Week 4: Similarity Analysis





Warm-up

- Computers store numbers (well everything) in binary
- In decimal, 45 means 4 x 10¹ + 5 x 10⁰
- In binary, 1011 means $1 \times 2^3 + 0 \times 2^2 + 1 \times 2^1 + 1 \times 2^0$
- Complete the table below with binary / decimal equivalences

Binary	Decimal
1011	11
101	
1001101	
	32
	100

A byte is 8 bits (where a bit is a 0 or 1). What's the largest number which can be stored in 1 byte? What's the largest number which can be stored in 4 bytes?

Next week labs and helpdesk

- Online support from TA Joseph Starkey in the module Zoom
 room (bring headphones if you want to access this from the lab computers)
 - Monday 24th Oct 10-12
 - Tuesday 25th Oct 9-11

- Adam Barrett in the lab in Chichester 1 to answer questions
 - Mon 24th Oct & Tues 25th Oct 9.30-10.30

Reminder: first assessment

- Opens at 9am on Thursday 27th Oct, and you must finish it before 5pm on Friday 28th Oct.
 This means that the latest you can start the assessment is 4pm on Friday 28th Oct.
- The assessment covers material from lectures 1-4, and is worth 10% of your mark for the module.

Week	Who	Topic
1	Barrett	Data structures and data formats
2	Barrett	Algorithmic complexity. Sorting.
3	Barrett	Matrices: Manipulation and computation
4	Barrett	Similarity analysis
5	Rosas	Processes and concurrency
6	Rosas	Distributed computation
7	Barrett	Map/reduce
8	Barrett	Clustering, graphs/networks
9	Barrett	Graphs/networks, PageRank algorithm
10	Barrett	Databases
11		independent study

Overview

- applications of similarity / near-neighbour search
- similarity and distance measures
- string similarity
- shingling
- Minhashing
- Locality sensitive hashing (LSH)

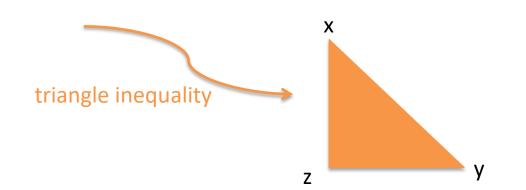
Applications of similarity

- similarity of documents
 - plagiarism
 - mirror pages
 - articles from the same source
- collaborative filtering
 - online purchases
 - movie ratings
- clustering
 - grouping objects in such a way that objects in the same group (called a cluster) are more similar to each other than to those in other clusters.

Similarity vs Distance

Distance measures measure dissimilarity

distance measures	similarity measures
$d(x,y) \geq 0$	$0 \le sim(x,y) \le 1$
d(x,y) = 0 iff x=y	sim(x,y)=1 iff x=y
d(x,y) = d(y,x)	sim(x,y) = sim(y,x)
$d(x,y) \le d(x,z) + d(z,y)$	

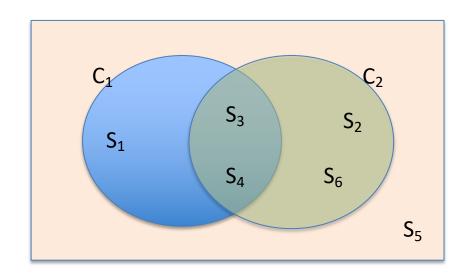


Example

- The 'objects' in which we are interested are customers
- We want to consider two customers similar if they have purchased similar items.
- If we have each customer's purchase history, how do we represent each customer?

Set-theoretic notions of similarity

 Boolean features (a customer C_i either has or hasn't purchased some item S_j) lead naturally to set—theoretic notions of similarity.



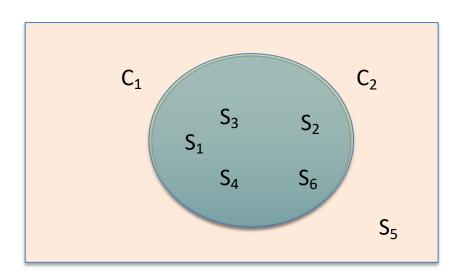
$$C_1 = \{S_1, S_3, S_4\}$$

 $C_2 = \{S_2, S_3, S_4, S_6\}$

Jaccard's measure is the ratio of the cardinality (size) of the intersection of two sets to the cardinality of the union of two sets

