

# CSE 5243 INTRO. TO DATA MINING

## Locality Sensitive Hashing (LSH) & Graph Data

Huan Sun, CSE@The Ohio State University

# Min-Hashing Example

Permutation  $\pi$

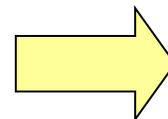
2	4	3
3	2	4
7	1	7
6	3	2
1	6	6
5	7	1
4	5	5

Input matrix (Shingles x Documents)

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

Signature matrix  $M$

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



Similarities:

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

# Implementation Trick

- **Permuting rows even once is prohibitive**
- **Row hashing!**
  - Pick  $K = 100$  hash functions  $k_i$
  - Ordering under  $k_i$  gives a random row permutation!
- **One-pass implementation**
  - For each column  $C$  and hash-func.  $k_i$  keep a “slot” for the min-hash value
  - Initialize all  $\text{sig}(C)[i] = \infty$
  - **Scan rows looking for 1s**
    - Suppose row  $j$  has 1 in column  $C$
    - Then for each  $k_i$ :
      - If  $k_i(j) < \text{sig}(C)[i]$ , then  $\text{sig}(C)[i] \leftarrow k_i(j)$

**How to pick a random hash function  $h(x)$ ?**

**Universal hashing:**

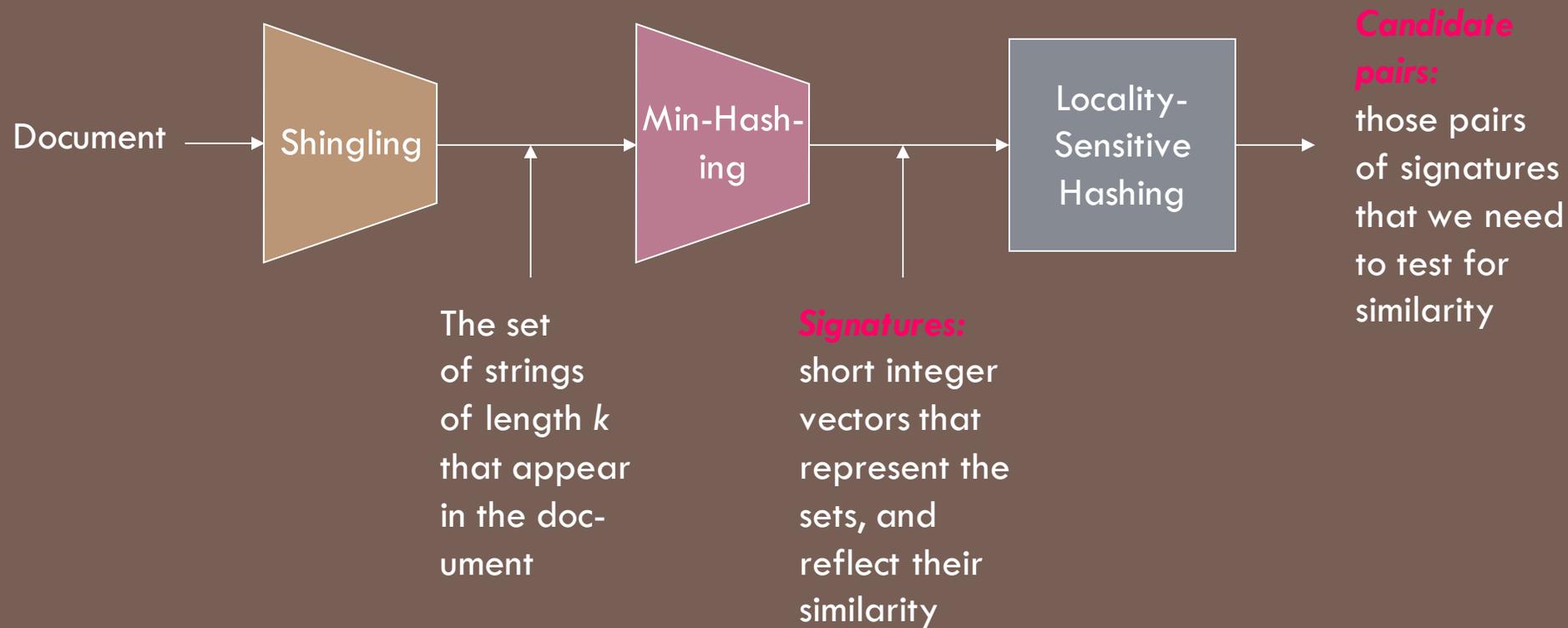
$h_{a,b}(x) = ((a \cdot x + b) \bmod p) \bmod N$   
where:

$a, b$  ... random integers

$p$  ... prime number ( $p > N$ )

More details:

Section 3.3.5 in J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>



## LOCALITY SENSITIVE HASHING

**Step 3: *Locality-Sensitive Hashing:*** Focus on pairs of signatures likely to be from similar documents **(Optional, See backup slides)**

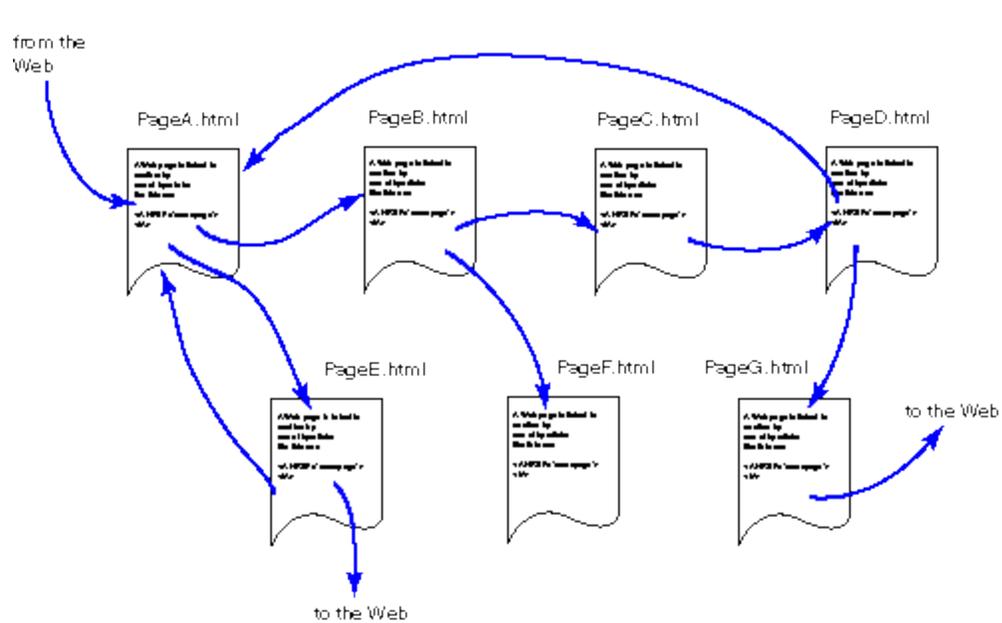
Chapter 4 Graph Data:

