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Theory of Locality Sensitive Hashing

CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
http://cs246.stanford.edu
Task: Given a large number ($N$ in the millions or billions) of documents, find “near duplicates”

Problem:
- Too many documents to compare all pairs

Solution: Hash documents so that similar documents hash into the same bucket
- Documents in the same bucket are then candidate pairs whose similarity is then evaluated
The set of strings of length $k$ that appear in the document

**Signatures:** short integer vectors that represent the sets, and reflect their similarity

**Candidate pairs:** those pairs of signatures that we need to test for similarity
Recap 1: Shingles

- A *k*-shingle (or *k*-gram) is a sequence of *k* tokens that appears in the document
  - **Example:** *k*=2; $D_1 = abcab$
    - Set of 2-shingles: $C_1 = S(D_1) = \{ab, bc, ca\}$
- Represent a doc by a set of hash values of its *k*-shingles
- A natural **similarity measure** is then the **Jaccard similarity**:
  $$sim(D_1, D_2) = \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|}$$
  - Similarity of two documents is the Jaccard similarity of their shingles
### Recap 2: Minhashing

**Min-Hashing**: Convert large sets into short signatures, while preserving similarity: \( \Pr[h(C_1) = h(C_2)] = \text{sim}(D_1, D_2) \)

<table>
<thead>
<tr>
<th>Permutation ( \pi )</th>
<th>Input matrix (Shingles x Documents)</th>
<th>Signature matrix ( M )</th>
</tr>
</thead>
</table>
| 2 4 3                  | \[
| 1 0 1 0               | \[2 1 2 1\]                        |
| 1 0 0 1               | | \[2 1 4 1\]                        |
| 0 1 0 1               | | \[1 2 1 2\]                        |
| 0 1 0 1               | |                                      |
| 1 0 1 0               | |                                      |
| 1 0 1 0               | |                                      |
| 1 0 1 0               | |                                      |

Similarities of columns and signatures (approx.) match!

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<th>Col/Col</th>
<th>Sig/Sig</th>
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<tbody>
<tr>
<td>1-3</td>
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<td>0.75</td>
<td>0.75</td>
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<td>0.67</td>
<td>1.00</td>
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</table>
Hash columns of the signature matrix $M$: Similar columns likely hash to same bucket

- Divide matrix $M$ into $b$ bands of $r$ rows ($M=b\cdot r$)
- **Candidate** column pairs are those that hash to the same bucket for $\geq 1$ band
Today: Generalizing Min-hash

Design a **locality sensitive hash function** (for a given distance metric)

Apply the “Bands” technique

**Signatures**: short integer signatures that reflect point similarity

**Candidate pairs**: those pairs of signatures that we need to test for similarity
The S-curve is where the “magic” happens

Remember: Probability of equal hash-values = similarity

Pr[hπ(C1) = hπ(C2)] = sim(D1, D2)

This is what 1 hash-code gives you

This is what we want!

How to get a step-function?
By choosing r and b!
How Do We Make the S-curve?

- **Remember:** \( b \) bands, \( r \) rows/band
- Let \( \text{sim}(C_1, C_2) = s \)

**What’s the prob. that at least 1 band is equal?**
- Pick some band (\( r \) rows)
  - Prob. that elements in a single row of columns \( C_1 \) and \( C_2 \) are equal \( = s \)
  - Prob. that all rows in a band are equal \( = s^r \)
  - Prob. that some row in a band is not equal \( = 1 - s^r \)
- Prob. that all bands are not equal \( = (1 - s^r)^b \)
- Prob. that at least 1 band is equal \( = 1 - (1 - s^r)^b \)

\[
P(C_1, C_2 \text{ is a candidate pair}) = 1 - (1 - s^r)^b
\]
Picking $r$ and $b$: The S-curve

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

![Graph showing the probability of sharing a bucket vs similarity](image-url)
S-curves as a func. of $b$ and $r$

Given a fixed threshold $t$.

We want choose $r$ and $b$ such that the $P(Candidate \ pair)$ has a “step” right around $t$. 

$$ prob = 1 - (1 - s^r)^b $$
Visualization of the effect of threshold, band size, and # of rows in LSH
by Trenton Chang (Thank you!!)
https://www.desmos.com/calculator/lzzvfjiujn
Signatures: short vectors that represent the sets, and reflect their similarity.

