# Finding Similar Items I 

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## TODAY

Features Today

- Lecture will be recorded, edited and posted
- Arsnova:
- Session ID: 50395809 (also pasted into Zoom chat today)
- Use Case: "Questions / Comments from Audience" (German: "Kummerkasten")
- Session will be active throughout semester
- I will (be happy to) respond whenever I can

Learning Goals

- Turning documents into sets shingles
- Computing the similarity of sets minhashing


# Finding Similar Items: Introduction 

## Finding Similar Items

Fundamental problem in data mining: retrieve pairs of similar elements of a dataset.

Applications

- Detecting plagiarism in a set of documents
- Identifying near-identical mirror pages during web searches
- Identifying documents from the same author
- Collaborative Filtering
- Online Purchases (Amazon: suggestions based on 'similar' customers)
- Movie Ratings (Netflix: suggestions based on 'similar' users)


## ISSUES

Consider a dataset of $N$ items, for example: $N$ webpages or $N$ text documents.

- Comparing all items requires $O\left(N^{2}\right)$ runtime.
- Ok for small $N$.
- If $N \approx 10^{6}$, we have $10^{12}$ comparisons. Maybe not OK!
- How to efficiently compute similarity if items themselves are large?
- Similarity works well for sets of items. How to turn data into sets of items?


## Overview



From mmds.org

- Shingling: turning text files into sets
- Minhashing: computing similarity for large sets
- Locality Sensitive Hashing: avoids $O\left(N^{2}\right)$ comparisons by determining candidate pairs


## Shingles <br> Turning Documents into Sets

## Jaccard Similarity

## Definition [Jaccard Similarity]

Consider two sets $S$ and $T$. The Jaccard similarity $\operatorname{SIM}(S, T)$ is defined as

$$
\begin{equation*}
\operatorname{SIM}(S, T)=\frac{|S \cap T|}{|S \cup T|} \tag{1}
\end{equation*}
$$

the ratio of elements in the intersection and in the union of $S$ and $T$.


## SHINGLES: DEFINITION

- Document = large string of characters
- $k$-shingle: a substring of a particular length $k$
- Idea: A document is set of $k$-shingles
- Example: document $=$ "acadacc",$k$-shingles:

$$
\{a c, a d, c a, c c, d a\}
$$

- We can now compute Jaccard similarity for two documents by considering them as sets of shingles.
- Example: documents $D_{1}=" a b c d ", D_{2}=" d b c d "$ using 2-shingles yields $D_{1}=\{a b, b c, c d\}, D_{2}=\{b c, c d, d b\}$, so $\operatorname{SIM}\left(D_{1}, D_{2}\right)=\frac{|\{b c, c d\}|}{|\{a b, b c, c d, d b\}|}=2 / 4=1 / 2$


## SHINGLES: DEFINITION

- Issue: Determining right size of $k$.
- $k$ large enough such that any particular $k$-shingle appears in document with low probability ( $k=5$, yielding $256^{5}$ different shingles on 256 different characters, ok for emails)
- too large $k$ yields too large universe of elements (example: $k=9$ means $256^{9}=\left(2^{8}\right)^{9}=2^{72}$ on the order of number of atoms in the universe)
- Solution if necessary $k$ is too large: hash shingles to buckets, such that buckets are evenly covered, and collisions are rare
- We would like to compute Jaccard similarity for pairs of sets
- But: even when hashed, size of the universe of elements (= \# buckets when hashed) may be prohibitive to do that fast
- What to do?


# Minhashing <br> Rapidly Computing Similarity of Sets 

## SETS As Bitvectors

- Representing sets as bitvectors
- Length of bitvectors is size of universal set
- For example, when hashed, length of bitvector = number of buckets
- Entries zero if element not in set, one if element in set
- Does not reflect to really store the sets, but nice visualization


## Sets as Bitvectors: the Characteristic Matrix

Definition [Characteristic Matrix]
Given $C$ sets over a universe $R$, the characteristic matrix
$M \in\{0,1\}^{|R| \times|C|}$ is defined to have entries

$$
M(r, c)= \begin{cases}0 & \text { if } r \notin c  \tag{2}\\ 1 & \text { if } r \in c\end{cases}
$$

for $r \in R, c \in C$.