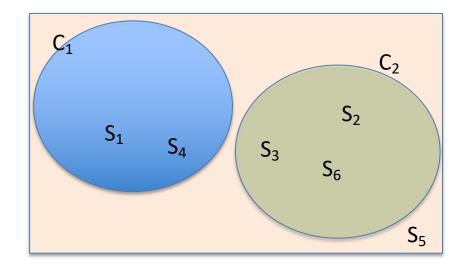
$$Jacc(C_1, C_2) = \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|} = \frac{|C_1 \cap C_2|}{|C_1| + |C_2| - |C_1 \cap C_2|} = \frac{2}{5}$$

Special cases



$$C_1=C_2=\{S_1, S_2, S_3, S_4, S_6\}$$

$$Jacc(C_1, C_2) = 5/5 = 1$$



$$C_1 = \{S_1, S_4\}$$

$$C_2 = \{S_2, S_3, S_6\}$$

$$Jacc(C_1, C_2) = 0/5 = 0$$

Algorithm for Jaccard's Measure

- What does the run-time for computing Jaccard similarity depend on?
- What are the possible worst-case performances in O notation?

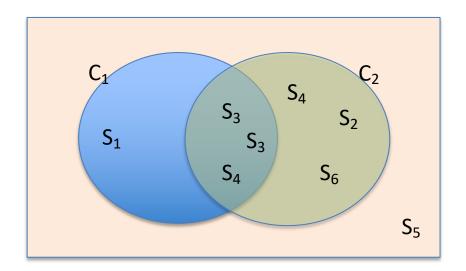
Algorithm for Jaccard's measure

Data stored in Python lists:

```
def jaccard(C1, C2):
    int=0
    union=0
    for item in C1:
        if item in C2:
            int+=1
    union=len(C1)+len(C2)-int
    return int/union
```

Assuming C1 and C2 have length O(n), then this is $O(n^2)$ because the if statement takes O(n) to execute (check every element).

Extending to Bags



$$C_1 = \{S_1, S_3, S_3, S_4\}$$

 $C_2 = \{S_2, S_3, S_3, S_4, S_4, S_6\}$

Can model duplicate items or even real-valued scores using bags.

The shared (minimum) part of the score goes in the intersection. All of it goes in the union

$$C_1$$
 C_2
 S_1 1 0
 S_2 0 1
 S_3 2 2
 S_4 1 2
 S_5 0 0
 S_6 0 1

$$Jacc(C_{1}, C_{2}) = \frac{|C_{1} \cap C_{2}|}{|C_{1}| + |C_{2}| - |C_{1} \cap C_{2}|} = \frac{\sum_{i} \min(S_{i1}, S_{i2})}{\sum_{i} S_{i1} + S_{i2} - \min(S_{i1}, S_{i2})} = \frac{3}{7}$$

Algorithm for Jaccard's measure

Data stored in a dictionary, bags version of Jaccard:

```
def maketotal(dict1):
    total=0
    for item in dict1:
        total += dict1[item]
    return total
def jaccard(dict1,dict2):
    intersection={}
    for item in dict1.keys():
        if item in dict2.keys():
            intersection[item]=min(dict1[item], dict2[item])
    intersectiontot=maketotal(intersection)
    union = maketotal(dict1)+maketotal(dict2)-intersectiontot
    return intersectiontot/union
```

Assuming dict1 and dict2 have O(n) item, then if we have no hash collisions:

the if statement takes O(1) to execute- just look at what is stored at the hash of the item.

Note

 Take care when using Jaccard similarity, to be clear whether you are using the measure applied to sets or to bags. In general, this choice affects the value you get.

Exercise

Consider the following 2 sets of items S1 and S2.

What is the Jaccard similarity of sets S1 and S2?

- (a) 3/4
- (b) 2/5
- (c) 2/7
- (d) 1/3

Exercise (Solution)

Consider the following 2 sets of items S1 and S2.

Compute the Jaccard similarity of sets S1 and S2.

```
Intersection = \{A2, A5\} size of intersection = 2
Union = \{A1,A2,A3,A5,A6\} size of union = 5
Jaccard similarity = |I| / |U| = 2/5 = 0.4
```

Compute the cosine similarity of sets S1 and S2.

