $\boldsymbol{p_2}$ is almost 0
- **The closer to 0 and 1 we get, the more hash functions must be used!**

LSH for other distance metrics

LSH for other Distance Metrics

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



Points

Hash func.

Signatures: short integer signatures that reflect their similarity

Locality-sensitive Hashing

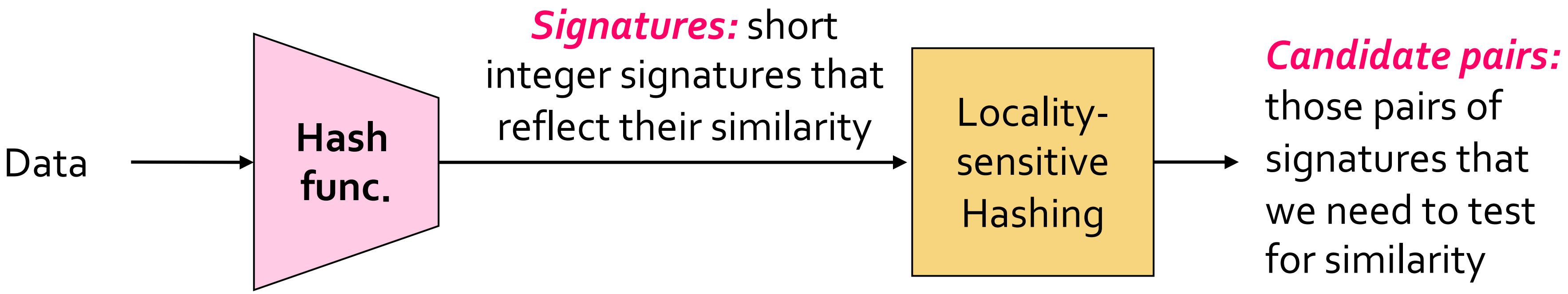
Candidate pairs: those pairs of signatures that we need to test for similarity

Design a ***(d_1, d_2, p_1, p_2)-sensitive*** family of hash functions **(for that particular distance metric)**

Depends on the distance function used

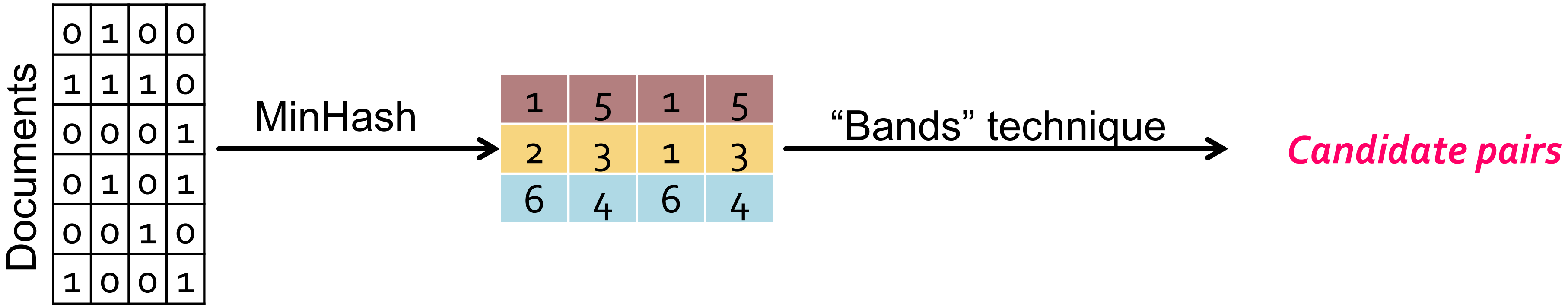
Amplify the family using *AND* and *OR* constructions

Summary of what we will learn



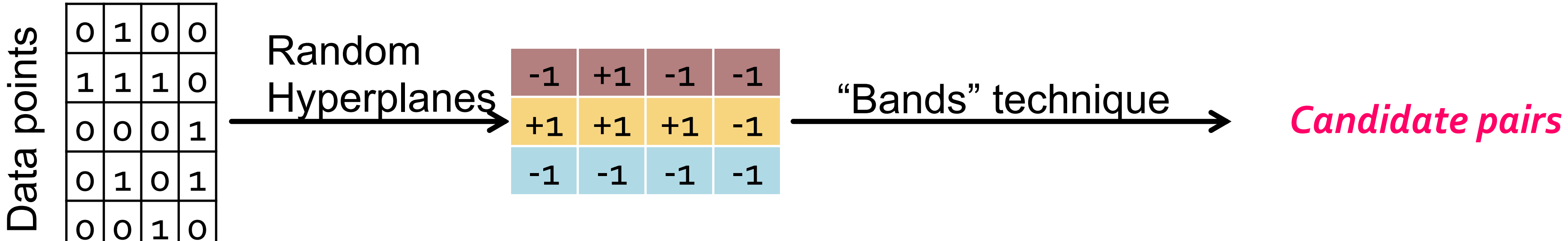
Signatures: short integer signatures that reflect their similarity