| Element | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :--- | :--- | :--- | :--- |
| $a$ | 1 | 0 | 0 | 1 |
| $b$ | 0 | 0 | 1 | 0 |
| $c$ | 0 | 1 | 0 | 1 |
| $d$ | 1 | 0 | 1 | 1 |
| $e$ | 0 | 0 | 1 | 0 |

Characteristic matrix of four sets $\left(S_{1}, S_{2}, S_{3}, S_{4}\right)$ over universal set $\{a, b, c, d, e\}$

## Permutations

Definition [Bijection,Permutation]

- A bijection is a map $\pi: S \rightarrow S$ such that
- $\pi(x)=\pi(y)$ implies $x=y$ ( $\pi$ is injective)
- For all $y \in S$ there is $x \in S$ such that $\pi(x)=y$ ( $\pi$ is surjective)
- A permutation is a bijection

$$
\begin{equation*}
\pi:\{1, \ldots, m\} \rightarrow\{1, \ldots, m\} \tag{3}
\end{equation*}
$$

Example: A permutation on $\{1,2,3,4,5\}$ may map

$$
1 \rightarrow 4,2 \rightarrow 3,3 \rightarrow 1,4 \rightarrow 5 \text { and } 5 \rightarrow 2
$$

## Permuting Rows of Characteristic Matrix

| Element | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |  |  |  |  |  |
| :---: | :--- | :--- | :--- | :--- | :---: | :--- | :--- | :--- | :--- |
| $a$ | 1 | 0 | 0 | 1 | Element | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| $b$ | 0 | 0 | 1 | 0 |  | 0 | 0 | 1 | 0 |
| $c$ | 0 | 1 | 0 | 1 |  | 0 | 0 | 1 | 0 |
| $d$ | 1 | 0 | 1 | 1 |  | 1 | 0 | 0 | 1 |
| $e$ | 0 | 0 | 1 | 0 | $c$ | 1 | 0 | 1 | 1 |
|  |  |  | $c$ | 0 | 1 | 0 | 1 |  |  |

A characteristic matrix of four sets $\left(S_{1}, S_{2}, S_{3}, S_{4}\right)$ over universal set $\{a, b, c, d, e\}$ and a permutation of its rows $1 \rightarrow 3,2 \rightarrow 1,3 \rightarrow 5,4 \rightarrow 4,5 \rightarrow 2$

## Minhash - Definition

Given

- a characteristic matrix with $m$ rows and a column $S$
- a permutation $\pi$ on the rows, that is $\pi:\{1, \ldots, m\} \rightarrow\{1, \ldots, m\}$ is a bijection

Definition [Minhash]
The minhash function $h_{\pi}$ on $S$ is defined by

$$
h_{\pi}(S)=\min _{i \in\{1, \ldots, m\}}\{\pi(i) \mid S[i]=1\}
$$

## Minhash - Definition

Definition [Minhash]
The minhash function $h_{\pi}$ on $S$ is defined by

$$
h_{\pi}(S)=\min _{i \in\{1, \ldots, m\}}\{\pi(i) \mid S[i]=1\}
$$

Explanation
The minhash of a column $S$ relative to permutation $\pi$ is

- after reordering rows according to the permutation $\pi$
- the first row in which a one in $S$ appears


## Minhash - Example

## Example

Let

- 1 corresponds to $a, 2$ to $b, \ldots$
- $\pi: 1 \rightarrow 3,2 \rightarrow 1,3 \rightarrow 5,4 \rightarrow 4,5 \rightarrow 2$ and


## Minhashing and Jaccard Similarity

Given

- two columns (sets) $S_{1}, S_{2}$ of a characteristic matrix
- a randomly picked permutation $\pi$ on the rows (on $\{1, \ldots, m\}$ )

Theorem [Minhash and Jaccard Similarity]:
The probability that $h_{\pi}\left(S_{1}\right)=h_{\pi}\left(S_{2}\right)$ is $\operatorname{SIM}\left(S_{1}, S_{2}\right)$.

