

# Similarity Search

**CSE545 - Spring 2022**  
Stony Brook University

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$A \cap B$

# Big Data Analytics, The Class

**Goal: Generalizations**  
*A model or summarization of the data.*

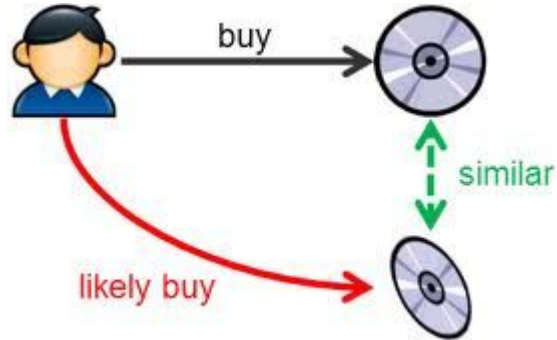
*Data Frameworks*

Hadoop File System ✓  
Streaming ✓  
MapReduce ✓  
Spark ✓  
Tensorflow ✓

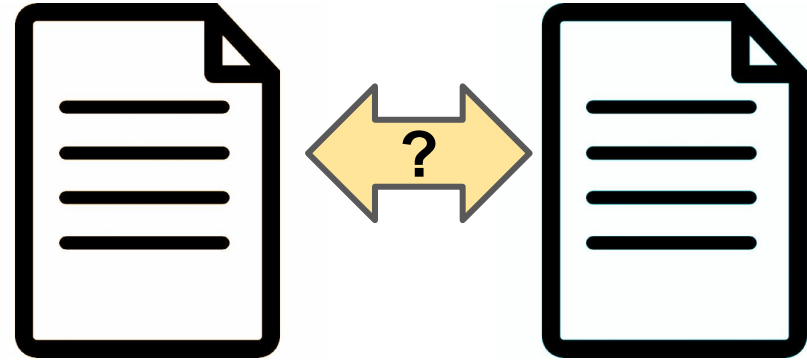
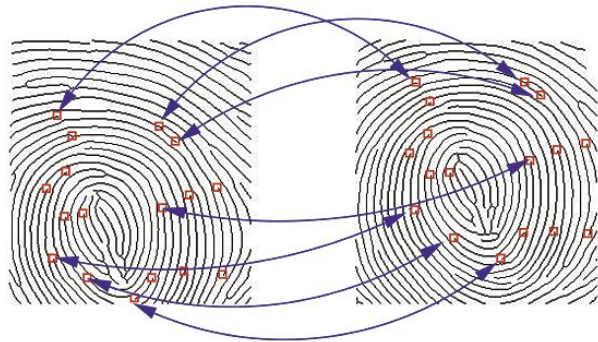
*Algorithms and Analyses*

Similarity Search  
Link Analysis  
Recommendation Systems  
Deep Learning  
Hypothesis Testing

# Finding Similar Items



(<http://blog.soton.ac.uk/hive/2012/05/10/recommendation-system-of-hive/>)



Real World



Digital World



(<http://www.datacommunitydc.org/blog/2013/08/entity-resolution-for-big-data>)

# Finding Similar Items: Topics

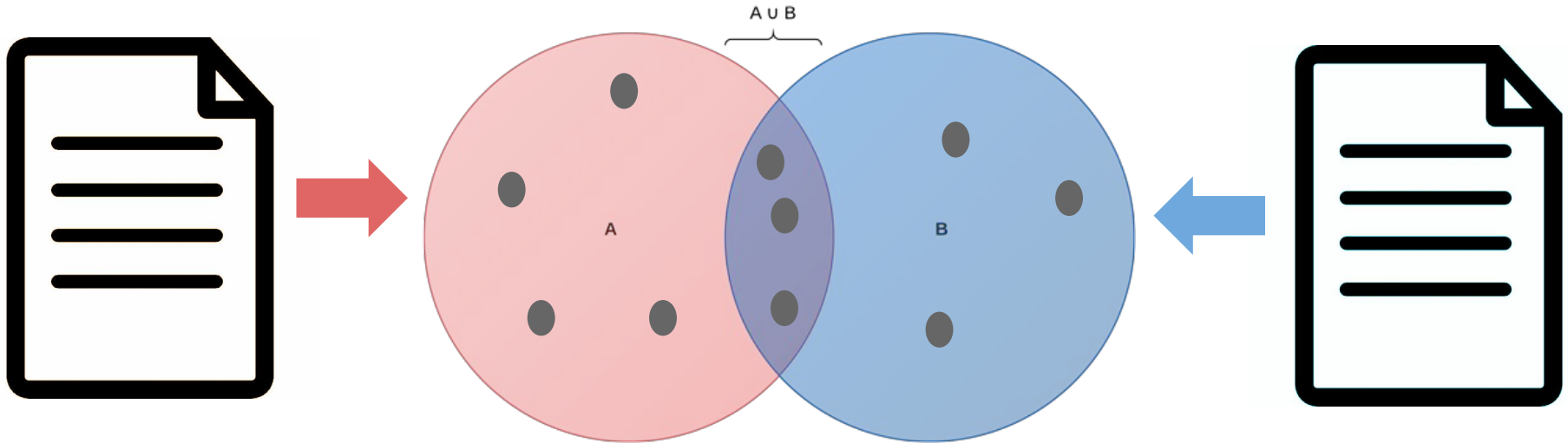
- Shingling
- Minhashing
- Locality-sensitive hashing
- Distance Metrics

# Document Similarity

**Challenge:** How to represent the document in a way that can be efficiently encoded and compared?

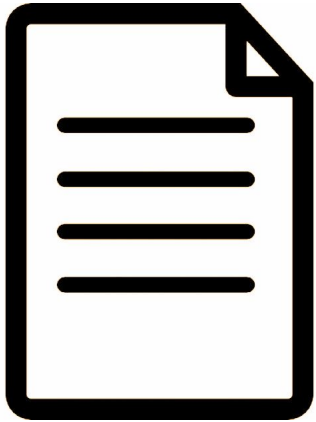
# Shingles

Goal: Convert documents to sets

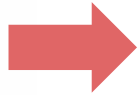


# Shingles

**Goal:** Convert documents to sets



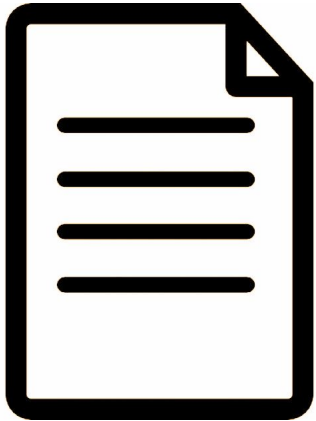
**k-shingles** (aka “character n-grams”)  
- sequence of  $k$  characters



E.g.  $k=2$  doc=“abcdabd”  
 $\text{singles}(\text{doc}, 2) = \{\text{ab}, \text{bc}, \text{cd}, \text{da}, \text{bd}\}$

# Shingles

Goal: Convert documents to sets



**k-shingles** (aka “character n-grams”)  
- sequence of  $k$  characters



E.g.  $k=2$  doc="abcdabd"  
 $\text{singles}(\text{doc}, 2) = \{\text{ab}, \text{bc}, \text{cd}, \text{da}, \text{bd}\}$

- Similar documents have many common shingles
- Changing words or order has minimal effect.
- In practice use  $5 < k < 10$



# Shingles

**Goal:** Convert documents to sets



Large enough that any given shingle appearing a document is highly unlikely (e.g.  $< .1\%$  chance)

Can hash large shingles to smaller (e.g. 9-shingles into 4 bytes)

*Can also use words (aka n-grams).*

- Similar documents have many common shingles
- Changing words or order has minimal effect.
- **In practice use  $5 < k < 10$**

# Shingles

**Problem:** Even if hashing, sets of shingles are large  
(e.g. 4 bytes  $\Rightarrow$  4x the size of the document).

# Minhashing

**Goal:** Convert sets to shorter ids, signatures

# Minhashing

**Goal:** Convert sets to shorter ids, “signatures”

Characteristic Matrix,  $X$ :