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



0	1	0	0
1	1	1	0
0	0	0	1
0	1	0	1
0	0	1	0
1	0	0	1

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

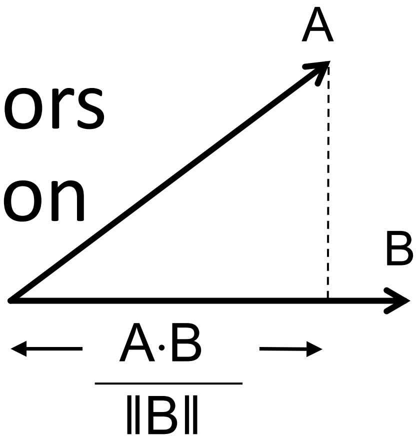


0	1	0	0
1	1	1	0
0	0	0	1
0	1	0	1
0	0	1	0

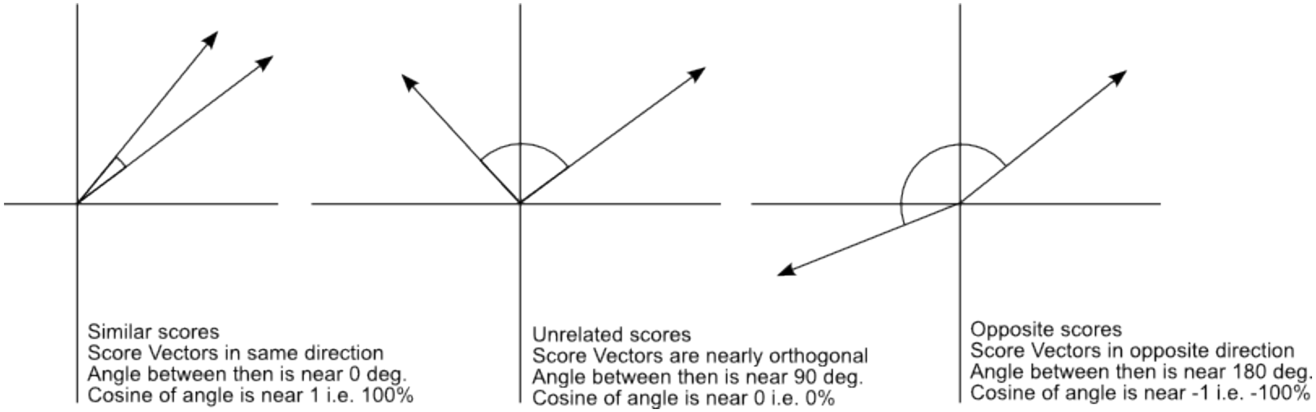
-1	+1	-1	-1
+1	+1	+1	-1
-1	-1	-1	-1

Cosine Distance

- ***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 $[\mathbf{0}, \boldsymbol{\pi}]$ (equivalently [0,180°])
  - Can divide θ by $\boldsymbol{\pi}$ to have distance in range [0,1]



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



Similar scores
Score Vectors in same direction
Angle between then is near 0 deg.
Cosine of angle is near 1 i.e. 100%

Unrelated scores
Score Vectors are nearly orthogonal
Angle between then is near 90 deg.
Cosine of angle is near 0 i.e. 0%

Opposite scores
Score Vectors in opposite direction
Angle between then is near 180 deg.
Cosine of angle is near -1 i.e. -100%

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

LSH for Cosine Distance

- For **cosine distance**, there is a technique called **Random Hyperplanes**
  - Technique similar to Min-Hashing

- **Random Hyperplanes** method is a ***$(d_1, d_2, (1-d_1/\pi), (1-d_2/\pi))$**-sensitive* family for any ***d_1*** and ***d_2***

- **Reminder:** *(d_1, d_2, p_1, p_2)-sensitive*
  1. If ***$d(x,y) \leq d_1$***, then prob. that ***$h(x) = h(y)$*** is at least ***p_1***
  2. If ***$d(x,y) \geq d_2$***, then prob. that ***$h(x) = h(y)$*** is at most **p_2**