<http://www.dataminingbook.info/pmwiki.php/Main/BookPathUploads?action=downloadman&upname=book-20160121.pdf> ,  
<http://www.dataminingbook.info/pmwiki.php>

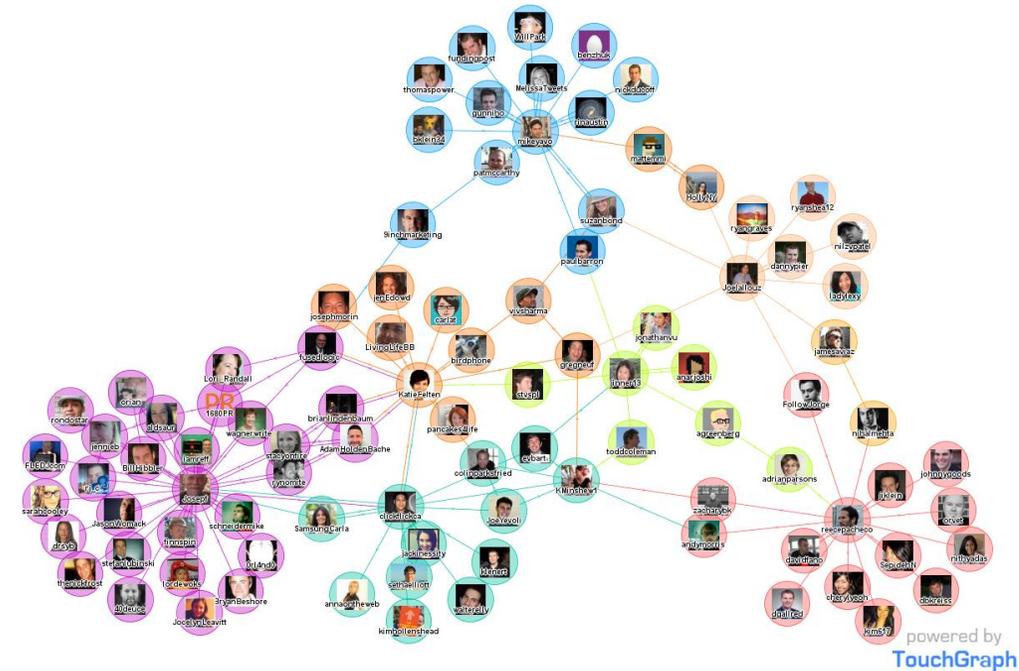
# GRAPH BASICS AND A GENTLE INTRODUCTION TO PAGERANK

Slides adapted from Prof. Srinivasan Parthasarathy @OSU

# Graphs from the Real World



The Web: hyperlinked docs



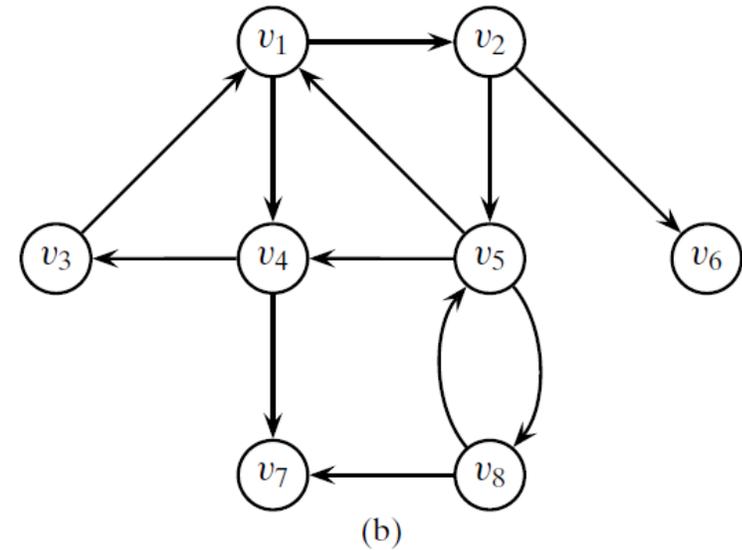
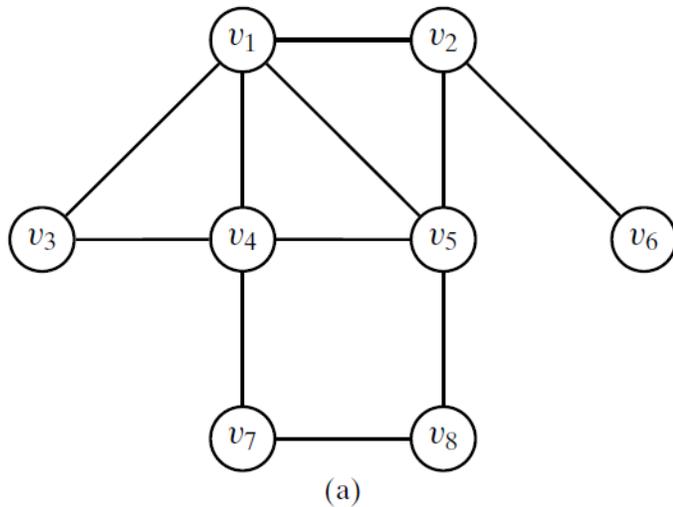
Social networks

[https://chortle.ccsu.edu/Java5/Notes/appendixA/htmlPart2\\_6.html](https://chortle.ccsu.edu/Java5/Notes/appendixA/htmlPart2_6.html)

<http://www.touchgraph.com/news>

# Primitives and Notations

- $G = (V, E)$ 
  - ▣  $E \subseteq V \times V$ , and can also be represented as an adjacency matrix.
- Undirected vs. directed graph

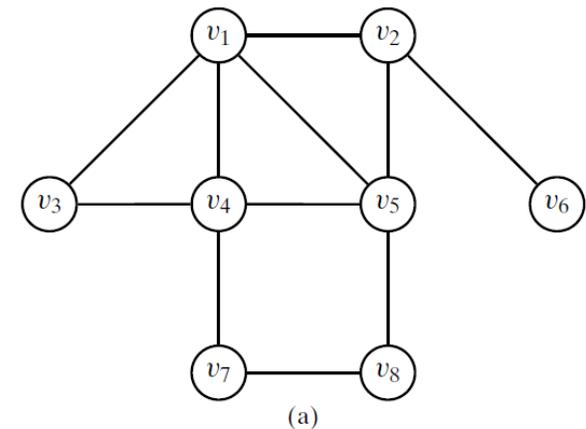


A directed edge  $(v_i, v_j)$  is also called an *arc*, and is said to be *from*  $v_i$  *to*  $v_j$ . We also say that  $v_i$  is the *tail* and  $v_j$  the *head* of the arc.