Candidate pairs: those pairs of signatures that we need to test for similarity.

Theory of LSH

General hashing vs. locality-sensitive hashing.
We have used LSH to find similar documents

- More generally, we found similar columns in large sparse matrices with high Jaccard similarity

Can we use LSH for other distance measures?

- e.g., Euclidean distances, Cosine distance
- Let’s generalize what we’ve learned!
Distance Measures

- $d(\cdot)$ is a **distance measure** if it is a function from pairs of points $x,y$ to real numbers such that:
  - $d(x, y) \geq 0$
  - $d(x, y) = 0$ if $x = y$
  - $d(x, y) = d(y, x)$
  - $d(x, y) \leq d(x, z) + d(z, y)$ (triangle inequality)

- **Jaccard distance** for sets = $1 - \text{Jaccard similarity}$
- **Cosine distance** for vectors = angle between the vectors
- **Euclidean distances**:
  - $L_2 \text{ norm}$: $d(x,y) = \sqrt{\text{sum of the squares of the differences between } x \text{ and } y \text{ in each dimension}}$
    - The most common notion of “distance”
  - $L_1 \text{ norm}$: sum of absolute value of the differences in each dimension
    - *Manhattan distance* = distance if you travel along axes only
Families of Hash Functions

- For Min-Hashing signatures, we got a Min-Hash function for each permutation of rows.
- A “hash function” is any function that allows us to say whether two elements are “equal”.
  - Shorthand: $h(x) = h(y)$ means “$h$ says $x$ and $y$ are equal”.
- A family of hash functions is any set of hash functions from which we can **efficiently pick one at random**.
  - Example: The set of Min-Hash functions generated from permutations of rows.
Locality-Sensitive (LS) Families

- Suppose we have a space $S$ of points with a distance measure $d(x,y)$

- A family $H$ of hash functions is said to be $(d_1, d_2, p_1, p_2)$-sensitive if for any $x$ and $y$ in $S$:
  1. If $d(x, y) \leq d_1$, then the probability over all $h \in H$, that $h(x) = h(y)$ is at least $p_1$
  2. If $d(x, y) \geq d_2$, then the probability over all $h \in H$, that $h(x) = h(y)$ is at most $p_2$

Critical assumption

With a LS Family we can do LSH!
A \((d_1, d_2, p_1, p_2)\)-sensitive function

Small distance, high probability

Large distance, low probability of hashing to the same value

Notice it’s distance, not similarity, hence the S-curve is flipped!
Let:

- $S =$ space of all sets,
- $d =$ Jaccard distance,
- $H$ is family of Min-Hash functions for all permutations of rows

Then for any hash function $h \in H$:

$$\Pr[h(x) = h(y)] = 1 - d(x, y)$$

Simply restates theorem about Min-Hashing in terms of distances rather than similarities
Claim: Min-hash $H$ is a $(1/3, 2/3, 2/3, 1/3)$-sensitive family for $S$ and $d$.

If distance $\leq 1/3$ (so similarity $\geq 2/3$)

Then probability that Min-Hash values agree is $> 2/3$

For Jaccard similarity, Min-Hashing gives a $(d_1, d_2, (1-d_1), (1-d_2))$-sensitive family for any $d_1 < d_2$
Can we reproduce the “S-curve” effect we saw before for any LS family?

The “bands” technique we learned for signature matrices carries over to this more general setting.

Can do LSH with any \((d_1, d_2, p_1, p_2)\)-sensitive family!

Two constructions:
- **AND** construction like “rows in a band”
- **OR** construction like “many bands”
Amplifying Hash Functions: AND and OR
AND of Hash Functions

- Given family $H$, construct family $H'$ consisting of $r$ functions from $H$
- For $h = [h_1,...,h_r]$ in $H'$, we say $h(x) = h(y)$ if and only if $h_i(x) = h_i(y)$ for all $i$ $1 \leq i \leq r$
  - Note this corresponds to creating a band of size $r$

**Theorem:** If $H$ is $(d_1, d_2, p_1, p_2)$-sensitive, then $H'$ is $(d_1, d_2, (p_1)^r, (p_2)^r)$-sensitive

**Proof:** Use the fact that $h_i$'s are independent

Also lowers probability for small distances (Bad)

Lowers probability for large distances (Good)
Independence of hash functions (HFs) really means that the prob. of two HFs saying “yes” is the product of each saying “yes”

- But two particular hash functions could be highly correlated
  - For example, in Min-Hash if their permutations agree in the first one million entries
- However, the probabilities in definition of a LSH-family are over all possible members of $H, H'$ (i.e., average case and not the worst case)
Given family $H$, construct family $H'$ consisting of $b$ functions from $H$.