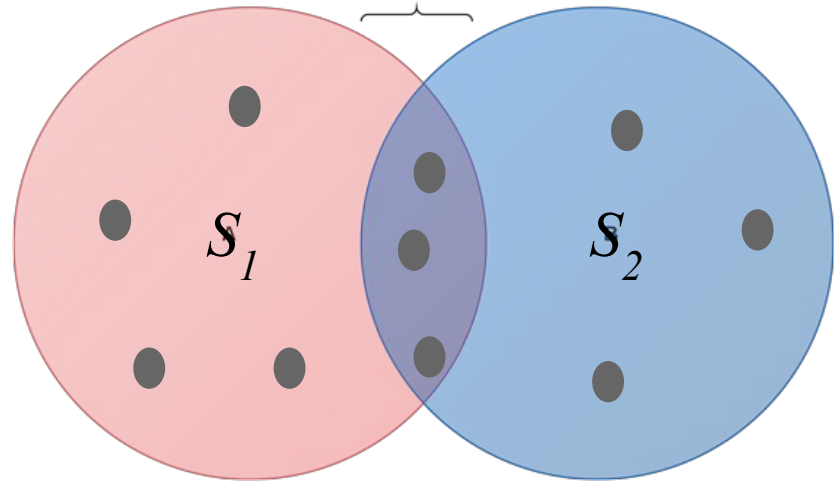
<i>Element</i>	$S_1$	$S_2$	$S_3$	$S_4$	.....
$a$	1	0	0	1	
$b$	0	0	1	0	
$c$	0	1	0	1	
$d$	1	0	1	1	
$e$	0	0	1	0	

(Leskovec et al., 2014; <http://www.mmms.org/>)

often very sparse! (lots of zeros)

Jaccard Similarity:

$$\text{sim}(S_1, S_2) = \frac{S_1 \cap S_2}{S_1 \cup S_2}$$



# Minhashing

Characteristic Matrix:

	$S_1$	$S_2$
ab	1	1
bc	0	1
de	1	0
ah	1	1
ha	0	0
ed	1	1
ca	0	1

Jaccard Similarity:

$$\text{sim}(S_1, S_2) = \frac{S_1 \cap S_2}{S_1 \cup S_2}$$

# Minhashing

Characteristic Matrix:

	$S_1$	$S_2$	
ab	1	1	**
bc	0	1	*
de	1	0	*
ah	1	1	**
ha	0	0	
ed	1	1	**
ca	0	1	*

Jaccard Similarity:

$$\text{sim}(S_1, S_2) = \frac{S_1 \cap S_2}{S_1 \cup S_2}$$

# Minhashing

Characteristic Matrix:

	$S_1$	$S_2$	
ab	1	1	**
bc	0	1	*
de	1	0	*
ah	1	1	**
ha	0	0	
ed	1	1	**
ca	0	1	*

Jaccard Similarity:

$$\text{sim}(S_1, S_2) = \frac{S_1 \cap S_2}{S_1 \cup S_2}$$

$$\text{sim}(S_1, S_2) = 3 / 6$$

# both have / # at least one has

# Minhashing

**Problem:** Even if hashing shingle contents,  
sets of shingles are large

e.g. 4 byte integer per shingle: assume all unique shingles,  
=> 4x the size of the document

(since there are as many shingles as characters and 1byte per char).



# Minhashing

**Goal:** Convert sets to shorter ids, “signatures”

Characteristic Matrix:  $X$

	$S_1$	$S_2$	$S_3$	$S_4$
ab	1	0	1	0
bc	1	0	0	1
de	0	1	0	1
ah	0	1	0	1
ha	0	1	0	1
ed	1	0	1	0
ca	1	0	1	0

(Leskovec et al., 2014; <http://www.mmms.org/>)

# Minhashing

**Goal:** Convert sets to shorter ids, “signatures”

Characteristic Matrix:  $X$

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ah	0	1	0	1
ha	0	1	0	1
ed	1	0	1	0
ca	1	0	1	0

## Approximate Approach:

1) Instead of keeping whole characteristic matrix, just keep first row where 1 is encountered.

2) Shuffle and repeat to get a “signature” for each set.

# Minhashing

**Goal:** Convert sets to shorter ids, “signatures”

Characteristic Matrix:  $X$

	$S_1$	$S_2$	$S_3$	$S_4$
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de	0	1	0	1
ah	0	1	0	1
ha	0	1	0	1
ed	1	0	1	0
ca	1	0	1	0

1 3 1 2

## Approximate Approach:

1) Instead of keeping whole characteristic matrix, just keep first row where 1 is encountered.

2) Shuffle and repeat to get a “signature”.

	$S_1$	$S_2$	$S_3$	$S_4$
ah	0	1	0	1
ca	1	0	1	0
ed	1	0	1	0
de	0	1	0	1
ab	1	0	1	0
bc	1	0	0	1

2 1 2 1

...

# Minhashing

**Goal:** Convert sets to shorter ids, “signatures”

Characteristic Matrix:  $X$

	$S_1$	$S_2$	$S_3$	$S_4$
ab	1	0	1	0
bc	1	0	0	1
de	0	1	0	1
ah	0	1	0	1
ha	0	1	0	1
ed	1	0	1	0
ca	1	0	1	0

1 3 1 2

## Approximate Approach:

1) Instead of keeping whole characteristic matrix, just keep first row where 1 is encountered.

2) Shuffle and repeat to get a “signature”.

	$S_1$	$S_2$	$S_3$	$S_4$
ah	0	1	0	1
ca	1	0	1	0
ed	1	0	1	0
de	0	1	0	1
ab	1	0	1	0
bc	1	0	0	1

2 1 2 1

signatures

$S_1$	$S_2$	$S_3$	$S_4$
1	3	1	2
2	1	2	1
...	...	...	...

...

# Minhashing

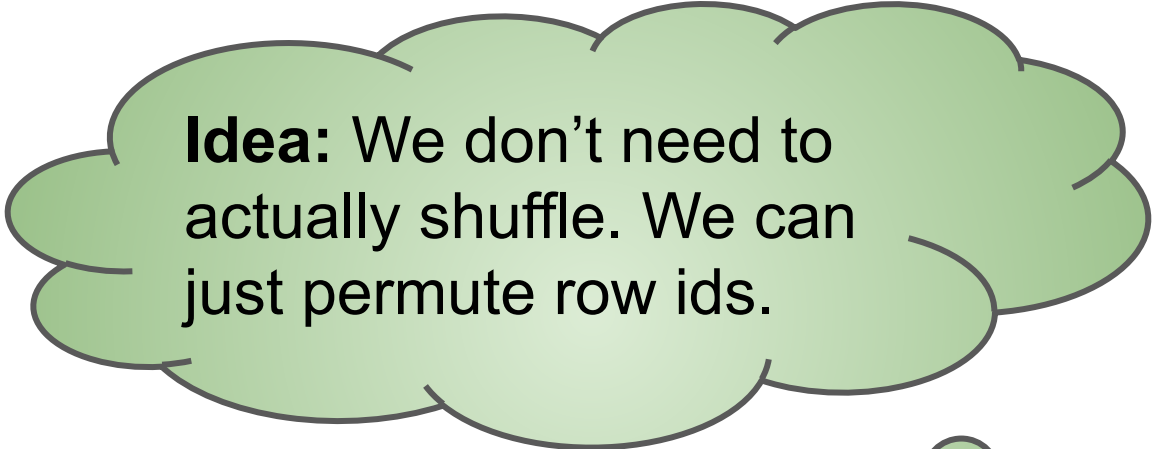
**Goal:** Convert sets to shorter ids, “signatures”

Characteristic Matrix:  $X$

	$S_1$	$S_2$	$S_3$	$S_4$
ab	1	0	1	0
bc	1	0	0	1
de	0	1	0	1
ah	0	1	0	1
ha	0	1	0	1
ed	1	0	1	0
ca	1	0	1	0

## Approximate Approach:

- 1) Instead of keeping whole characteristic matrix, just keep first row where 1 is encountered.
- 2) Shuffle and repeat to get a “signature” for each set.



**Idea:** We don't need to actually shuffle. We can just permute row ids.

# Minhashing

Characteristic Matrix:

	$S_1$	$S_2$	$S_3$	$S_4$
ab	1	0	1	0
bc	1	0	0	1
de	0	1	0	1
ah	0	1	0	1
ha	0	1	0	1
ed	1	0	1	0
ca	1	0	1	0

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to first row where set appears.