# Primitives and Notations

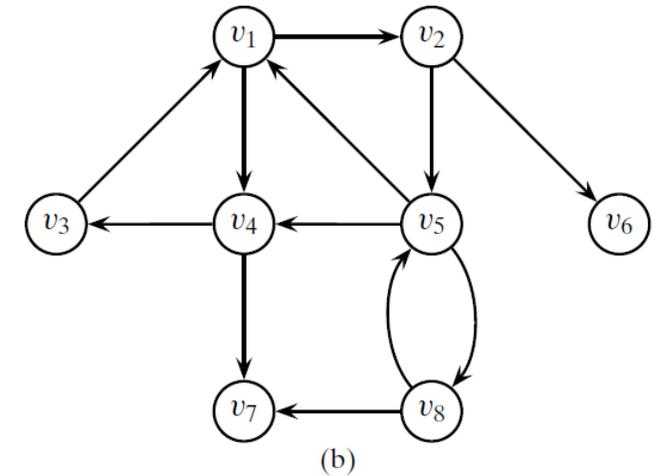
- $G = (V, E)$ 
  - ▣  $E$  can also be represented as an adjacency matrix
- Undirected vs. directed graph
- Degree

The *degree* of a node  $v_i \in V$  is the number of edges incident with it



# Primitives and Notations

- $G = (V, E)$ 
  - ▣  $E$  can also be represented as an adjacency matrix
- Undirected vs. directed graph
- Degree



For directed graphs, the *indegree* of node  $v_i$ , denoted as  $id(v_i)$ , is the number of edges with  $v_i$  as head, that is, the number of incoming edges at  $v_i$ . The *outdegree* of  $v_i$ , denoted  $od(v_i)$ , is the number of edges with  $v_i$  as the tail, that is, the number of outgoing edges from  $v_i$ .

# Primitives and Notations

- $G = (V, E)$ 
  - ▣  $E$  can also be represented as an adjacency matrix
- Undirected vs. directed graph
- Degree
- (Shortest) distance between two vertices

The *eccentricity* of a node  $v_i$  is the maximum distance from  $v_i$  to any other node in the graph:

$$\text{Eccentricity}(v) = \max_{u \neq v} \text{dist}(u, v)$$

# Primitives and Notations

- $G = (V, E)$ 
  - ▣  $E$  can also be represented as an adjacency matrix
- Undirected vs. directed graph
- Degree
- (Shortest) distance between two vertices

The *eccentricity* of a node  $v_i$  is the maximum distance from  $v_i$  to any other node in the graph:

$$\text{Eccentricity}(v) = \max_{u \neq v} \text{dist}(u, v)$$

# Primitives and Notations

- $G = (V, E)$ 
  - ▣  $E$  can also be represented as an adjacency matrix
- Undirected vs. directed graph
- Degree
- (Shortest) distance between two vertices

The *radius* of a connected graph, denoted  $r(G)$ , is the minimum eccentricity of any node in the graph:

$$\text{Radius}(G) = \min_{v \in V} \text{Eccentricity}(v)$$

# Primitives and Notations

- $G = (V, E)$ 
  - ▣  $E$  can also be represented as an adjacency matrix
- Undirected vs. directed graph
- Degree
- (Shortest) distance between two vertices

The *diameter*, denoted  $d(G)$ , is the maximum eccentricity of any vertex in the graph:

$$\text{Diameter}(G) = \max_{v \in V} \text{Eccentricity}(v)$$

# Properties of Nodes

- Centrality: how “central” or important a node is in the graph
  - ▣ How close the node is to all other nodes?

$$\text{Closeness Centrality}(v) = \frac{1}{\sum_{u \neq v} \text{dist}(u, v)}$$

A node  $v_i$  with the smallest total distance,  $\sum_j d(v_i, v_j)$ , is called the *median node*.

# Properties of Nodes

- Centrality: how “central” or important a node is in the graph
  - ▣ How close the node is to all other nodes?
  - ▣ How much is a node a “choke point”?

Betweenness centrality: How many shortest paths between all pairs of vertices include  $v_i$ .

$$\gamma_{jk}(v_i) = \frac{\eta_{jk}(v_i)}{\eta_{jk}} : \text{the fraction of shortest paths between vertices } v_j \text{ and } v_k \text{ through } v_i$$

The betweenness centrality for a node  $v_i$  is defined as

$$c(v_i) = \sum_{j \neq i} \sum_{\substack{k \neq i \\ k > j}} \gamma_{jk}(v_i) = \sum_{j \neq i} \sum_{\substack{k \neq i \\ k > j}} \frac{\eta_{jk}(v_i)}{\eta_{jk}}$$

# Properties of Nodes

- Clustering coefficient: how much does a node cluster with neighbors

- ▣ Local clustering coefficient

The **local clustering coefficient** of a vertex (node) in a graph quantifies how close its neighbors are to being a clique (complete graph).

The proportion of links between the vertices within its neighbourhood divided by the number of links that could possibly exist between them.

# Background

---

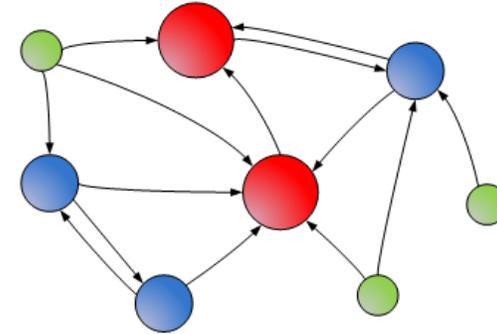
- Besides the keywords, what other evidence can one use to rate the importance of a webpage?

# Background

- Besides the keywords, what other evidence can one use to rate the importance of a webpage?
- Solution: Use the hyperlink structure
- E.g. a webpage linked by many webpages is probably important.
  - ▣ but this method is not global (comprehensive).
- PageRank is developed by Larry Page in 1998.

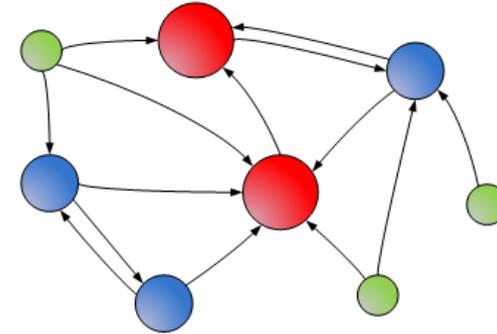
# Idea

- A graph representing WWW
  - ▣ Node: webpage
  - ▣ Directed edge: hyperlink



# Idea

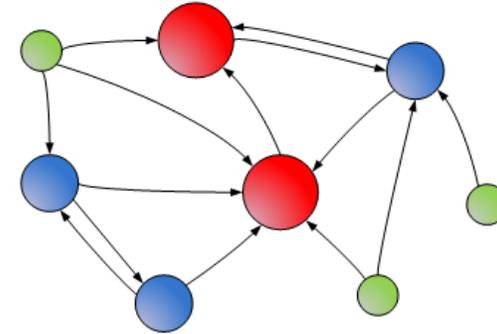
- A graph representing WWW
  - ▣ Node: webpage
  - ▣ Directed edge: hyperlink



- A user randomly clicks the hyperlink to surf WWW.
  - ▣ The probability a user stop in a particular webpage is the PageRank value.

# Idea

- A graph representing WWW
  - ▣ Node: webpage
  - ▣ Directed edge: hyperlink
- A user randomly clicks the hyperlink to surf WWW.
  - ▣ The probability a user stop in a particular webpage is the PageRank value.
- A node that is linked by many nodes with high PageRank value receives a high rank itself;  
If there are no links to a node, then there is no support for that page.



