CS60021: Scalable Data Mining

Similarity Search and Hashing

Sourangshu Bhattacharya

GENERALIZATION OF LSH

Locality Sensitive Hashing

[Indyk Motwani]

- Hash family H is *locality sensitive* if

$\Pr[h(x) = h(y)]$ is high if x is close to y

$\Pr[h(x) = h(y)]$ is low if x is far from y

- Not clear such functions exist for all distance functions

Locality sensitive hashing

- Originally defined in terms of a similarity function [C'02]

- Given universe U and a similarity $s: U \times U \rightarrow [0,1]$, does there exist a prob distribution over some hash family H such that

$$\Pr_{h \in H}[h(x) = h(y)] = s(x,y)$$

$$s(x,y) = 1 \rightarrow x = y$$
$$s(x,y) = s(y,x)$$

Hamming distance

- Points are bit strings of length d
- $H(x,y) = |\{i, x_i \neq y_i\}|$

Hamming distance

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- $H(x, y) = |\{i, x_i \neq y_i\}|$ $\quad S_H(x, y) = 1 - \frac{H(x,y)}{d}$
  - $x = 1011010001, y = 0111010101$
  - $H(x, y) = 3 \quad S_H(x, y) = 1 - \frac{3}{10} = 0.7$

Hamming distance

- Points are bit strings of length d
- $H(x, y) = |\{i, x_i \neq y_i\}|$ $\quad S_H(x, y) = 1 - \frac{H(x,y)}{d}$
- Define a hash function h by sampling a set of positions
  - $x = 1011010001, y = 0111010101$
  - $S = \{1,5,7\}$
  - $h(x) = 100, h(y) = 100$

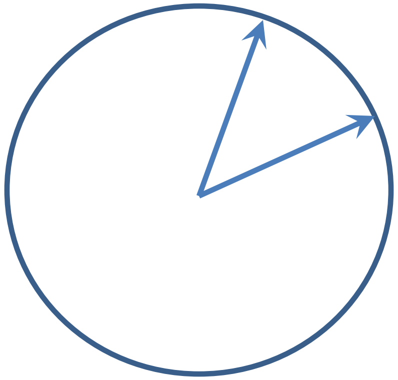
Existence of LSH

- The above hash family is locality sensitive, $k = |S|$

$$\Pr[h(x) = h(y)] = \left(1 - \frac{H(x, y)}{d}\right)^k$$

LSH for angle distance

- x, y are unit norm vectors
- $d(x, y) = \cos^{-1}(x \cdot y) = \theta$
- $S(x, y) = 1 - \theta/\pi$



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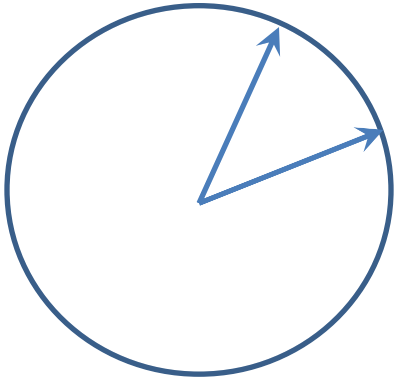
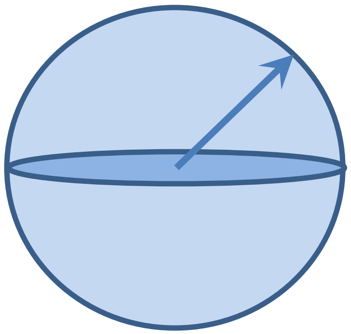


- Choose direction v uniformly at random
  - $h_v(x) = sign(v \cdot x)$
  - $\Pr[h_v(x) = h_v(y)] = 1 - \theta/\pi$

Aside: picking a direction u.a.r.

- How to sample a vector $x \in R^d, |x|_2 = 1$ and the direction is uniform among all possible directions



- Generate $x = (x_1, \ldots . x_d)$, $x_i \sim N(0,1)$ iid
- Normalize $\frac{x}{|x|_2}$
  – By writing the pdf of the d-dimensional Gaussian in polar form, easy to see that this is uniform direction on unit sphere

Jaccard distance: minhashing

- Pick a uniform permutation of the element universe U
- For any set S,
  - $h(S) = min_{x \in S}\, h(x)$

- Often easier to visualize if we think of the collection of sets as a $\{0,1\}$ matrix

Example

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

A
C
G
F
B
E
D

		S_1	S_2	S_3	S_4
1	**A**	1	0	1	0
2	**C**	0	1	0	1
3	**G**	1	0	1	0
4	**F**	1	0	1	0
5	**B**	1	0	0	1
6	**E**	0	1	0	1
7	**D**	0	1	0	1

1	**2**	**1**	**2**

[Slide from Evimaria Terzi]

Example

	S_1	S_2	S_3	S_4
A	1	0	1	0
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D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

→

D
B
A
C
F
G
E

→

		S_1	S_2	S_3	S_4
1	**D**	0	1	0	1
2	**B**	1	0	0	1
3	**A**	1	0	1	0
4	**C**	0	1	0	1
5	**F**	1	0	1	0
6	**G**	1	0	1	0
7	**E**	0	1	0	1
		2	1	3	1

Why is this LSH?