# Minhashing

Characteristic Matrix:

	$S_1$	$S_2$	$S_3$	$S_4$
ab	1	0	1	0
bc	1	0	0	1
de	0	1	0	1
ah	0	1	0	1
ha	0	1	0	1
ed	1	0	1	0
ca	1	0	1	0

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to first row where set appears.

permuted order
1 ha
2 ed
3 ab
4 bc
5 ca
6 ah
7 de



# Minhashing

Characteristic Matrix:

		$S_1$	$S_2$	$S_3$	$S_4$
3	ab	1	0	1	0
4	bc	1	0	0	1
7	de	0	1	0	1
6	ah	0	1	0	1
1	ha	0	1	0	1
2	ed	1	0	1	0
5	ca	1	0	1	0

permuted order
1 ha
2 ed
3 ab
4 bc
5 ca
6 ah
7 de

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to first row where set appears.

# Minhashing

Characteristic Matrix:

		$S_1$	$S_2$	$S_3$	$S_4$
3	ab	1	0	1	0
4	bc	1	0	0	1
7	de	0	1	0	1
6	ah	0	1	0	1
1	ha	0	1	0	1
2	ed	1	0	1	0
5	ca	1	0	1	0

permuted order
1 ha
2 ed
3 ab
4 bc
5 ca
6 ah
7 de

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to first row where set appears.

$$h(S_1) = ed \text{ \#permuted row 2}$$

$$h(S_2) = ha \text{ \#permuted row 1}$$

$$h(S_3) =$$

# Minhashing

Characteristic Matrix:

		$S_1$	$S_2$	$S_3$	$S_4$
3	ab	1	0	1	0
4	bc	1	0	0	1
7	de	0	1	0	1
6	ah	0	1	0	1
1	ha	0	1	0	1
2	ed	1	0	1	0
5	ca	1	0	1	0

permuted order
1 ha
2 ed
3 ab
4 bc
5 ca
6 ah
7 de

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to first row where set appears.

$$h(S_1) = ed \text{ \#permuted row 2}$$

$$h(S_2) = ha \text{ \#permuted row 1}$$

$$h(S_3) = ed \text{ \#permuted row 2}$$

$$h(S_4) =$$

# Minhashing

Characteristic Matrix:

		$S_1$	$S_2$	$S_3$	$S_4$
3	ab	1	0	1	0
4	bc	1	0	0	1
7	de	0	1	0	1
6	ah	0	1	0	1
1	ha	0	1	0	1
2	ed	1	0	1	0
5	ca	1	0	1	0

permuted order
1 ha
2 ed
3 ab
4 bc
5 ca
6 ah
7 de

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to first row where set appears.

$$h(S_1) = ed \text{ \#permuted row 2}$$

$$h(S_2) = ha \text{ \#permuted row 1}$$

$$h(S_3) = ed \text{ \#permuted row 2}$$

$$h(S_4) = ha \text{ \#permuted row 1}$$

# Minhashing

Characteristic Matrix:

		$S_1$	$S_2$	$S_3$	$S_4$
3	ab	1	0	1	0
4	bc	1	0	0	1
7	de	0	1	0	1
6	ah	0	1	0	1
1	ha	0	1	0	1
2	ed	1	0	1	0
5	ca	1	0	1	0

(Leskovec et al., 2014; <http://www.mmms.org/>)

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to rows.

Signature matrix:  $M$

- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1

$h_1(S_1) = ed$  #permuted row 2

$h_1(S_2) = ha$  #permuted row 1

$h_1(S_3) = ed$  #permuted row 2

$h_1(S_4) = ha$  #permuted row 1

# Minhashing

Characteristic Matrix:

		$S_1$	$S_2$	$S_3$	$S_4$
3	ab	1	0	1	0
4	bc	1	0	0	1
7	de	0	1	0	1
6	ah	0	1	0	1
1	ha	0	1	0	1
2	ed	1	0	1	0
5	ca	1	0	1	0

(Leskovec et al., 2014; <http://www.mmhds.org/>)

Minhash function:  $h$

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Signature matrix:  $M$

- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1

$$h_1(S_1) = \text{ed} \text{ \#permutated row}$$

2

$$h_1(S_2) = \text{ha} \text{ \#permutated row}$$

1

$$h(S_3) = \text{ed} \text{ \#permutated row}$$

# Minhashing

Characteristic Matrix:

		$S_1$	$S_2$	$S_3$	$S_4$
3	ab	1	0	1	0
4	bc	1	0	0	1
7	de	0	1	0	1
6	ah	0	1	0	1
1	ha	0	1	0	1
2	ed	1	0	1	0
5	ca	1	0	1	0

(Leskovec et al., 2014; <http://www.mmms.org/>)

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to rows.

Signature matrix:  $M$

- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1

$h_1(S_1) = ed$  #permutated row

2

$h_1(S_2) = ha$  #permutated row

1

$h(S_3) = ed$  #permutated row

# Minhashing

Characteristic Matrix:

			$S_1$	$S_2$	$S_3$	$S_4$
4	3	ab	1	0	1	0
2	4	bc	1	0	0	1
1	7	de	0	1	0	1
3	6	ah	0	1	0	1
6	1	ha	0	1	0	1
7	2	ed	1	0	1	0
5	5	ca	1	0	1	0

Minhash function:  $h$

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Signature matrix:  $M$

- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$				



# Minhashing

Characteristic Matrix:

			$S_1$	$S_2$	$S_3$	$S_4$
4	3	ab	1	0	1	0
2	4	bc	1	0	0	1
1	7	de	0	1	0	1
3	6	ah	0	1	0	1
6	1	ha	0	1	0	1
7	2	ed	1	0	1	0
5	5	ca	1	0	1	0

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to rows.

Signature matrix:  $M$

- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$	2	1	4	1

# Minhashing

Characteristic Matrix:

				$S_1$	$S_2$	$S_3$	$S_4$
1	4	3	ab	1	0	1	0
3	2	4	bc	1	0	0	1
7	1	7	de	0	1	0	1
6	3	6	ah	0	1	0	1
2	6	1	ha	0	1	0	1
5	7	2	ed	1	0	1	0
4	5	5	ca	1	0	1	0

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to rows.

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- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$	2	1	4	1
$h_3$				

# Minhashing

Characteristic Matrix:

				$S_1$	$S_2$	$S_3$	$S_4$
1	4	3	ab	1	0	1	0
3	2	4	bc	1	0	0	1
7	1	7	de	0	1	0	1
6	3	6	ah	0	1	0	1
2	6	1	ha	0	1	0	1
5	7	2	ed	1	0	1	0
4	5	5	ca	1	0	1	0

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to rows.

Signature matrix:  $M$

- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$	2	1	4	1
$h_3$	1	2	1	2

# Minhashing

Characteristic Matrix:

				$S_1$	$S_2$	$S_3$	$S_4$
1	4	3	ab	1	0	1	0
3	2	4	bc	1	0	0	1
7	1	7	de	0	1	0	1
6	3	6	ah	0	1	0	1
2	6	1	ha	0	1	0	1
5	7	2	ed	1	0	1	0
4	5	5	ca	1	0	1	0

(Leskovec et al., 2014; <http://www.mmms.org/>)

Minhash function:  $h$

- Based on permutation of rows in the characteristic matrix,  $h$  maps sets to rows.

Signature matrix:  $M$

- Record first row where each set had a 1 in the given permutation

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$	2	1	4	1
$h_3$	1	2	1	2
...				
...				

# Minhashing

**Property of signature matrix:**  
The probability for any  $h_i$  (i.e. any row), that  $h_i(S_1) = h_i(S_2)$  is the same as  $\text{Sim}(S_1, S_2)$

Characteristic Matrix:

				$S_1$	$S_2$	$S_3$	$S_4$
1	4	3	ab	1	0	1	0
3	2	4	bc	1	0	0	1
7	1	7	de	0	1	0	1
6	3	6	ah	0	1	0	1
2	6	1	ha	0	1	0	1
5	7	2	ed	1	0	1	0
4	5	5	ca	1	0	1	0

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$	2	1	4	1
$h_3$	1	2	1	2
...				
...				

# Minhashing

Characteristic Matrix:

				$S_1$	$S_2$	$S_3$	$S_4$
1	4	3	ab	1	0	1	0
3	2	4	bc	1	0	0	1
7	1	7	de	0	1	0	1
6	3	6	ah	0	1	0	1
2	6	1	ha	0	1	0	1
5	7	2	ed	1	0	1	0
4	5	5	ca	1	0	1	0

**Property of signature matrix:**

The probability for any  $h_i$  (i.e. any row), that  $h_i(S_1) = h_i(S_2)$  is the same as  $\text{Sim}(S_1, S_2)$

Thus, similarity of signatures  $S_1, S_2$  is the fraction of minhash functions (i.e. rows) in which they agree.