# Formal Formulation

Let  $G = (V, E)$  be a directed graph, with  $|V| = n$ . The adjacency matrix of  $G$  is an  $n \times n$  asymmetric matrix  $\mathbf{A}$  given as

$$\mathbf{A}(u, v) = \begin{cases} 1 & \text{if } (u, v) \in E \\ 0 & \text{if } (u, v) \notin E \end{cases}$$

Let  $p(u)$  be a positive real number, called the *prestige* score for node  $u$ .

$$\begin{aligned} p(v) &= \sum_u \mathbf{A}(u, v) \cdot p(u) \\ &= \sum_u \mathbf{A}^T(v, u) \cdot p(u) \end{aligned}$$

the prestige of a node depends on the prestige of other nodes pointing to it.

# Formal Formulation

Let  $p(u)$  be a positive real number, called the *prestige* score for node  $u$ .

$$\begin{aligned} p(v) &= \sum_u \mathbf{A}(u, v) \cdot p(u) \\ &= \sum_u \mathbf{A}^T(v, u) \cdot p(u) \end{aligned}$$

the prestige of a node depends on the prestige of other nodes pointing to it.

Across all the nodes, we can recursively express the prestige scores as

$$\mathbf{p}' = \mathbf{A}^T \mathbf{p}$$

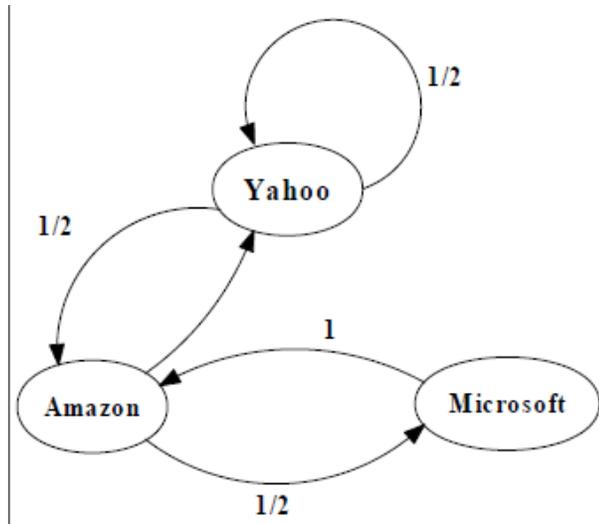
where  $\mathbf{p}$  is an  $n$ -dimensional column vector corresponding to the prestige scores for each vertex.

# Iterative Computation

$$\begin{aligned}\mathbf{p}_k &= \mathbf{A}^T \mathbf{p}_{k-1} \\ &= \mathbf{A}^T (\mathbf{A}^T \mathbf{p}_{k-2}) = (\mathbf{A}^T)^2 \mathbf{p}_{k-2} \\ &= (\mathbf{A}^T)^2 (\mathbf{A}^T \mathbf{p}_{k-3}) = (\mathbf{A}^T)^3 \mathbf{p}_{k-3} \\ &= \vdots \\ &= (\mathbf{A}^T)^k \mathbf{p}_0\end{aligned}$$

where  $\mathbf{p}_0$  is the initial prestige vector. It is well known that the vector  $\mathbf{p}_k$  converges to the dominant eigenvector of  $\mathbf{A}^T$  with increasing  $k$ .

# Example 1



$$M = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix}$$

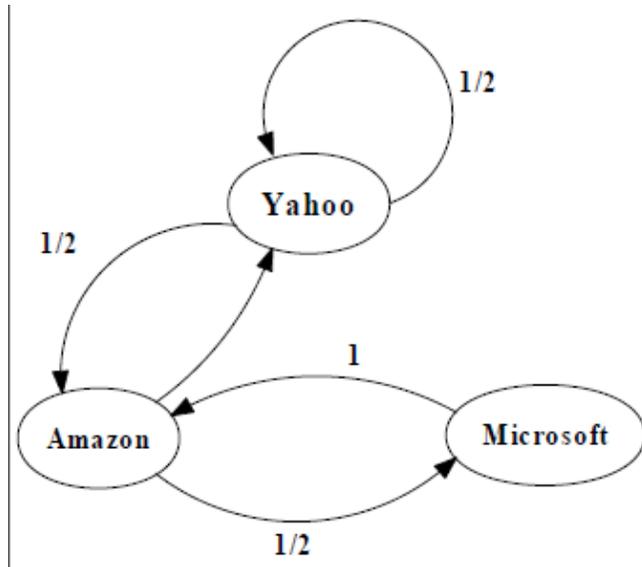
=the transpose of A  
(adjacency matrix)

$$\begin{bmatrix} \text{yahoo} \\ \text{Amazon} \\ \text{Microsoft} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

$$\begin{bmatrix} 1/3 \\ 1/2 \\ 1/6 \end{bmatrix} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix} \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

PageRank Calculation: first iteration

# Example 1



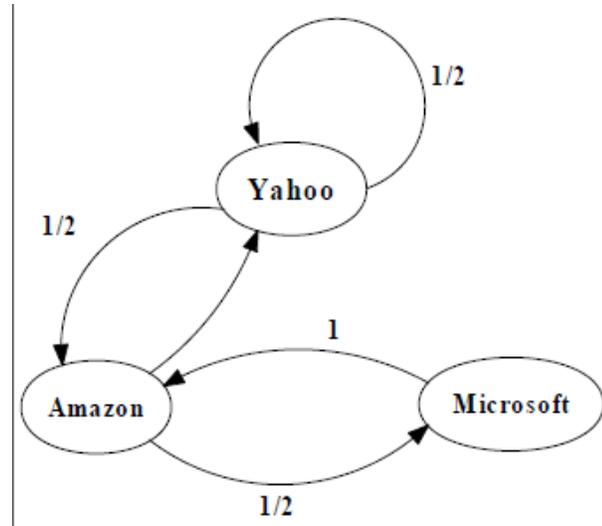
$$M = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix}$$

$$\begin{bmatrix} \text{yahoo} \\ \text{Amazon} \\ \text{Microsoft} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

$$\begin{bmatrix} 5/12 \\ 1/3 \\ 1/4 \end{bmatrix} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix} \begin{bmatrix} 1/3 \\ 1/2 \\ 1/6 \end{bmatrix}$$

PageRank Calculation: second iteration

# Example 1



$$M = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix}$$

$$\begin{bmatrix} \text{yahoo} \\ \text{Amazon} \\ \text{Microsoft} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

$$\begin{bmatrix} 3/8 \\ 11/24 \\ 1/6 \end{bmatrix} \quad \begin{bmatrix} 5/12 \\ 17/48 \\ 11/48 \end{bmatrix} \quad \dots \quad \begin{bmatrix} 2/5 \\ 2/5 \\ 1/5 \end{bmatrix}$$

Convergence after some iterations

# A simple version

$$R(u) = \sum_{v \in B_u} \frac{R(v)}{N_v}$$

- $u$ : a webpage
- $B_u$ : the set of  $u$ 's backlinks
- $N_v$ : the number of forward links of page  $v$
  
- Initially,  $R(u)$  is  $1/N$  for every webpage
- Iteratively update each webpage's PR value until convergence.