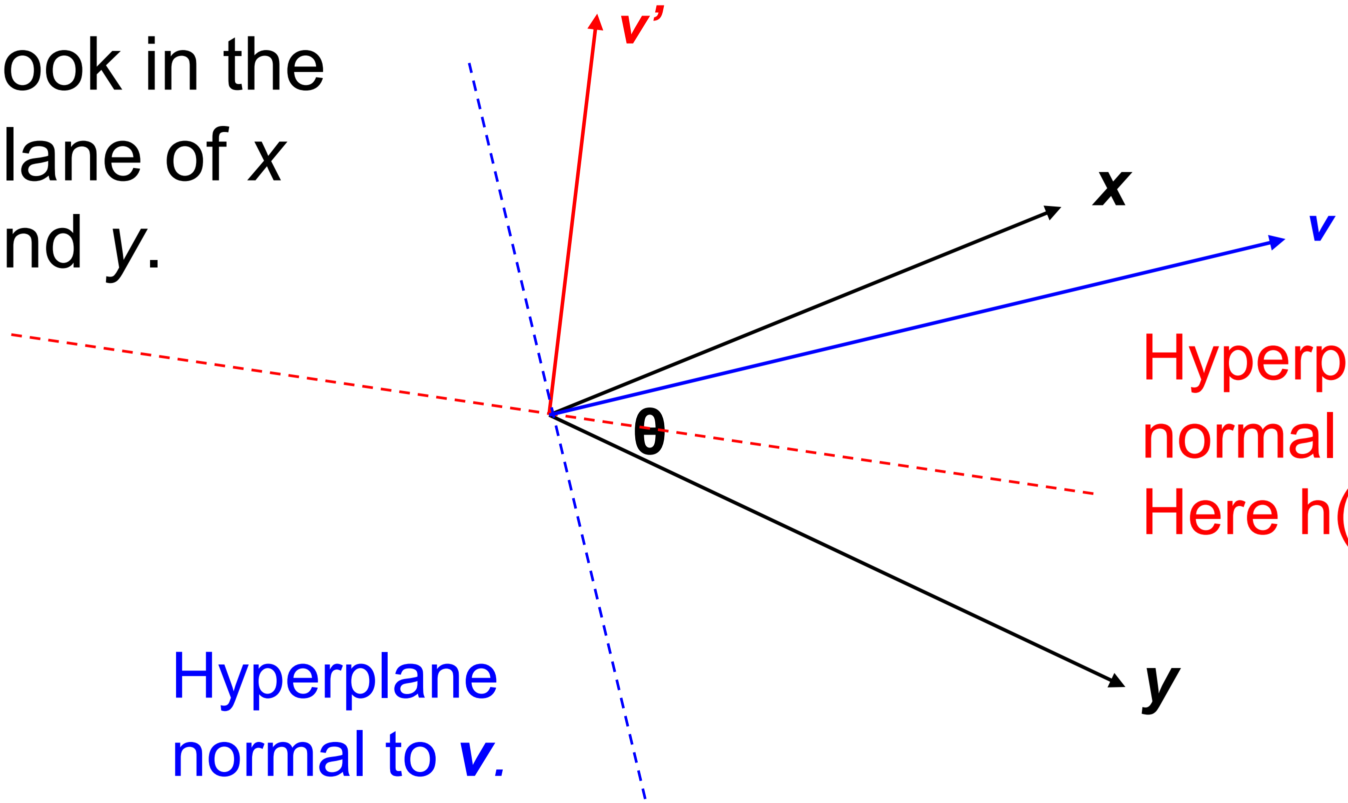
Random Hyperplanes

- Each vector ***v*** determines a hash function $\boldsymbol{h_v}$ with two buckets
- $\mathbf{h_v(x) = +1}$ if $\mathbf{v \cdot x} \geq \mathbf{0}$; $\mathbf{= -1}$ if $\mathbf{v \cdot x < 0}$
- LS-family ***H*** = set of all functions derived from any vector
- **Claim:** For points **x** and **y**,

$$\mathbf{Pr[h(x) = h(y)] \;=\; 1 - d(x,y) / \pi}$$

Proof of Claim

Look in the plane of *x* and *y*.