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$	2	1	4	1
$h_3$	1	2	1	2
...				
...				

# Minhashing

Characteristic Matrix:

				$S_1$	$S_2$	$S_3$	$S_4$
1	4	3	ab	1	0	0	0
3	2	4	an	0	1	0	0
7	1	5	ar	0	0	1	0
6	3	6	an	0	1	0	0
2	6	1	ha	0	1	0	1
5	7	2	ed	1	0	1	0
4	5	5	ca	1	0	1	0

Estimate with a random sample of permutations (i.e. ~100)

	$S_1$	$S_2$	$S_3$	$S_4$
$h_1$	2	1	2	1
$h_2$	2	1	4	1
$h_3$	1	2	1	2
...				
...				

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# Minhashing

Characteristic Matrix:

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1	4	3	ab	1	0	0	0
3	2	4	ba	0	1	1	0
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6	3	6	ac	0	1	0	1
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Estimate with a random sample of permutations (i.e. ~100)

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Standard Error of Mean =  $\text{std}/\sqrt{N}$

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Solution: Use “random” hash functions.

- Setup:
  - Pick  $\sim 100$  hash functions, hashes
  - Store  $M[i][s] = \text{a potential minimum } h_i(r)$   
*#initialized to infinity (num hashes x num sets)*



# Minhashing

Solution: Use “random” hash functions.

Setup:

```
hashes = [getHfunc(i) for i in rand(1, num=100)]
```

*#100 hash functions, seeded random*

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for i in hashes: for s in sets:
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    Sig[i][s] = np.inf #represents a potential minimum  $h_i(r)$  ; initially infinity
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Algorithm (“efficient minhashing”):

```
for r in rows of cm: #cm is characteristic matrix
```

```
    compute  $h_i(r)$  for all i in hashes #precompute 100 values
```

```
    for each set s in sets: #columns of cm
```

```
        if cm[r][s] == 1:
```

```
            for i in hashes: #check which hash produces smallest value
```

```
                if  $h_i(r) < \text{Sig}[i][s]$ :  $\text{Sig}[i][s] = h_i(r)$ 
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Algorithm (“efficient minhashing”) without charact matrix:

```
for feat in shins: #shins is all unique shingles
```

```
    compute  $h_i(\textit{feat})$  for all i in hashes #precompute 100 values
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```
    for each set s in sets: #sets is list of shingle sets
```

```
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```

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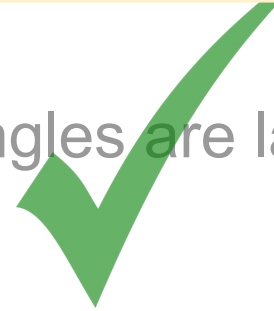
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**Problem:** Even if hashing, sets of shingles are large (e.g. 4 bytes => 4x the size of the document).

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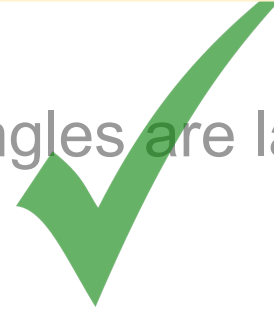


**New Problem:** Even if the size of signatures are small, it can be computationally expensive to find similar pairs.

E.g. 1m documents;  $1,000,000 \text{ choose } 2 = 500,000,000,000$  pairs!

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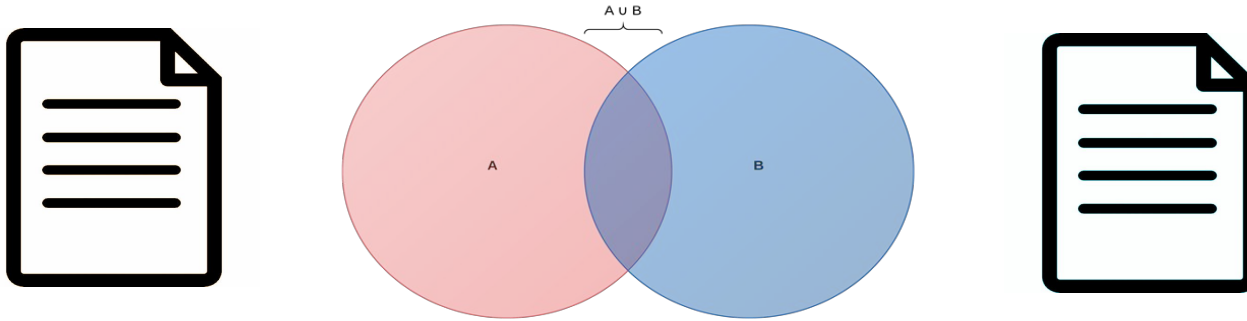


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E.g. 1m documents; 1,000,000 choose 2 = 500,000,000,000 pairs!

(1m documents isn't even "big data")

# Document Similarity



Duplicate web pages (useful for ranking

Plagiarism

Cluster News Articles

Anything similar to documents: movie/music/art tastes, product characteristics

COVID-19 Report matching

# Locality-Sensitive Hashing

**Goal:** find pairs of minhashes *likely* to be similar (in order to then test more precisely for similarity).

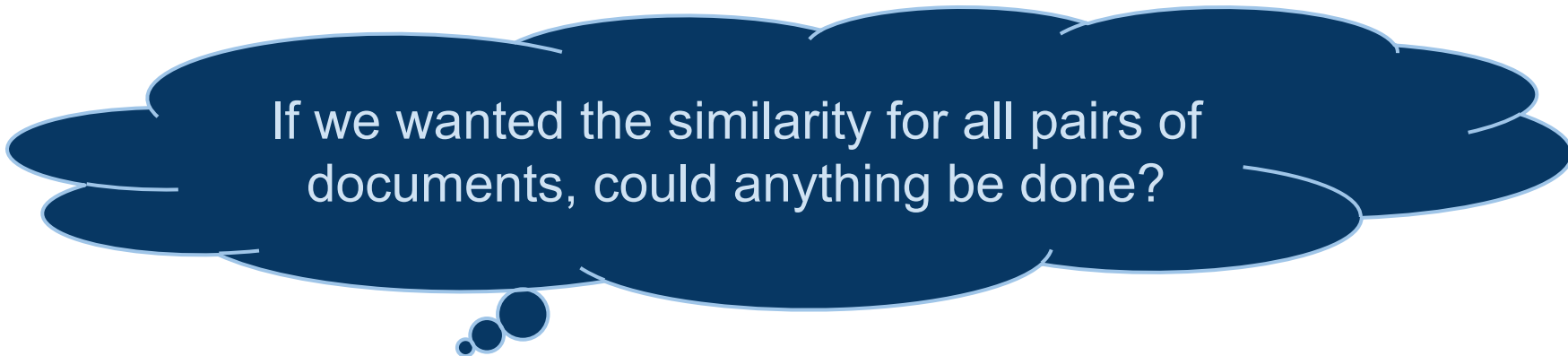
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If we wanted the similarity for all pairs of documents, could anything be done?