# A little more advanced version

- Adding a **damping factor  $d$**
- Imagine that a surfer would stop clicking a hyperlink with probability  $1-d$

$$R(u) = \frac{(1-d)}{N-1} + d \sum_{v \in B_u} \frac{R(v)}{N_v}$$

- $R(u)$  is at least  $(1-d)/(N-1)$ 
  - ▣  $N$  is the total number of nodes.

# Other applications

- Social network (Facebook, Twitter, etc)
  - ▣ Node: Person; Edge: Follower / Followee / Friend
  - ▣ Higher PR value: Celebrity
- Citation network
  - ▣ Node: Paper; Edge: Citation
  - ▣ Higher PR values: Important Papers.
- Protein-protein interaction network
  - ▣ Node: Protein; Edge: Two proteins bind together
  - ▣ Higher PR values: Essential proteins.

43

# Backup slides

# LSH: First Cut

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

- **Goal:** Find documents with Jaccard similarity at least  $s$  (for some similarity threshold, e.g.,  $s=0.8$ )
- **LSH – General idea:** Use a function  $f(x,y)$  that tells whether  $x$  and  $y$  is a **candidate pair**: a pair of elements whose similarity must be evaluated
- **For Min-Hash matrices:**
  - Hash columns of **signature matrix  $M$**  to many buckets
  - Each pair of documents that hashes into the same bucket is a **candidate pair**

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

# Candidates from Min-Hash

- Pick a similarity threshold  $s$  ( $0 < s < 1$ )
- Columns  $x$  and  $y$  of  $M$  are a **candidate pair** if their signatures agree on at least fraction  $s$  of their rows:  
 $M(i, x) = M(i, y)$  for at least frac.  $s$  values of  $i$ 
  - We expect documents  $x$  and  $y$  to have the same (Jaccard) similarity as their signatures

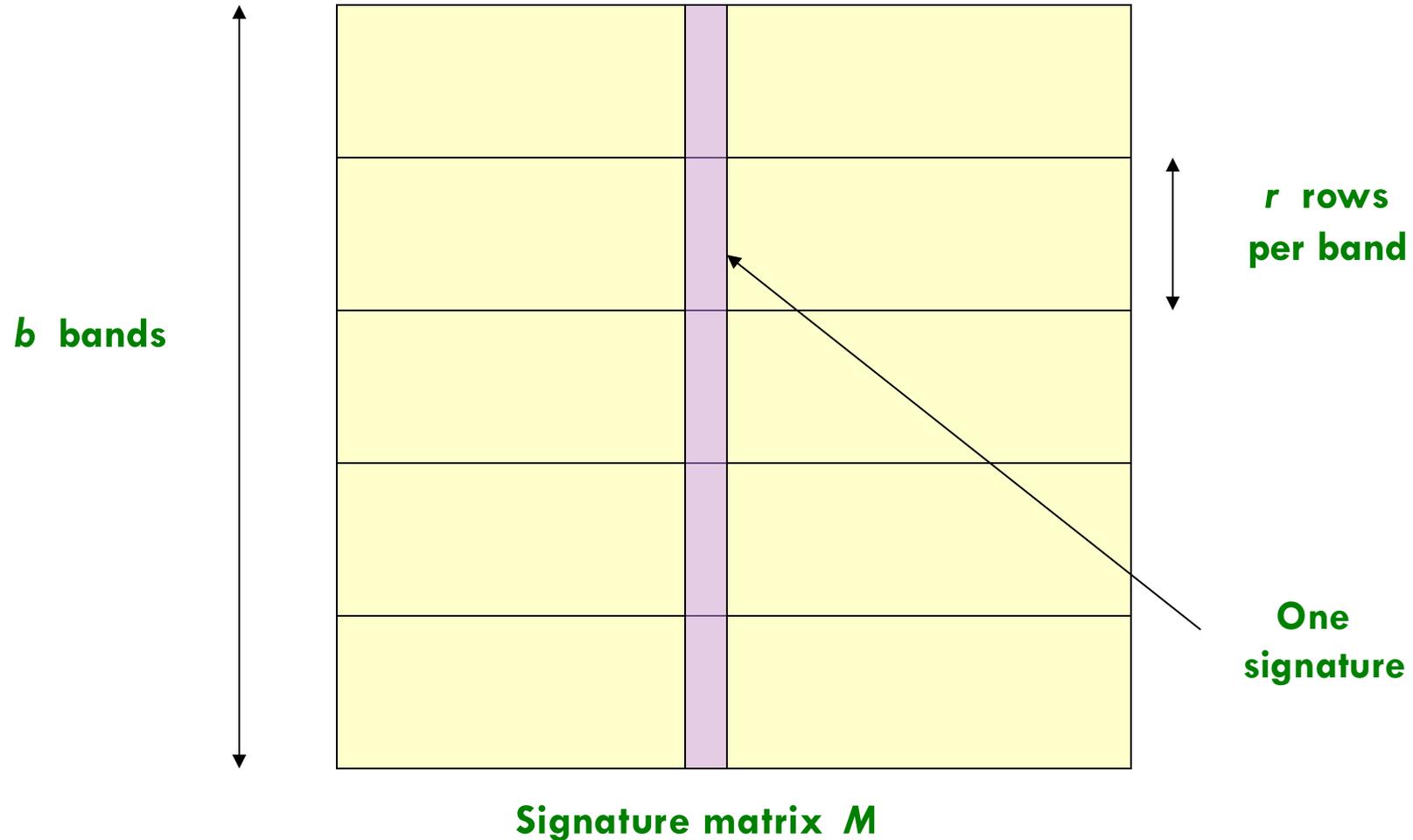
2	1	4	1
1	2	1	2
2	1	2	1

# LSH for Min-Hash

- **Big idea: Hash columns of signature matrix  $M$  several times**
- Arrange that (only) **similar columns** are likely to **hash to the same bucket**, with high probability
- **Candidate pairs are those that hash to the same bucket**