- For sets S and T,
  - The first row where one of the two has a 1 belong to $S \cup T$
  - We have equality $h(S) = h(T)$, only if both the rows contain 1
  - This means that this row belongs to $S \cap T$

- Hence, the event $h(S) = h(T)$ is same as the event that a row in $S \cap T$ appears first among all rows in $S \cup T$

$$\Pr[h(S) = h(T)] = \frac{|S \cap T|}{|S \cup T|}$$

Aside: How to choose random permutations

- Picking a uniform at random permutation is expensive
- In theory, need to choose from a family of min-wise independent permutations

- In practice, can use standard hash functions, hash all the values and then sort

Which similarities admit LSH?

- There are various similarities and distance that are used in scientific literature
  - Encyclopedia of distances DL’11

- Will there be an LSH for each one of them?
  - Similarity is LSHable if there exists an LSH for it

[slide courtesy R. Kumar]

LSHable similarities

- <u>Thm</u>: S is LSHable → 1 – S is a metric

$$d(x,y) = 0 \ \rightarrow x = y$$
$$d(x,y) = d(y,x)$$
$$d(x,y) + d(y,z) \geq d(x,z)$$

Fix hash function $h \in H$ and define

$$\Delta_h(A,B) = [h(A) \neq h(B)]$$
$$1 \ - \mathrm{S}(\mathrm{A},\mathrm{B}) = \Pr_h[\Delta_h(A,B)]$$

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$$\Delta_h(A,B) = [h(A) \neq h(B)]$$
$$1 \ - \mathrm{S}(\mathrm{A},\mathrm{B}) = \Pr_h[\Delta_h(A,B)]$$

Also

$$\Delta_h(A,B) + \Delta_h(B,C) \geq \Delta_h(A,C)$$

Example of non-LSHable similarities

- $d(A, B) = 1 - s(A, B)$
- Sorenson-Dice : $s(A, B) = \frac{2|A \cap B|}{|A| + |B|}$
  - Ex: $A = \{a\}, B = \{b\}, C = \{a, b\}$
  - $s(A, B) = 0, s(B, C) = s(A, C) = 2/3$

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  - $s(A,B) = 0, s(B,C) = s(A,C) = \frac{2}{3}$
- Overlap: $s(A,B) = \frac{|A \cap B|}{\min(|A|,|B|)}$
  - $s(A,B) = 0, s(A,C) = 1 = s(B,C)$

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- Overlap: $s(A, B) = \frac{|A \cap B|}{\min(|A|, |B|)}$
  - $s(A, B) = 0, s(A, C) = 1 = s(B, C)$

These similarities are not LSHable

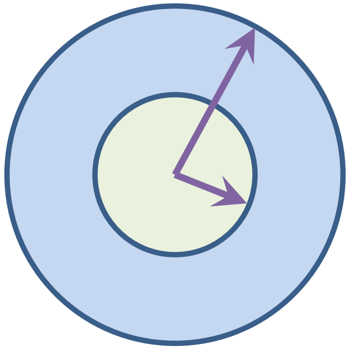
Gap Definition of LSH

IMRS'97, IM'98, GIM'99

- A family is (r, R, p, P) LSH if

$$\Pr_{h \in H}[h(x) = h(y)] \geq p \; if \; d(x,y) \leq r$$

$$\Pr_{h \in H}[h(x) = h(y)] \leq P \; if \; d(x,y) \geq R$$



Gap LSH

- All the previous constructions satisfy the gap definition
  - Ex: for $JS(S,T) = \frac{|S \cap T|}{|S \cup T|}$

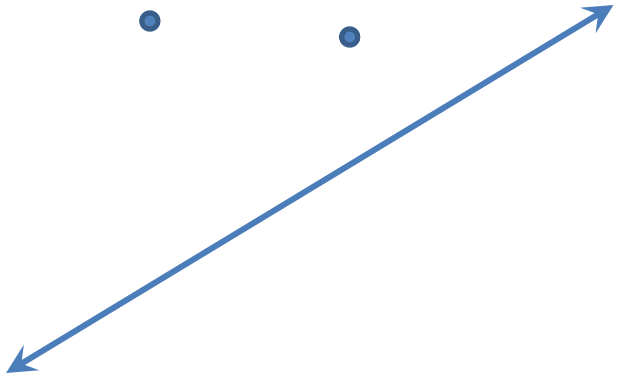
$$JD(S,T) \leq r \rightarrow JS(S,T) \geq 1 - r \rightarrow \Pr[h(S) = h(T)] = JS(S,T) \geq 1 - r$$

$$JD(S,T) \geq R \rightarrow JS(S,T) \leq 1 - R \rightarrow \Pr[h(S) = h(T)] = JS(S,T) \leq 1 - R$$