## Minhash and Jaccard Similarity - Proof

Theorem [Minhash and Jaccard Similarity]:
The probability that $h_{\pi}\left(S_{1}\right)=h_{\pi}\left(S_{2}\right)$ is $\operatorname{SIM}\left(S_{1}, S_{2}\right)$.
Proof.
Distinguish three different classes of rows:

- Type X rows have a 1 in both $S_{1}, S_{2}$
- Type $Y$ rows have a 1 in only one of $S_{1}, S_{2}$
- Type Z rows have a 0 in both $S_{1}, S_{2}$

Let $x$ be the number of type $X$ rows and $y$ the number of type Y rows.

- So $x=\left|S_{1} \cap S_{2}\right|$ and $x+y=\left|S_{1} \cup S_{2}\right|$
- Hence

$$
\begin{equation*}
\operatorname{SIM}\left(S_{1}, S_{2}\right)=\frac{\left|S_{1} \cap S_{2}\right|}{\left|S_{1} \cup S_{2}\right|}=\frac{x}{x+y} \tag{4}
\end{equation*}
$$

## Minhash and Jaccard Similarity - Proof

Proof. (CONT.)

- Consider the probability that $h\left(S_{1}\right)=h\left(S_{2}\right)$
- Imagine rows to be permuted randomly, and proceed from the top
- The probability to encounter type X before type Y is

$$
\begin{equation*}
\frac{x}{x+y} \tag{5}
\end{equation*}
$$

- If first non type Z row is type X , then $h\left(S_{1}\right)=h\left(S_{2}\right)$
- If first non type Z row is type Y , then $h\left(S_{1}\right) \neq h\left(S_{2}\right)$
- So $h\left(S_{1}\right)=h\left(S_{2}\right)$ happens with probability (5), which by (4) concludes the proof.


## Minhash - Intermediate Summary / Expansion of Idea

- Computing a minhash means turning a set into one number
- For different sets, numbers agree with probability equal to their Jaccard similarity.
- Can we expand on this idea? Can we compute (ensembles of) numbers that enable us to determine their Jaccard similarity?
- Immediate idea: compute several minhashes. The fraction of times the minhashes of two sets agree equals their Jaccard similarity.
- Several sufficiently well chosen minhashes yield a minhash signature.


## Minhash Signatures

Consider

- the $m$ rows of the characteristic matrix
- $n$ permutations $\{1, \ldots, m\} \rightarrow\{1, \ldots, m\}$
- the corresponding minhash functions $h_{1}, \ldots, h_{n}:\{0,1\}^{m} \rightarrow\{1, \ldots, m\}$
- and a particular column $S \in\{0,1\}^{m}$ $h_{i}(S) \in\{1, \ldots, m\}$ for any $1 \leq i \leq n$

Definition [Minhash Signature]
The minhash signature SIG of $S$ given $h_{1}, \ldots, h_{n}$ is the array

$$
\left[h_{1}(S), \ldots, h_{n}(S)\right] \in\{1, \ldots, m\}^{n}
$$

## Minhash Signatures

Definition [Minhash Signature]
The minhash signature SIG ${ }_{S}$ of $S$ given $h_{1}, \ldots, h_{n}$ is the array

$$
\left[h_{1}(S), \ldots, h_{n}(S)\right] \in\{1, \ldots, m\}^{n}
$$

Meaning: Computing the minhash signature for a column $S$ turns

- the binary-valued array of length $m$ that represents $S$

$$
\leftrightarrow S \in\{0,1\}^{m}
$$

- into an $m$-valued array of length $n$

$$
\leftrightarrow\left[h_{1}(S), \ldots, h_{n}(S)\right] \in\{1, \ldots, m\}^{n}
$$

Because $n<m$ (often $n \ll m$ ), the minhash signature is a reduced representation of a set.

## SIGNATURE MATRIX

Consider a characteristic matrix, and $n$ permutations $h_{1}, \ldots, h_{n}$.
Definition [Signature Matrix]
The signature matrix SIG is a matrix with $n$ rows and as many columns as the characteristic matrix (i.e. the number of sets), where entries SIG $_{i j}$ are defined by

$$
\begin{equation*}
\operatorname{SIG}_{i j}=h_{i}\left(S_{j}\right) \tag{6}
\end{equation*}
$$

where $S_{j}$ refers to the $j$-th column in the characteristic matrix.