# Partition $M$ into $b$ Bands

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



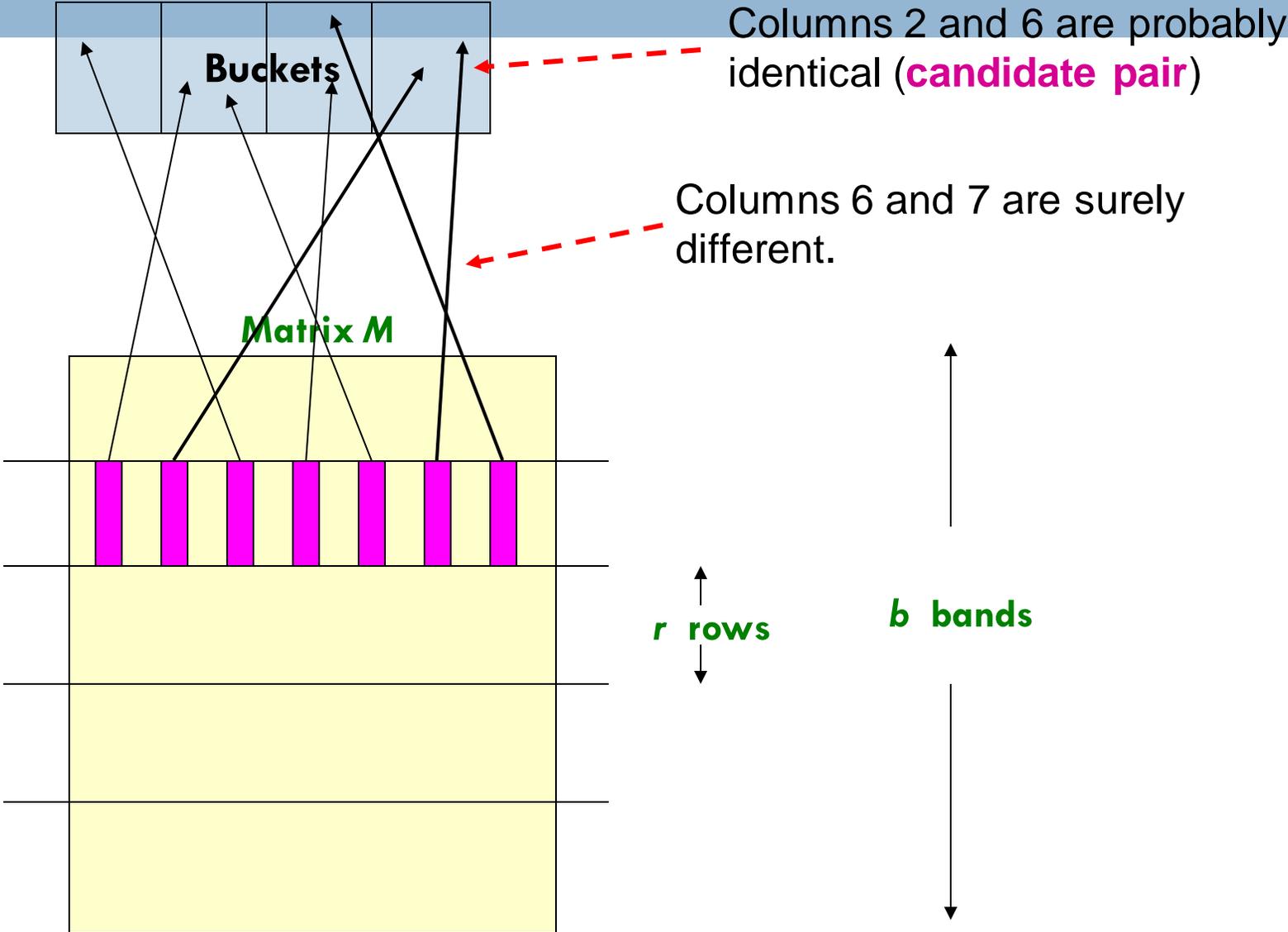
# Partition $M$ into Bands

- Divide matrix  $M$  into  $b$  bands of  $r$  rows
- For each band, hash its portion of each column to a hash table with  $k$  buckets
  - Make  $k$  as large as possible

# Partition $M$ into Bands

- Divide matrix  $M$  into  $b$  bands of  $r$  rows
- For each band, hash its portion of each column to a hash table with  $k$  buckets
  - Make  $k$  as large as possible
- **Candidate** column pairs are those that hash to the same bucket for  $\geq 1$  band
- Tune  $b$  and  $r$  to catch most similar pairs, but few non-similar pairs

# Hashing Bands



# Simplifying Assumption

- There are **enough buckets** that columns are unlikely to hash to the same bucket unless they are **identical** in a particular band
- Hereafter, we assume that “**same bucket**” means “**identical in that band**”
- Assumption needed only to simplify analysis, not for correctness of algorithm

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

# Example of Bands

## Assume the following case:

- Suppose 100,000 columns of  $M$  (100k docs)
- Signatures of 100 integers (rows)
- Therefore, signatures take 40Mb
- Choose  $b = 20$  bands of  $r = 5$  integers/band
- **Goal:** Find pairs of documents that are at least  $s = 0.8$  similar

# $C_1, C_2$ are 80% Similar

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

- Find pairs of  $\geq s=0.8$  similarity, set  $b=20, r=5$
- Assume:  $\text{sim}(C_1, C_2) = 0.8$ 
  - Since  $\text{sim}(C_1, C_2) \geq s$ , we want  $C_1, C_2$  to be a **candidate pair**: We want them to hash to at **least 1 common bucket** (at least one band is identical)

# $C_1, C_2$ are 80% Similar

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

- Find pairs of  $\geq s=0.8$  similarity, set  $b=20, r=5$
- **Assume:**  $\text{sim}(C_1, C_2) = 0.8$ 
  - Since  $\text{sim}(C_1, C_2) \geq s$ , we want  $C_1, C_2$  to be a **candidate pair**: We want them to hash to at **least 1 common bucket** (at least one band is identical)
- **Probability  $C_1, C_2$  identical in one particular band:**  $(0.8)^5 = 0.328$
- Probability  $C_1, C_2$  are **not** similar in all of the 20 bands:  $(1 - 0.328)^{20} = 0.00035$ 
  - i.e., about 1/3000th of the 80%-similar column pairs are **false negatives** (we miss them)
  - We would find **99.965%** pairs of truly similar documents

# $C_1, C_2$ are 30% Similar

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

- Find pairs of  $\geq s=0.8$  similarity, set  $b=20, r=5$
- **Assume:**  $\text{sim}(C_1, C_2) = 0.3$ 
  - Since  $\text{sim}(C_1, C_2) < s$  we want  $C_1, C_2$  to hash to **NO common buckets** (all bands should be different)

# $C_1, C_2$ are 30% Similar

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

- Find pairs of  $\geq s=0.8$  similarity, set  $b=20, r=5$
- **Assume:**  $\text{sim}(C_1, C_2) = 0.3$ 
  - Since  $\text{sim}(C_1, C_2) < s$  we want  $C_1, C_2$  to hash to **NO common buckets** (all bands should be different)
- **Probability  $C_1, C_2$  identical in one particular band:**  $(0.3)^5 = 0.00243$
- Probability  $C_1, C_2$  identical in at least 1 of 20 bands:  $1 - (1 - 0.00243)^{20} = 0.0474$ 
  - In other words, approximately 4.74% pairs of docs with similarity 30% end up becoming **candidate pairs**
    - They are **false positives** since we will have to examine them (they are candidate pairs) but then it will turn out their similarity is below threshold  $s$