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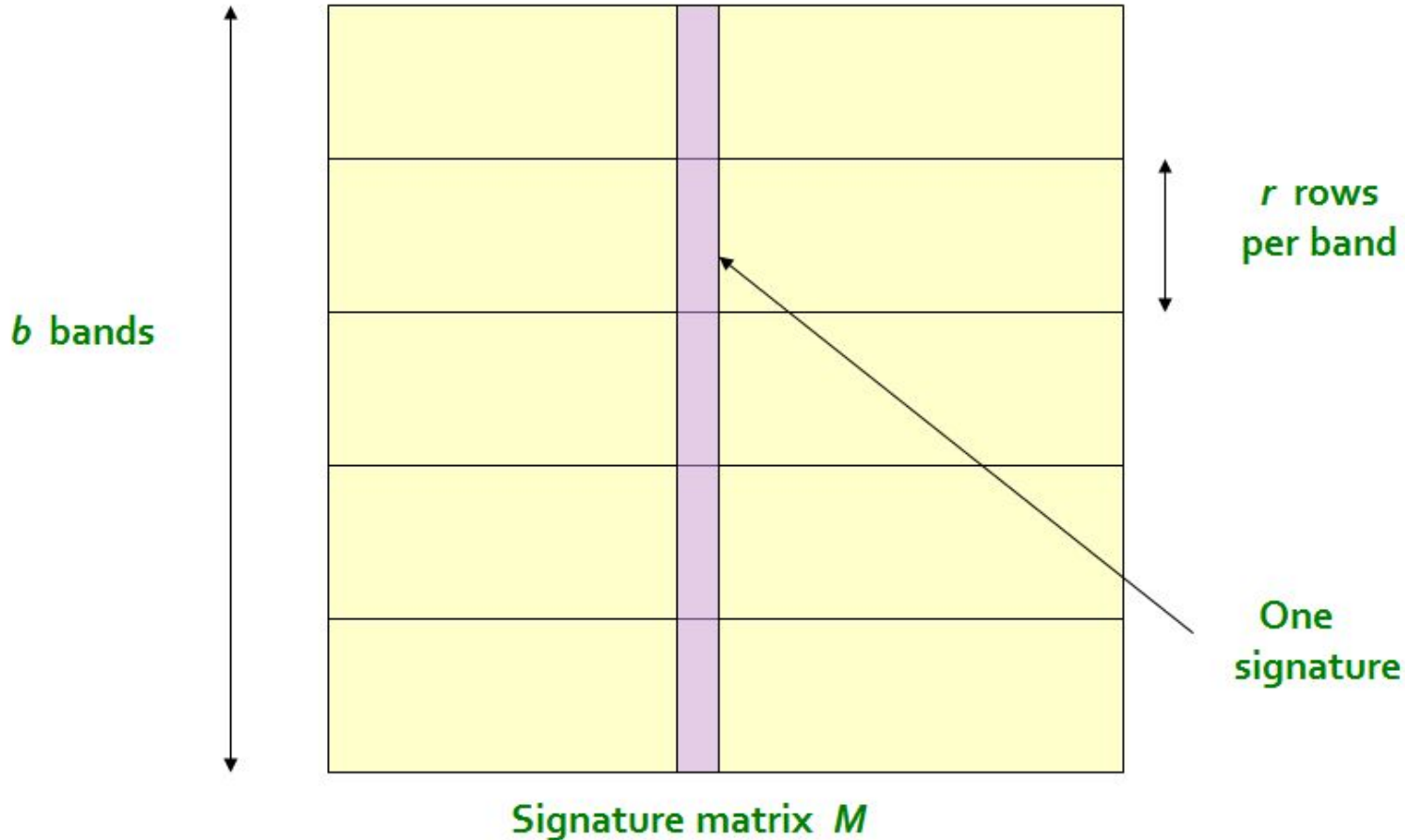
**Approach:** Hash multiple times over subsets of data: similar items are likely in the same bucket once.

**Approach from MinHash:** Hash columns of signature matrix

➡ Candidate pairs end up in the same bucket.

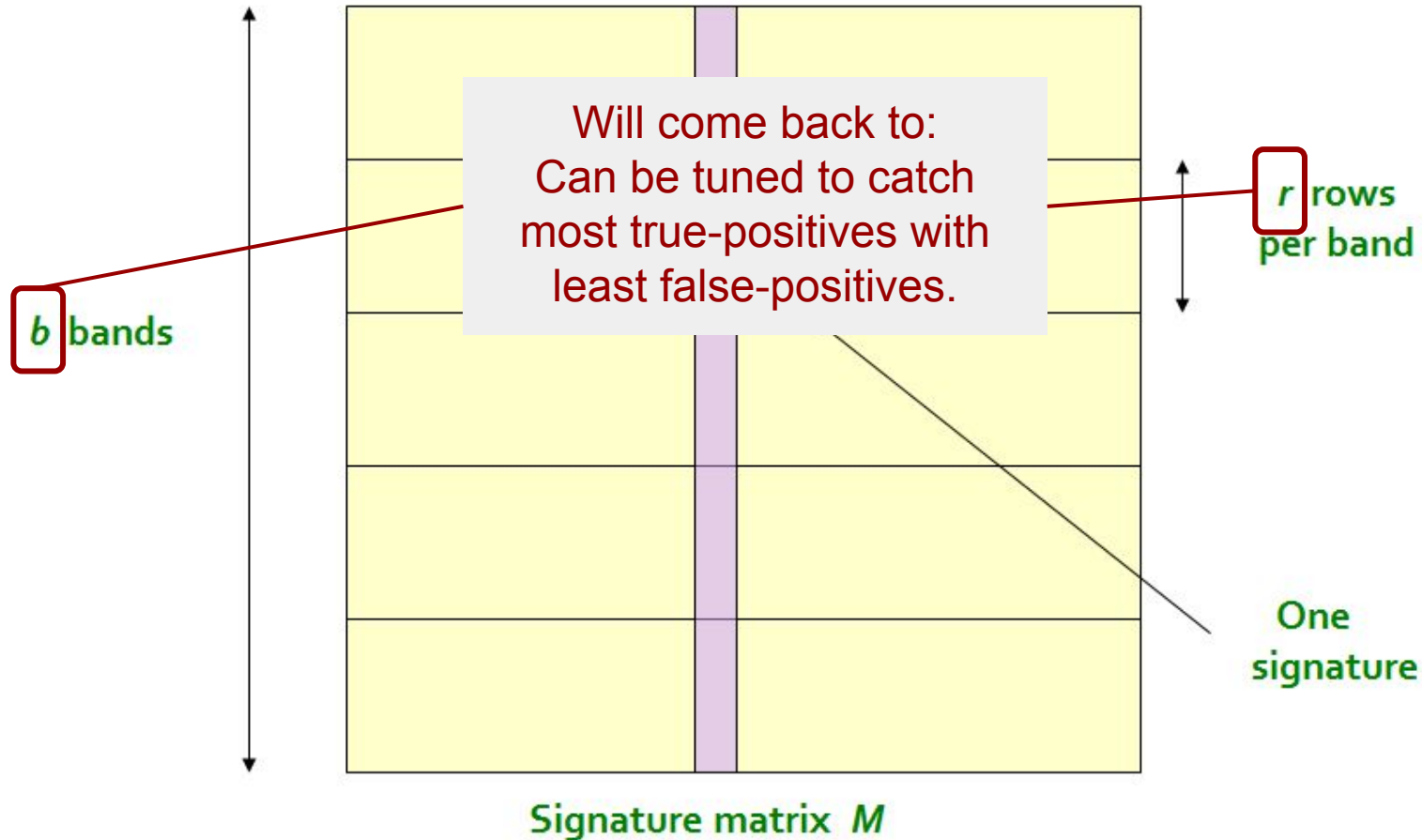
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Step 1: Divide signature matrix into  $b$  bands



