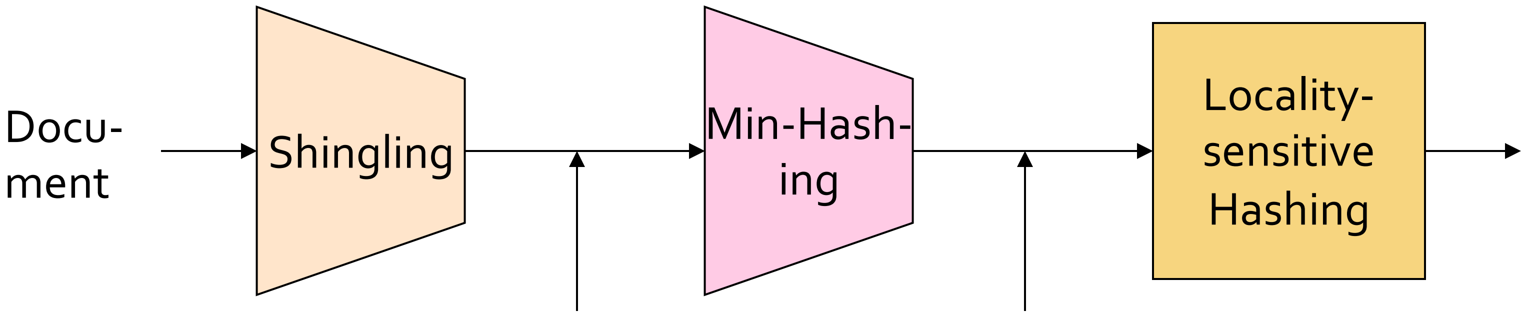
Theory of Locality Sensitive Hashing

CSEP590A Machine Learning for Big Data
Tim Althoff
PAUL G. ALLEN SCHOOL
OF COMPUTER SCIENCE & ENGINEERING

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



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**

Recap: 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: 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*

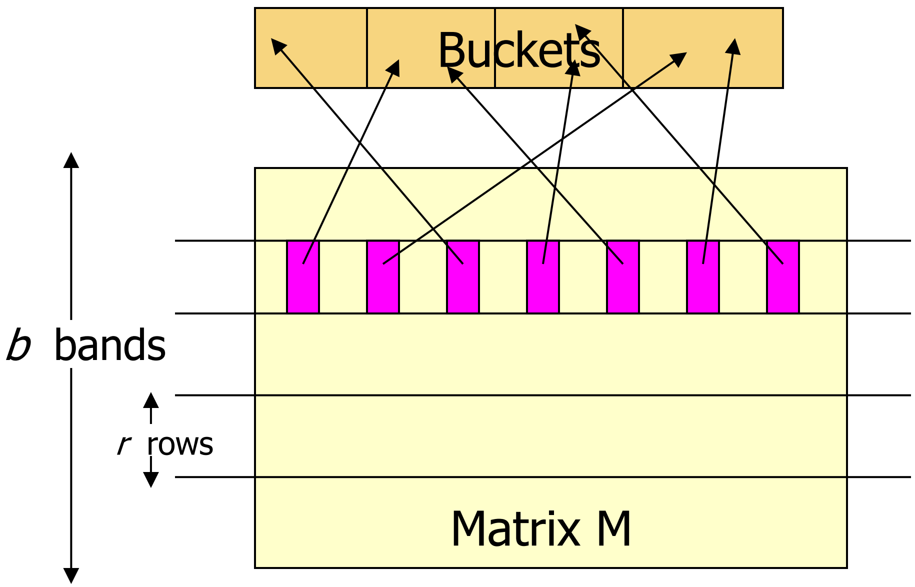
2	1	2	1
2	1	4	1
1	2	1	2

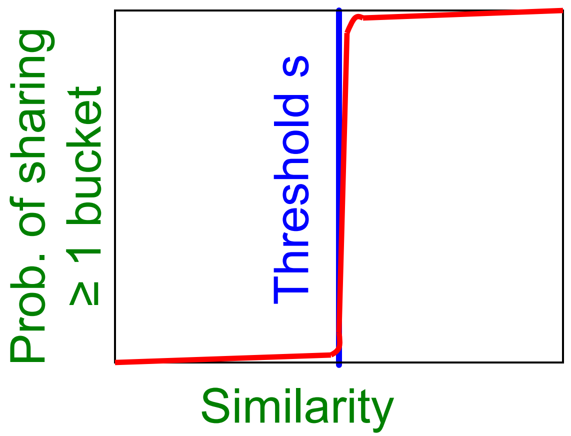
Similarities of columns and signatures (approx.) match!