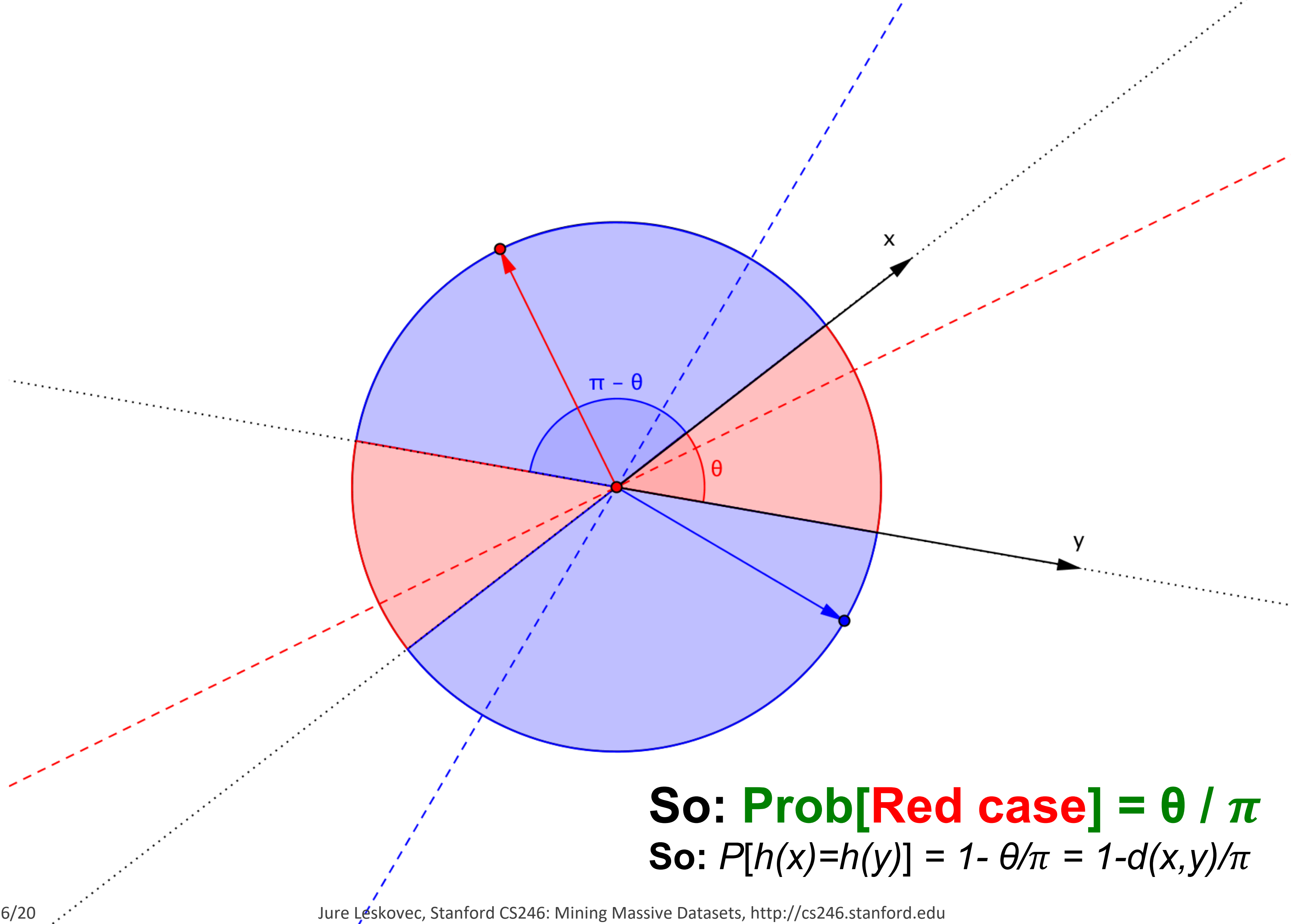


Hyperplane normal to ***v'***. Here h(x) ≠ h(y)

Hyperplane normal to ***v***. Here h(x) = h(y)

Note: what is important is that hyperplane is outside the angle, not that the vector is inside.

Proof of Claim



So: Prob[Red case] = θ / π

So: $P[h(x)=h(y)] = 1- \theta/\pi = 1-d(x,y)/\pi$

Signatures for Cosine Distance

- 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

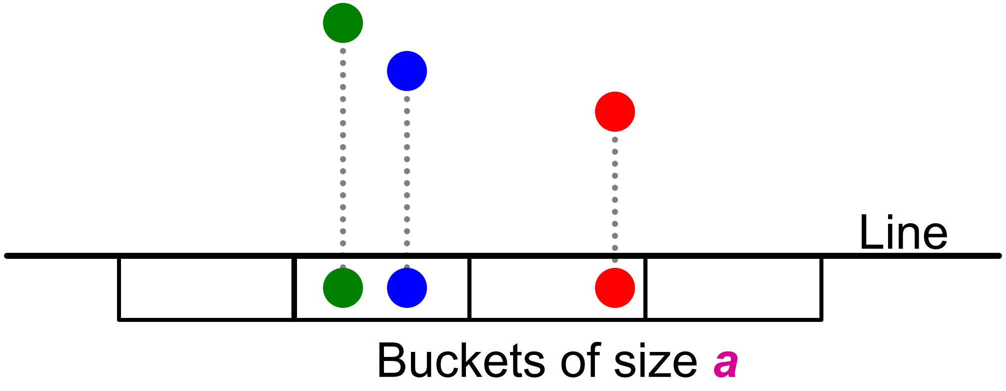
How to pick random vectors?

