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Theory of Locality Sensitive Hashing

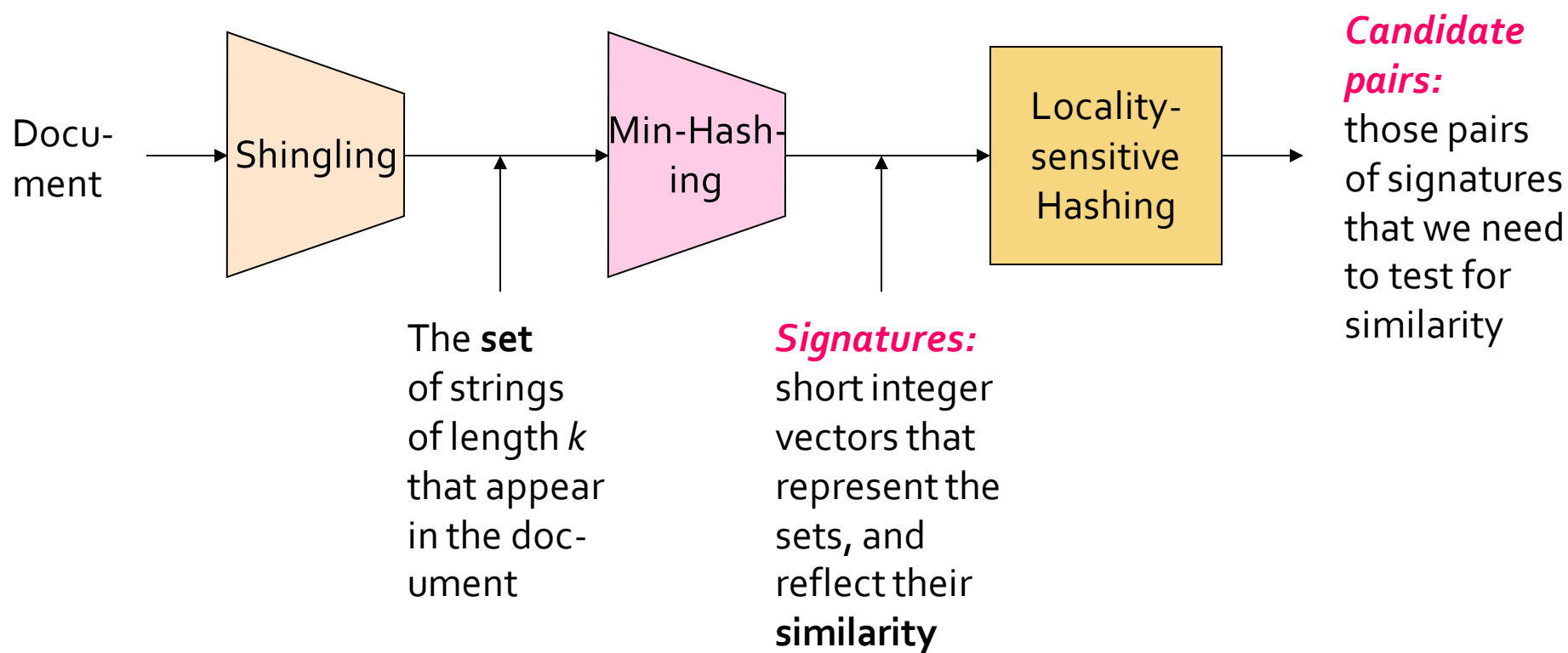
CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
<http://cs246.stanford.edu>



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



Recap 1: Shingles

- A ***k*-shingle** (or ***k*-gram**) is a sequence of k tokens that appears in the document
 - **Example:** $k=2$; $D_1 = \text{abcab}$
Set of 2-shingles: $C_1 = S(D_1) = \{\text{ab}, \text{bc}, \text{ca}\}$
- Represent a doc by a set of hash values of its k -shingles
- A natural **similarity measure** is then the **Jaccard similarity**:
$$\text{sim}(D_1, D_2) = |C_1 \cap C_2| / |C_1 \cup C_2|$$
 - Similarity of two documents is the Jaccard similarity of their shingles

Recap 2: Minhashing

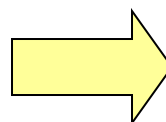
- **Min-Hashing**: Convert large sets into short signatures, while preserving similarity: $\Pr[h(C_1) = h(C_2)] = \text{sim}(D_1, D_2)$

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

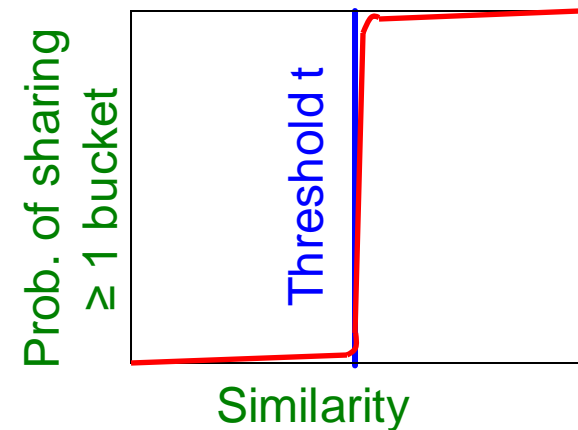
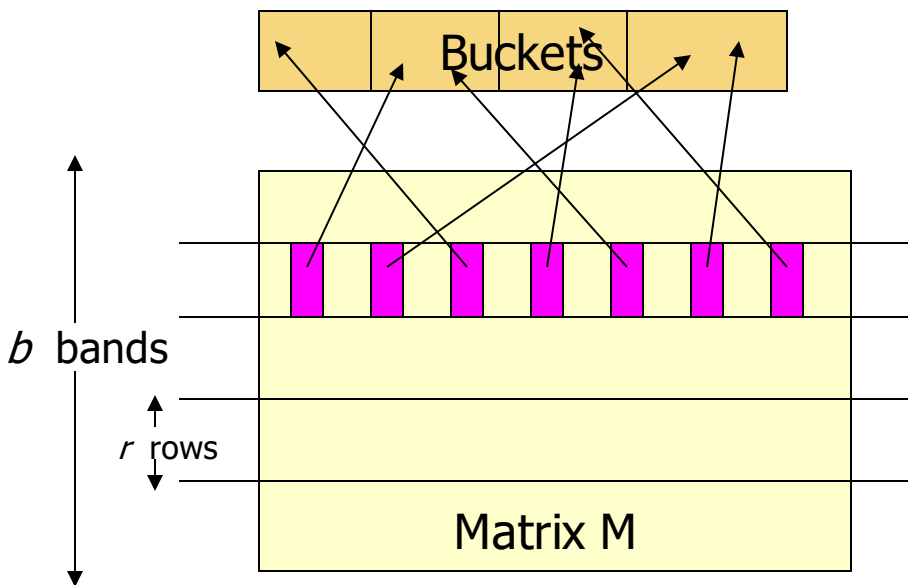
2	1	2	1
2	1	4	1
1	2	1	2

Similarities of columns and signatures (approx.) match!

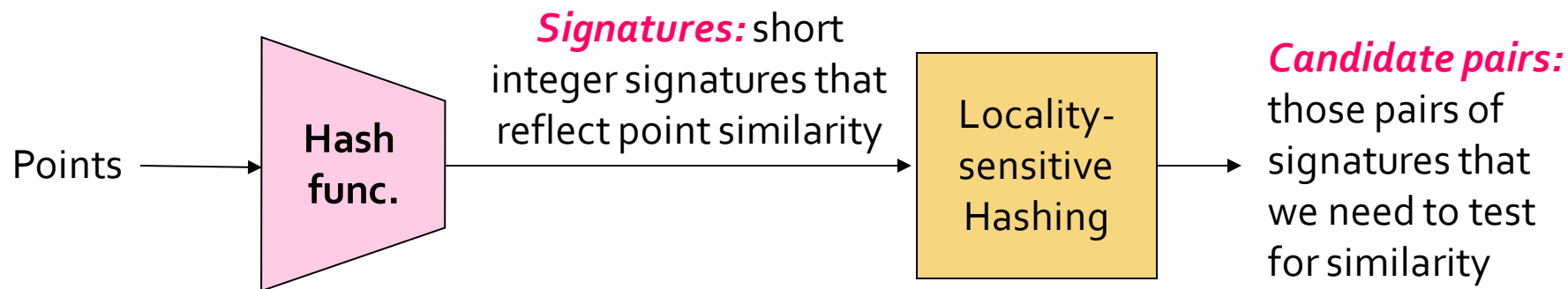
	1-3	2-4	1-2	3-4
Col/Col	0.75	0.75	0	0
Sig/Sig	0.67	1.00	0	0

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 ($M=b \cdot r$)
 - **Candidate** column pairs are those that hash to the same bucket for ≥ 1 band



Today: Generalizing Min-hash

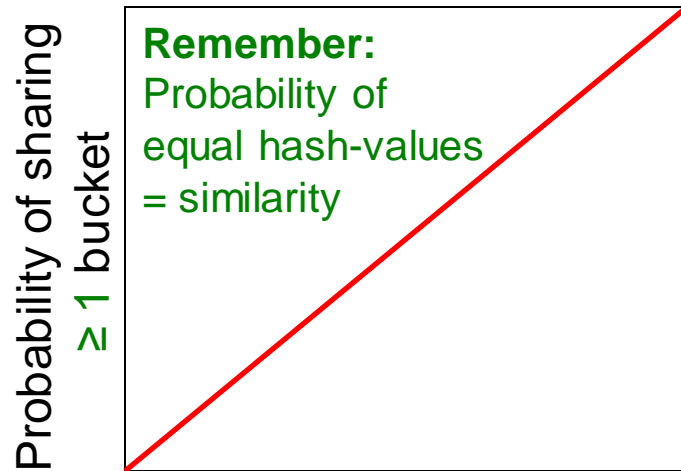


Design a **locality sensitive hash function** (for a given distance metric)

Apply the **“Bands”** technique

The S-Curve

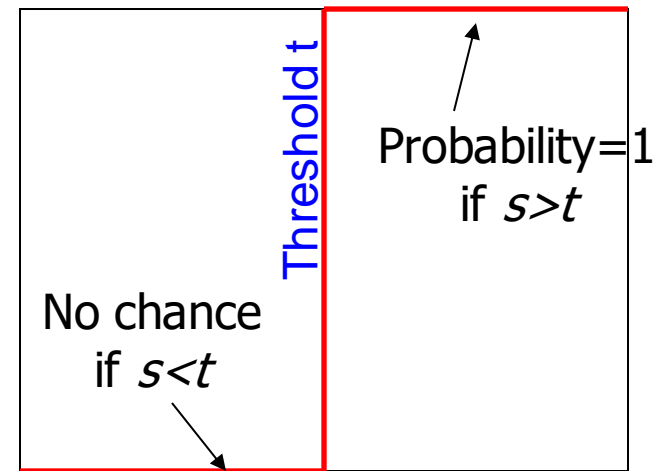
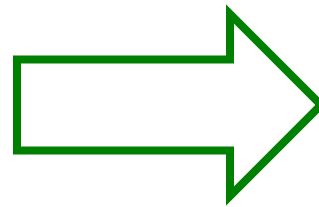
- The S-curve is where the “magic” happens



Similarity s of two sets

This is what 1 hash-code gives you

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



Similarity s of two sets

This is what we want!