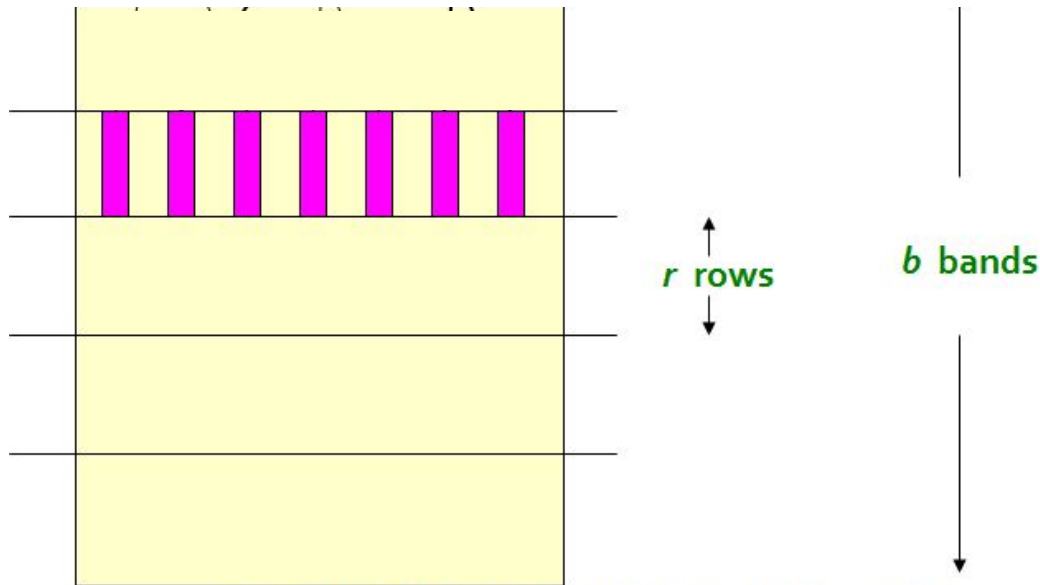
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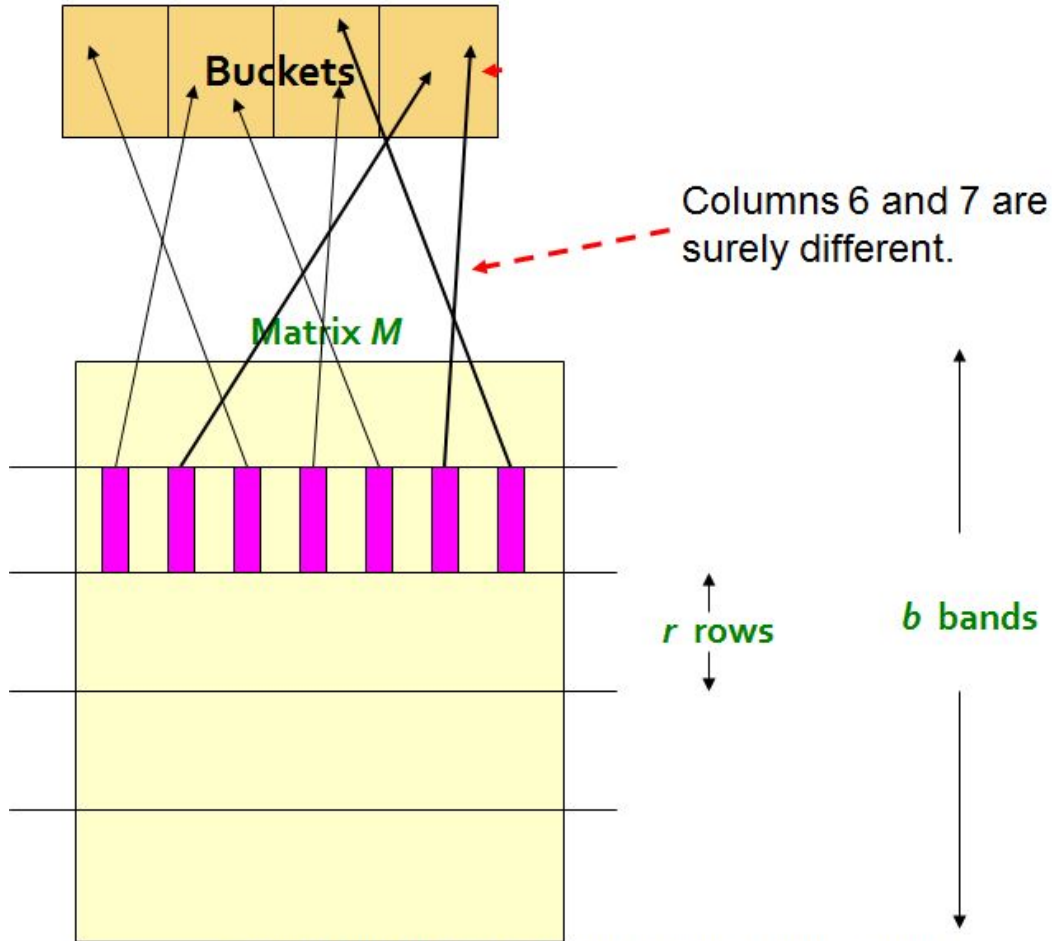
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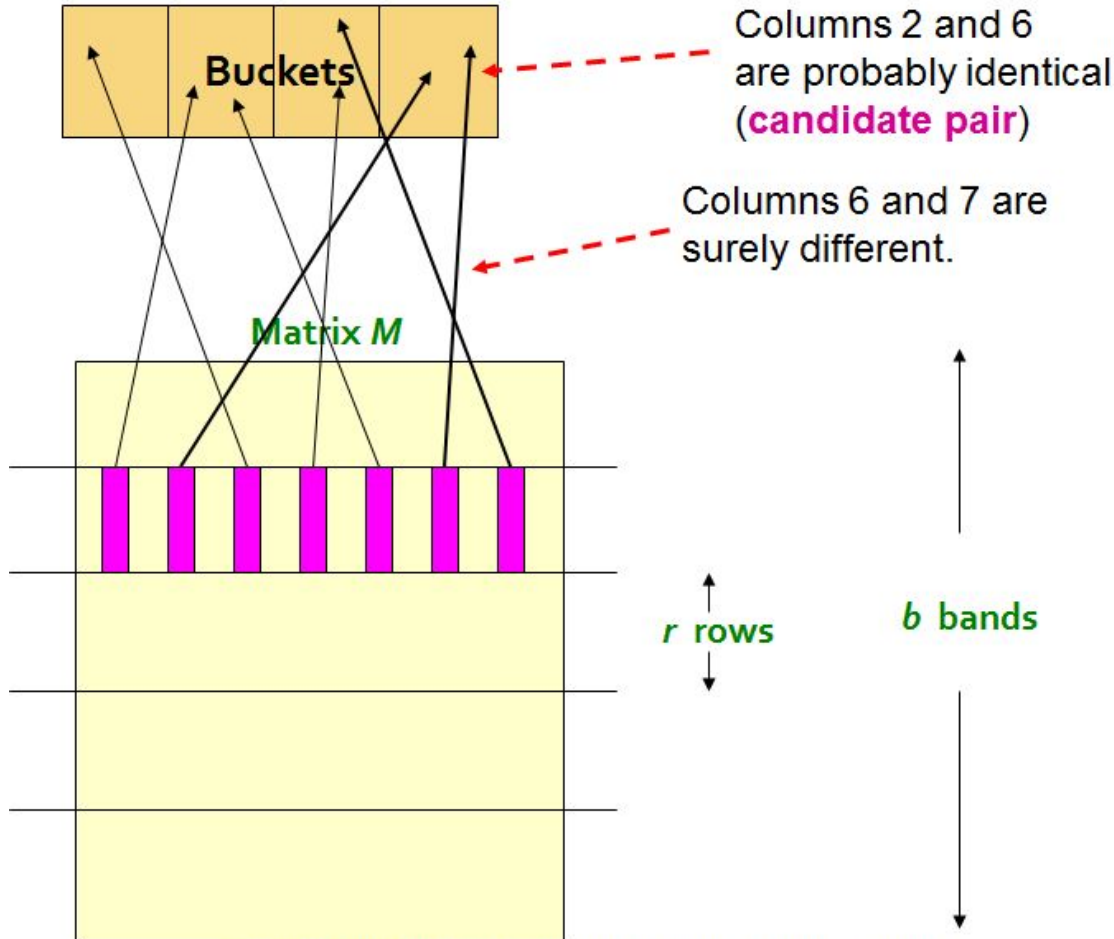
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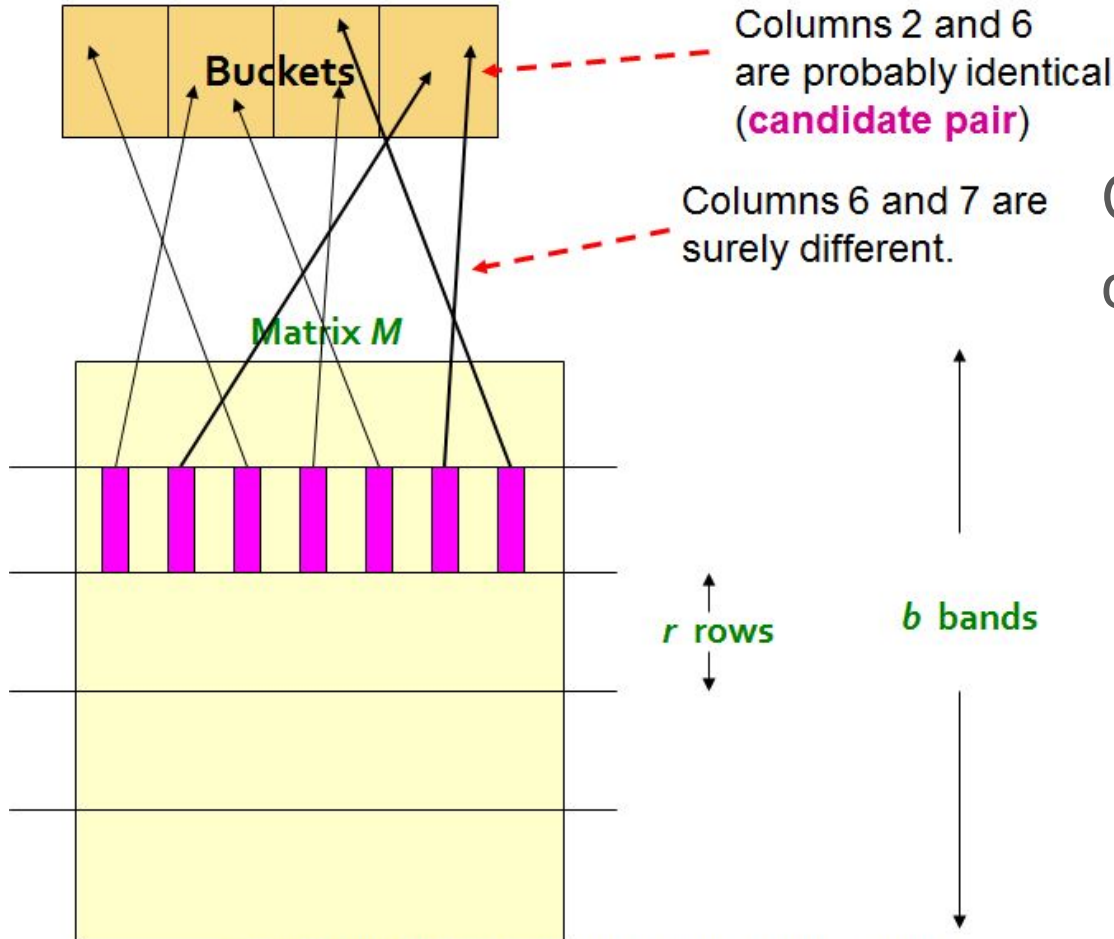
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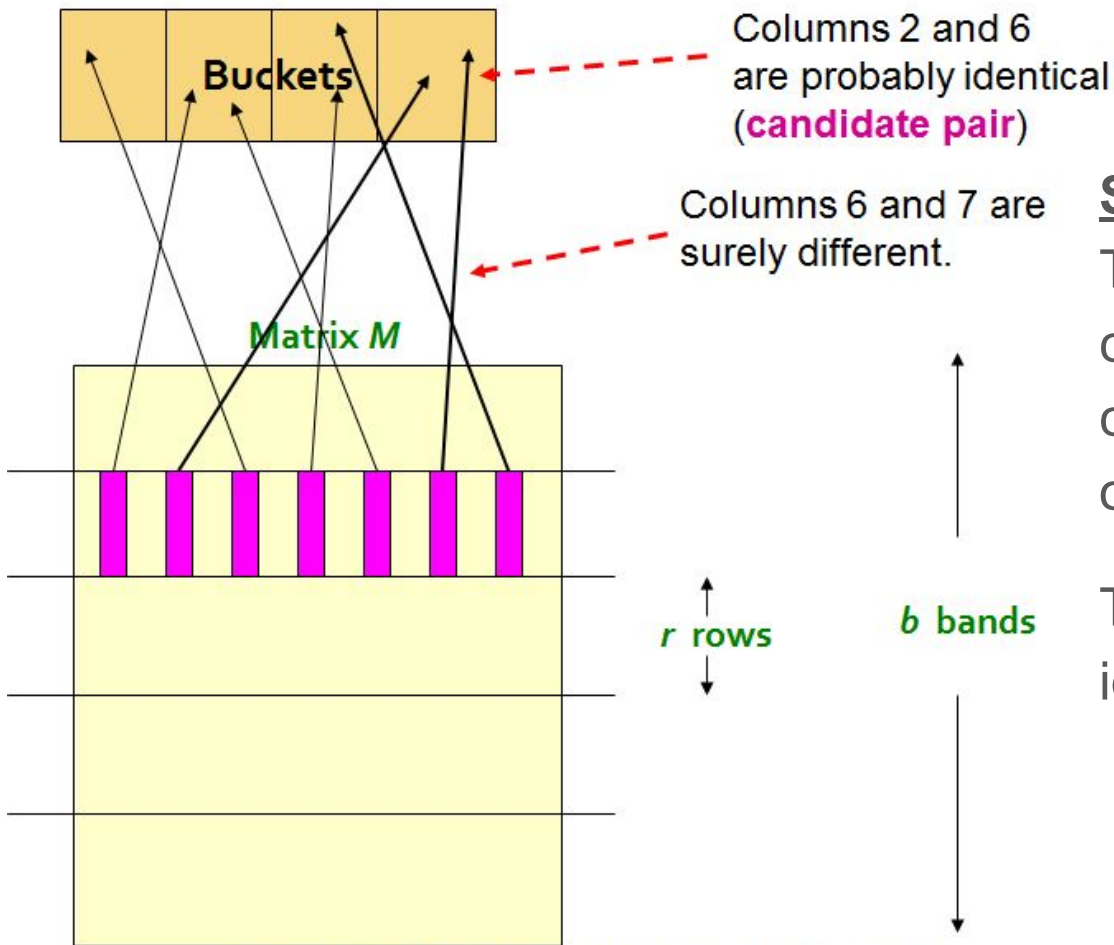