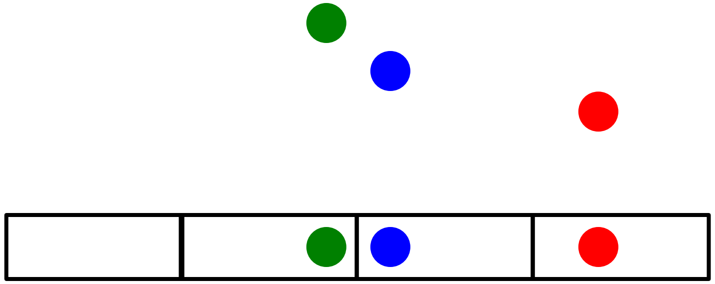
- Expensive to pick a random vector in ***M*** dimensions for large ***M***
  - Would have to generate ***M*** random numbers
- **A more efficient approach**
  - It suffices to consider only vectors ***v*** consisting of +1 and –1 components
    - **Why?** Assuming data is random, then vectors of +/-1 cover the entire space evenly (and does not bias in any way)

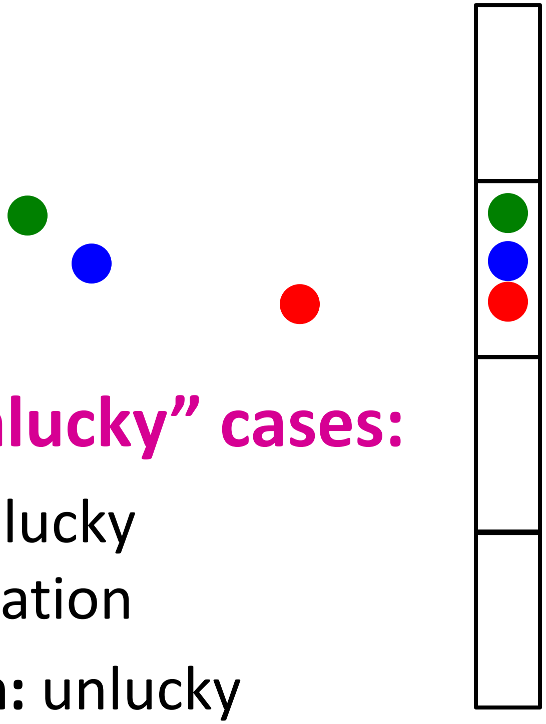