How to get a step-function?

By choosing r and b !

How Do We Make the S-curve?

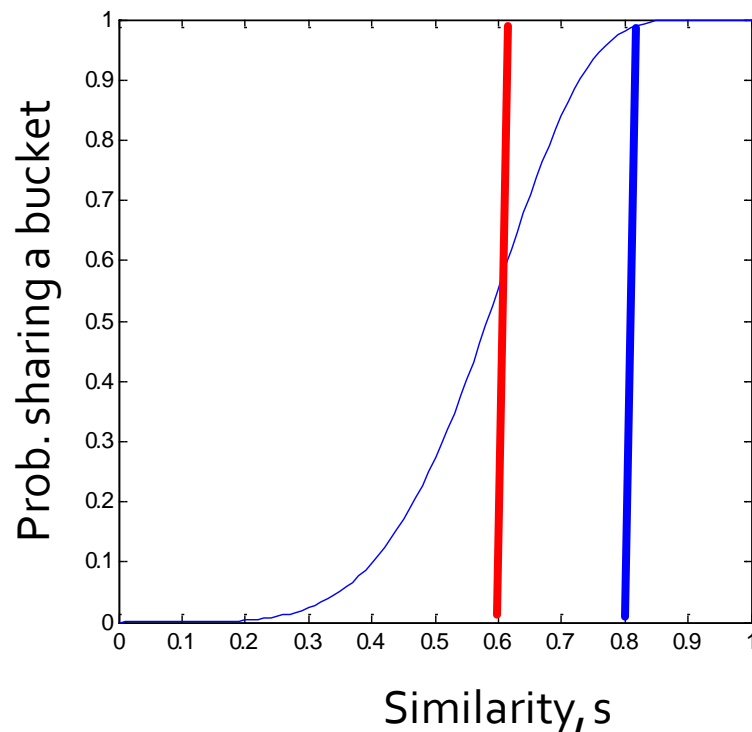
- **Remember:** b bands, r rows/band
- Let $\text{sim}(\mathbf{C}_1, \mathbf{C}_2) = s$

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 \mathbf{C}_1 and \mathbf{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 $= 1 - (1 - s^r)^b$
- $P(\mathbf{C}_1, \mathbf{C}_2 \text{ is a candidate pair}) = 1 - (1 - s^r)^b$**

Picking r and b : The S-curve

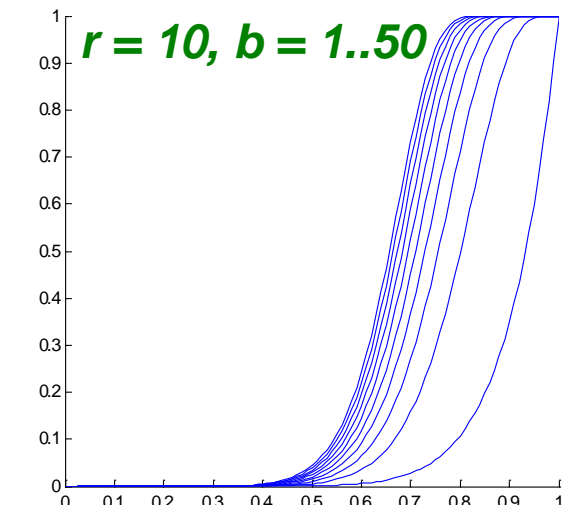
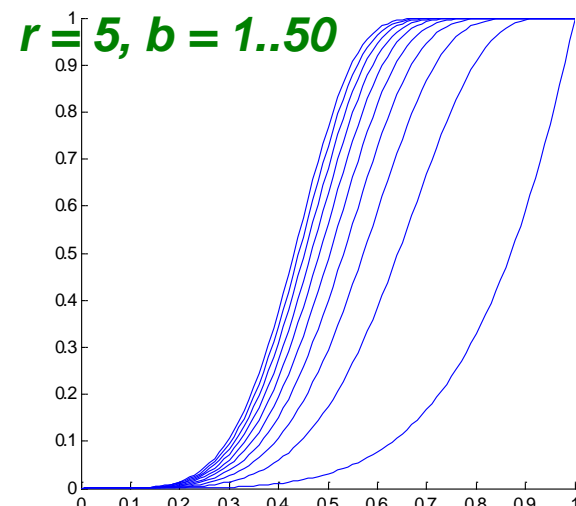
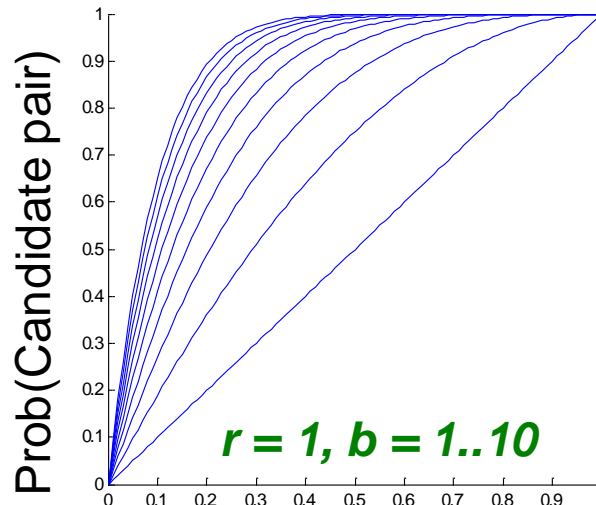
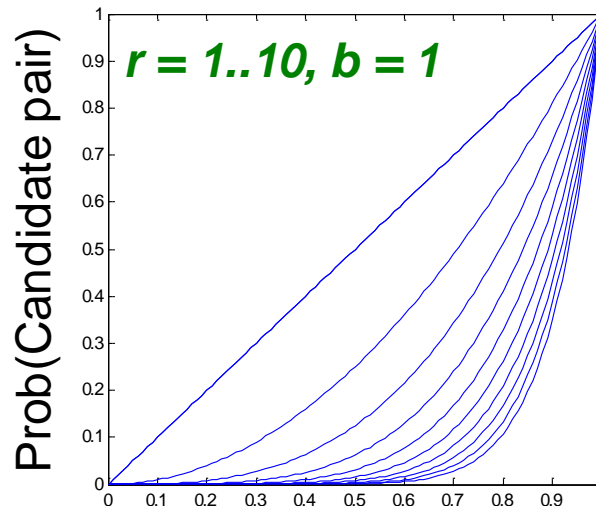
- Picking r and b to get the best S-curve
 - 50 hash-functions ($r=5$, $b=10$)



S-curves as a func. of b and r

Given a fixed threshold t .

We want choose r and b such that the $P(\text{Candidate pair})$ has a “step” right around t .