S1 S2
$$S1.S2 = 0 + 1 + 0 + 1 + 0 = 2$$

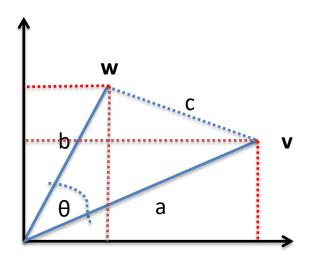
A1 1 0 $S1.S1 = 4$
A2 1 1 $S2.S2 = 3$
A3 0 1 $S3.S2 = 3$
A5 1 1 $S3.S2 = 3$
A6 1 0 $S3.S2 = 3$
 $S3.S3 =$

Cosine similarity

This makes use of the **dot product** for vectors:

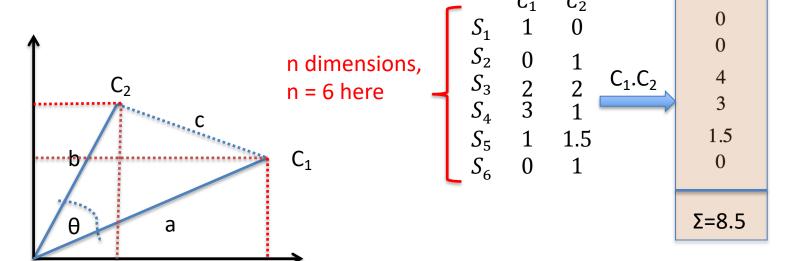
$$v \cdot w = \sum_{i=1}^{n} v_i w_i$$

$$\cos(\theta) = \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{\sqrt{(\boldsymbol{v} \cdot \boldsymbol{v})(\boldsymbol{w} \cdot \boldsymbol{w})}}$$



Cosine similarity

 Real valued 'vector' representations of objects lead naturally to geometric notions of similarity



$$\cos(C_1, C_2) = \frac{C_1.C_2}{\sqrt{C_1.C_1 \times C_2.C_2}}$$

 $C_1.C_2$ is the dot product. Also known as the inner product $< C_1, C_2 >$ or the scalar product

Algorithm for Cosine Measure

- What does the running time of this algorithm depend on?
- Give an estimate of its worst-case performance in O notation

```
def naiveCosine (a , b):
    num=0
    d1=0
    d2=0
    for i in range len( a ) :
        num += a [ i ] *b [ i ]
        d1 += a [ i ] *a [ i ]
        d2 += b [ i ] *b [ i ]
    return num / ( d1*d2 ) **0.5
```

Correlation vs Cosine Similarity

To compute correlation of 2 variables X and Y

- Subtract the mean of X from each value X_i and the mean of Y from each value Y_i
- Compute the dot-product of the transformed X and Y. This is the covariance of X and Y
- Divide by the square root of the product of cov(X,X) and cov(Y,Y)

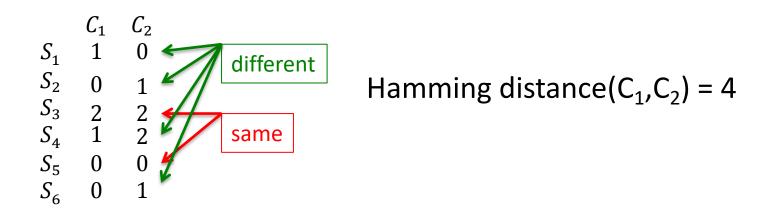
To compute cosine similarity between 2 vectors X and Y

- Compute the dot product of X and Y: <X,Y>
- Divide by the square root of the product of <X,X> and <Y,Y>

The only difference is that when computing correlation, we compute covariance rather than a simple dot product i.e., we standardize by subtracting the means first.

Other measures: Hamming distance

- The number of vector components (dimensions) in which two objects differ.
- Usually only applied to Boolean vectors (e.g., sets) but can be applied to bags

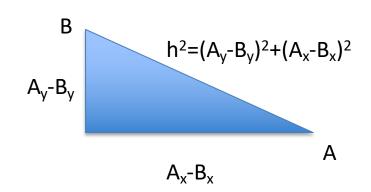


L Norms

Most people are familiar with the L₂ Norm (also known as the **Euclidean distance**), which is Pythagoras theorem in n-dimensions:

$$L_2(A,B) = \sqrt{\sum_{i=1}^n (A_i - B_i)^2}$$

In general, the L_k Norm is given by



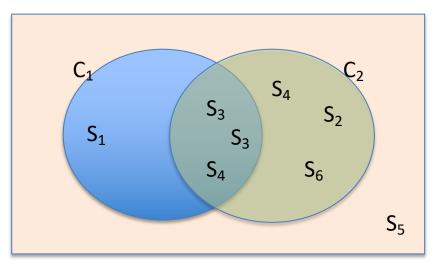
$$L_k(A,B) = \sqrt[k]{\sum_{i=1}^n |A_i - B_i|^k}$$