Criteria for being candidate pair:

- They end up in same bucket for at least 1 band.

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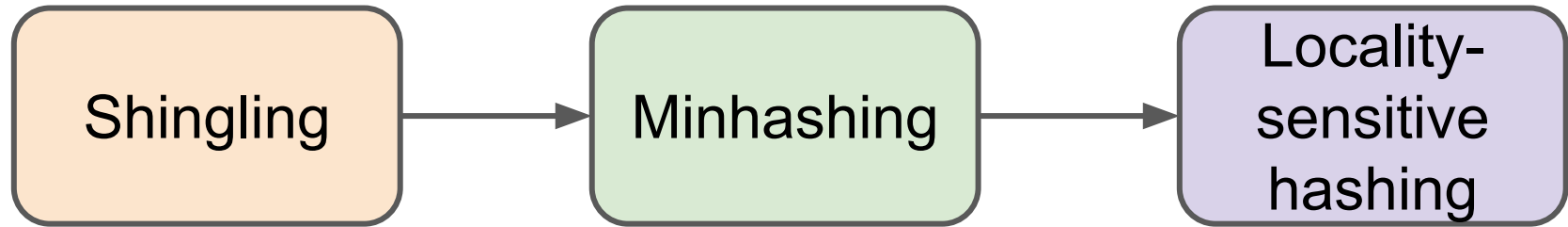


## Simplification:

There are enough buckets compared to rows per band that columns must be identical in order to hash into same bucket.

Thus, we only need to check if identical within a band.