Similarity

Similarity

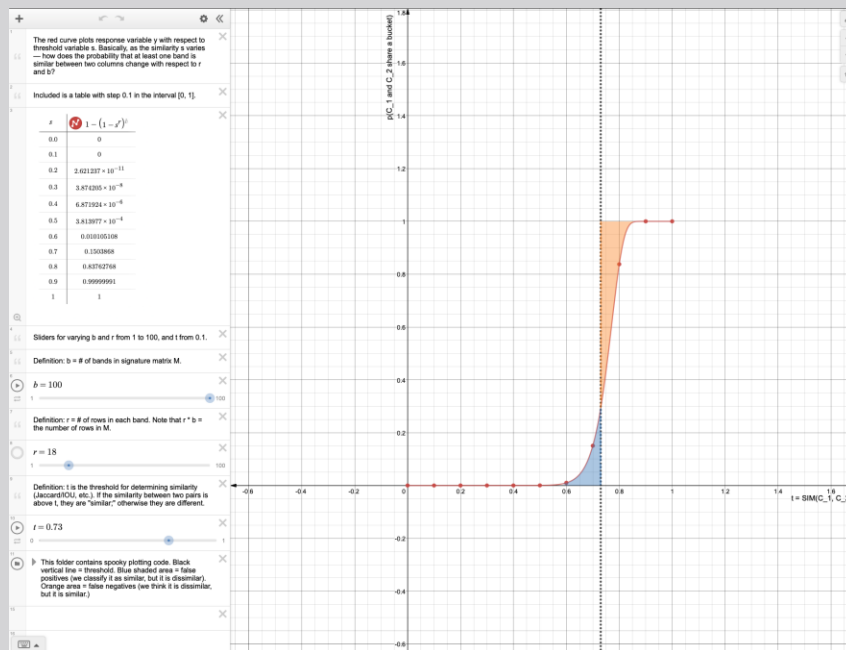
$$\text{prob} = 1 - (1 - s^r)^b$$

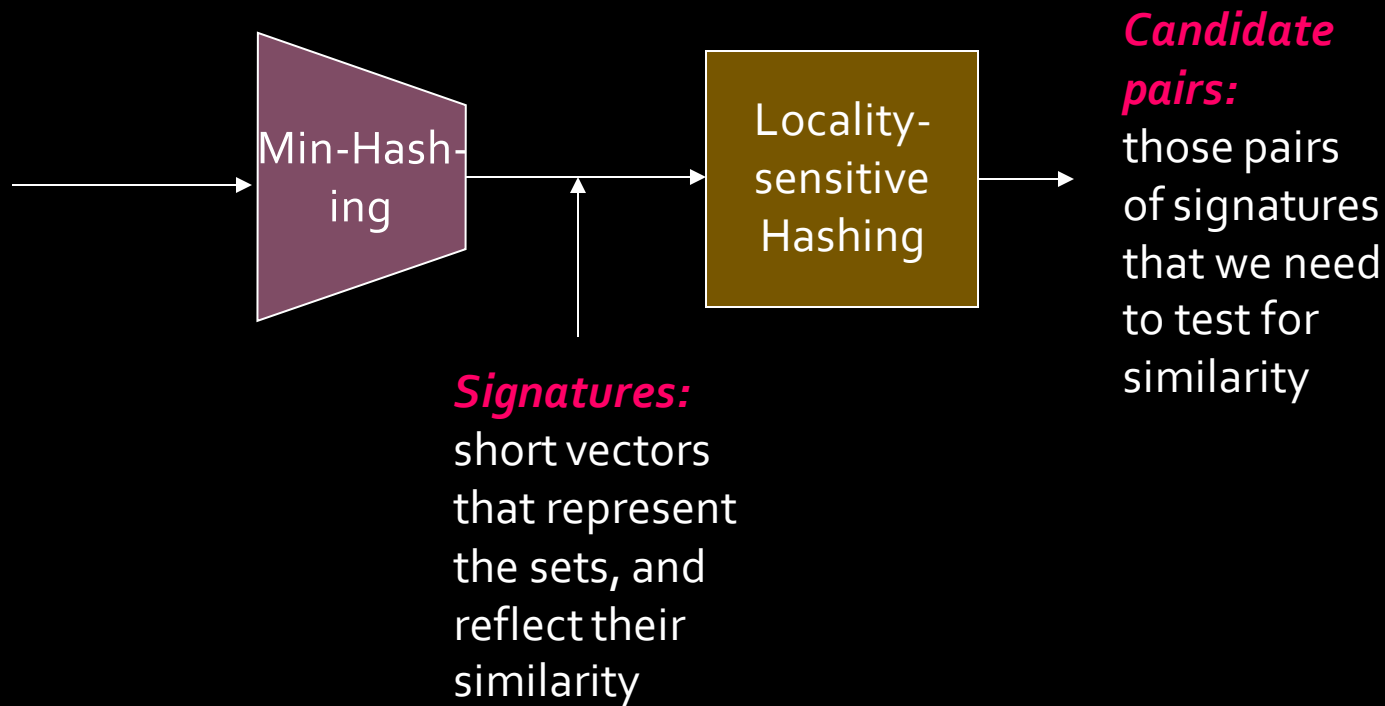
Visualizing S-Curves

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

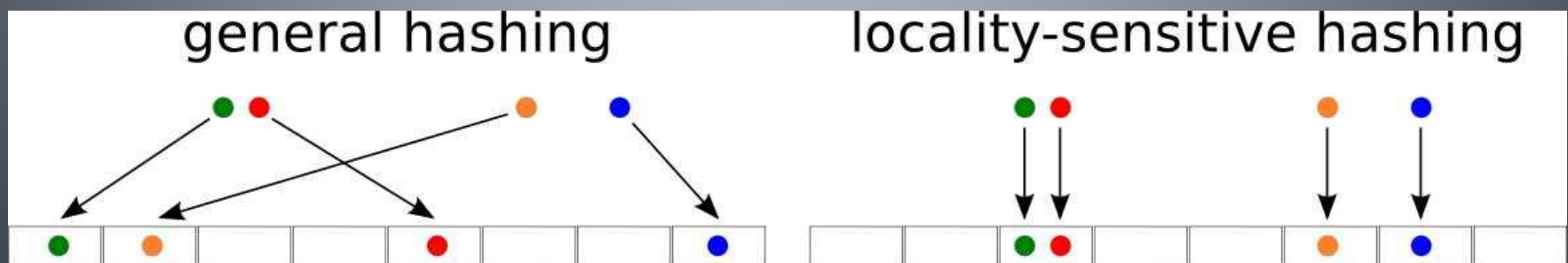
by Trenton Chang (Thank you!!)

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





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

- $d(\cdot)$ is a **distance measure** if it is a function from pairs of points \mathbf{x}, \mathbf{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 = $1 - \text{Jaccard similarity}$
- **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

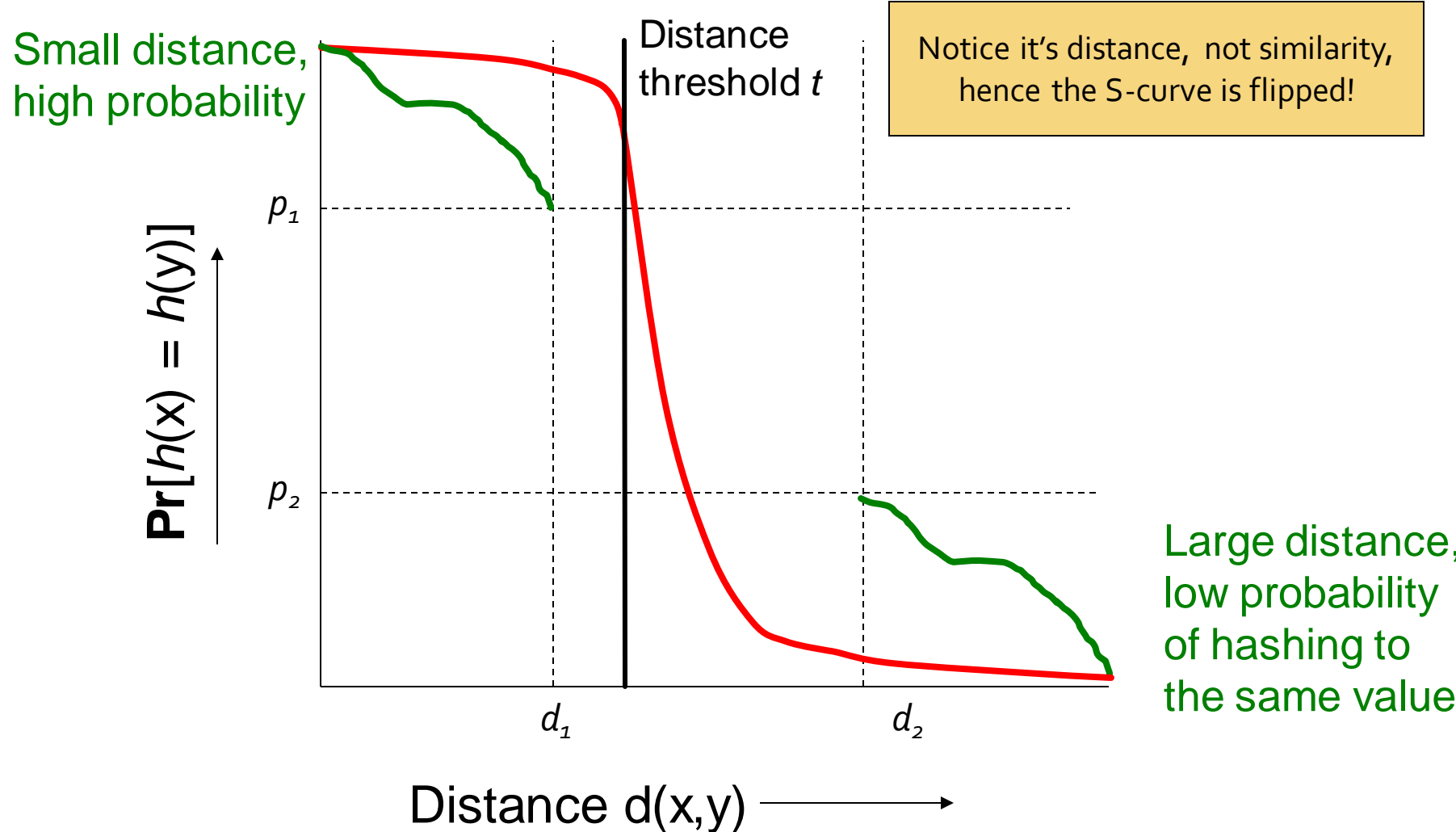
- Suppose we have a space S of points with a distance measure $d(x,y)$

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



Example of LS Family: Min-Hash

- **Let:**
 - \mathcal{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 $h \in H$:
$$\Pr[h(x) = h(y)] = 1 - d(x, y)$$
 - Simply restates theorem about Min-Hashing in terms of distances rather than similarities

Example: LS Family – (2)

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

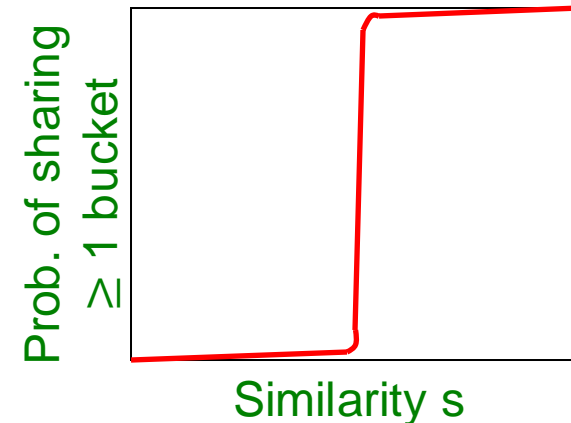
If distance $\leq 1/3$
(so similarity $\geq 2/3$)

Then probability
that Min-Hash values
agree is $\geq 2/3$

- 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 $h_i(x) = h_i(y)$ for **all** i $1 \leq i \leq r$
 - 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**)

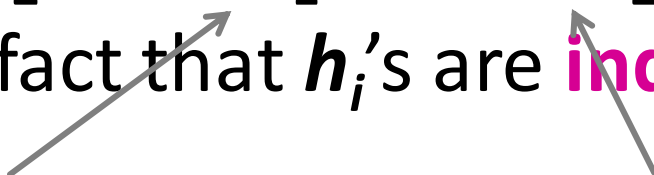
Lowers probability for
large distances (**Good**)

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 $h_i(x) = h_i(y)$ for **at least 1** i
- **Theorem:** If H is (d_1, d_2, p_1, p_2) -sensitive, then H' is $(d_1, d_2, 1-(1-p_1)^b, 1-(1-p_2)^b)$ -sensitive
- **Proof:** Use the fact that h_i 's are **independent**

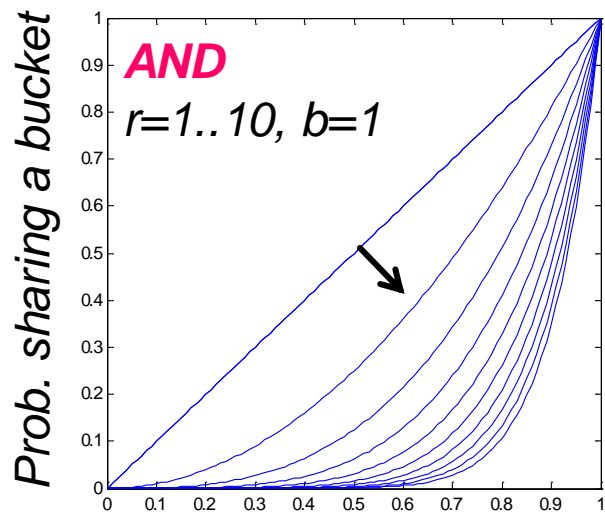


Raises probability for
small distances (Good)