Hence is a $(r, R, 1-r, 1-R)$ LSH

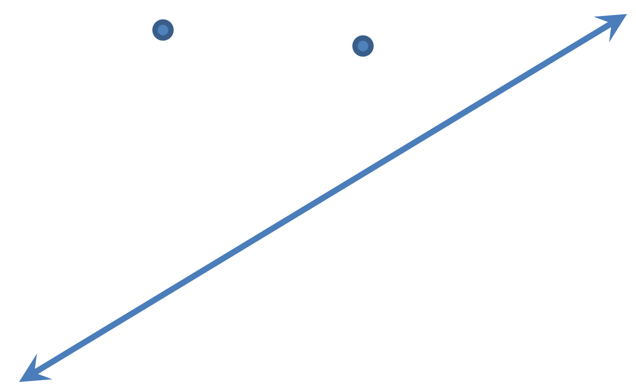
L2 norm

- $d(x, y) = \sqrt{(\sum_i (x_i - y_i)^2}$
- u = random unit norm vector, $w \in R$ parameter, $b \sim Unif[0, w]$
- $h(x) = \lfloor \frac{u \cdot x + b}{w} \rfloor$



L2 norm

- $d(x, y) = \surd(\sum_i(x_i - y_i)^2$
- $u =$ random unit norm vector, $w \in R$ parameter, $b \sim Unif[0, w]$
- $h(x) = \lfloor \frac{u \cdot x + b}{w} \rfloor$
- If $|x - y|_2 < \frac{w}{2}$, $\Pr[h(x) = h(y)] \geq \frac{1}{3}$
- If $|x - y|_2 > 4w$, $\Pr[h(x) = h(y)] \leq \frac{1}{4}$



Solving the near neighbour

- (r, c) $-$near neighbour problem
  - Given query point q, return all points p such that $d(p, q) < r$ and none such that $d(p, q) > cr$
  - Solving this gives a subroutine to solve the "nearest neighbour", by building a data-structure for each r , in powers of $(1 + \epsilon)$

How to actually use it?

- Need to amplify the probability of collisions for “near” points

Band construction

- AND-ing of LSH
  - Define a composite function $H(x) = (h_1(x), \ldots h_k(x))$
  - $\Pr[H(x) = H(y)] = \Pi_{\mathrm{i}} \Pr[h_i(x) = h_i(y)] = \Pr[h_1(x) = h_1(y)]^k$

Band construction

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  - Define a composite function $H(x) = (h_1(x), \dots h_k(x))$
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- OR-ing
  - Create L independent hash-tables for $H_1, H_2, \dots H_L$
  - Given query q, search in $\cup_j H_j(q)$

Example

	S_1	S_2	S_3	S_4
A	1	0	1	0
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C	0	1	0	1
D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

	S1	S2	S3	S3
h1	1	2	1	2
h2	2	1	3	1

	S1	S2	S3	S3
h3	3	1	2	1
h4	1	3	2	2

Why is this better?

- Consider q, y with $\Pr[h(q) = h(y)] = 1 - d(x, y)$
- Probability of not finding y as one of the candidates in $\cup_j H_j(q)$

$$1 - \left(1 - (1 - d)^k\right)^L$$

Creating an LSH

- If we have a (r, cr, p, q) LSH
- For any y, with $|q - y| < r$,
  - Prob of y as candidate in $\cup_j H_j(q) \geq 1 - \left(1 - p^k\right)^L$
- For any z, $|q - z| > cr$,
  - Prob of z as candidate in any fixed $H_j(q) \leq q^k$
  - Expected number of such $z \leq Lq^k$

Creating an LSH

- If we have a (r, cr, p, q) LSH $\rho = \frac{\log(p)}{\log(q)}$ $L = n^\rho$ $k = \log(n)/\log\left(\frac{1}{q}\right)$
- For any y, with $|q - y| < r$,
  - Prob of y as candidate in $\cup_j H_j(q) \geq 1 - \left(1 - p^k\right)^L \geq 1 - \frac{1}{e}$
- For any z, $|q - z| > cr$,
  - Prob of z as candidate in any fixed $H_j(q) \leq q^k$
  - Expected number of such $z \leq Lq^k \leq L = n^\rho$

Runtime

- Space used = $n^{1+\rho}$
- Query time = n^{ρ}

- We can show that for Hamming, angle etc, $\rho \approx \frac{1}{c}$
  - Can get 2-approx near neighbors in $O\left(\sqrt{n}\right)$ query time

LSH: theory vs practice

- In order to design LSH in practice, the theoretical parameter values are only a guidance
  - Typically need to search over the parameter space to find a good operating point
  - Data statistics can provide some guidance (will see in next class)

Summary

- Locality sensitive hashing is a powerful tool for near neighbour problems
- Trades off space with query time
- Practical for medium to large datasets with fairly large number of dimensions
  - However, doesn't really work very well for sparse, very very high dimensional datasets
- LSH and extensions are an area of active research and practice

References:

- Primary references for this lecture
  - Modern Massive Datasets, Rajaraman, Leskovec, Ullman.
  - Survey by Andoni et al. (CACM 2008) available at www.mit.edu/~andoni/LSH