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

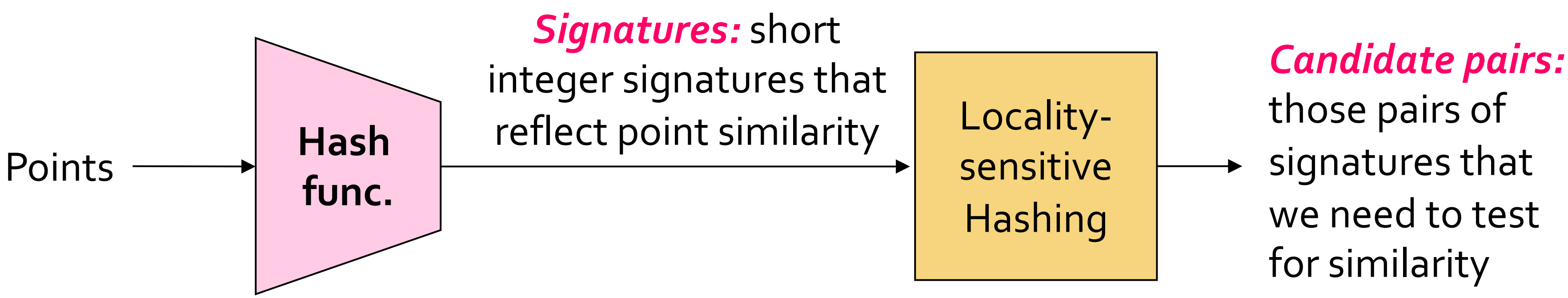
Recap: LSH

- **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

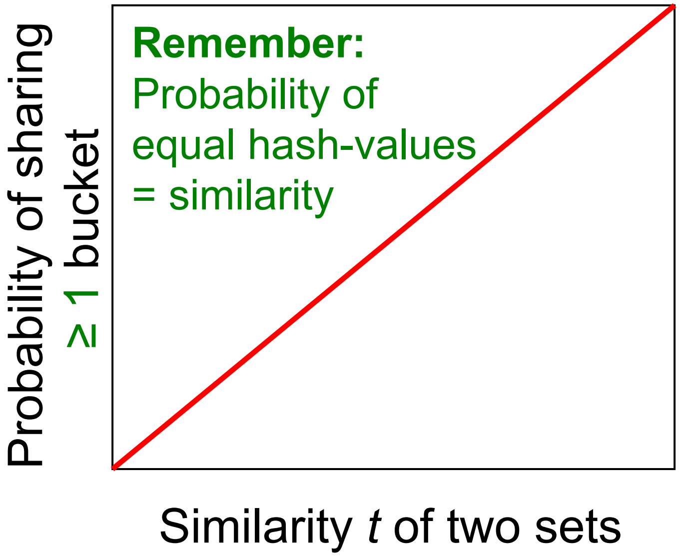


Design a **locality sensitive hash function (for a given distance metric)**

Apply the "Bands" technique

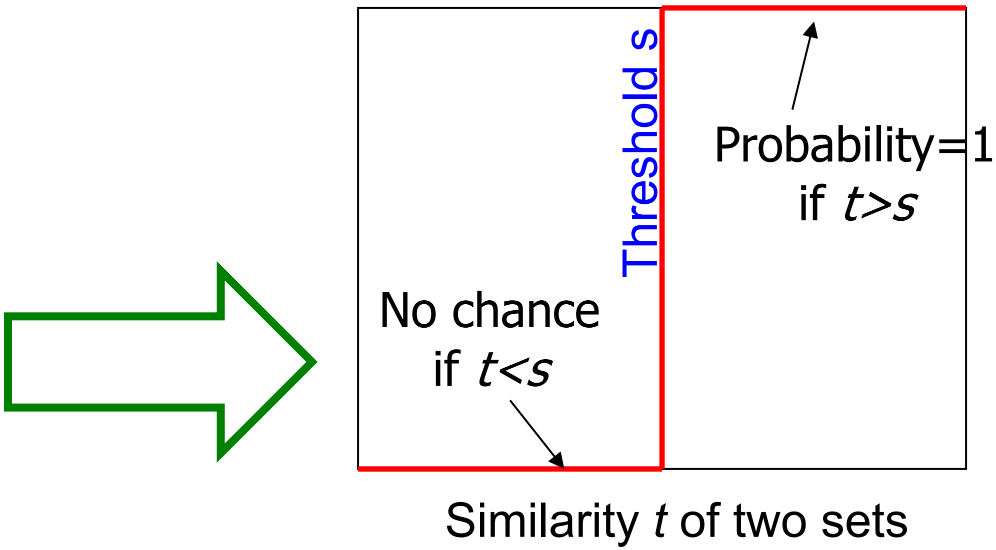
The S-Curve

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



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 $sim(C_1, C_2) = s$

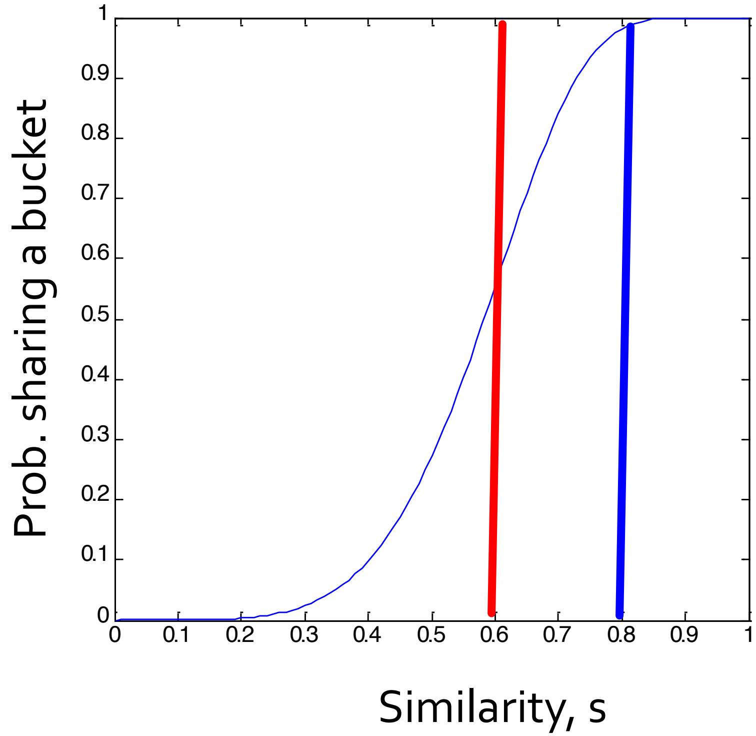
What's the prob. that at least 1 band is equal?

- Pick some band (***r*** rows)
  - Prob. that elements in a single row of columns $\mathbf{C_1}$ 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 $= 1 - (1 - s^r)^b$

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

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

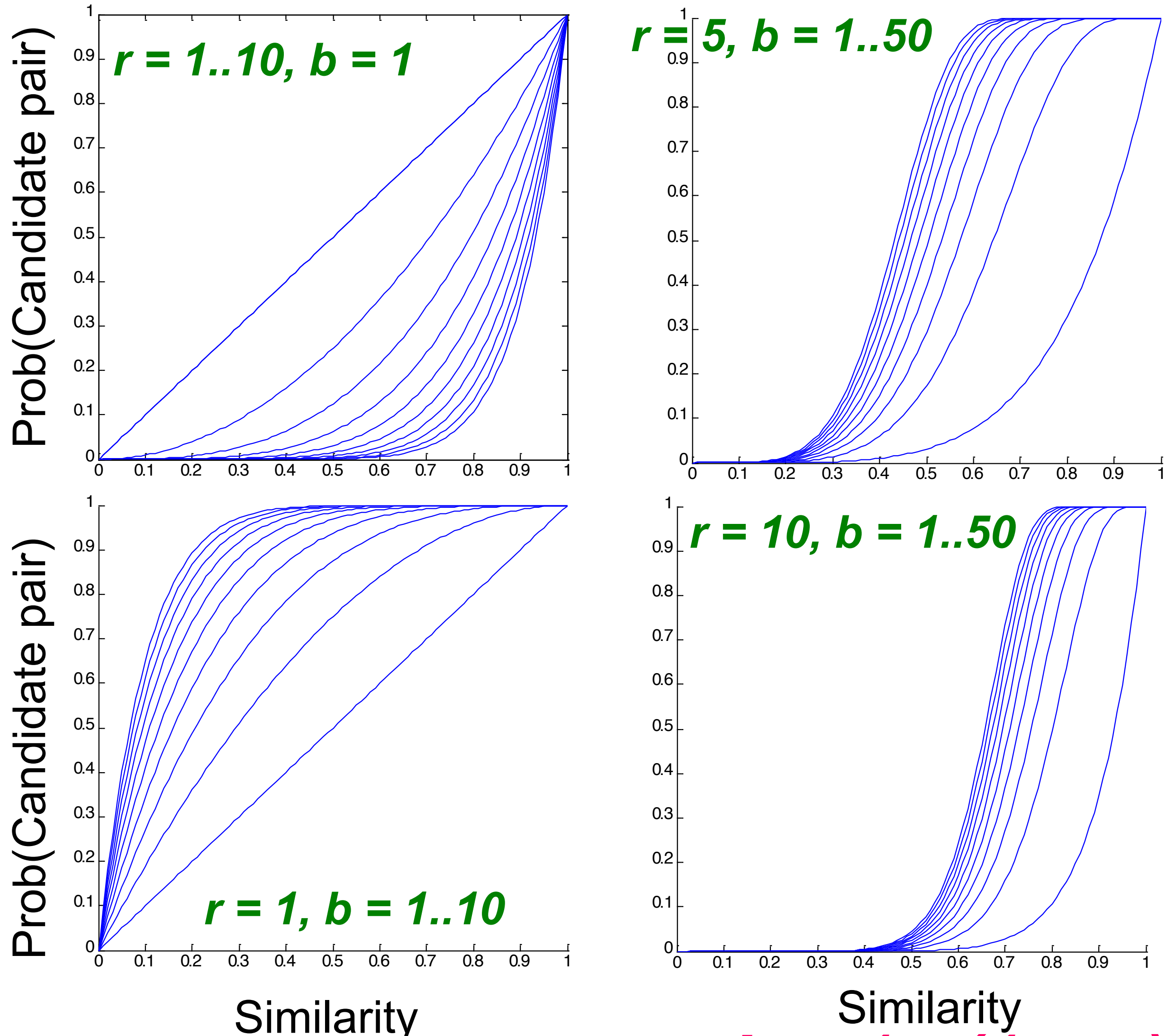
- **Picking *r* and *b* to get the best S-curve**
  - 50 hash-functions (r=5, b=10)



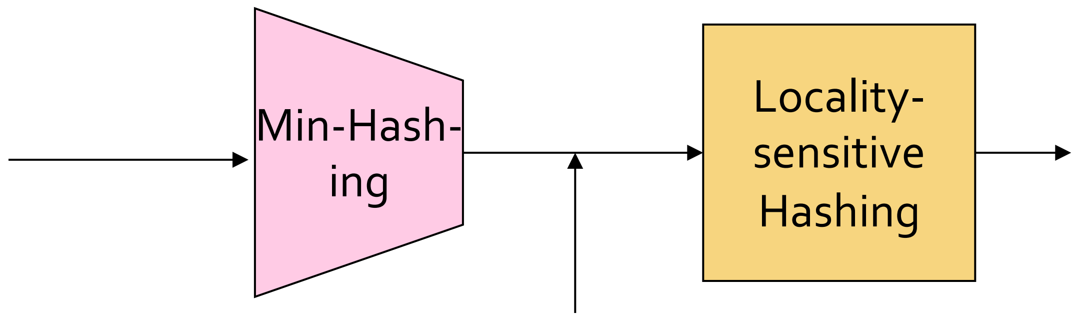
S-curves as a func. of *b* and *r*

Given a fixed threshold ***s***.

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



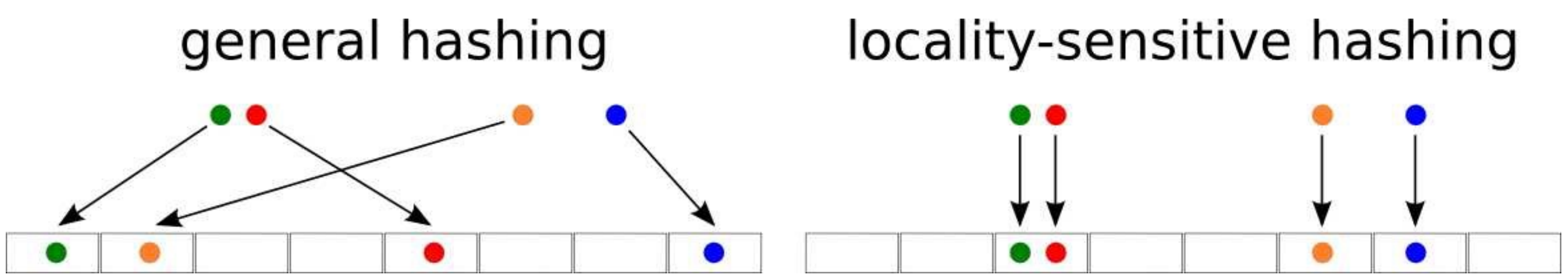
prob = 1 - (1 - t ^{r})^b



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

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

Theory of LSH



Theory of LSH

- **We have used LSH to find similar documents**
  - More specifically, 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 Metric

- **d()** is a **distance metric** 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 coordinates 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 ***pick one at random efficiently***
  - **Example:** The set of Min-Hash functions generated from permutations of rows (e.g. Universal Hashing)