LSH for Euclidean Distance

- **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

Projection of Points

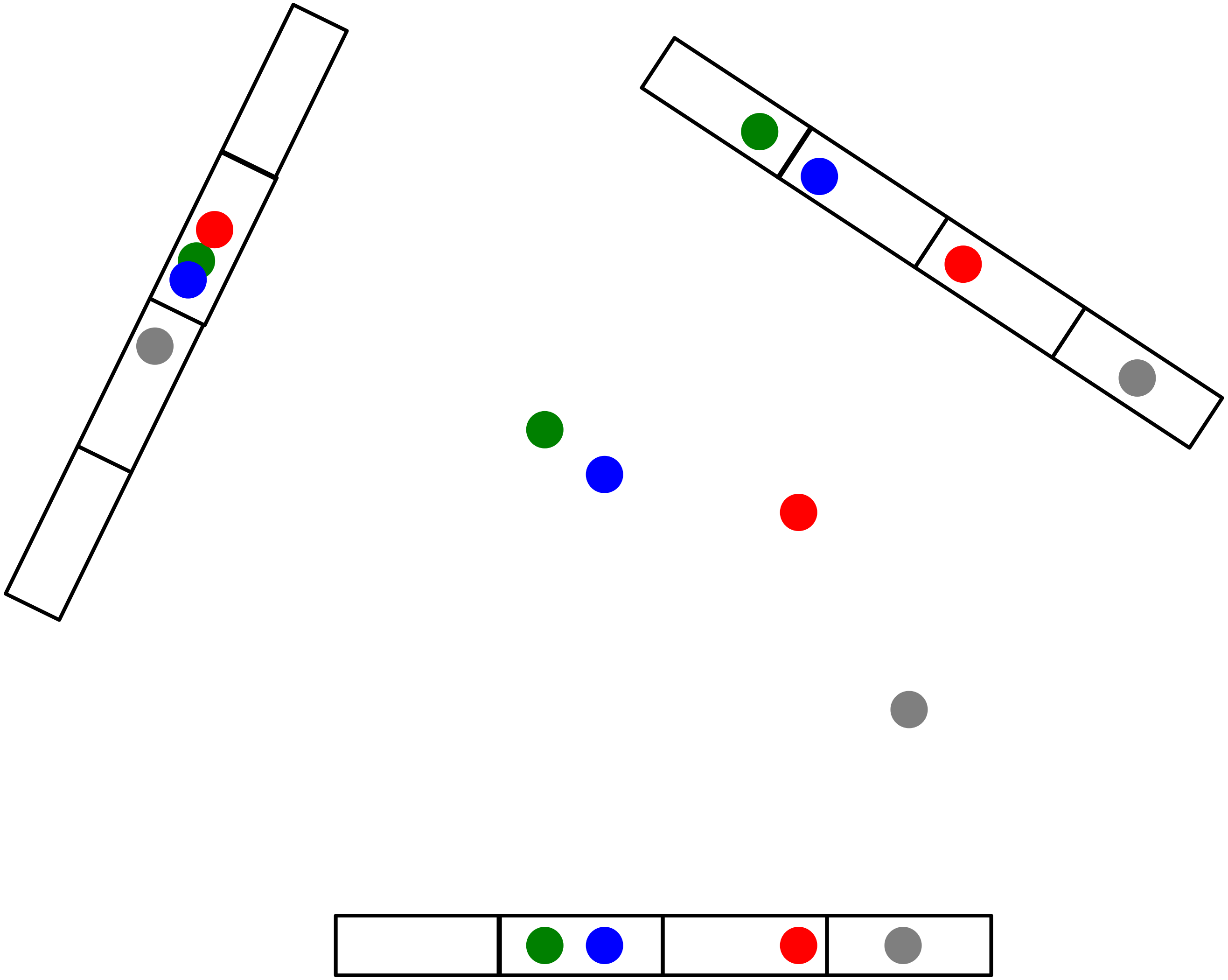




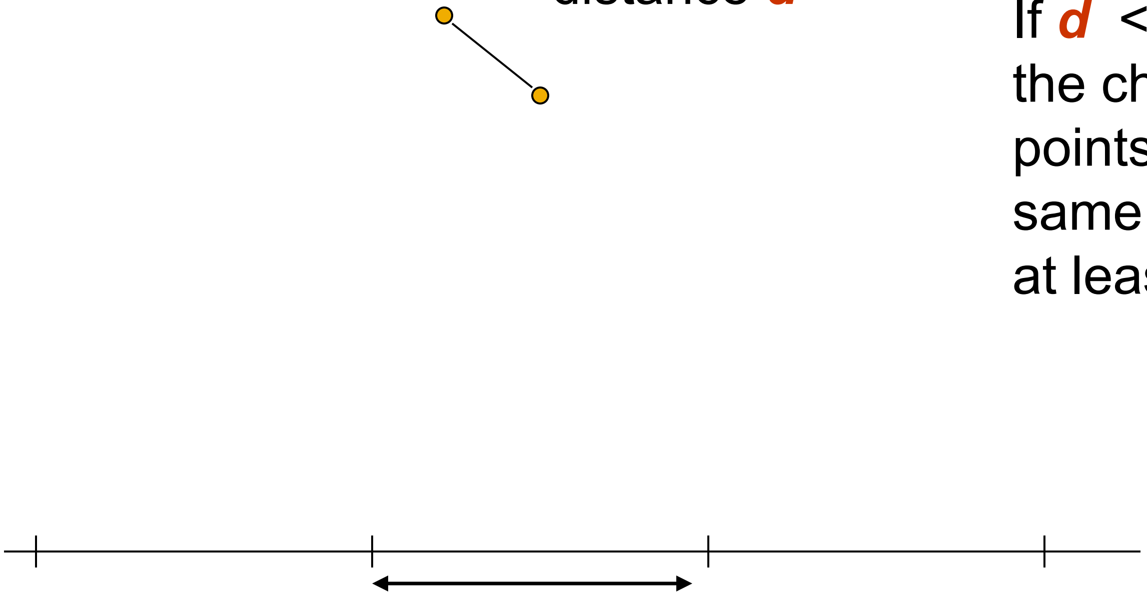


- **“Lucky” case:**
  - Points that are close hash in the same bucket
  - Distant points end up in different buckets
- **Two “unlucky” cases:**
  - **Top:** unlucky quantization
  - **Bottom:** unlucky projection

Multiple Projections



Projection of Points (1)