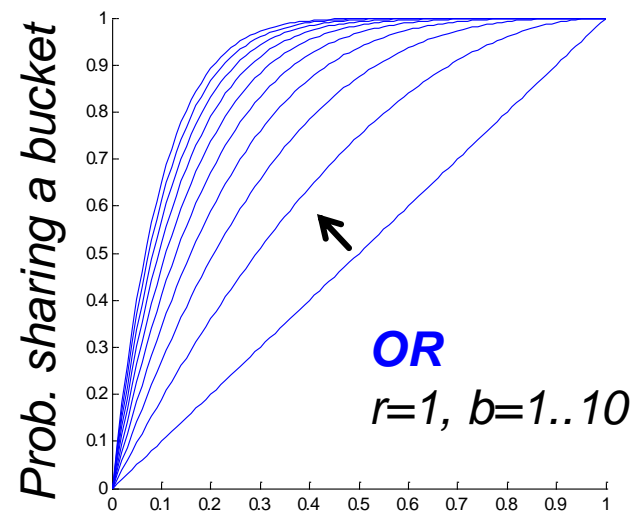
Raises probability for
large distances (Bad)

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



Similarity of a pair of items



Similarity of a pair of items

Combine AND and OR Constructions

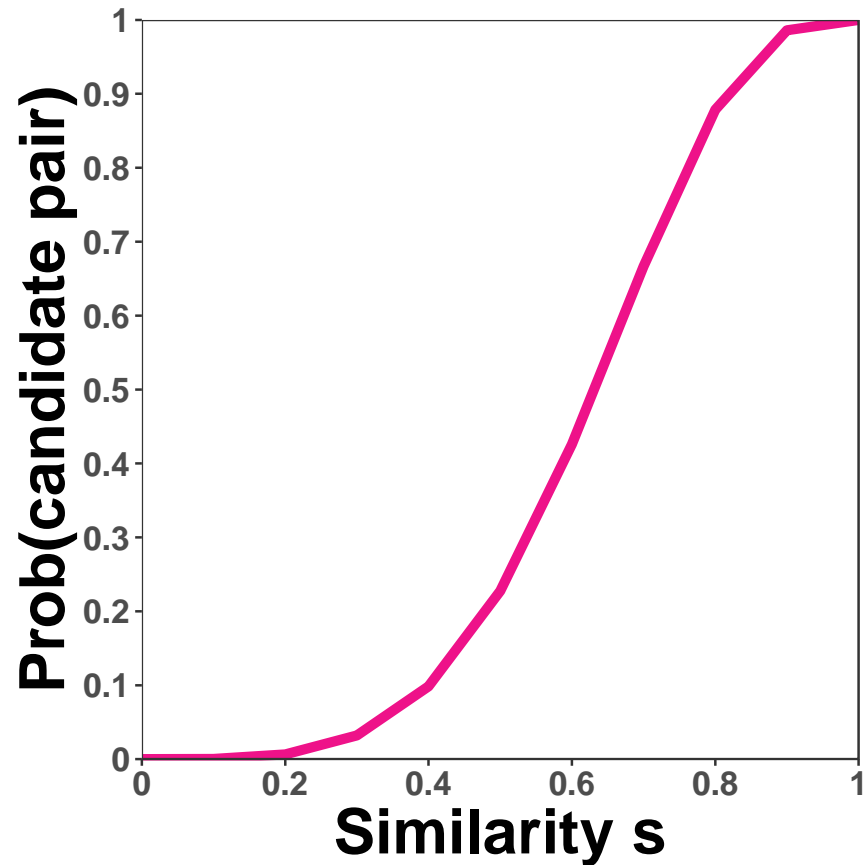
- By choosing \mathbf{b} and \mathbf{r} correctly, we can make the lower probability approach 0 while the higher approaches 1
- As for the signature matrix, we can use the AND construction followed by the OR construction
 - Or vice-versa
 - Or any sequence of AND's and OR's alternating

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 \rightarrow **Candidate**
- Take points \mathbf{x} and \mathbf{y} s.t. $\Pr[h(\mathbf{x}) = h(\mathbf{y})] = s$
 - H will make (\mathbf{x}, \mathbf{y}) a candidate pair with prob. s
- Construction makes (\mathbf{x}, \mathbf{y}) a candidate pair with probability $1 - (1 - s^r)^b$ **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 $1-(1-s^4)^4$

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

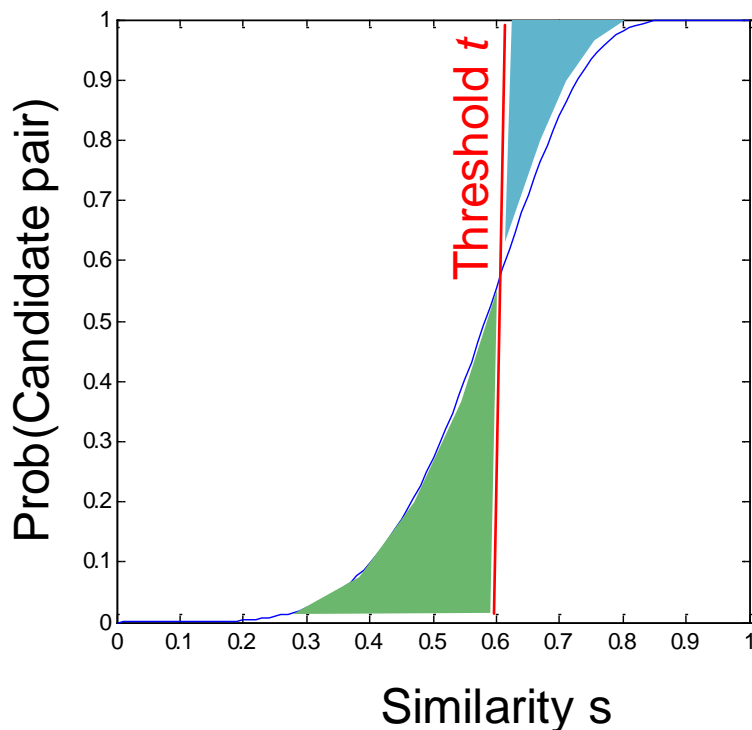


$r = 4, b = 4$ transforms a
(.2,.8,.8,.2)-sensitive family into a
(.2,.8,.8785,.0064)-sensitive family.

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

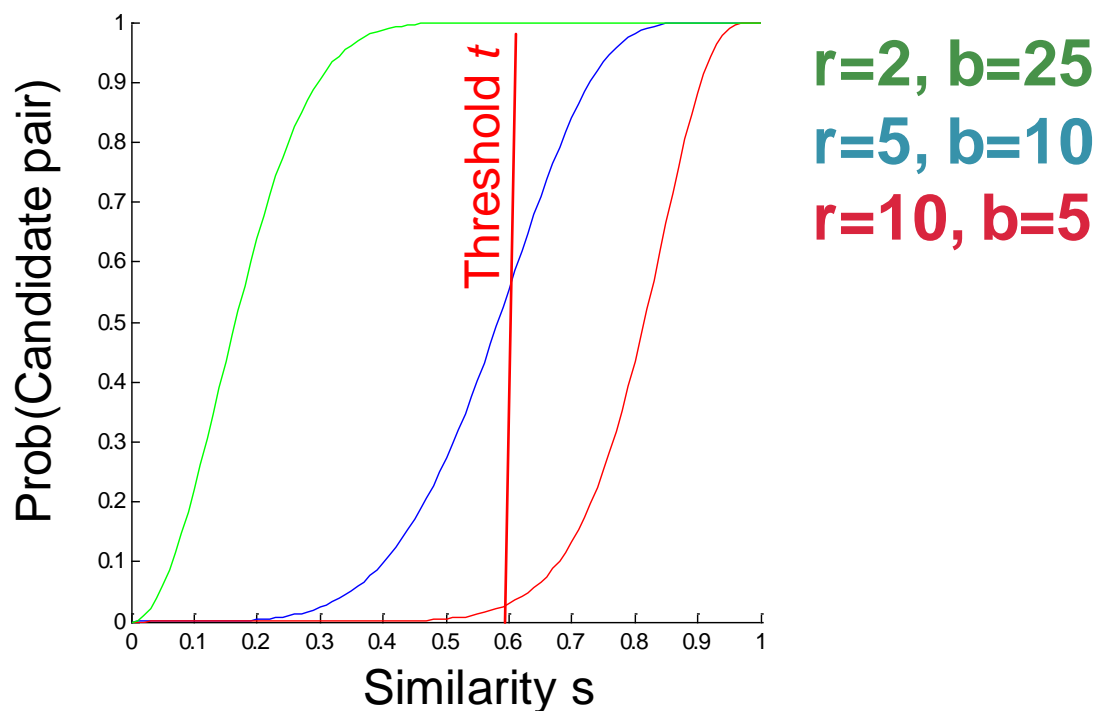
These are pairs with $\text{sim} > t$ but the **X** fraction won't share a band and then will **never become candidates**. This means we will never consider these pairs for (slow/exact) similarity calculation!