Locality-Sensitive (LS) Families

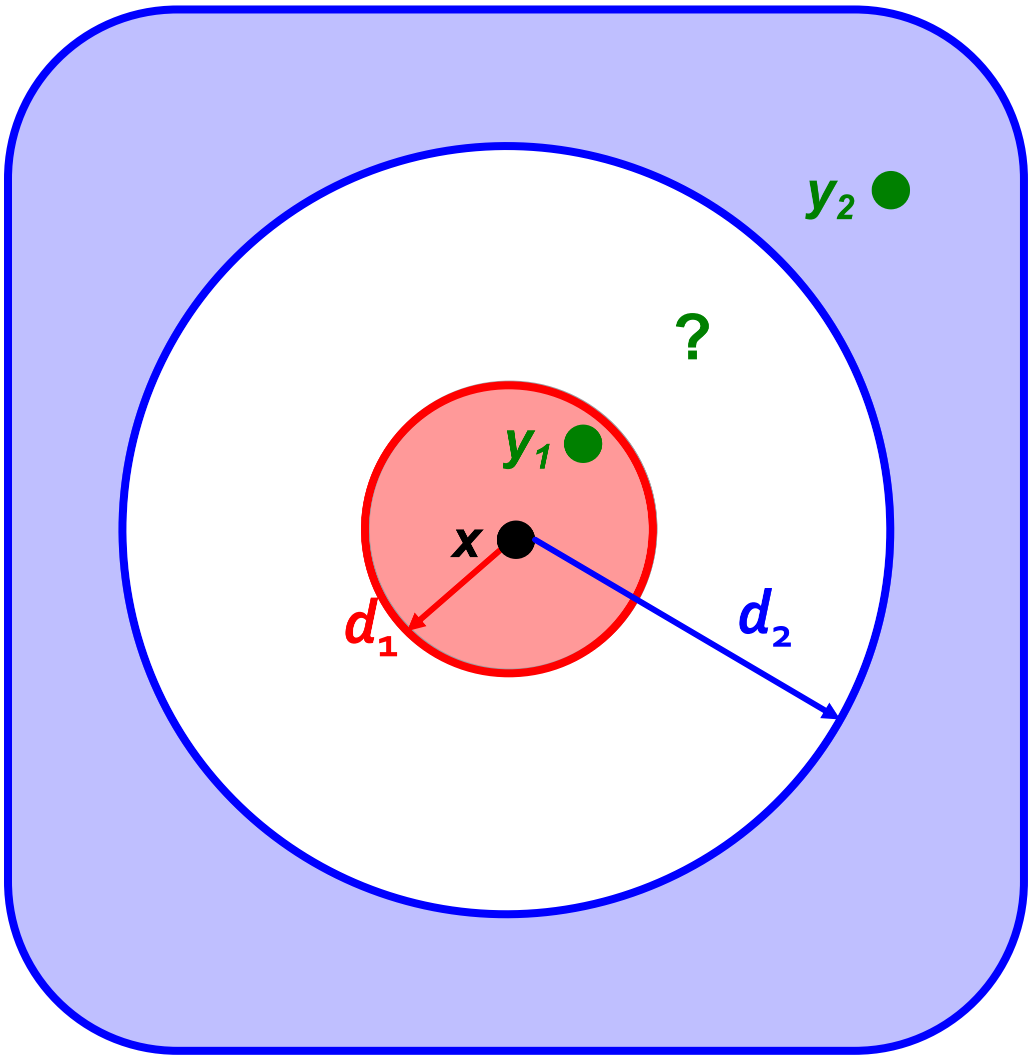
- **Suppose we have a space S of points with a <u>distance</u> metric $d(x,y)$**

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

<u>With a LS Family we can do LSH!</u>

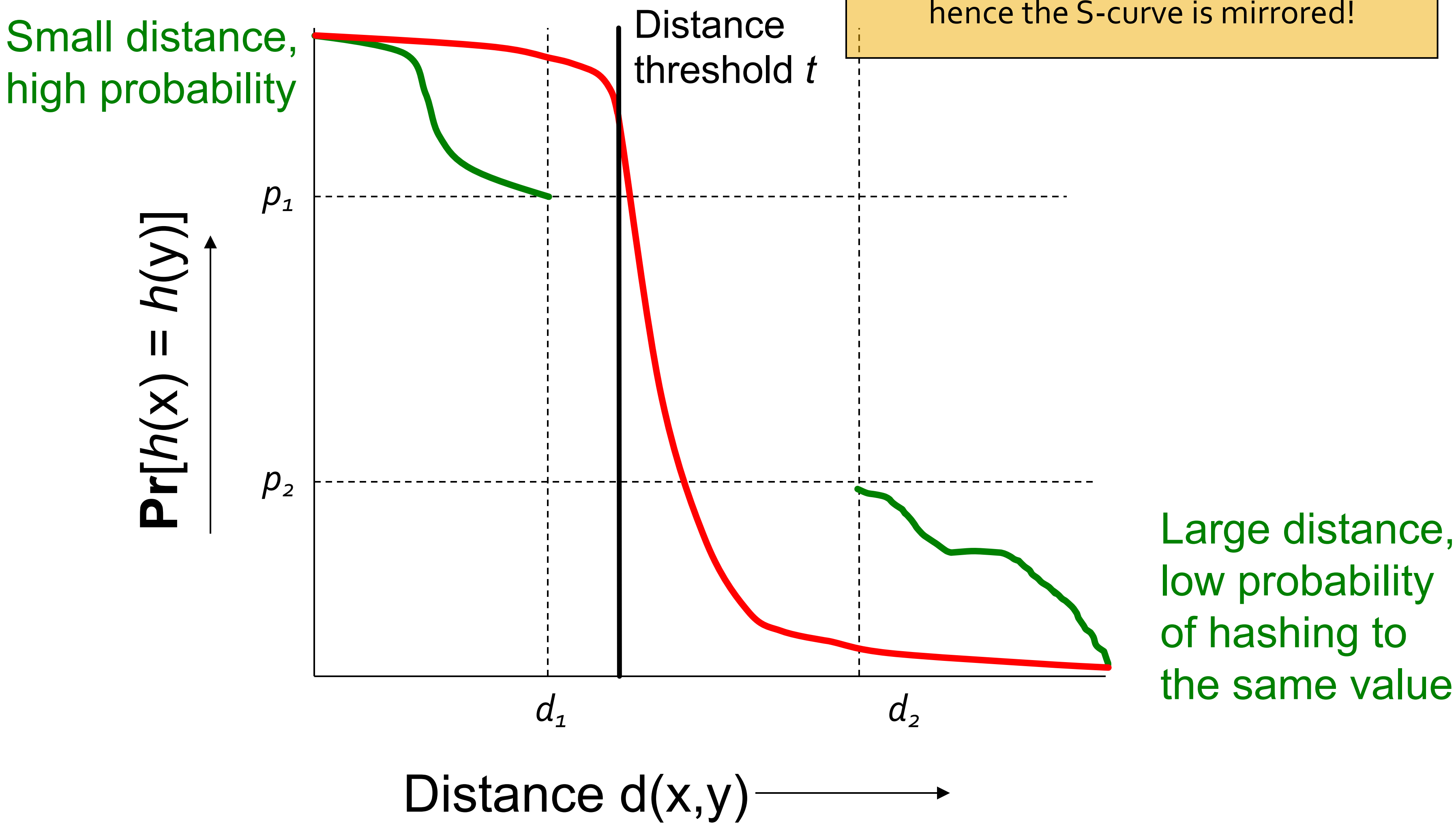
A (d_1,d_2,p_1,p_2)-sensitive function



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

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

Notice distance on x-axis, not similarity, hence the S-curve is mirrored!



Example of LS Family: Min-Hash

- **Let:**
  - ***S*** = space of all sets,
  - ***d*** = Jaccard distance,
  - ***H*** is family of Min-Hash functions for all permutations of rows
- Then for any hash function $h \in H$:

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

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

Example: LS Family – (2)

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

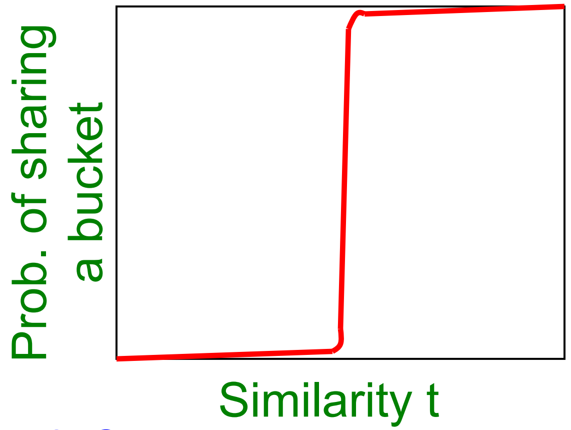
If distance $\leq$ 1/3
(so similarity ≥ 2/3)

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*** independent functions from ***H***
- For $h = [h_1,\dots,h_r]$ in **H'**, we say
  $\mathbf{h(x) = h(y)}$ 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 99% of 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