The L₁ Norm (or Manhattan or City Block) distance is

$$L_1(A,B) = \sum_{i=1}^{n} |A_i - B_i|$$

Probabilistic measures of similarity

Frequencies can be easily converted into probabilities



 \mathcal{C}_1 \mathcal{C}_2 \mathcal{C}_1 C_2 S_1 0.25 0 $\begin{array}{ccc} 0 & 1 \\ 2 & 2 \\ 1 & 2 \end{array} \rightarrow$ 0.166 0.5 0.333 0.25 0.333 S_5 S_5 0.166

What is the probability that a randomly chosen item is S_i given it is in the set / bag C_i ?

Probabilistic measures of similarity

Most well-known 'distance' measure for probability distributions is the Kullback-Leibler divergence measure

$$D_{KL}(C_1 \parallel C_2) = \sum_{i} p_{i1} \times \log \frac{p_{i1}}{p_{i2}}$$

What is the average penalty (i.e., difference in log probabilities) if you use the distribution for C_1 in place of the distribution for C_2 ?

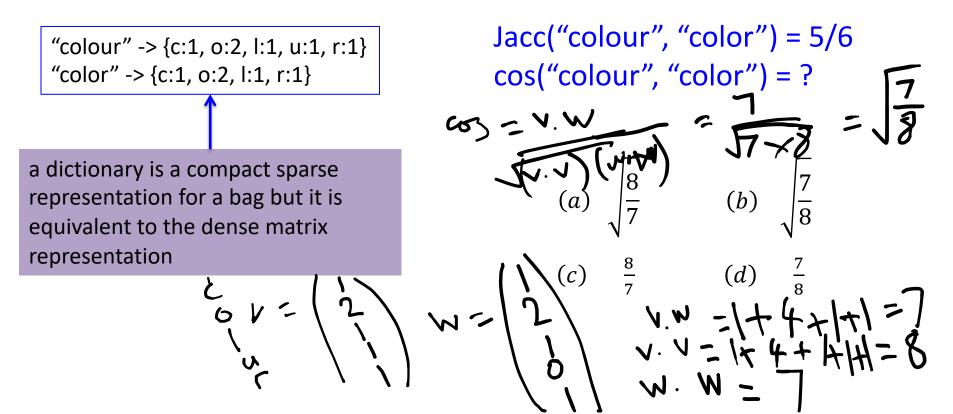
This is not strictly a distance measure because it is not symmetric. The Jenson-Shannon divergence measure is the symmetric version, which measures distance as the average Kullback-Leibler divergence to the centroid of the distributions.

$$JS(A,B) = \frac{1}{2} (KL(A,M) + KL(B,M))$$

where
$$M = \frac{1}{2}(A+B)$$

Finding similarity of two strings

- Strings can be modelled as bags-of-characters
- Long strings (documents!) can be modelled as bags-of-words



Disadvantages of Using Bags for Text

- Not sensitive to order
 - "brag" = "grab"
- If applied to documents where the atomic units are words
 - does not capture relationships between different words

The old man chased the small dog that bit a naughty child.





The old dog chased the naughty small child that bit a man.

Edit distance

- The edit distance between strings X and Y is the smallest number of operations required to transform X into Y, where the operations allowed are insertion and deletion (and also sometimes transposition and mutation).
- There are variants where the different operations have different costs but lets assume cost of each operation = 1

X	Υ		d(X,1)
colour	color	delete c ₅	1
doggy	daddy	delete c_2 , delete c_3 , delete c_4 , insert 'a' at c_2 , insert 'd' at c_3 , insert 'd' at c_4	6
brag	grab	??	4
house	home	??	?

Shingling

The old man chased the small dog that bit a naughty child.





The old dog chased the naughty small child that bit a man.