Green area Y: False Positive rate

These are pairs with $\text{sim} < t$ 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 ($r * b = 50$)

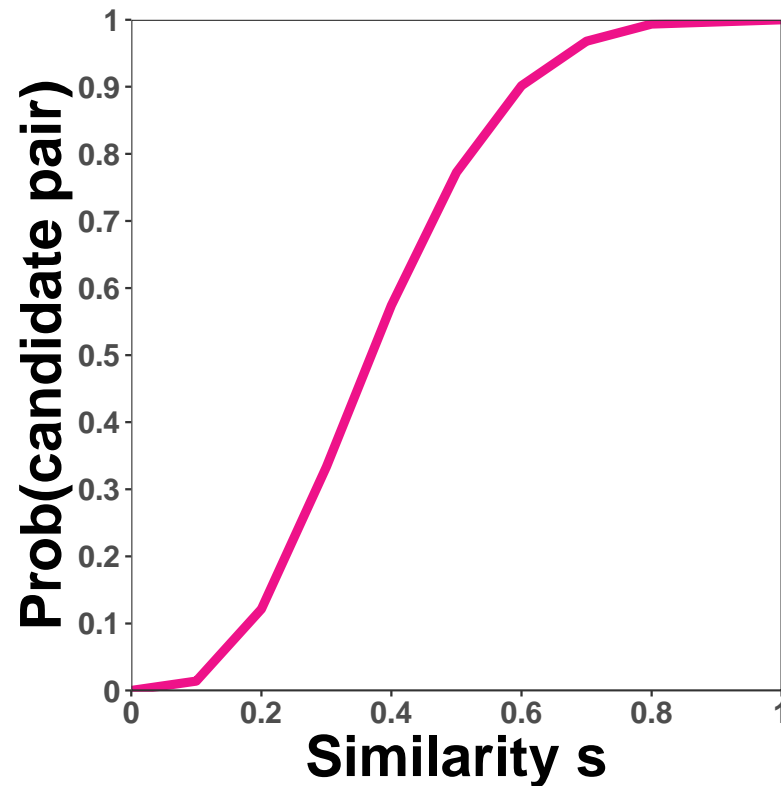


OR-AND Composition

- Apply a ***b***-way **OR** construction followed by an ***r***-way **AND** construction
- Transforms similarity ***s*** (probability *p*) into $(1-(1-s)^b)^r$
 - 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

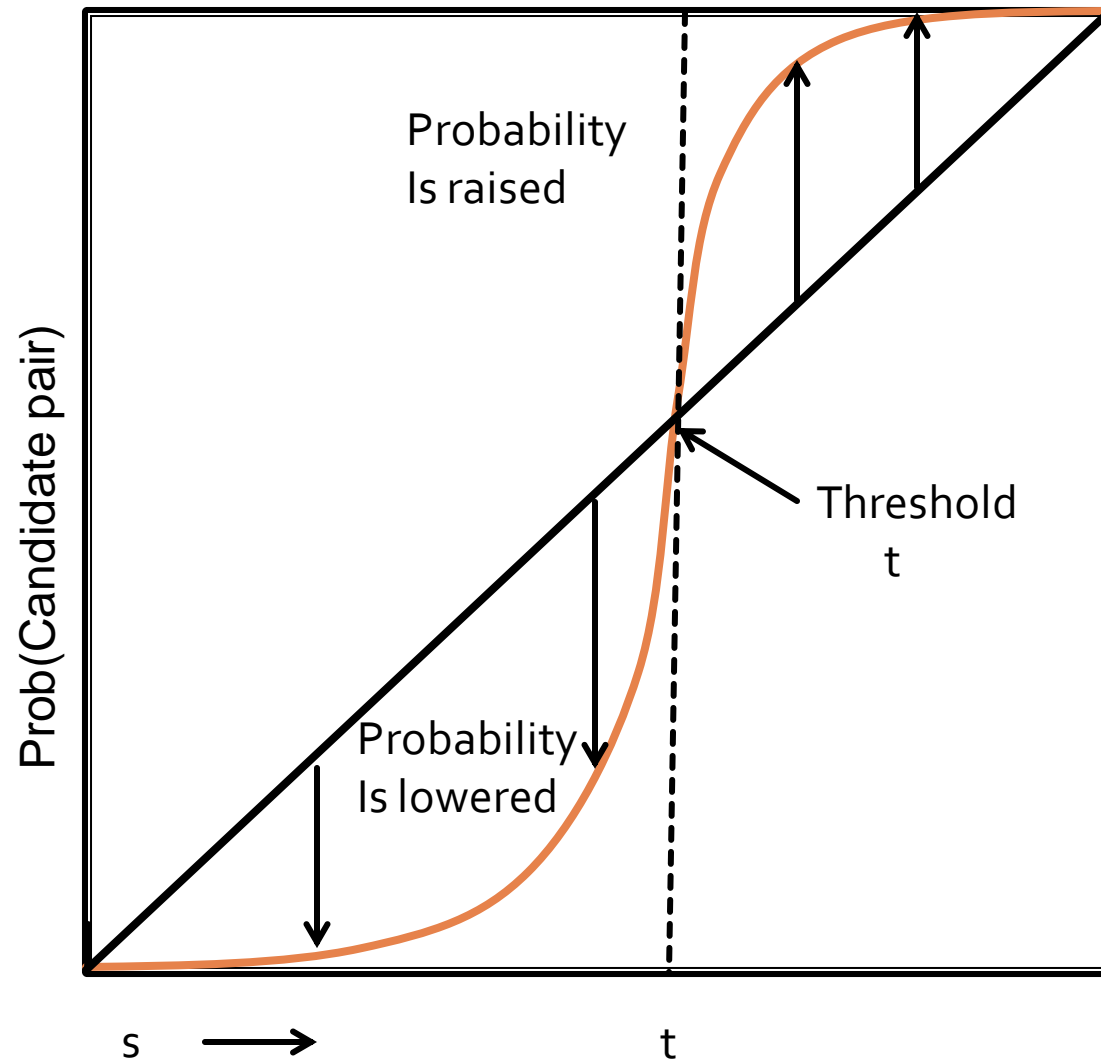
Cascading Constructions

- **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



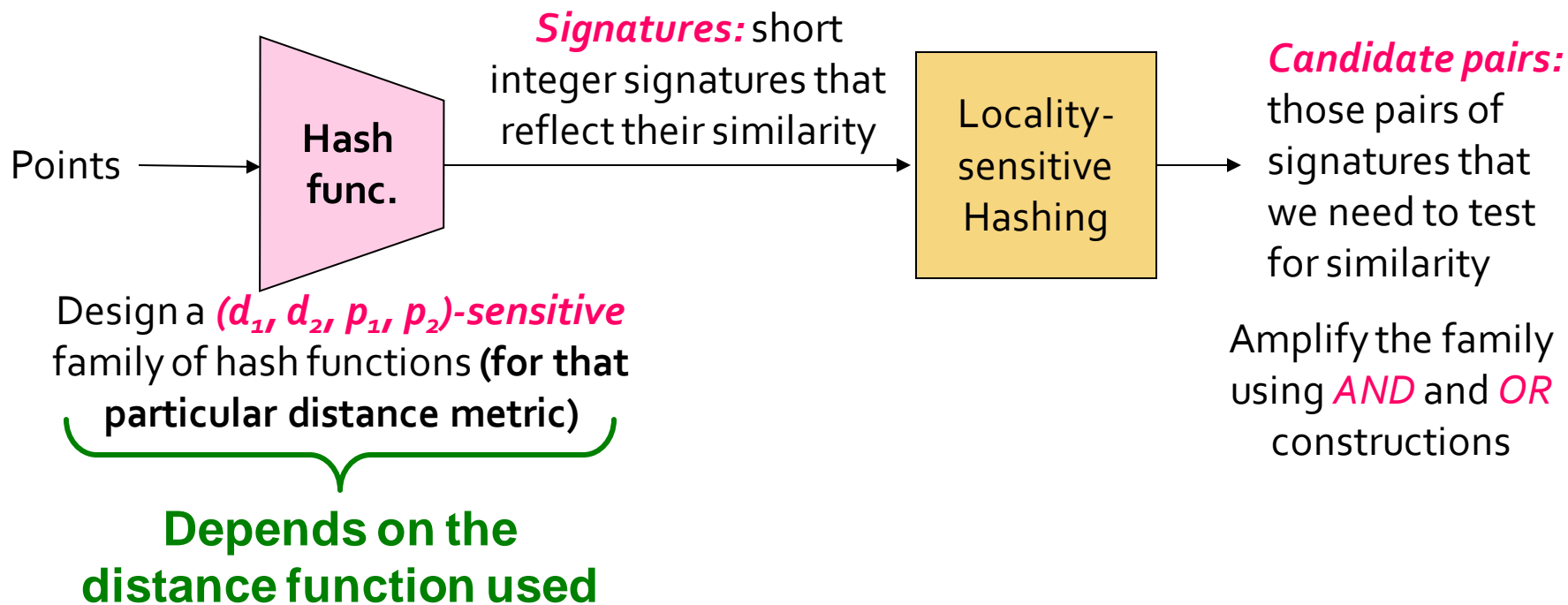
Summary

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

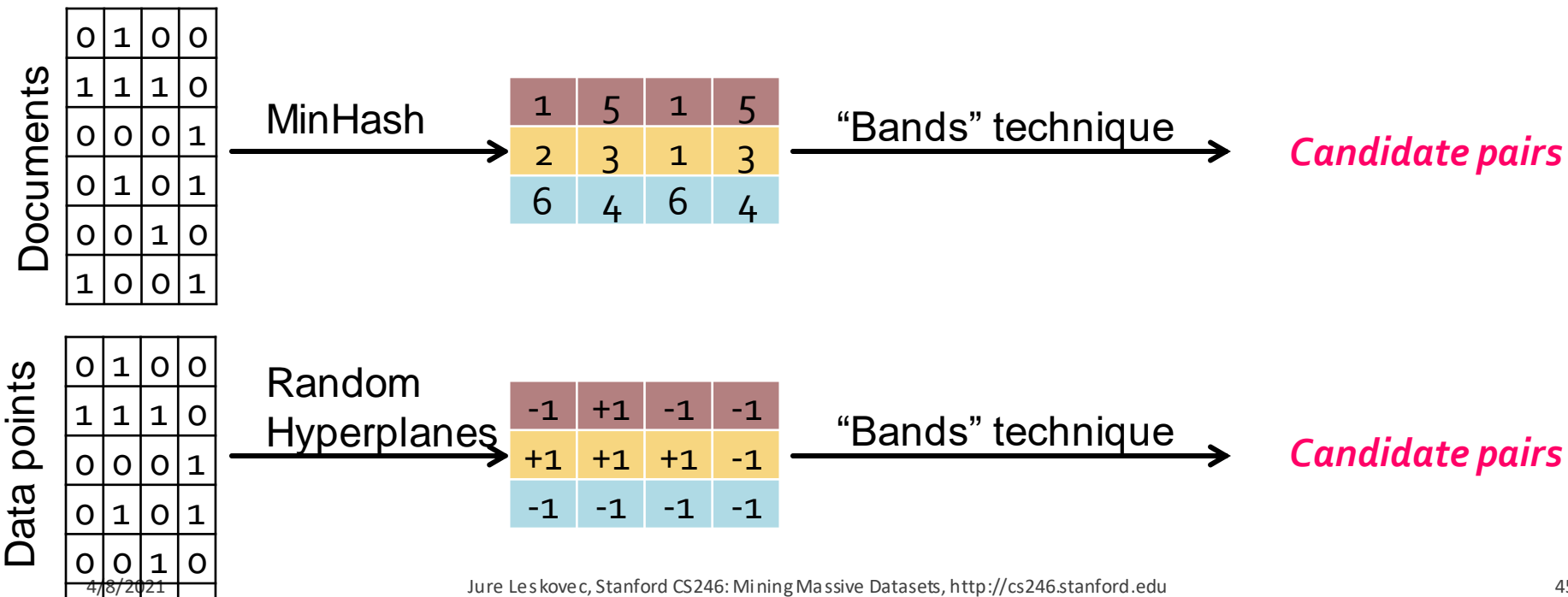
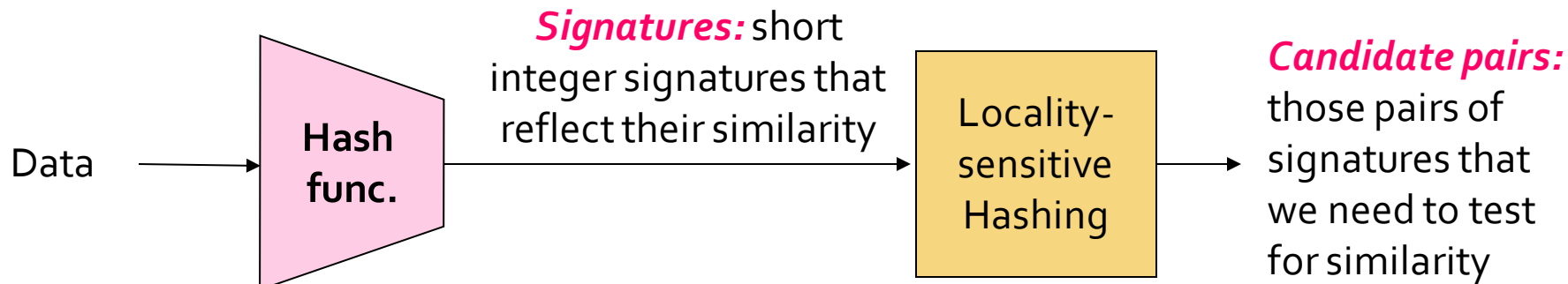
LSH for other distance metrics