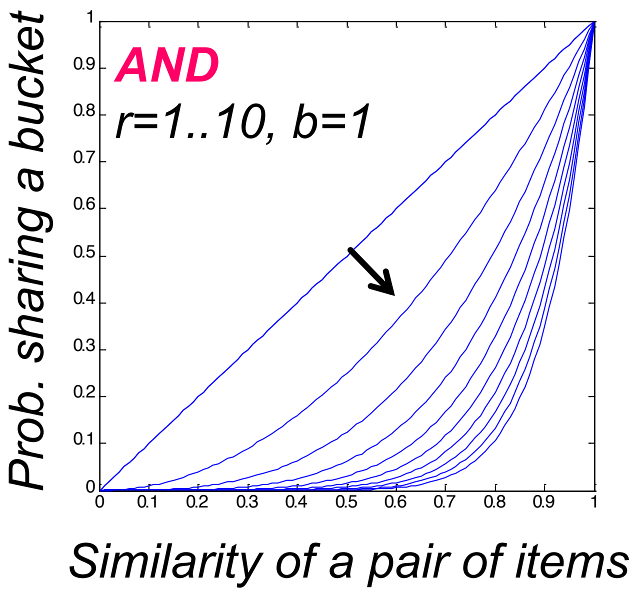
- Given family $\boldsymbol{H}$, construct family $\boldsymbol{H'}$ consisting of $\boldsymbol{b}$ independent functions from $\boldsymbol{H}$
- For $\boldsymbol{h} = [\boldsymbol{h_1},\ldots,\boldsymbol{h_b}]$ in $\boldsymbol{H'}$,
  h(x) = h(y) if and only if $\mathbf{h_i(x) = h_i(y)}$ for **at least 1** $\boldsymbol{i}$
- **Theorem:** If $\boldsymbol{H}$ is $(\boldsymbol{d_1, d_2, p_1, p_2})$-sensitive,
  then $\boldsymbol{H'}$ is $(\boldsymbol{d_1, d_2, 1\text{-}(1\text{-}p_1)^b, 1\text{-}(1\text{-}p_2)^b})$-sensitive
- **Proof:** Use the fact that $\boldsymbol{h_i}$'s are **independent**

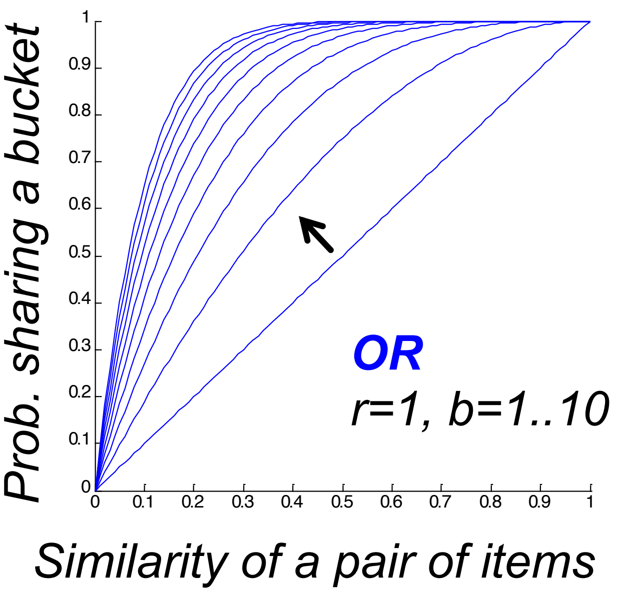
Raises probability for small distances (Good)

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

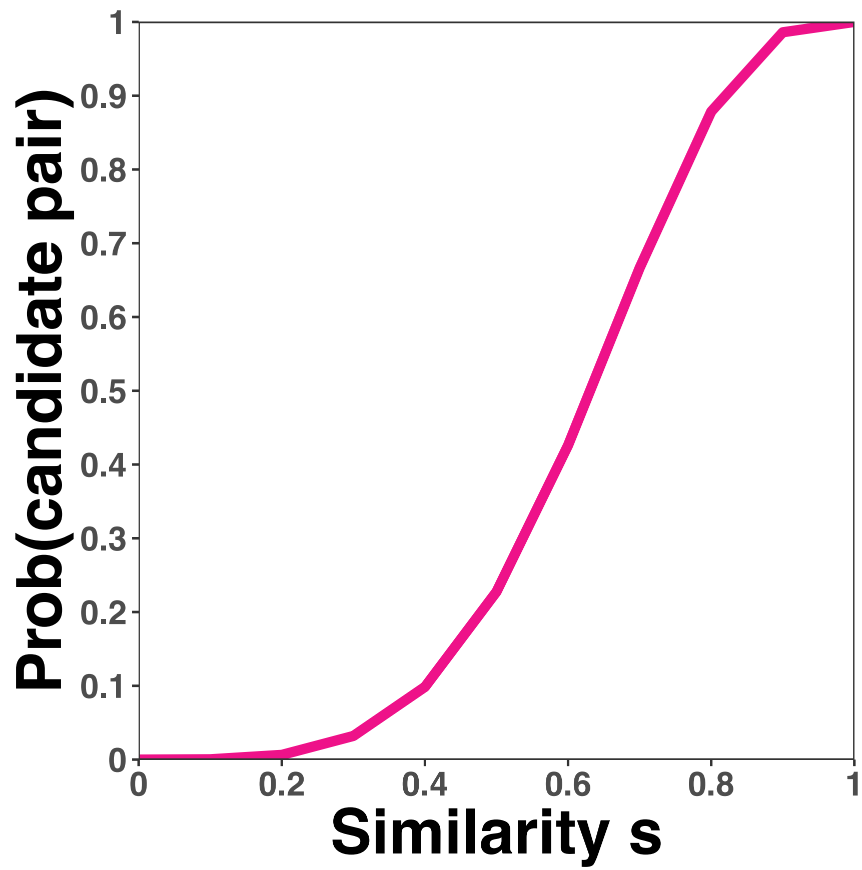
- As for the signature matrix, we can use the AND construction followed by the OR construction
  - Or vice-versa
  - Or any sequence of AND's and OR's alternating

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 $\geq$ 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 $1-(1-s^r)^b$ **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

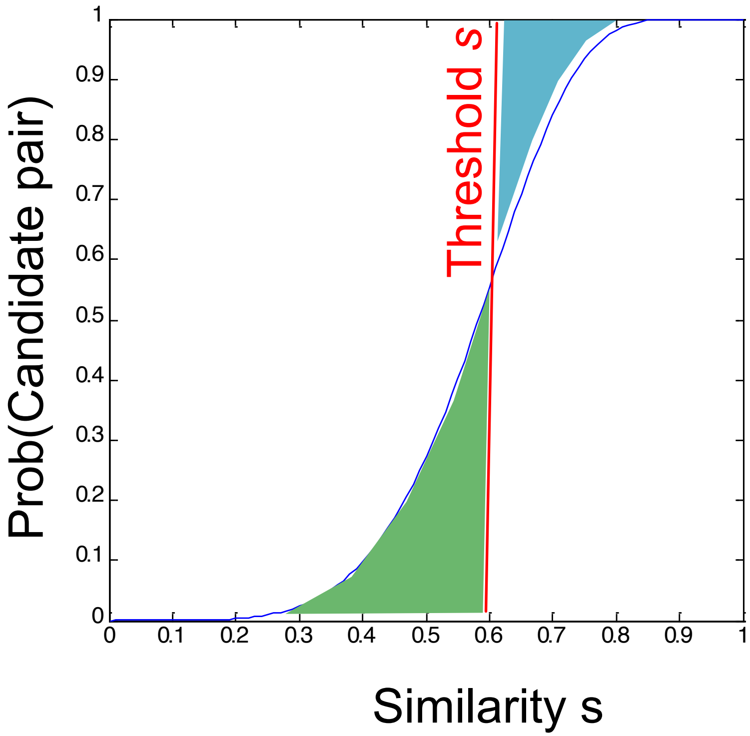


***r* = 4, *b* = 4** transforms a (.2,.8,.8,.2)-sensitive family into a (.2,.8,.8785,.0064)-sensitive family.

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*)

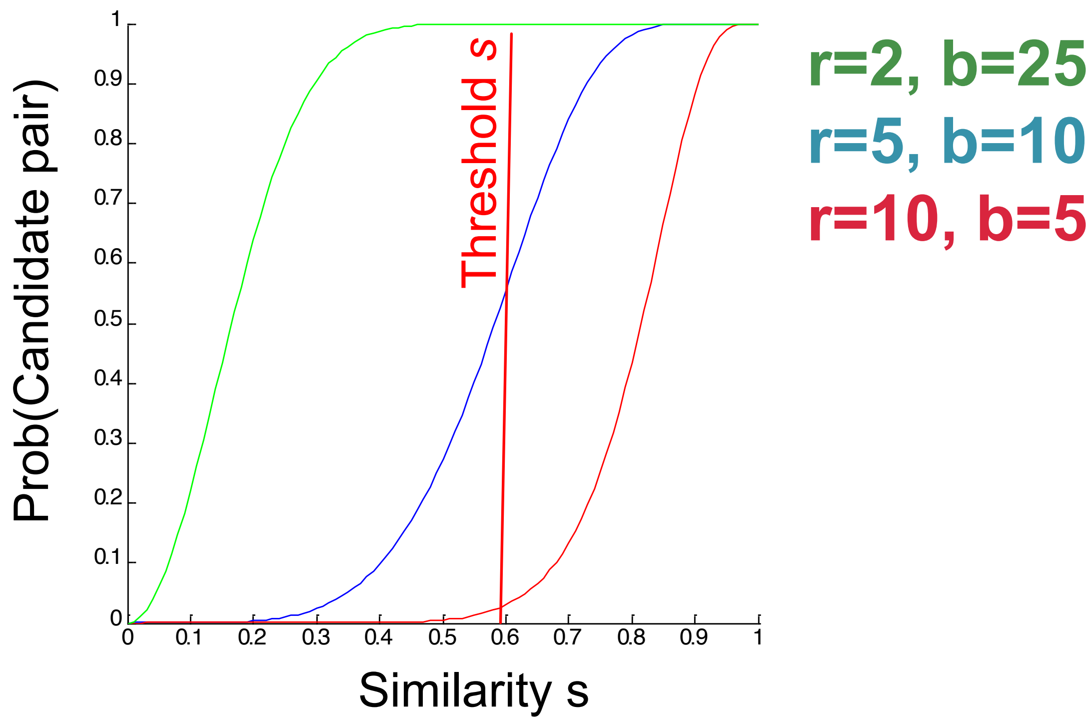


Blue area *X*: False Negative rate
These are pairs with ***sim* > *s*** but the ***X*** fraction won't share a band and then will **never become candidates.** This means we will never consider these pairs for (slow/exact) similarity calculation!