- A bag-of-words (or bag of characters) representation will lead to these strings being considered identical.
- We could use a bag-of-ngrams :
 - unigram = 1 word, bigram = 2 words, trigram = 3 words,
 ngram = n words
 - What would be the Jaccard similarity if we used a bag of bigrams?
- Alternative is to use a set or bag of shingles. A k-shingle for a document is any string of length k found in the document

Shingling

Example: What are the sets of 3-shingles for the strings "john loves mary" and "mary loves john"?

If a string has m characters, it will have at most m-k distinct shingles

A: john loves mary		B: mary loves john			
joh	ohn	hn_	mar	ary	ry_
n_l	_lo	lov	y_l	_lo	lov
ove	ves	es_	ove	ves	es_
s_m	_ma	mar	s_j	_jo	joh
ary			ohn		

$$Jacc(A,B) = 9/(13+13-9) = 9/17$$

Similarity for large collection of documents

documents

	C1	C2	C3	C4
S1	1	0	0	1
S2	0	0	1	0
S3	0	1	0	1
S4	1	0	1	1
S5	0	0	1	0

...

. . .

shingles

. . .

. .

- We're going to see an efficient way of analysing similarity for all pairs of documents in a collection.
- It will use the set version of Jaccard similarity.
 - So want to choose a shingle length where most shingles don't occur in most documents, so very different documents have very different shingle sets.

Choosing the shingle size

- k should be picked large enough that the probability of any given shingle appearing in any given document is low
- depends on the length of the typical document and the size of the character set

Example: if our corpus of documents is emails then k=5 is probably appropriate. Why?

- Assume number of characters is 27.
- Number of shingles = 27^5 = 14, 348, 907
- Typical email length << 14, 348 907 characters ☺
- In practice, there are more than 27 characters but many are very rare which increases probability of shingles of more common letters
- So actually better to assume number of characters for English ≈

Shingles vs Bags-of-words

Representation	parameters	dimensionality
shingles	characters = 27 k = 5	$27^5 \approx 1.4 \times 10^7$
shingles	characters = 20 k = 9	$20^9 = 5.12 \times 10^{11}$
bag-of-words	vocabulary = 500K	5 x 10 ⁵
bag-of-ngrams	vocabulary = 500K n = 2	$500,000^2 = 2.5 \times 10^{11}$

Shingles are fixed length whereas words are variable in length

Hashing shingles

- The ASCII character set has 128 characters
- If we use 1 byte per character, a 9-shingle will take 9 bytes
- And many of the possible shingles will never occur
- Use a hash function which maps 9-shingles to numbers in range $0 \rightarrow 2^{32} 1$
- Then likelihood of each hashed value occurring much more equal.
- And such a number can be stored in 4 bytes
- However, still have several times more shingles per document as individual characters – need compression if lots of documents to analyse.

Minhashing

 A technique for constructing small signatures from large sets whilst preserving estimates of similarity.

Algorithm for minhashing a set represented by a column of a characteristic matrix:

- 1. pick a permutation of the rows
- 2. The minhash value of any column is the first row in the permuted order in which the column has a 1.
- 3. Repeat m times to get a minhash signature of length m

	C1	C2	C3	C4
S1	1	0	0	1
S2	0	0	1	0
S3	0	1	0	1
S4	1	0	1	1
S5	0	0	1	0

permutation 2

	C1	C2	C3	C4
S2	0	0	1	0
S 5	0	0	1	0
S3	0	1	0	1
S1	1	0	0	1
S4	1	0	1	1
МН	4	3	1	3

permutation 1

	C1	C2	C3	C4
S4	1	0	1	1
S3	0	1	0	1
S2	0	0	1	0
S1	1	0	0	1
S 5	0	0	1	0
МН	1	2	1	1

How many permutations?

- In practice, m will be much less than the dimensionality of the matrix (and much much less than the number of possible permutations)
- How large should m be? Say m = 100
- By minhashing we have reduced the dimensionality of the characteristic matrix :
- Originally: e.g. 2³² Boolean values, each Boolean takes 1 bit so 2²⁴ bytes (=17MB) per column
- In minhash signature: each integer < 2³² so can be stored in 4 bytes so 400 bytes per column

Computing Minhash Signatures

- Not feasible to permute a large matrix explicitly
 - would have to pick a random permutation of billions of rows
 - then sort all of those rows ...
- Simulate the effect of a random permutation using a hash function, h(r)
- Same number of buckets as rows
- Whilst there will be some collisions, we can maintain the fiction that our hash function h permutes row r to position h(r)
- So instead of m random permutations, randomly choose m hash functions on the rows