## Signature Matrices: Facts

Let $M$ be a signature matrix.

- Because usually $n \ll m$, that is $n$ is much smaller than $m$, a signature matrix is much smaller than the original characteristic matrix.
- The probability that SIG $_{i j_{1}}=$ SIG $_{i j_{2}}$ for two sets $S_{j_{1}}, S_{j_{2}}$ equals the Jaccard similarity $\operatorname{SIM}\left(S_{j_{1}}, S_{j_{2}}\right)$
- The expected number of rows where columns $j_{1}, j_{2}$ agree, divided by $n$, is $\operatorname{SIM}\left(S_{j_{1}}, S_{j_{2}}\right)$.


## Signature Matrices: Issues

Issue:

- For large $m$, it is time-consuming / storage-intense to determine permutations

$$
\pi:\{1, \ldots, m\} \rightarrow\{1, \ldots, m\}
$$

- Re-sorting rows relative to a permutation is even more expensive

Solution:

- Instead of permutations, use hash functions (watch the index shift!)

$$
h:\{0, \ldots, m-1\} \rightarrow\{0, \ldots, m-1\}
$$

- Likely, a hash function is not a bijection, so at times
- places two rows in the same bucket
- leaves other buckets empty
- Effects are negligible for our purposes, however


## Computing Signature Matrices in Practice

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        \(\operatorname{SIG}(i, c)=\infty\)
        end for
end for
for each row \(r\) do
    for each column \(c\) do
        if \(M(r, c)=1\) then
        for \(\mathrm{i}=1\) to n do
        \(\operatorname{SIG}(i, c)=\)
                \(\min \left(\operatorname{SIG}(i, c), h_{i}(r)\right)\)
            end for
        end if
        end for
end for
```


## Computing Signature Matrices: Example

| Row | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ | $x+1 \bmod 5$ | $3 x+1 \bmod 5$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 2 | 4 |
| 2 | 0 | 1 | 0 | 1 | 3 | 2 |
| 3 | 1 | 0 | 1 | 1 | 4 | 0 |
| 4 | 0 | 0 | 1 | 0 | 0 | 3 |

Hash functions computed for a characteristic matrix, with rows indexed from 0 to 4

## Computing Signature Matrices in Practice

- Consider $n$ hash functions
$h_{i}:\{0, \ldots, m-1\} \rightarrow$
$\{0, \ldots, m-1\}, i=1, \ldots, n$
- Let $r$ and $c$ index rows and columns in the characteristic matrix $M \in\{0,1\}^{m \times|C|}$
- So $c$ also index columns, while $i$ indexes rows in the signature matrix SIG $\in\{1, \ldots, m\}^{n \times|C|}$

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        \(\operatorname{SIG}(i, c)=\infty\)
    end for
end for
for each row \(r\) do
    for each column \(c\) do
        if \(M(r, c)=1\) then
        for \(\mathrm{i}=1\) to n do
                \(\operatorname{SIG}(i, c)=\)
                \(\min \left(S I G(i, c), h_{i}(r)\right)\)
            end for
            end if
    end for
end for
```


## Computing Signature Matrices: Example

| Row | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ | $x+1 \bmod 5$ | $3 x+1 \bmod 5$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 2 | 4 |
| 2 | 0 | 1 | 0 | 1 | 3 | 2 |
| 3 | 1 | 0 | 1 | 1 | 4 | 0 |
| 4 | 0 | 0 | 1 | 0 | 0 | 3 |

Hash functions computed for a characteristic matrix, with rows indexed from 0 to 4

|  | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $h_{1}$ | $\infty$ | $\infty$ | $\infty$ | $\infty$ |
| $h_{2}$ | $\infty$ | $\infty$ | $\infty$ | $\infty$ |