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

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

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

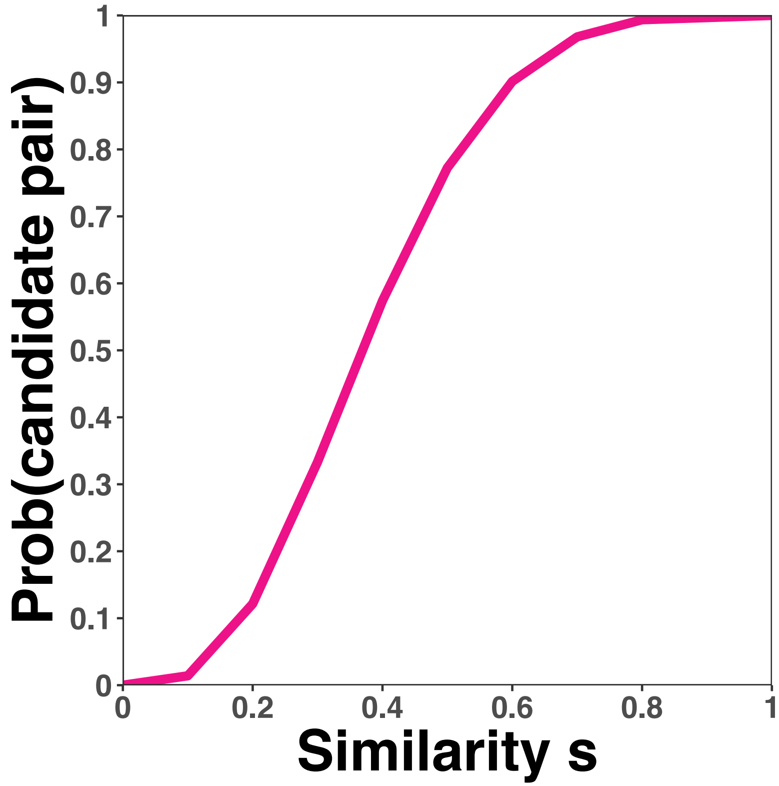


OR-AND Composition

- 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**

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 want to 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**

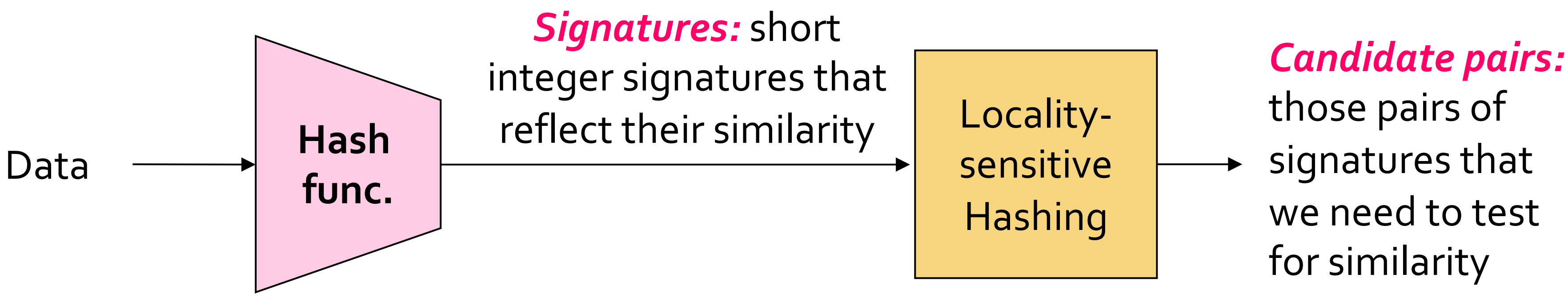
Points → **Hash func.** → ***Signatures:*** short integer signatures that reflect their similarity → Locality-sensitive Hashing → ***Candidate pairs:*** those pairs of signatures that we need to test for similarity

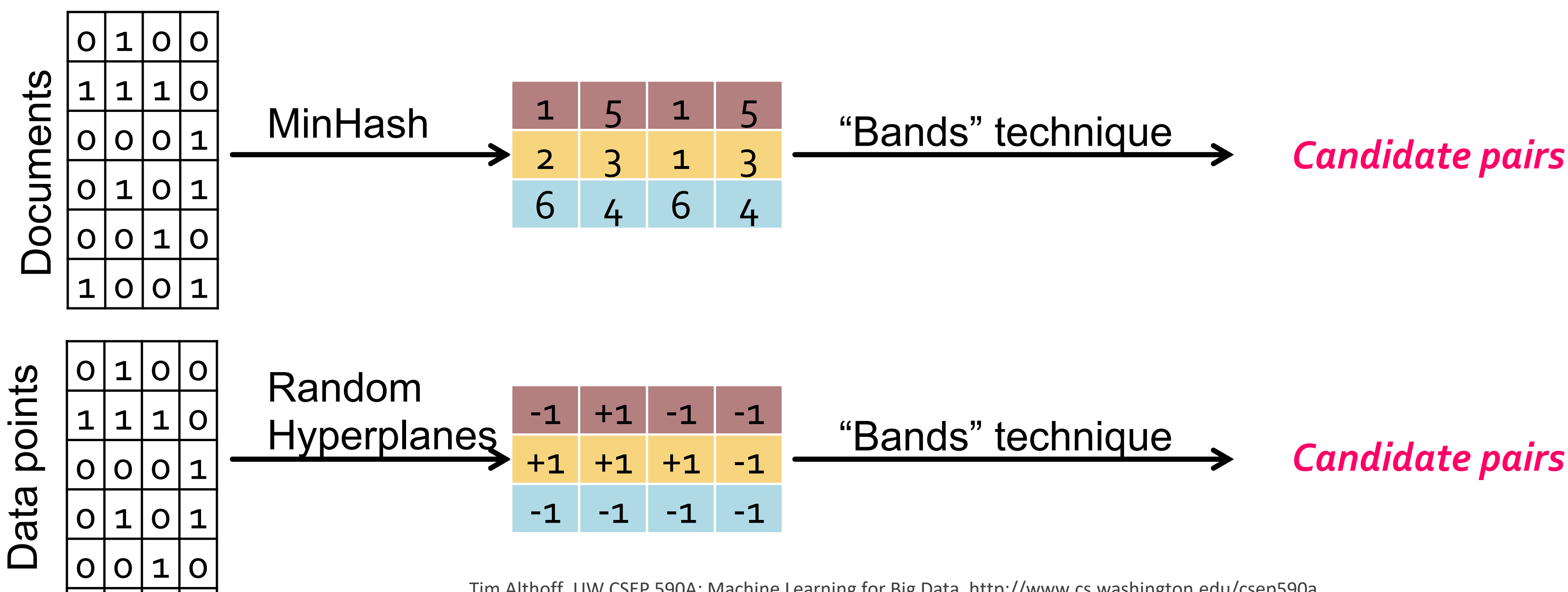
Design a ***(d_1, d_2, p_1, p_2)-sensitive*** family of hash functions **(for that particular distance metric)**

Depends on the distance function used

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

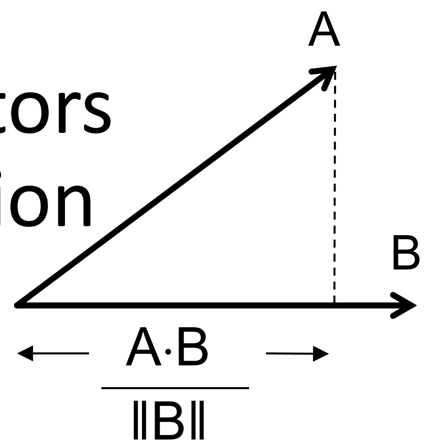
Summary of what we will learn



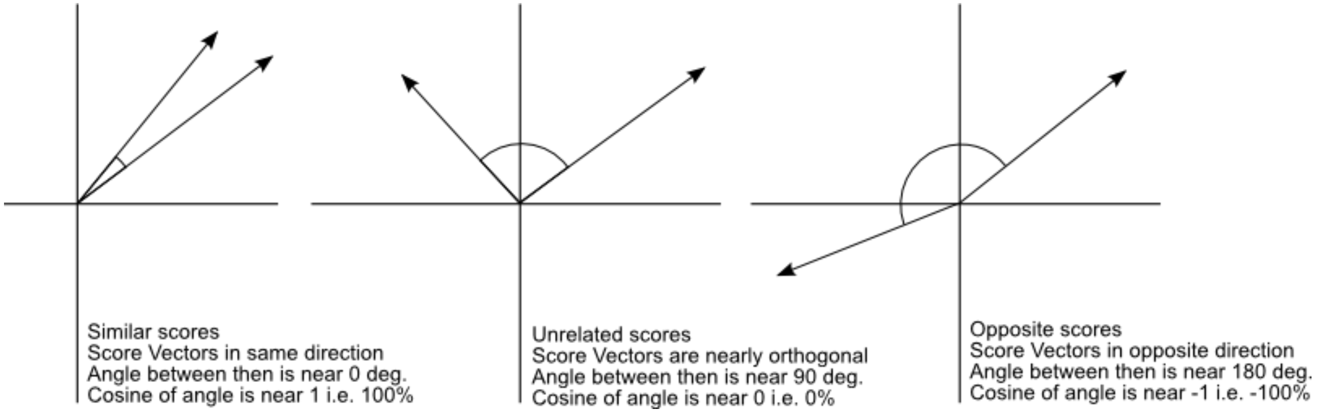


Cosine Distance

- ***Cosine distance*** = angle between vectors from the origin to the points in question
  d(A, B) = θ = arccos(A·B / ‖A‖·‖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)/ $\boldsymbol{\pi}$**
  - 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