Computing Minhash signatures

- 1. LET $M_{r,c}$ be element of the characteristic matrix for the rth element for cth set.
- 2. Let $SIG_{i,c}$ be the element of the signature matrix for the *i*th hash function and column c.
- 3. Initialise SIG_{i,c} to ∞ for all i and c
- 4. FOR each row r:

```
FOR each hash function h_i: compute h_i(r)
```

FOR each column c:

IF c has a 0 in row r: do nothing ELSE: $SIG_{i,c} = MIN(SIG_{i,c}, h_i(r))$

Minhashing and Jaccard Similarity

The probability that the minhash function for a random permutation of rows produces the same value for two sets equals the Jaccard similarity of those sets.

M	C1	C2	C3	C4
S1	1	0	0	1
S2	0	0	1	0
S3	0	1	0	1
S4	1	0	1	1
S5	0	0	1	0



SIG	C1	C2	C3	C4	
MH1	4	3	1	3	
MH2	1	2	1	1	

Why?

Minhashing and Jaccard

	C1	C2	C3	C4
S1	1	0	0	1
S2	0	0	1	0
S3	0	1	0	1
S4	1	0	1	1
S 5	0	0	1	0

For any given pair of columns:

- Type X rows have a 1 in both
- Type Y rows have different values
- Type Z rows have a 0 in both

For sparse matrices, most rows for most pairings will be type Z

It is the ratio of type X to type Y rows that determine $Jacc(C_i, C_j)$ and also the probability that $h(C_i) = h(C_i)$

$$Jacc(C_3, C_4) = \frac{X_{3,4}}{X_{3,4} + Y_{3,4}} = \frac{1}{5}$$

	C1	C2	C3	C4
S4	1	0	1	1
S 3	0	1	0	1
S2	0	0	1	0
S1	1	0	0	1
S5	0	0	1	0
МН	1	2	1	1

In a random permutation, the probability that we meet a type X row before we meet a type Y row is also $X_{3,4}/(X_{3,4}+Y_{3,4})$

If we do meet a type X row before we meet a type Y row, then we get $MH(C_3) = MH(C_4)$

	C1	C2	C3	C4
S2	0	0	1	0
S5	0	0	1	0
S3	0	1	0	1
S1	1	0	0	1
S4	1	0	1	1
МН	4	3	1	3

However, if we meet a type Y row before we meet a type X row then we get $MH(C_3) \neq MH(C_4)$

Minhashing and Jaccard Similarity

SIG	C1	C2	C3	C4
MH1	4	3	1	3
MH2	1	2	1	1

So, if we carried out ALL random permutations, the proportion of matches in the minhash signatures for 2 objects would equal Jaccard similarity

For a random selection of permutations, proportion of matches will estimate the Jaccard similarity

estimate of Jaccard	C1	C2	C3	C4
C1	1	0	0.5	0.5
C2	0	1	0	0.5
C3	0.5	0	1	0.5
C4	0.5	0.5	0.5	1

Efficient similarity analysis: Summary

- 1. Construct a characteristic matrix:
 - columns are population members e.g. documents, customers
 - rows are items, e.g. hashed k-shingles, items for sale
- 2. Compute *m* minhash signatures.

Jaccard similarity of C_i and C_j is approximately the proportion of minhash signatures which agree in column i and column j

But if n is the size of the population (number of documents / customers etc), this is still $O(n^2)$.

Locality-Sensitive Hashing (LSH)

- A technique for efficiently finding nearest neighbours without computing all-pairs similarities.
- General approach is to hash items several times in such a way that similar items are more likely to be hashed to the same bucket than dissimilar items
- Any pair hashed to the same bucket for any of the hashings is then considered a candidate pair
- Only compute similarities for candidate pairs.
- There will be false positives but these will be found whilst computing similarities
- There will be false negatives (candidate pairs completely missed) – need to minimise these as no way of recovering them.