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

# LSH Involves a Tradeoff

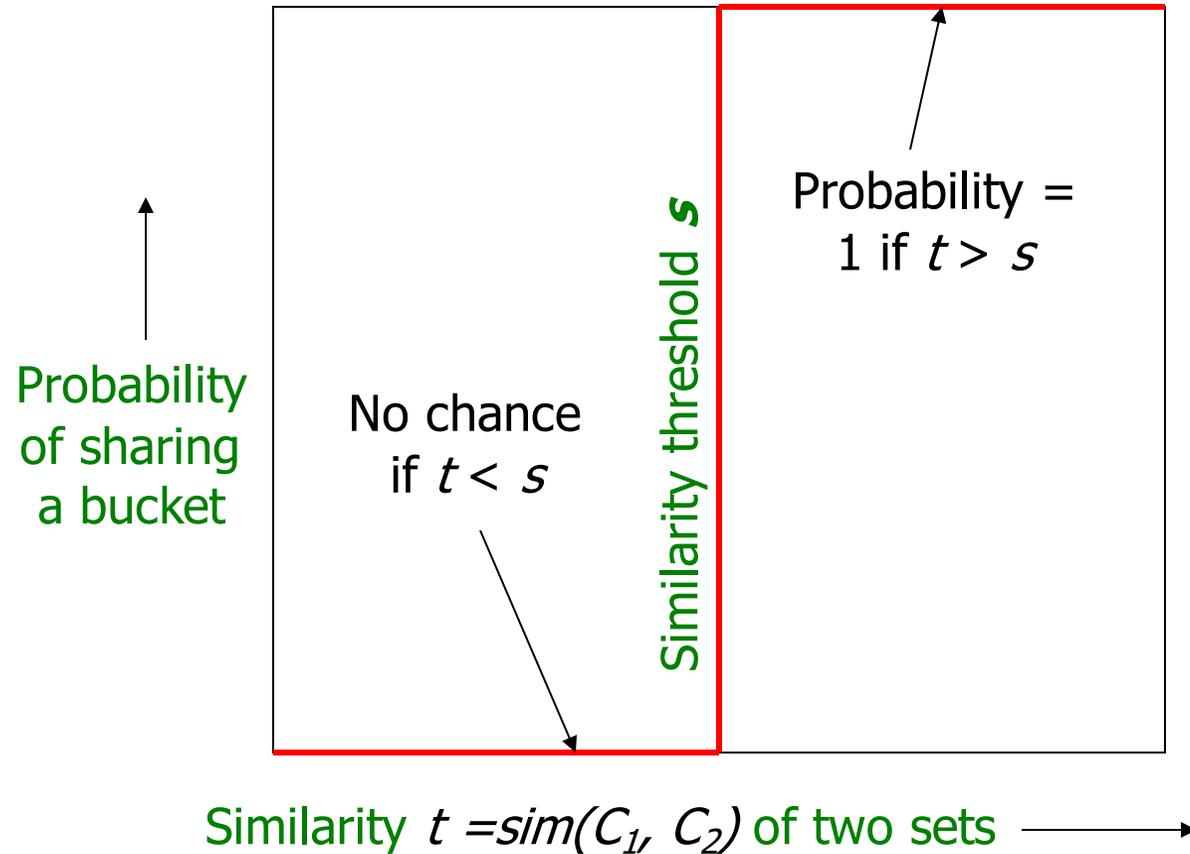
## □ Pick:

- The number of Min-Hashes (rows of  $M$ )
- The number of bands  $b$ , and
- The number of rows  $r$  per band

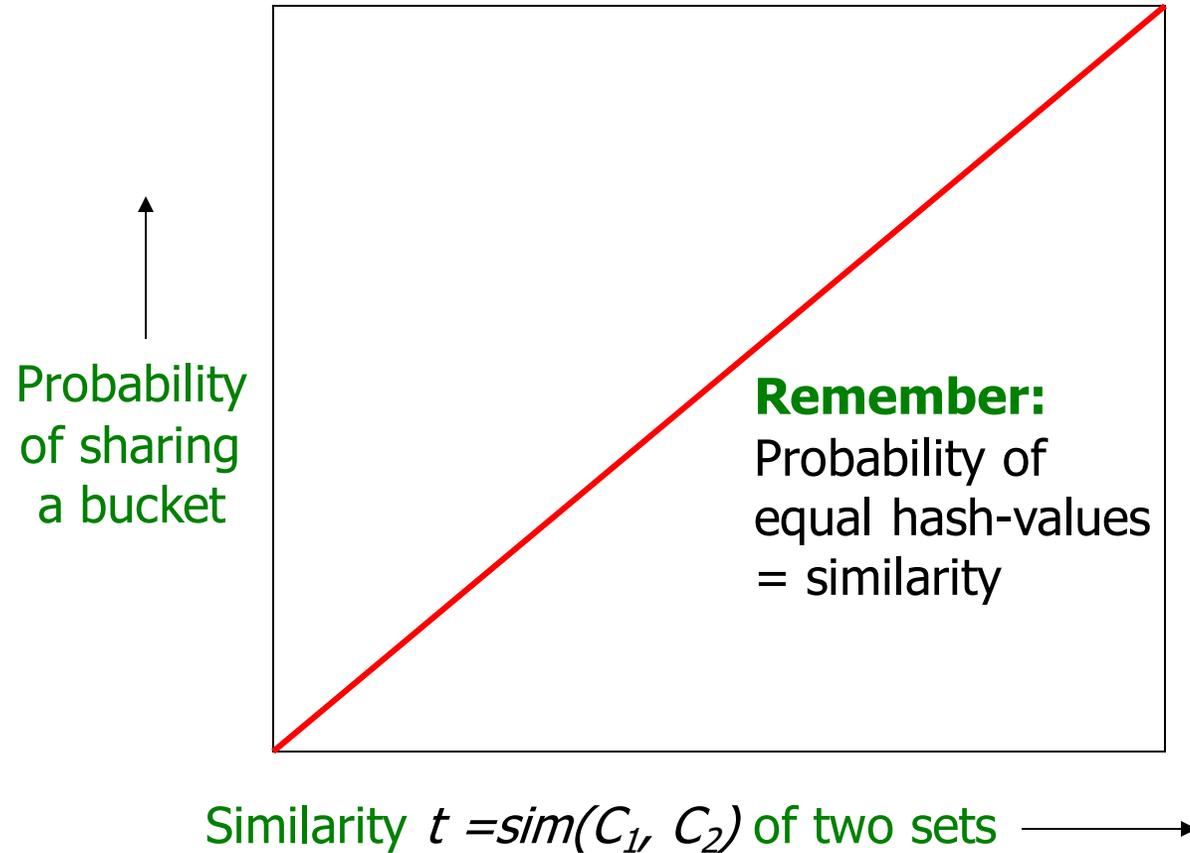
to balance false positives/negatives

- **Example:** If we had only 15 bands of 5 rows, the number of false positives would go down, but the number of false negatives would go up