LSH for other Distance Metrics

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



Summary of what we will learn

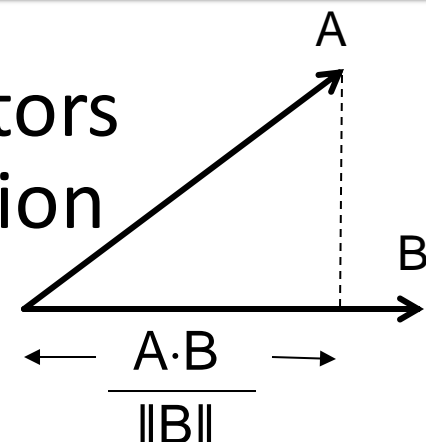


LSH for Cosine Distance

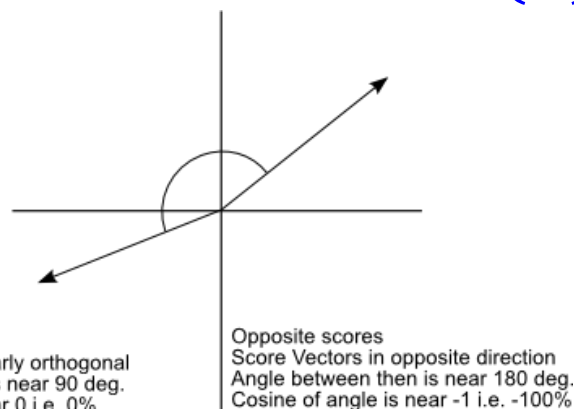
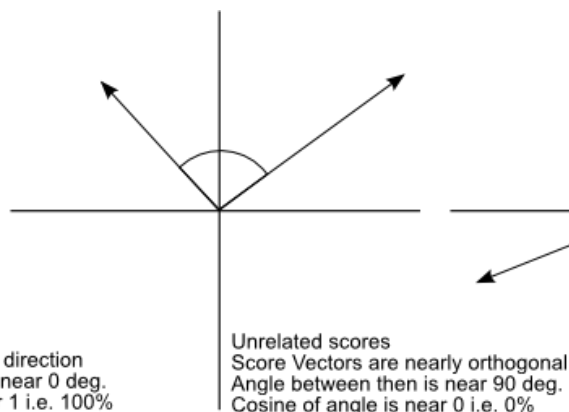
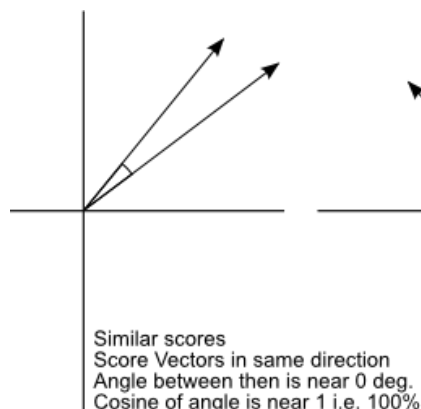
Cosine Distance

- **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 $[0, \pi]$ (equivalently $[0, 180^\circ]$)
 - 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°)

LSH for Cosine Distance

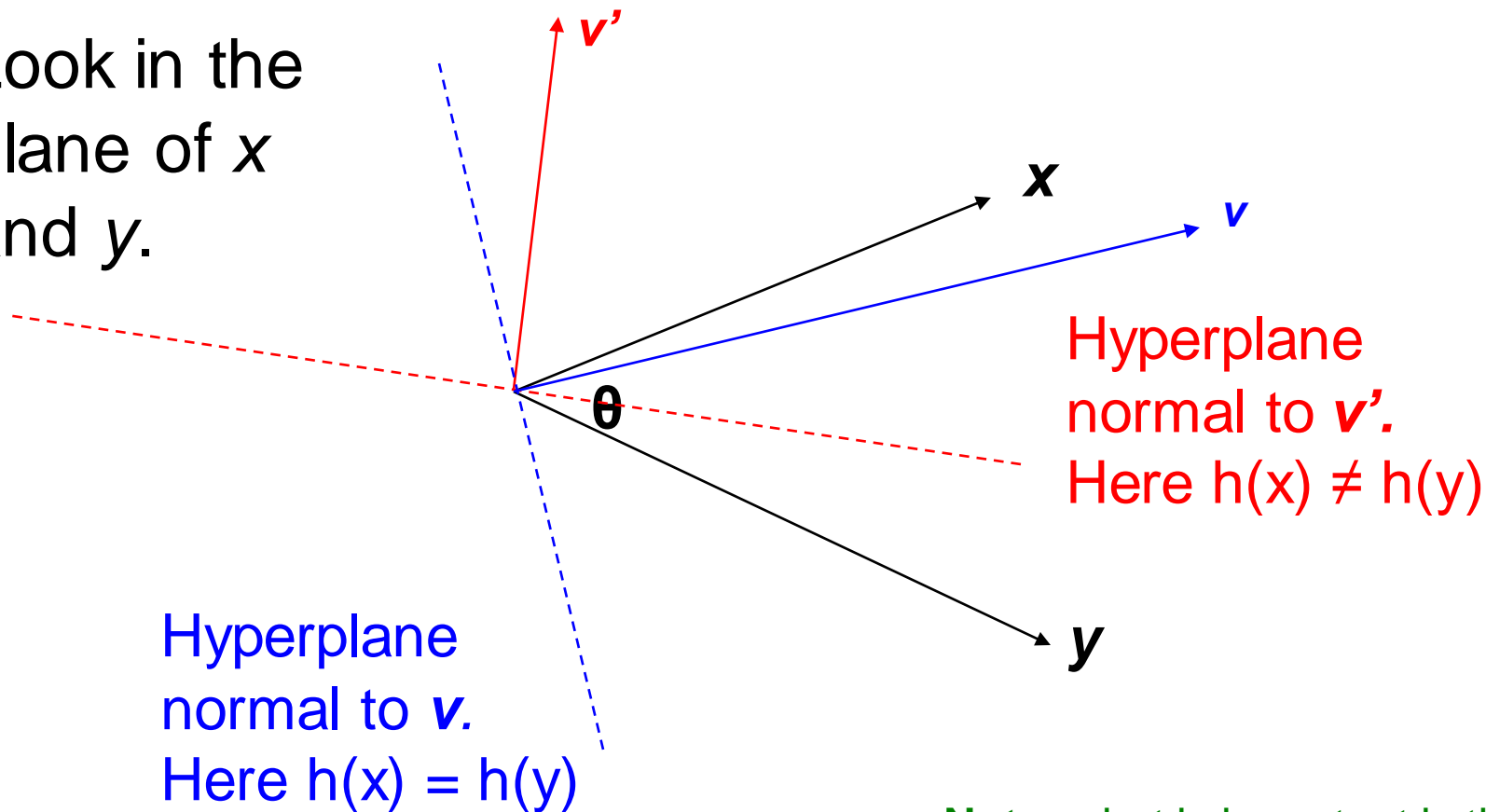
- For **cosine distance**, there is a technique called **Random Hyperplanes**
 - Technique similar to Min-Hashing
- **Random Hyperplanes** method is a $(d_1, d_2, (1-d_1/\pi), (1-d_2/\pi))$ -sensitive family for any d_1 and d_2
- **Reminder:** (d_1, d_2, p_1, p_2) -sensitive
 1. If $d(x, y) \leq d_1$, 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 \mathbf{v} determines a hash function $h_{\mathbf{v}}$ with **two buckets**
- $h_{\mathbf{v}}(\mathbf{x}) = +1$ if $\mathbf{v} \cdot \mathbf{x} \geq 0$; $= -1$ if $\mathbf{v} \cdot \mathbf{x} < 0$
- LS-family H = set of all functions derived from any vector
- **Claim:** For points \mathbf{x} and \mathbf{y} ,
$$\Pr[h(\mathbf{x}) = h(\mathbf{y})] = 1 - d(\mathbf{x}, \mathbf{y}) / \pi$$