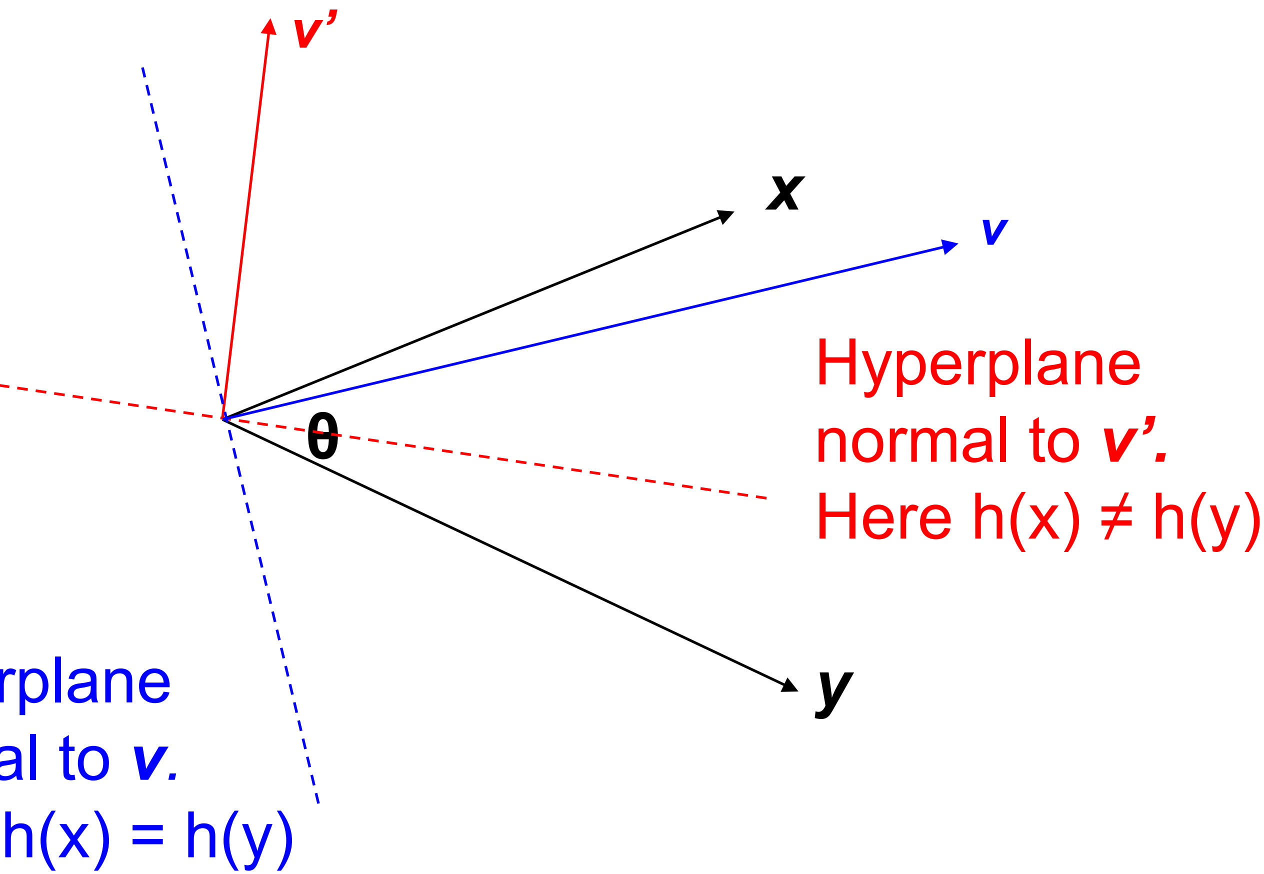
Random Hyperplanes

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

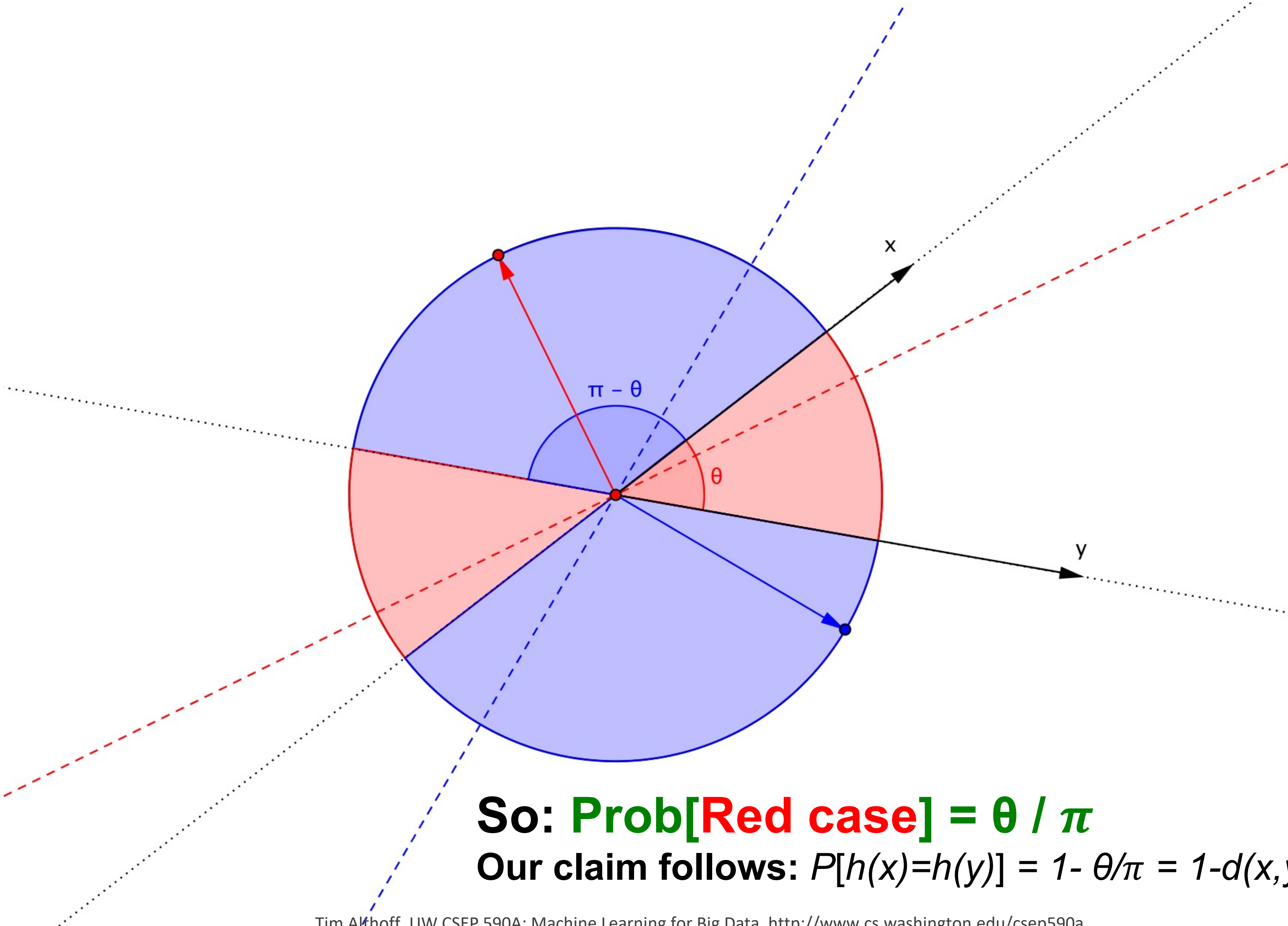
  $$\mathbf{Pr[h(x) = h(y)] \ = \ 1 - d(x,y) / \pi}$$

Proof of Claim

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



Proof of Claim



So: Prob[Red case] = θ / π

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

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

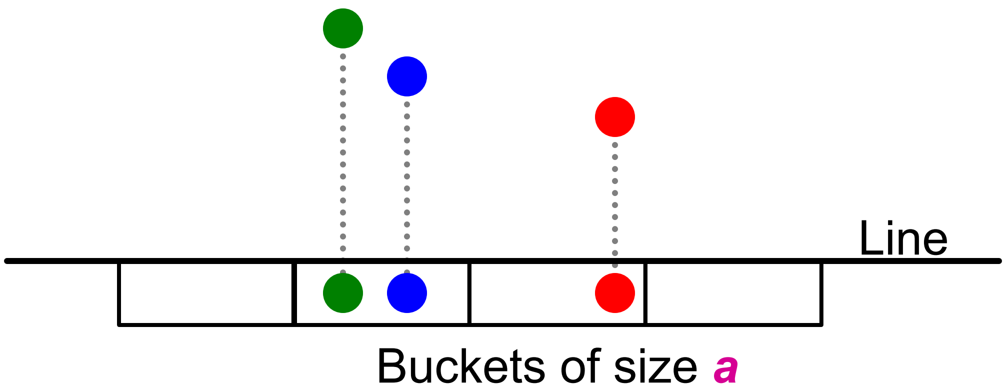
How to pick random vectors?