# Document-Similarity Pipeline



# Probability of Agreement

- 100,000 documents
- 100 random permutations/hash functions/rows
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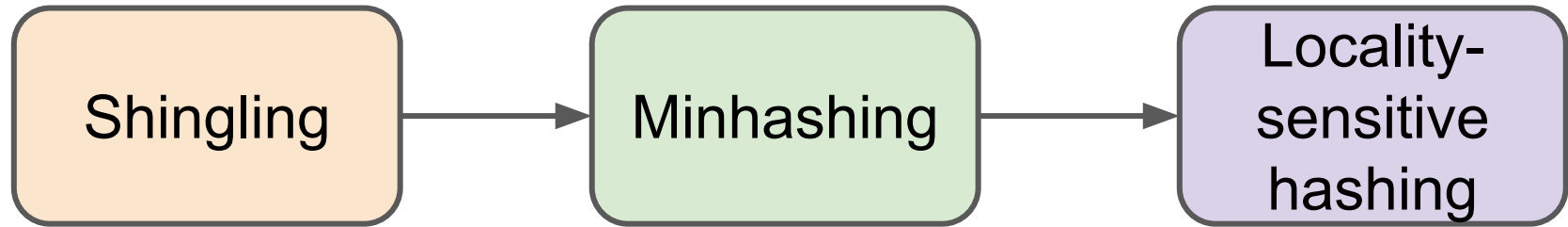
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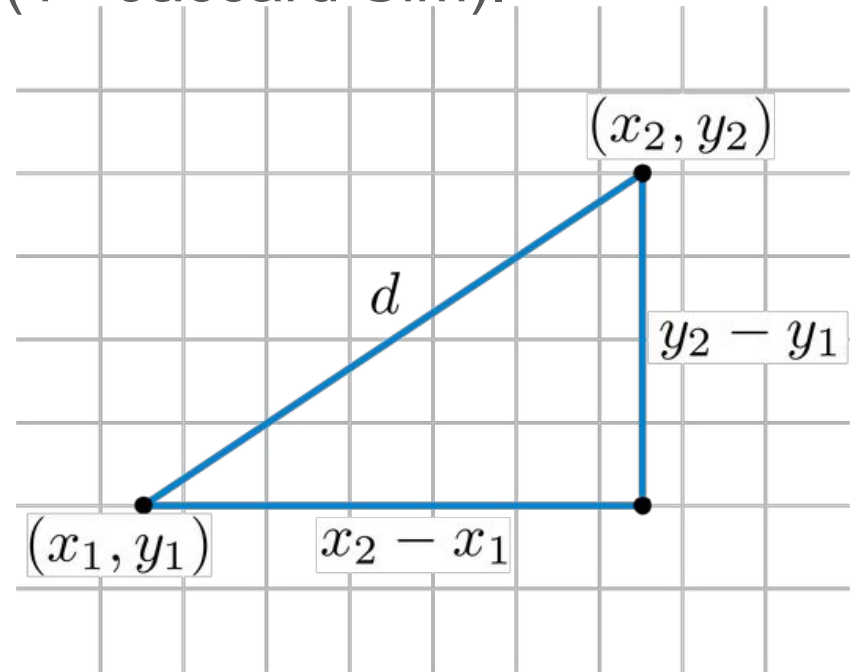
What if wanting 40% Jaccard Similarity?

# Similarity Search



# Distance Metrics

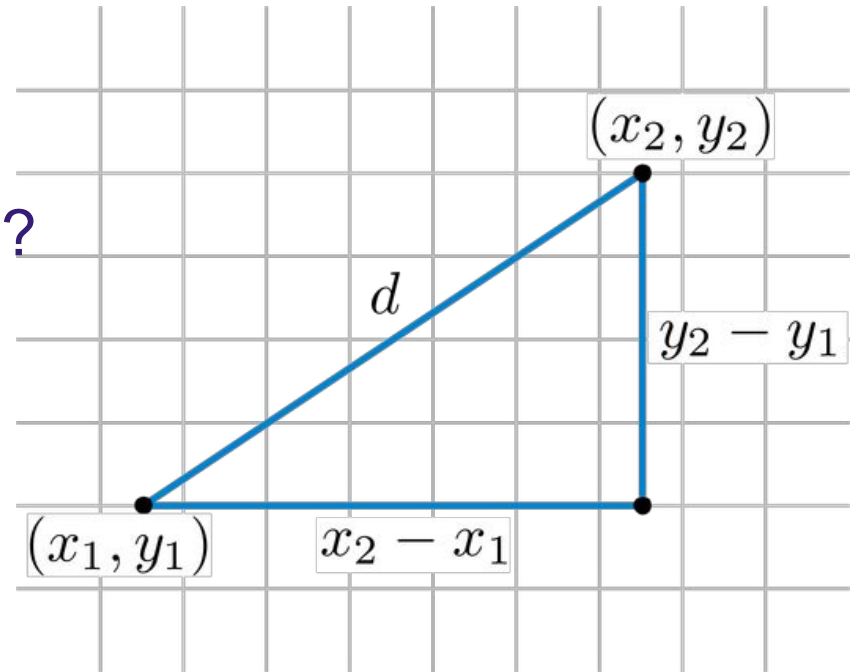
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Typical properties of a distance metric,  $d(\text{point1}, \text{point2})$ ?



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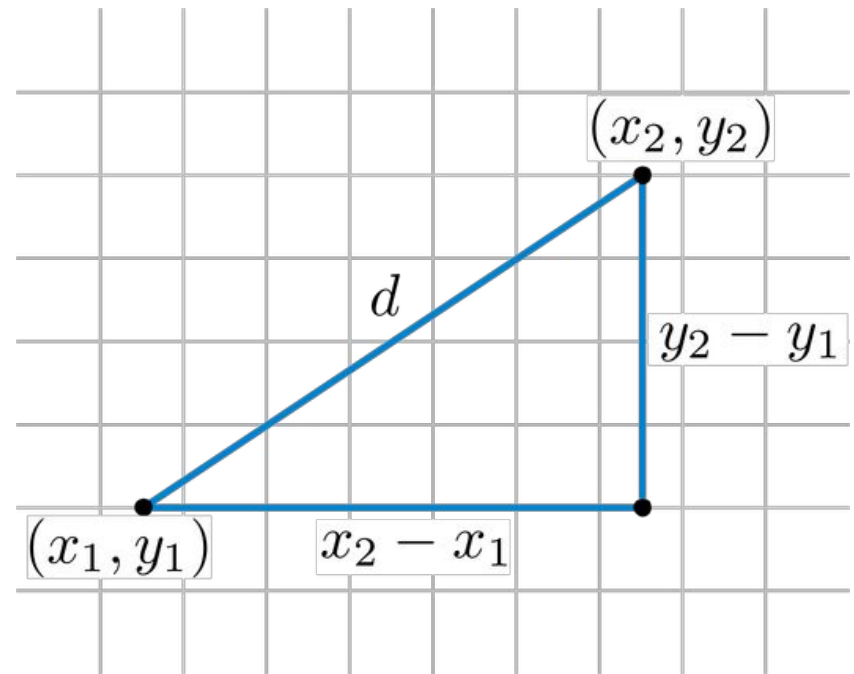
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Typical properties of a distance metric,  $d$ :

$$d(a, a) = 0$$

$$d(a, b) = d(b, a)$$

$$d(a, b) \leq d(a, c) + d(c, b)$$



# Distance Metrics

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There are other metrics of similarity. e.g:

- Euclidean Distance
- Cosine Distance
- ...
- Edit Distance
- Hamming Distance



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$$distance(X, Y) = \sqrt{\sum_i^n (x_i - y_i)^2} \quad (\text{"L2 Norm"})$$

- Cosine Distance

...

- Edit Distance

- Hamming Distance

# Distance Metrics

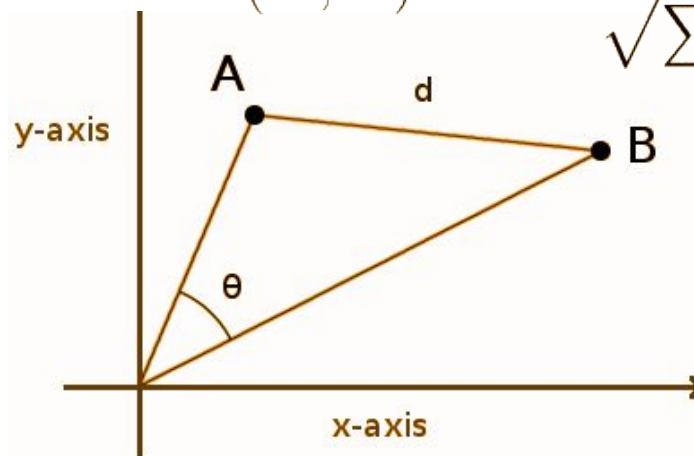
Pipeline gives us a way to find *near-neighbors* in *high-dimensional space* based on Jaccard Distance (1 - Jaccard Sim).

There are other metrics of similarity. e.g:

- Euclidean Distance
- Cosine Distance
- ...
- Edit Distance
- Hamming Distance

$$distance(X, Y) = \sqrt{\sum_i^n (x_i - y_i)^2} \quad (\text{"L2 Norm"})$$

$$distance(X, Y) = 1 - \frac{\sum x_i y_i}{\sqrt{\sum x_i^2} \sqrt{\sum y_i^2}}$$



# Distance Metrics

## Locality Sensitive Hashing - Theory

LSH Can be generalized to many distance metrics by converting output to a probability and providing a lower bound on probability of being similar.

E.g. for euclidean distance:

- Choose random lines (analogous to hash functions in minhashing)
- Project the two points onto each line; match if two points within an interval