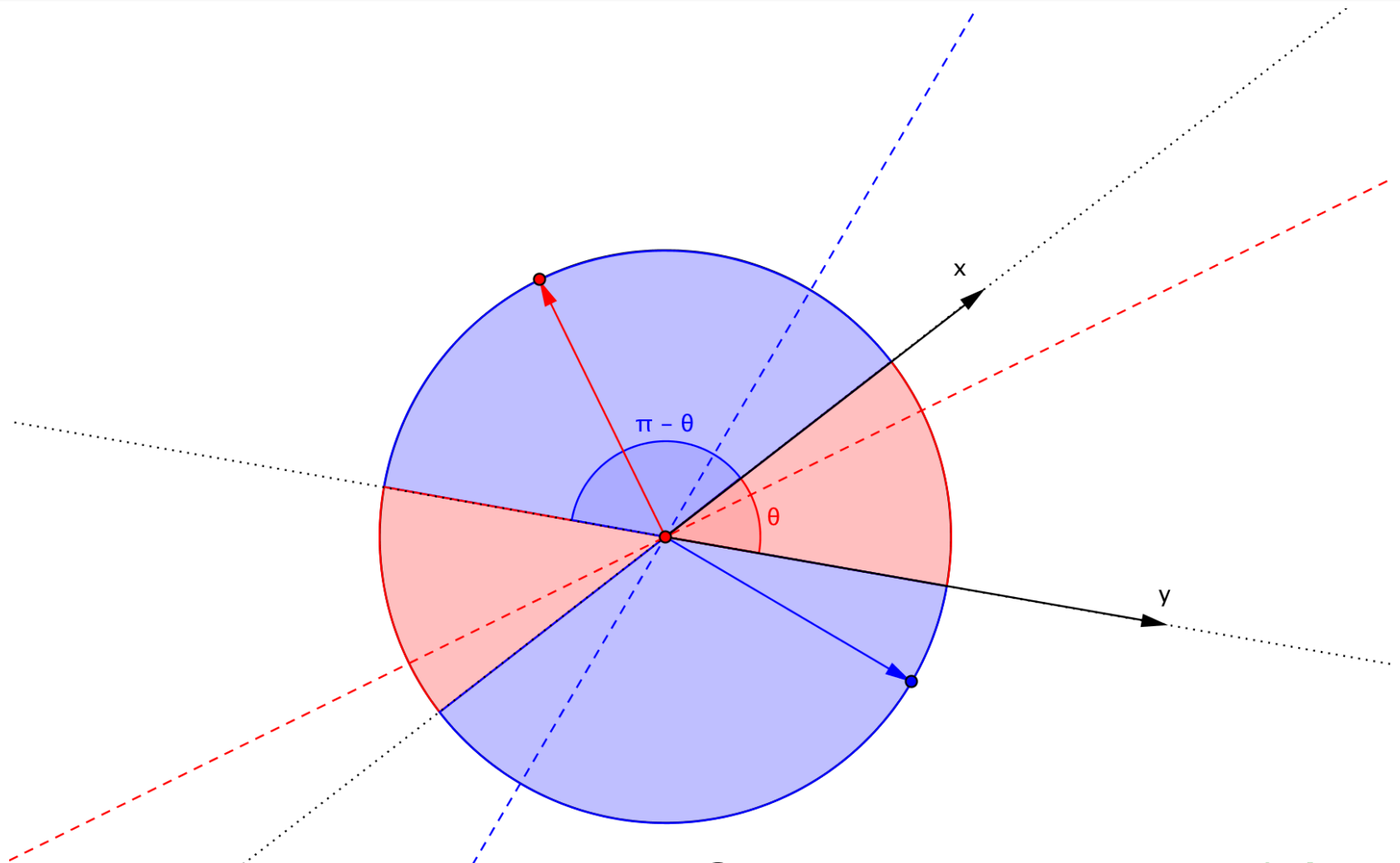
Proof of Claim

Look in the
plane of x
and 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?

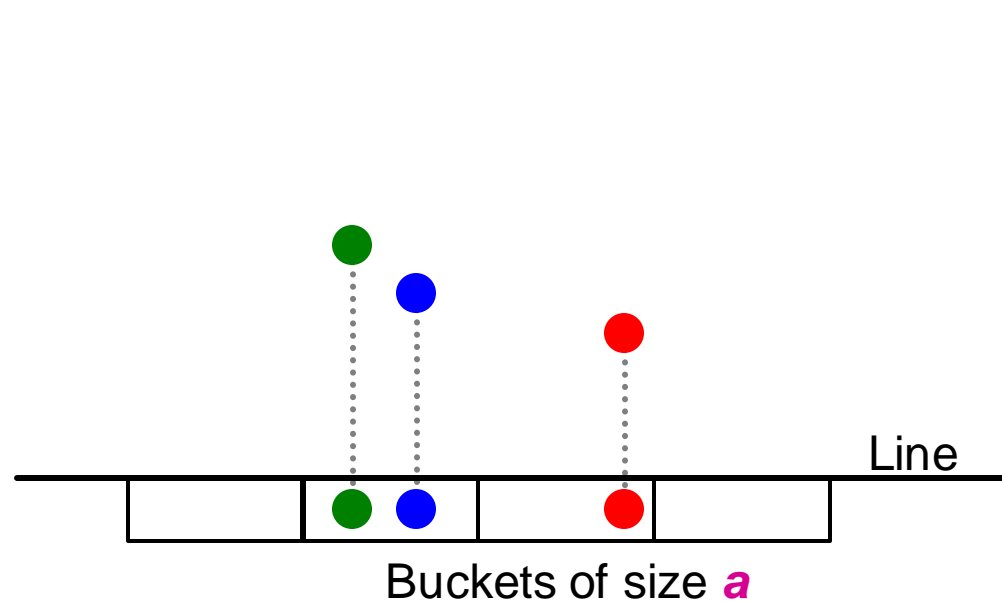
- Expensive to pick a random vector in M dimensions for large M
 - Would have to generate M random numbers
- **A more efficient approach**
 - It suffices to consider only vectors \mathbf{v} consisting of +1 and -1 components
 - **Why?** Assuming data is random, then vectors of +/-1 cover the entire space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

LSH for Euclidean Distance

LSH for Euclidean Distance

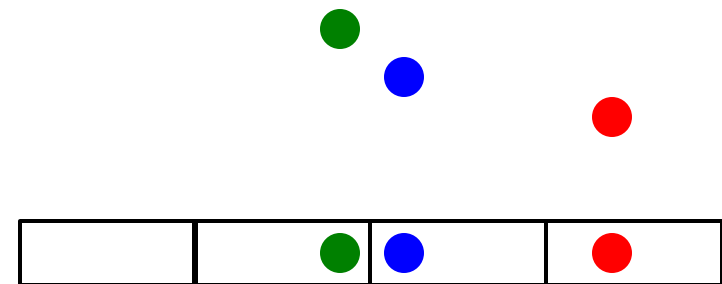
- **Idea:** Hash functions correspond to lines
- Partition the line into buckets of size a
- **Hash each point to the bucket containing its projection onto the line**
 - An element of the “Signature” is a bucket id for that given projection line
- **Nearby points are always close;**
distant points are rarely in same bucket

Projection of Points



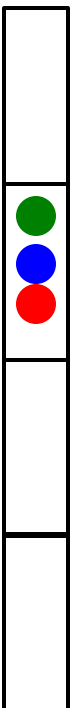
- “Lucky” case:

- Points that are close hash in the same bucket
- Distant points end up in different buckets

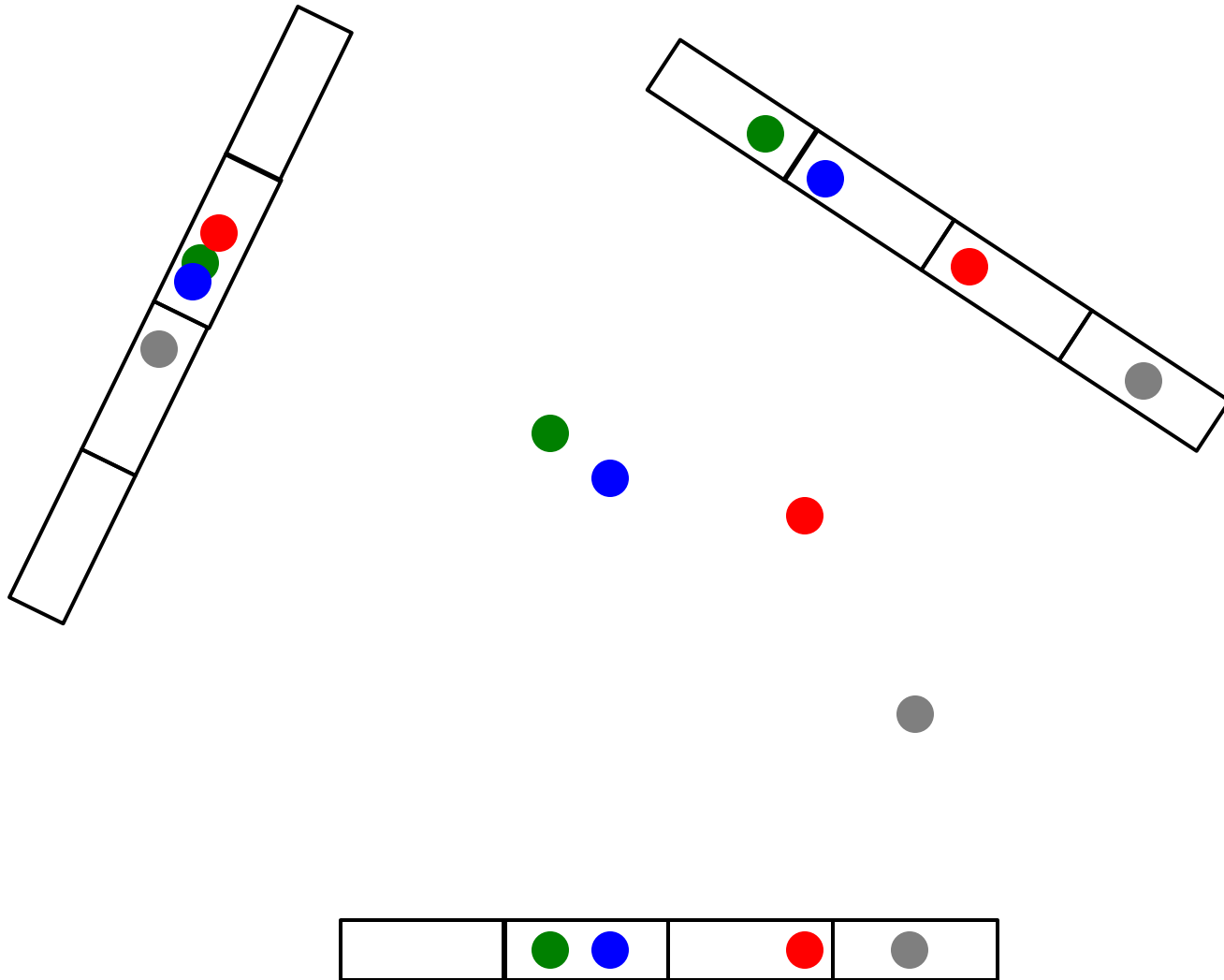


- Two “unlucky” cases:

- **Top:** unlucky quantization
- **Bottom:** unlucky projection

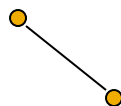


Multiple Projections

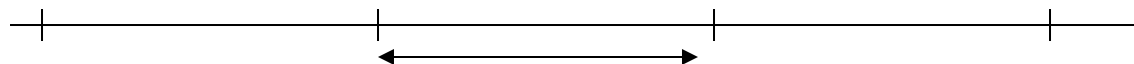


Projection of Points (1)

Points at
distance d



If $d \ll a$, then
the chance the
points are in the
same bucket is
at least $1 - d/a$.