Signature matrix SIG: after initialization

## Computing Signature Matrices in Practice

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        SIG \((i, c)=\infty\)
    end for
end for
for each row \(r\) do
    for each column \(c\) do
        if \(M(r, c)=1\) then
        for \(\mathrm{i}=1\) to n do
        \(\operatorname{SIG}(i, c)=\)
                \(\min \left(\operatorname{SIG}(i, c), h_{i}(r)\right)\)
            end for
        end if
        end for
end for
```


## Computing Signature Matrices in Practice

- Consider $n$ hash functions
$h_{i}:\{0, \ldots, m-1\} \rightarrow$
$\{0, \ldots, m-1\}, i=1, \ldots, n$
- Let $r$ and $c$ index rows and columns in the characteristic matrix $M \in\{0,1\}^{m \times|C|}$
- So $c$ also index columns, while $i$ indexes rows in the signature matrix $\operatorname{SIG} \in\{1, \ldots, m\}^{n \times|C|}$

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        \(\operatorname{SIG}(i, c)=\infty\)
    end for
end for
for each row \(r\) do
    / / Iteration 1: first row
    for each column \(c\) do
        if \(M(r, c)=1\) then
            for \(\mathrm{i}=1\) to n do
                \(\operatorname{SIG}(i, c)=\)
                \(\min \left(S I G(i, c), h_{i}(r)\right)\)
                end for
        end if
        end for
    / / End first row
end for
```


## Computing Signature Matrices: Example

| Row | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ | $x+1 \bmod 5$ | $3 x+1 \bmod 5$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 2 | 4 |
| 2 | 0 | 1 | 0 | 1 | 3 | 2 |
| 3 | 1 | 0 | 1 | 1 | 4 | 0 |
| 4 | 0 | 0 | 1 | 0 | 0 | 3 |

Hash functions computed for a characteristic matrix, with rows indexed from 0 to 4
First iteration: row \# 0 has 1's in $S_{1}$ and $S_{4}$, so put $S_{I G} G_{11}=$ SIG $_{14}=0+1 \bmod 5=1$ and SIG $_{21}=$ SIG $_{24}=3 \cdot 0+1$ $\bmod 5=1$

|  | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $h_{1}$ | 1 | $\infty$ | $\infty$ | 1 |
| $h_{2}$ | 1 | $\infty$ | $\infty$ | 1 |

## Computing Signature Matrices in Practice

- Consider $n$ hash functions
$h_{i}:\{0, \ldots, m-1\} \rightarrow$
$\{0, \ldots, m-1\}, i=1, \ldots, n$
- Let $r$ and $c$ index rows and columns in the characteristic matrix $M \in\{0,1\}^{m \times|C|}$
- So $c$ also index columns, while $i$ indexes rows in the signature matrix $\operatorname{SIG} \in\{1, \ldots, m\}^{n \times|C|}$

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        \(\operatorname{SIG}(i, c)=\infty\)
    end for
end for
for each row \(r\) do
    / / Iteration 2: second row
    for each column \(c\) do
        if \(M(r, c)=1\) then
            for \(\mathrm{i}=1\) to n do
                    \(\operatorname{SIG}(i, c)=\)
                \(\min \left(S I G(i, c), h_{i}(r)\right)\)
                end for
        end if
        end for
    / / End second row
end for
```


## Computing Signature Matrices: Example

| Row | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ | $x+1 \bmod 5$ | $3 x+1 \bmod 5$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 2 | 4 |
| 2 | 0 | 1 | 0 | 1 | 3 | 2 |
| 3 | 1 | 0 | 1 | 1 | 4 | 0 |
| 4 | 0 | 0 | 1 | 0 | 0 | 3 |

Hash functions computed for a characteristic matrix, with rows indexed from 0 to 4
Second iteration: row \#1 has 1 in $S_{3}$, so put SIG $_{31}=1+1 \bmod 5=2$ and SIG $_{32}=3+1 \bmod 5=4$.

|  | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $h_{1}$ | 1 | $\infty$ | 2 | 1 |
| $h_{2}$ | 1 | $\infty$ | 4 | 1 |

## Computing Signature Matrices in Practice

- Consider $n$ hash functions
$h_{i}:\{0, \ldots, m-1\} \rightarrow$
$\{0, \ldots, m-1\}, i=1, \ldots, n$
- Let $r$ and $c$ index rows and columns in the characteristic matrix $M \in\{0,1\}^{m \times|C|}$
- So $c$ also index columns, while $i$ indexes rows in the signature matrix $\operatorname{SIG} \in\{1, \ldots, m\}^{n \times|C|}$

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        \(\operatorname{SIG}(i, c)=\infty\)
    end for
end for
for each row \(r\) do
    / / Iteration 3: third row
    for each column \(c\) do
        if \(M(r, c)=1\) then
            for \(\mathrm{i}=1\) to n do
                    \(\operatorname{SIG}(i, c)=\)
                \(\min \left(S I G(i, c), h_{i}(r)\right)\)
                end for
        end if
        end for
    / / End third row
end for
```