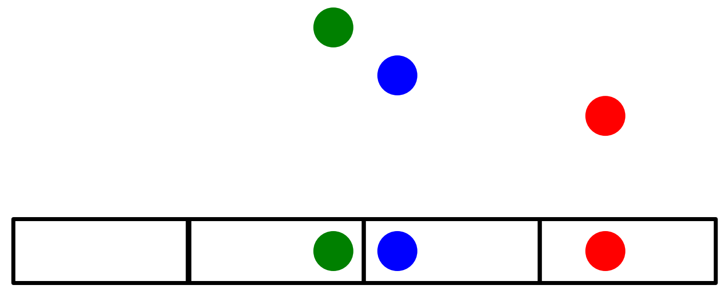
- Expensive to pick a random vector in ***M*** dimensions for large ***M***
  - Would have to generate ***M*** random numbers
- **A more efficient approach**
  - It suffices to consider only vectors ***v*** consisting of +1 and –1 components
    - **Why?** Assuming data is random, then vectors of +/-1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

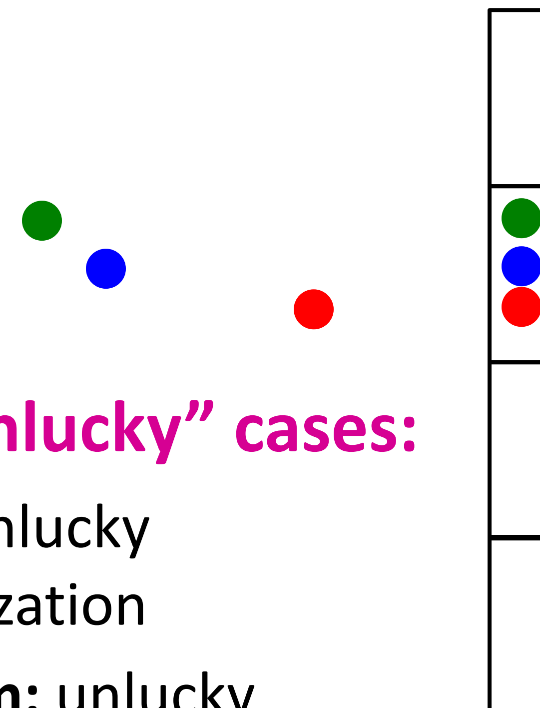
LSH for Euclidean Distance

- **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

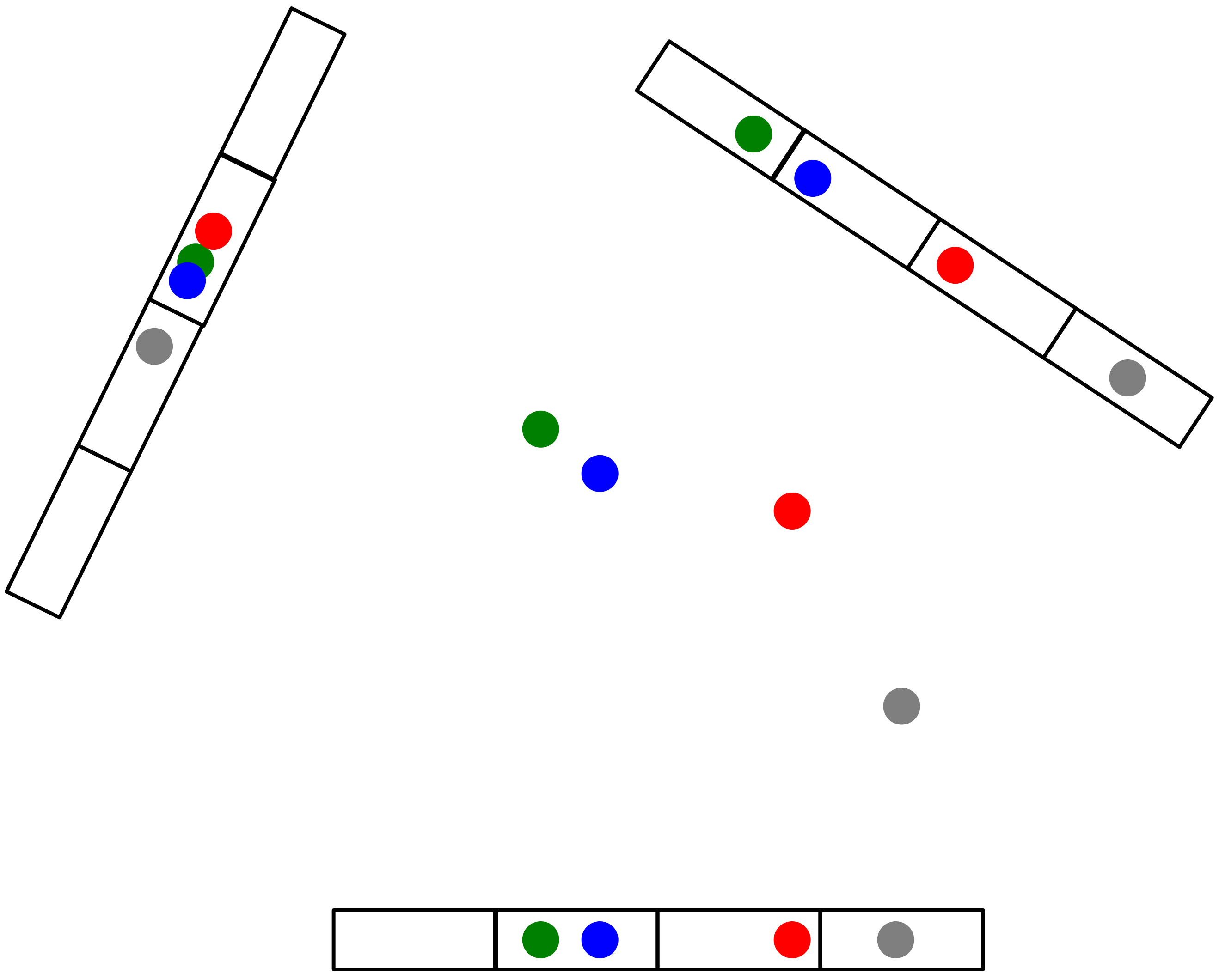






- **"Lucky" case:**
  - Points that are close hash in the same bucket
  - Distant points end up in different buckets
- **Two "unlucky" cases:**
  - **Top:** unlucky quantization
  - **Bottom:** unlucky projection