# Analysis of LSH – What We Want



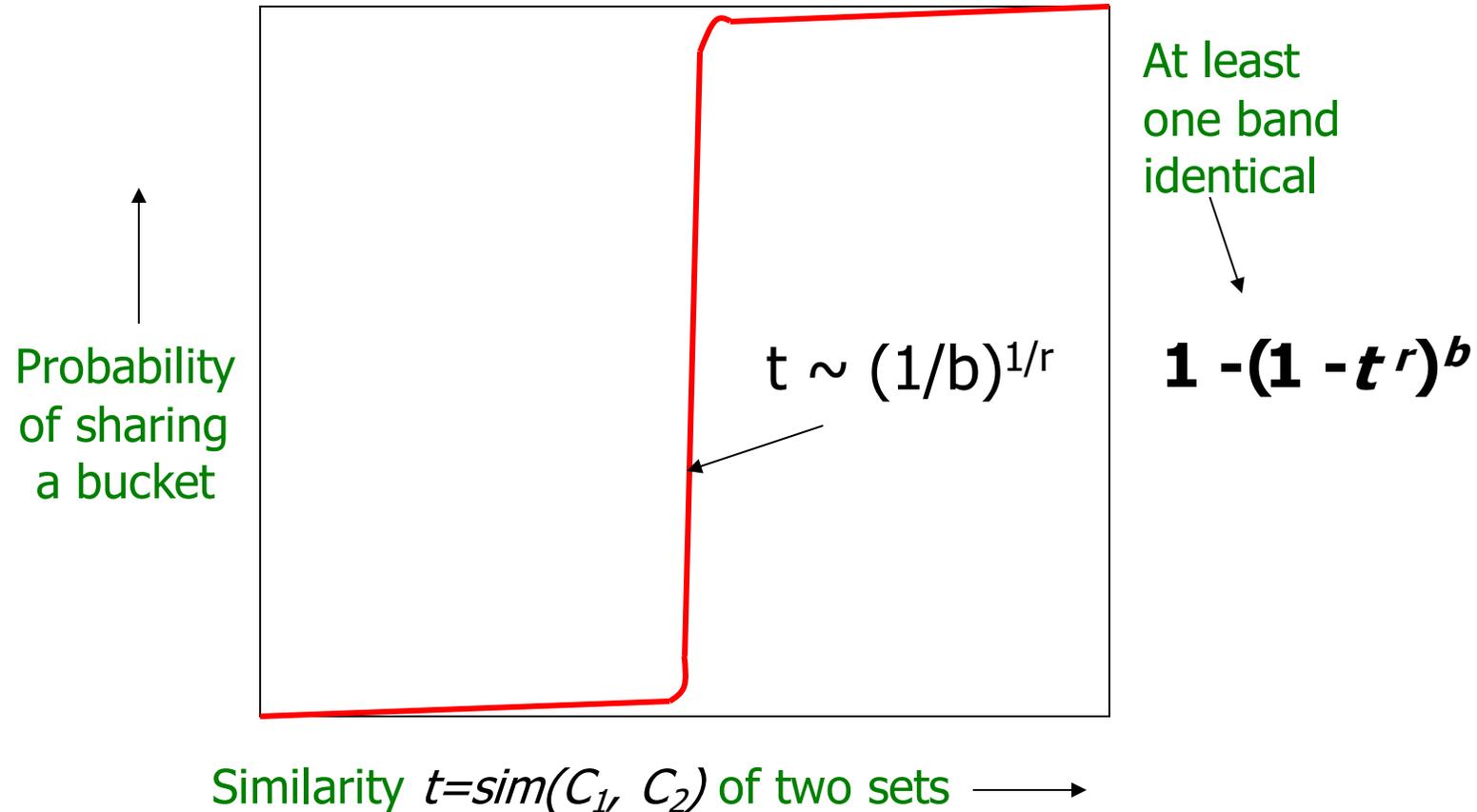
# What 1 Band of 1 Row Gives You



# $b$ bands, $r$ rows/band

- Columns  $C_1$  and  $C_2$  have similarity  $t$
- Pick any band ( $r$  rows)
  - ▣ Prob. that all rows in band equal =  $t^r$
  - ▣ Prob. that some row in band unequal =  $1 - t^r$
- Prob. that no band identical =  $(1 - t^r)^b$
- Prob. that at least 1 band identical =  $1 - (1 - t^r)^b$

# What $b$ Bands of $r$ Rows Gives You



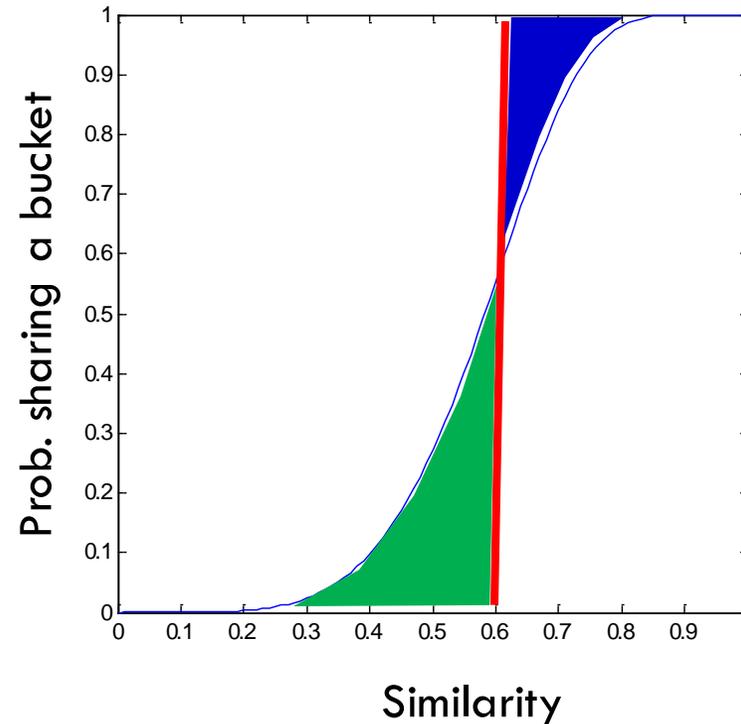
# Example: $b = 20; r = 5$

- **Similarity threshold  $s$**
- **Prob. that at least 1 band is identical:**

$s$	$1-(1-s^r)^b$
.2	.006
.3	.047
.4	.186
.5	.470
.6	.802
.7	.975
.8	.9996

# Picking $r$ and $b$ : The S-curve

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



**Blue area:** False Negative rate  
**Green area:** False Positive rate

# LSH Summary

- Tune  $M, b, r$  to get almost all pairs with similar signatures, but eliminate most pairs that do not have similar signatures
- Check in main memory that **candidate pairs** really do have **similar signatures**
- **Optional:** In another pass through data, check that the remaining candidate pairs really represent similar documents

# Summary: 3 Steps

- **Shingling:** Convert documents to sets
  - We used hashing to assign each shingle an ID
- **Min-Hashing:** Convert large sets to short signatures, while preserving similarity
  - We used **similarity preserving hashing** to generate signatures with property  $\Pr[h_\pi(\mathbf{C}_1) = h_\pi(\mathbf{C}_2)] = \text{sim}(\mathbf{C}_1, \mathbf{C}_2)$
  - We used hashing to get around generating random permutations
- **Locality-Sensitive Hashing:** Focus on pairs of signatures likely to be from similar documents
  - We used hashing to find **candidate pairs** of similarity  $\geq s$