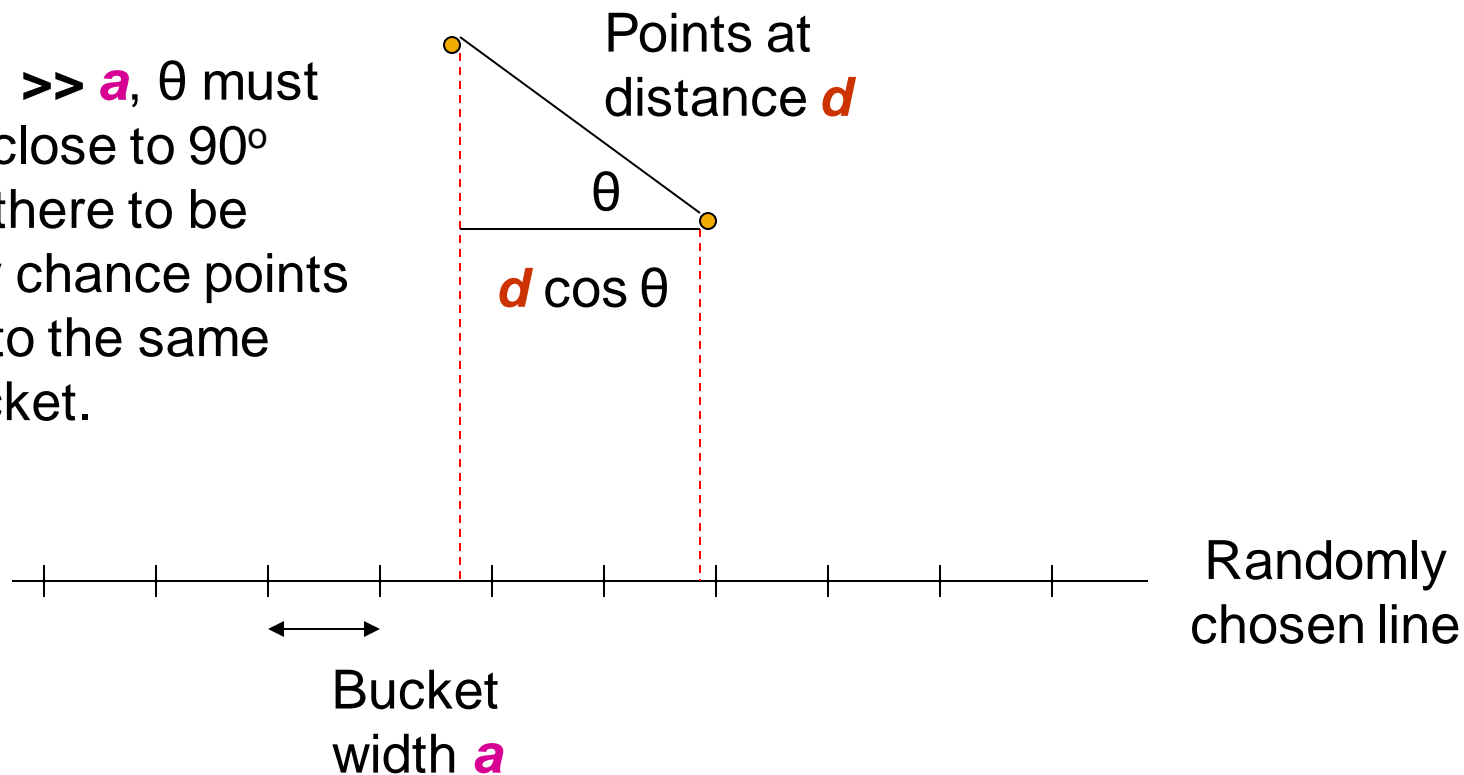


Bucket
width a

Randomly
chosen line

Projection of Points (2)

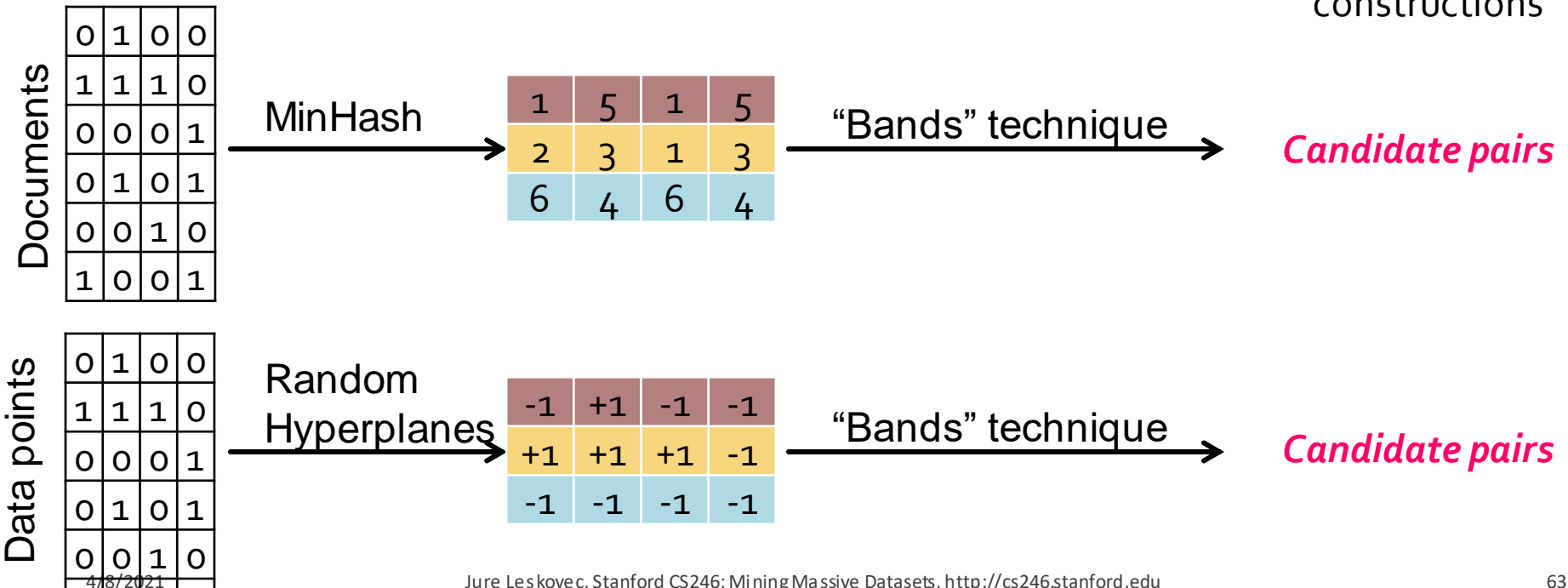
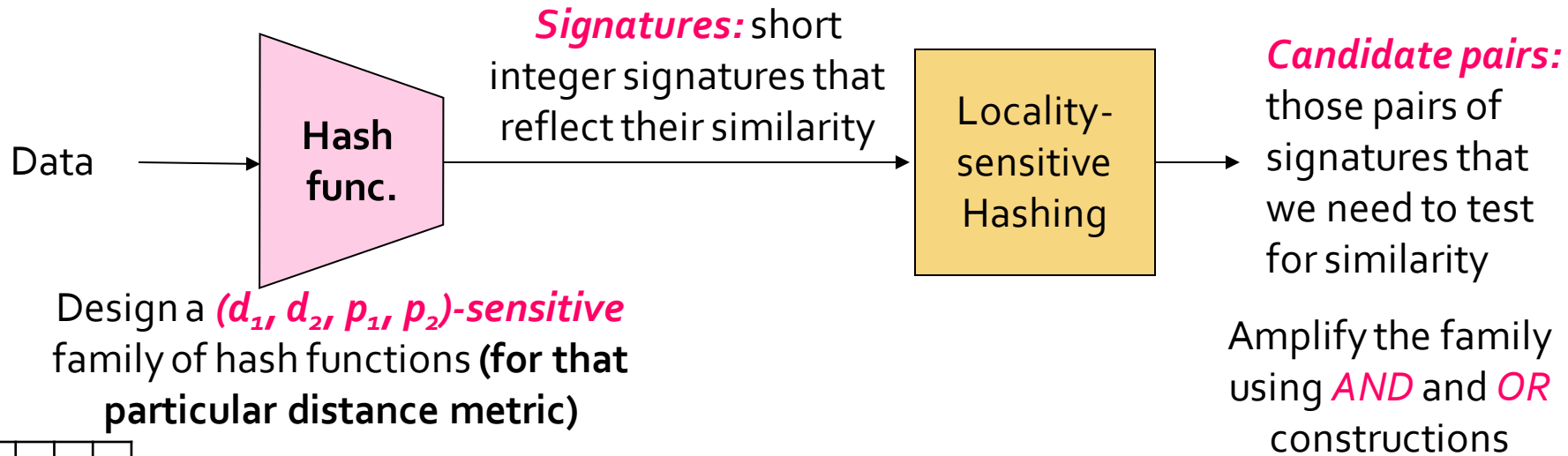
If $d \gg a$, θ must be close to 90° for there to be any chance points go to the same bucket.



A LS-Family for Euclidean Distance

- If points are distance $d \leq a/2$, prob. they are in same bucket $\geq 1 - d/a = 1/2$
- If points are distance $d \geq 2a$ apart, then they can be in the same bucket only if $d \cos \theta \leq a$
 - $\cos \theta \leq 1/2$
 - $60 \leq \theta \leq 90$, 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



Two Important Points

- Property $P(h(C_1)=h(C_2))=\text{sim}(C_1,C_2)$ 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