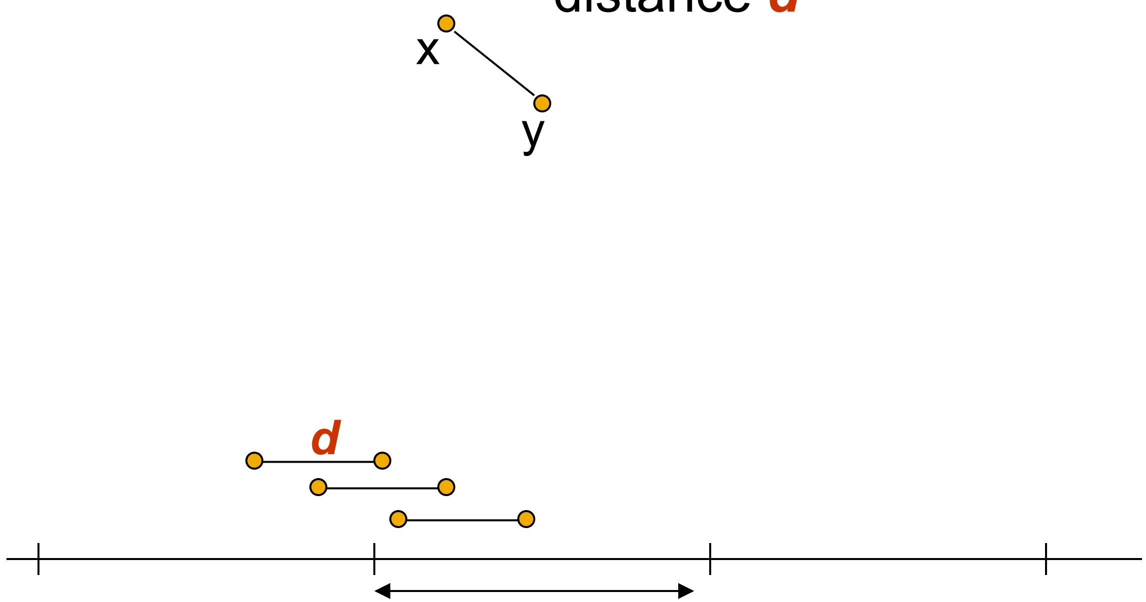
Multiple Projections



Projection of Points

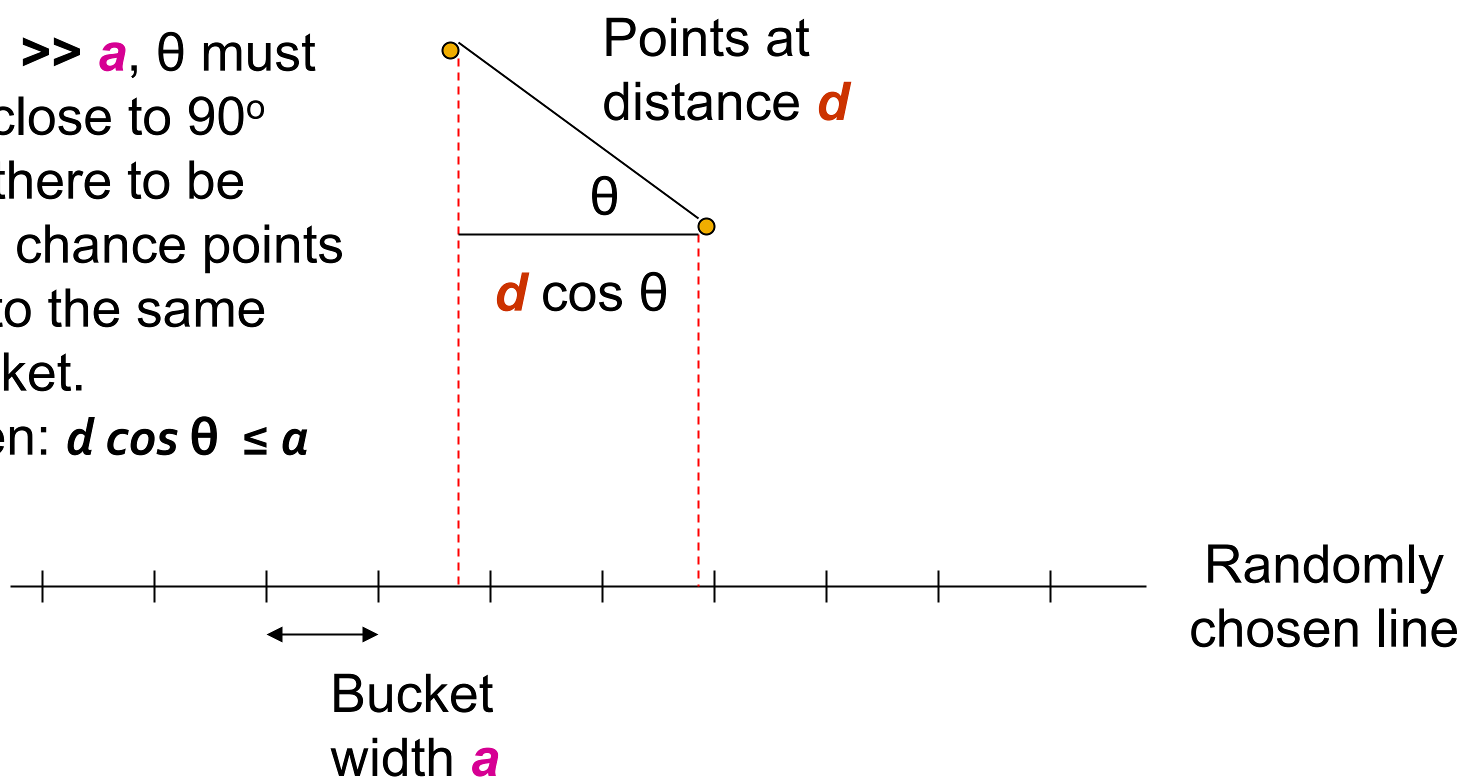
If ***d*** << ***a***, then the chance the points are in the same bucket is at least **1 – *d*/*a***.

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



Projection of Points

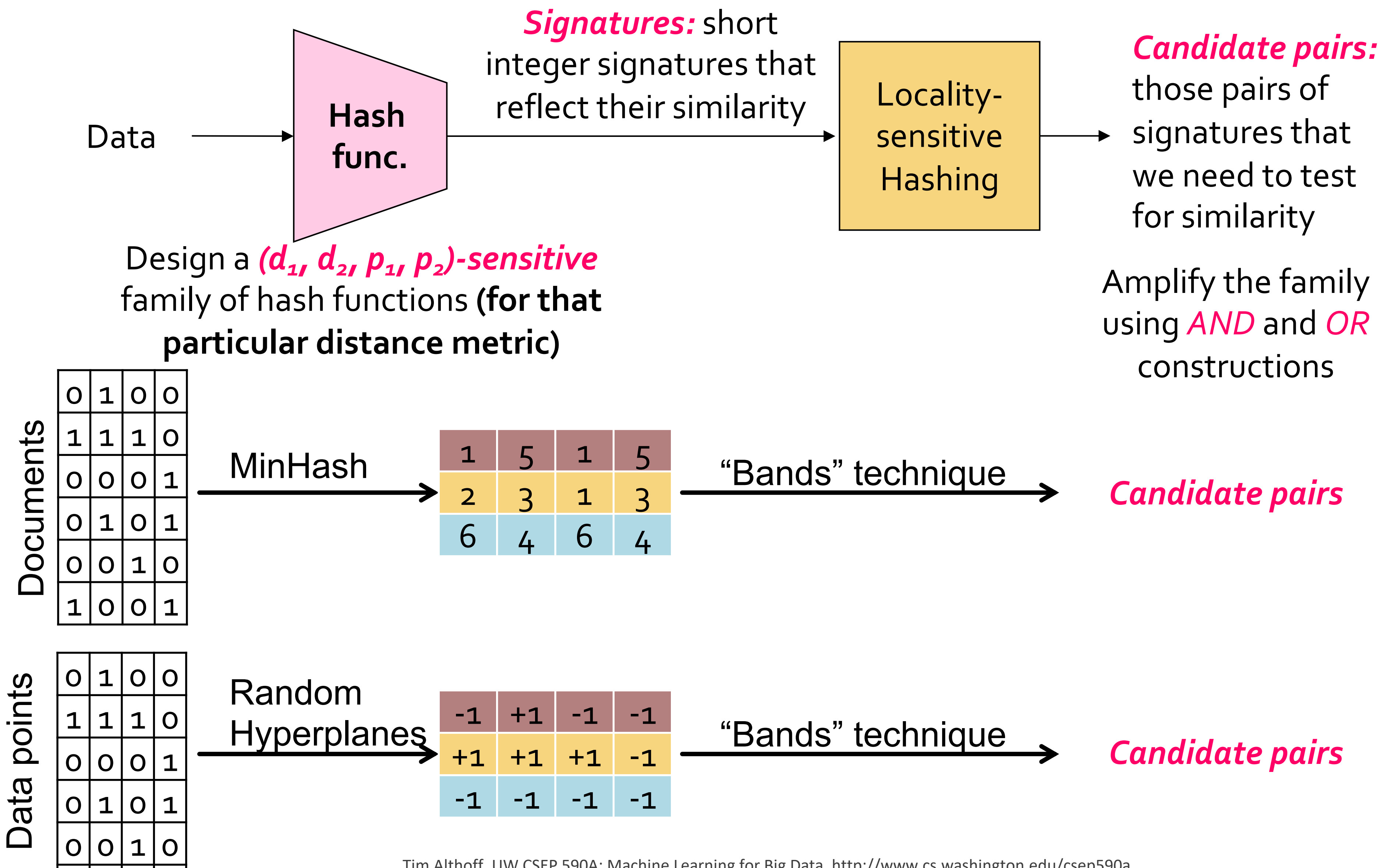
If ***d*** **>>** ***a***, θ must be close to 90°
for there to be any chance points go to the same bucket.
Then: $d \cos\theta \le a$



A LS-Family for Euclidean Distance

- If points are distance $d \leq a/2$, prob. they are in same bucket $\geq 1 - d/a = ½$
- If points are distance $d \geq 2a$ apart, then they can be in the same bucket only if $d \cos \theta \leq a$
  - $\cos \theta \leq ½$
  - $60 \leq \theta \leq 90$, 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



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 (d1, d2, p1, p2)-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

Announcements

Ed Discussion Board

Recitation sessions:
- Review of proof techniques and probability
  - **Location: Thursday, April 7, 7:30-8:30 PM, Zoom**

Deadlines next Wed, 6 PM:
- HW1
- Colab 2 (You can submit many times and will get immediate feedback)

For office hours – please check our website

How to find teammates for project?
- Ed Discussion Board
- Make sure you have a good dataset **accessible**

If you cannot attend our final project presentations (Monday, June 7, 6:30-9:20pm), please email course staff. Attendance is required.

Please give us feedback (Link to Google form on Ed)

Concern about workload: We respect everyone's time and responsibilities. Relative to the non-PMP version of the course we have reduced homework requirements. Most (theory) questions have partial credit opportunities. Nobody expects 100/100 homeworks. Grades will be curved in the end. What is most important to us, is to support your learning.