Points at distance ***d***

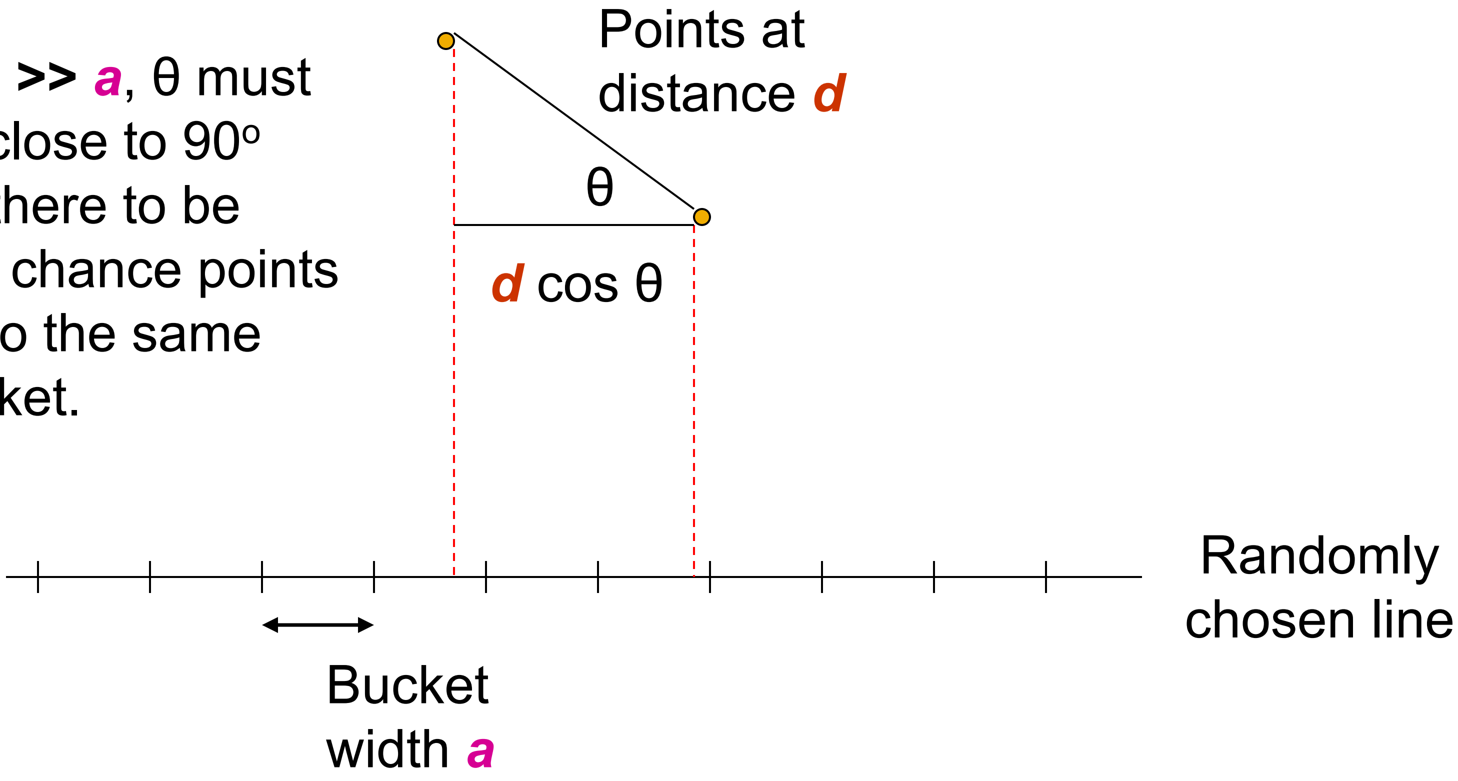
If ***d*** << ***a***, then the chance the points are in the same bucket is at least **1 –** ***d*/*a***.

Randomly chosen line

Bucket width ***a***

Projection of Points (2)