## Computing Signature Matrices: Example

| Row | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ | $x+1 \bmod 5$ | $3 x+1 \bmod 5$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 2 | 4 |
| 2 | 0 | 1 | 0 | 1 | 3 | 2 |
| 3 | 1 | 0 | 1 | 1 | 4 | 0 |
| 4 | 0 | 0 | 1 | 0 | 0 | 3 |

Hash functions computed for a characteristic matrix, with rows indexed from 0 to 4
Third iteration: row \# 2 has 1's in $S_{2}$ and $S_{4}$, so put SIG $_{21}=2+1$ $\bmod 5=3$, SIG $_{41}=\min (1,2+1 \bmod 5=3)=1$ and $S I G_{22}=6+1$ $\bmod 5=2$ and SIG $_{42}=\min (1,6+1 \bmod 5=2)=1$

|  | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $h_{1}$ | 1 | 3 | 2 | 1 |
| $h_{2}$ | 1 | 2 | 4 | 1 |

## Computing Signature Matrices in Practice

- Consider $n$ hash functions
$h_{i}:\{0, \ldots, m-1\} \rightarrow$
$\{0, \ldots, m-1\}, i=1, \ldots, n$
- Let $r$ and $c$ index rows and columns in the characteristic matrix $M \in\{0,1\}^{m \times|C|}$
- So $c$ also index columns, while $i$ indexes rows in the signature matrix $\operatorname{SIG} \in\{1, \ldots, m\}^{n \times|C|}$

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        \(\operatorname{SIG}(i, c)=\infty\)
    end for
end for
for each row \(r\) do
    / / Iteration 4: fourth row
    for each column \(c\) do
        if \(M(r, c)=1\) then
            for \(\mathrm{i}=1\) to n do
                \(\operatorname{SIG}(i, c)=\)
                \(\min \left(S I G(i, c), h_{i}(r)\right)\)
                end for
        end if
        end for
    / / End fourth row
end for
```


## Computing Signature Matrices: Example

| Row | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ | $x+1 \bmod 5$ | $3 x+1 \bmod 5$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 2 | 4 |
| 2 | 0 | 1 | 0 | 1 | 3 | 2 |
| 3 | 1 | 0 | 1 | 1 | 4 | 0 |
| 4 | 0 | 0 | 1 | 0 | 0 | 3 |

Hash functions computed for a characteristic matrix, with rows indexed from 0 to 4

|  | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $h_{1}$ | 1 | 3 | 2 | 1 |
| $h_{2}$ | 0 | 2 | 0 | 0 |

Signature matrix after considering fourth row

## Computing Signature Matrices in Practice

- Consider $n$ hash functions
$h_{i}:\{0, \ldots, m-1\} \rightarrow$
$\{0, \ldots, m-1\}, i=1, \ldots, n$
- Let $r$ and $c$ index rows and columns in the characteristic matrix $M \in\{0,1\}^{m \times|C|}$
- So $c$ also index columns, while $i$ indexes rows in the signature matrix $\operatorname{SIG} \in\{1, \ldots, m\}^{n \times|C|}$