LSH for a Minhash Signature

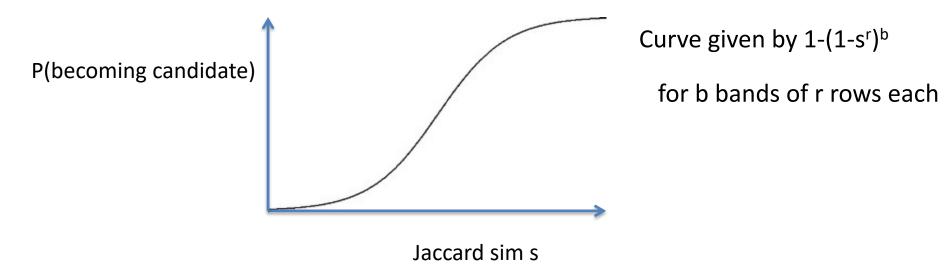
	C1	C2	C3	C4	C5
	4	3	1	3	1
band 1	1	2	1	1	1
	0	1	3	1	3
band 2					
band 3					
band 4					

- Each hash function only considers a band of rows.
- Columns which are identical in the rows of a particular band must be hashed to the same bucket for that band
- There will be accidental collisions (leading to false positives)
- However, similar items will probably be identical in at least 1 band

Analysis of Banding Technique

- Suppose we use b bands of r rows each and that a particular pair of documents have Jaccard similarity s
- P(sigs agree in all rows of a particular band) = s^r
- P(sigs do not agree in all rows of a particular band) = 1 s^r
- P(sigs do not agree in all rows of any band) = (1 s^r)^b
- P(sigs agree in all rows of at least one band) = 1-(1-s^r)^b

Analysis of Banding Technique



- The threshold Jaccard similarity at which it becomes likely that the pair will become a candidate depends on b and r.
- The more rows per band, the higher this threshold is.
- An approximation to the threshold (where Prob=1/2) is threshold similarity = (1/b)^{1/r}
- If 100 rows are divided into 20 bands of 5, what will the threshold similarity be?
- What if we use 5 bands of 20?

Complexity of LSH

 Assuming that parameters have been chosen so that only 10% of pairs are considered to be candidate pairs by LSH, how much efficiency saving do you get for finding the k-nearest neighbours?

Efficient similarity analysis: Summary

- 1. Construct a characteristic matrix:
 - columns are population members e.g. documents, customers
 - rows are items, e.g. hashed k-shingles, items for sale
- 2. Compute *m* minhash signatures.

Jaccard similarity of C_i and C_j is approximately the proportion of minhash signatures which agree in column i and column j

- 1. Choose a similarity threshold, t
- 2. Construct candidate pairs by applying LSH
- 3. Compute similarities for candidate pairs from minhash signatures
- 4. Check similarity for a few original documents (to verify nothing went wrong).

Bonus material: Other Similarity Measures and LSH

- No guarantee that a particular distance / similarity measure has a locality-sensitive family of hash functions
- However possible to do so for:-
 - Hamming distance
 - Cosine distance
 - Euclidean distance

Bonus material: LSH for Cosine

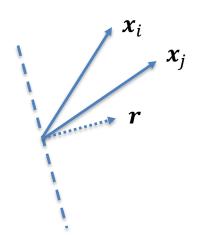
- Consider two points (described by position vectors) and a random hyperplane through the Origin
- The two points are either on the same side of the hyperplane or on different sides of the hyperplane
- If we take the dot product of each vector with the normal vector to the plane
 - Same sign -> same side of hyperplane
 - Different signs -> different sides of hyperplane

Bonus material: LSH for Cosine

 The probability that a random hyperplane separates two unit vectors depends on the angle between them:

$$\Pr[\operatorname{sign}(\boldsymbol{x}_i^T\boldsymbol{r}) = \operatorname{sign}(\boldsymbol{x}_j^T\boldsymbol{r})] = 1 - \frac{1}{\pi} \cos^{-1}(\boldsymbol{x}_i^T\boldsymbol{x}_j)$$

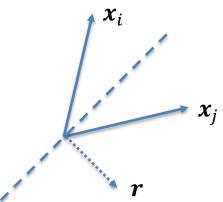
High dot product: unlikely to split



Corresponding hash function:

Lower dot product: likely to split

$$h_{r}(x) = \begin{cases} 1, & \text{if } r^{T}x \geq 0 \\ 0, & \text{otherwise} \end{cases}$$



What have you learnt about the following topics?

- applications of near-neighbour search
- similarity and distance measures
- string similarity
- shingling
- min-hashing
- LSH