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

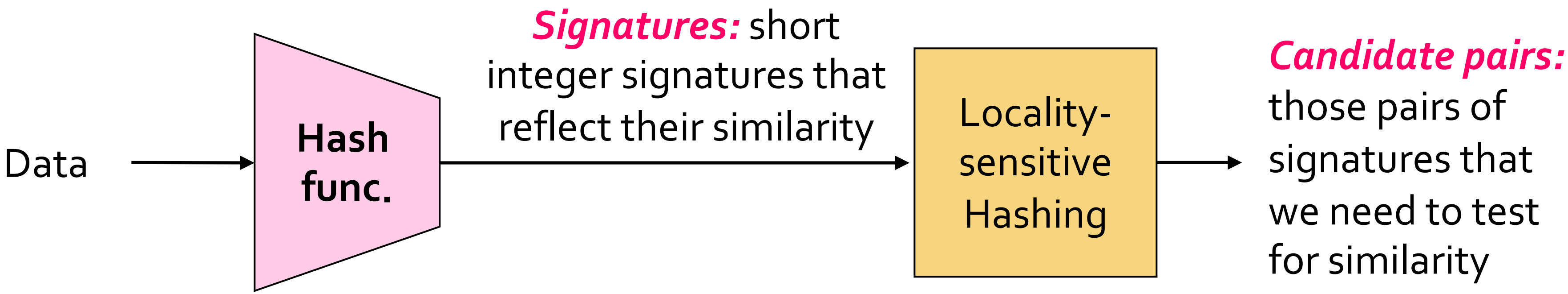


A LS-Family for Euclidean Distance

- If points are distance ***d* ≤ *a*/2**, prob. they are in same bucket **≥ *1- d/a* = ½**
- If points are distance ***d* ≥ 2*a*** apart, then they can be in the same bucket only if ***d* cos θ ≤ *a***
  - cos θ ≤ ½
  - 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**

Summary



Data

Hash func.

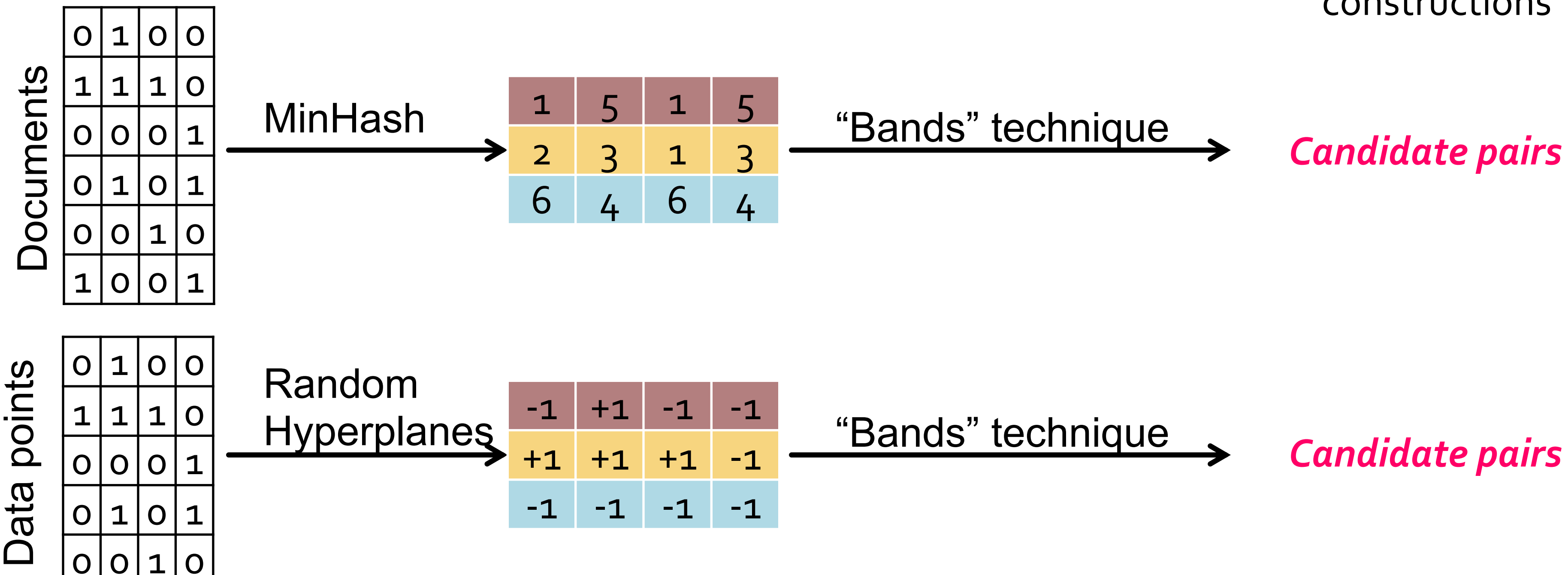
Signatures: short integer signatures that reflect their similarity

Locality-sensitive Hashing

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

Design a ***(d_1, d_2, p_1, p_2)-sensitive*** family of hash functions **(for that particular distance metric)**

Amplify the family using *AND* and *OR* constructions



Documents

0	1	0	0
1	1	1	0
0	0	0	1
0	1	0	1
0	0	1	0
1	0	0	1

MinHash

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

"Bands" technique

Candidate pairs

Data points

0	1	0	0
1	1	1	0
0	0	0	1
0	1	0	1
0	0	1	0

Random Hyperplanes

-1	+1	-1	-1
+1	+1	+1	-1
-1	-1	-1	-1

"Bands" technique

Candidate pairs

Two Important Points

- Property $P(h(C_1)=h(C_2))=sim(C_1,C_2)$ of hash function h is the essential part of LSH, without which we can't do anything

- LS-hash functions transform data to signatures so that the bands technique (AND, OR constructions) can then be applied