```
for each \(c\) do
    for \(0 \leq i \leq n\) do
        \(\operatorname{SIG}(i, c)=\infty\)
    end for
end for
for each row \(r\) do
    / / Iteration 5: fifth (final) row
    for each column \(c\) do
        if \(M(r, c)=1\) then
        for \(\mathrm{i}=1\) to n do
                        \(\operatorname{SIG}(i, c)=\)
                \(\min \left(\operatorname{SIG}(i, c), h_{i}(r)\right)\)
                end for
        end if
        end for
    / / End fifth (final) row
end for
```


## Computing Signature Matrices: Example

| Row | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ | $x+1 \bmod 5$ | $3 x+1 \bmod 5$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 2 | 4 |
| 2 | 0 | 1 | 0 | 1 | 3 | 2 |
| 3 | 1 | 0 | 1 | 1 | 4 | 0 |
| 4 | 0 | 0 | 1 | 0 | 0 | 3 |

Hash functions computed for a characteristic matrix, with rows indexed from 0 to 4

|  | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $h_{1}$ | 1 | 3 | 0 | 1 |
| $h_{2}$ | 0 | 2 | 0 | 0 |

Signature matrix after considering fifth row: final signature matrix

## Computing Signature Matrices: Example

|  | $S_{1}$ | $S_{2}$ | $S_{3}$ | $S_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $h_{1}$ | 1 | 3 | 0 | 1 |
| $h_{2}$ | 0 | 2 | 0 | 0 |

Signature matrix after considering fifth row: final signature matrix

- Estimates for Jaccard similarity: $\operatorname{SIM}\left(S_{1}, S_{3}\right)=\frac{1}{2}, \operatorname{SIM}\left(S_{1}, S_{4}\right)=1$
- True Jaccard similarities: $\operatorname{SIM}\left(S_{1}, S_{3}\right)=\frac{1}{3}, \operatorname{SIM}\left(S_{1}, S_{4}\right)=\frac{2}{3}$
- Estimates will be better when raising number of hash functions that is increasing number of rows of the signature matrix


## Minhashing - Issues Remaining

- Minhashing is time-consuming, because iterating through all $m$ rows of $M$ necessary, and $m$ is large (huge!)
- Thought experiment:
- Imagine using real permutations
- Recall: minhash is first row in permuted order with a 1
- Consider permutations $\pi:\{1, \ldots, \bar{m}\} \rightarrow\{1, \ldots, \bar{m}\}$ for $\bar{m}<m$
- Consider only examining the first $\bar{m}$ of the permuted rows
- Speed up of a factor of $\frac{m}{\bar{m}}$
- However, all first $\bar{m}$ rows may have 0 in some columns
- How to deal with that? Can we nevertheless work with only $\bar{m}<m$ rows and compute sufficiently accurate estimates for the Jaccard similarity of two columns?


## Speeding Up Minhashing: Motivation

- Continue thought experiment
- Consider computing signature matrices by only examining $\bar{m}<m$ rows in the characteristic matrix, and using permutations $\pi:\{1, \ldots, \bar{m}\} \rightarrow\{1, \ldots, \bar{m}\}$ where
- the chosen $\bar{m}$ rows need not be the first $\bar{m}$ rows
- For each permutation where no 1 shows, keep $\infty$ as symbol in the signature matrix SIG
- Situation: Much faster to compute SIG, but $\operatorname{SIG}(i, c)=\infty$ in some places (how many? is this bad?)
- Consider computing Jaccard similarities for pairs of columns


## Speeding Up Minhashing: Motivation

## Situation:

- Compute Jaccard similarities for pairs of columns, while possibly
- $\operatorname{SIG}(i, c)=\infty$ for some $(i, c)$
- Algorithm for estimating Jaccard similarity:
- Row by row, by iterative updates,
- maintain count of rows $a$ where columns agree
- maintain count of rows $d$ where columns disagree
- Estimate SIM as $\frac{a}{a+d}$


## Three cases:

1. Both columns do not contain $\infty$ in row: update counts as usual (either $a \rightarrow a+1$ or $d \rightarrow d+1$
2. Only one column has $\infty$ in row:

- Let two rows be $c_{1}, c_{2}$, and $\operatorname{SIG}\left(i, c_{1}\right)=\infty$, but $\operatorname{SIG}\left(i, c_{2}\right) \neq \infty$ :
- It follows that $\operatorname{SIG}\left(i, c_{1}\right)>\operatorname{SIG}\left(i, c_{2}\right)$
- So increase count of disagreeing rows by one $(d \rightarrow d+1)$


## Speeding up Minhashing: Motivation

Summary: One determines $\frac{a}{a+d}$ as estimate for $\operatorname{SIM}\left(c_{1}, c_{2}\right)$

- Counts rely on less rows than before. How reliable are they?
- However, since each permutation only refers to $\bar{m}<m$ rows, we can afford more permutations
- The one makes counts less reliable, while the other compensates for it
- Can we control the corresponding trade-off to our favour?
- What are the consequences in practice when using real hash functions and not permutations?


## Speeding up Minhashing: Issues to Resolve

- Let $T$ be the set of elements of the universal set that correspond to the initial $\bar{m}$ rows in the characteristic matrix.
- When executing the above algorithm on only these $\bar{m}$ rows, we determine

$$
\begin{equation*}
\frac{\left|S_{1} \cap S_{2} \cap T\right|}{\left|\left(S_{1} \cup S_{2}\right) \cap T\right|} \tag{7}
\end{equation*}
$$

as an estimate for the true Jaccard similarity $\frac{\left|S_{1} \cap S_{2}\right|}{\mid S_{1} \cup S_{2}}$.

- If $T$ is chosen randomly, the expected value of (7) is the Jaccard similarity $\operatorname{SIM}\left(S_{1}, S_{2}\right)$
- But: there may be some disturbing variation to this estimate


## Speeding up Minhashing: Strategy

Idea in practice using hash functions

- Divide $m$ rows into $\frac{m}{\bar{m}}$ blocks of $\bar{m}$ rows each
- For each hash function $h:\{0, \ldots, \bar{m}-1\} \rightarrow\{0, \ldots, \bar{m}-1\}$, compute minhash values for each block of $\bar{m}$ rows
- Yields $\frac{m}{\bar{m}}$ minhash values for a single hash function, instead of just one
- Extreme: If $\frac{m}{\bar{m}}$ is large enough, only one hash function may be necessary
- Possible advantage: By using all $m$ rows, one balances out errors in the particular estimates on only $\bar{m}$ of the $m$ rows:
- The overall $x$ of the type X rows are distributed across blocks of $\bar{m}$ rows
- Likewise, the overall $y$ type Y rows are distributed across the blocks


## Speeding up Minhashing: Example

| $S_{1}$ | $S_{2}$ | $S_{3}$ |
| :---: | :---: | :---: |
| 0 | 0 | 0 |
| 0 | 0 | 0 |
| 0 | 0 | 1 |
| 0 | 1 | 1 |
| 1 | 1 | 1 |
| 1 | 1 | 0 |
| 1 | 0 | 0 |
| 0 | 0 | 0 |

Characteristic matrix for three sets $S_{1}, S_{2}, S_{3} . m=8, \bar{m}=4$.

- Truth: $\operatorname{SIM}\left(S_{1}, S_{2}\right)=\frac{1}{2}, \operatorname{SIM}\left(S_{1}, S_{3}\right)=$ $\frac{1}{5}, \operatorname{SIM}\left(S_{2}, S_{3}\right)=\frac{1}{2}$
- Estimate for first four rows: $\operatorname{SIM}\left(S_{1}, S_{2}\right)=0$
- Estimate for last four rows: $\operatorname{SIM}\left(S_{1}, S_{2}\right)=\frac{2}{3}$ on average across randomly picked hash functions
- Overall estimate (expected across randomly picked hash functions): $\operatorname{SIM}\left(S_{1}, S_{2}\right)=\frac{1}{3}$, Ok estimate for two hash functions


## Current Status: Issues Still Remaining

- Estimating similarity for each pair of sets may be infeasible even when using minhash signatures just because number of pairs is too large
- Apart from parallelism nothing can help
- Question/Idea: Can we determine candidate pairs, and only compute similarity for them, knowing similarity will be small for all others?
- Solution: Locality Sensitive Hashing (a.k.a. Near Neighbor Search)


## Summary of Current Status



From mmds.org

- Shingling: turning text files into sets Done!
- Minhashing: computing similarity for large sets Done!
- Locality Sensitive Hashing: avoids $O\left(N^{2}\right)$ comparisons by determining candidate pairs next lecture!


## Materials / Outlook

- See Mining of Massive Datasets, chapter 3.1-3.3
- As usual, see http://www.mmds.org/in general for further resources
- Next lecture: "Finding Similar Items II"
- See Mining of Massive Datasets 3.4-3.6