For $h = [h_1, ..., h_b]$ in $H'$, $h(x) = h(y)$ if and only if $h_i(x) = h_i(y)$ for at least 1 $i$.

**Theorem:** If $H$ is $(d_1, d_2, p_1, p_2)$-sensitive, then $H'$ is $(d_1, d_2, 1-(1-p_1)^b, 1-(1-p_2)^b)$-sensitive.

**Proof:** Use the fact that $h_i$'s are independent.

- Raises probability for small distances (Good)
- Raises probability for large distances (Bad)
**Effect of AND and OR Constructions**

- **AND** makes all probs. **shrink**, but by choosing $r$ correctly, we can make the lower prob. approach 0 while the higher does not.

- **OR** makes all probs. **grow**, but by choosing $b$ correctly, we can make the higher prob. approach 1 while the lower does not.
By choosing \( b \) and \( r \) correctly, we can make the lower probability approach 0 while the higher approaches 1.

As for the signature matrix, we can use the AND construction followed by the OR construction:
- Or vice-versa
- Or any sequence of AND’s and OR’s alternating
Composing Constructions

- **r-way AND** followed by **b-way OR** construction
  - **Exactly what we did with Min-Hashing**
    - **AND:** If bands match in **all** $r$ values hash to same bucket
    - **OR:** Cols that have $\geq 1$ common bucket $\Rightarrow$ **Candidate**

- Take points $x$ and $y$ s.t. $Pr[h(x) = h(y)] = s$
  - $H$ will make $(x,y)$ a candidate pair with prob. $s$
  - Construction makes $(x,y)$ a candidate pair with probability $1-(1-s^r)^b$ **The S-Curve!**

- **Example:** Take $H$ and construct $H'$ by the **AND** construction with $r = 4$. Then, from $H'$, construct $H''$ by the **OR** construction with $b = 4$
Table for Function $1-(1-s^4)^4$

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<tr>
<th>s</th>
<th>$p=1-(1-s^4)^4$</th>
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<td>.2</td>
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$r = 4, b = 4$ transforms a (.2,.8,.8,.2)-sensitive family into a (.2,.8,.8785,.0064)-sensitive family.
How to choose $r$ and $b$
Picking $r$ and $b$: The S-curve

- **Picking $r$ and $b$ to get desired performance**
  - 50 hash-functions ($r = 5$, $b = 10$)

**Blue area X:** False Negative rate
These are pairs with $\text{sim} > t$ but the $X$ fraction won’t share a band and then will **never become candidates**. This means we will never consider these pairs for (slow/exact) similarity calculation!

**Green area Y:** False Positive rate
These are pairs with $\text{sim} < t$ but we will consider them as candidates. This is not too bad, we will consider them for (slow/exact) similarity computation and discard them.
Picking $r$ and $b$: The S-curve

- Picking $r$ and $b$ to get desired performance
  - 50 hash-functions ($r \times b = 50$)

![Graph showing the S-curve with different values of $r$ and $b$.]

- $r=2, b=25$
- $r=5, b=10$
- $r=10, b=5$
OR-AND Composition

- Apply a $b$-way OR construction followed by an $r$-way AND construction
- Transforms similarity $s$ (probability $p$) into $(1-(1-s)^b)^r$
  - The same S-curve, mirrored horizontally and vertically

**Example:** Take $H$ and construct $H'$ by the OR construction with $b = 4$. Then, from $H'$, construct $H''$ by the AND construction with $r = 4
The example transforms a (.2,.8,.8,.2)-sensitive family into a (.2,.8,.9936,.1215)-sensitive family.
Example: Apply the (4,4) OR-AND construction followed by the (4,4) AND-OR construction

Transforms a (.2, .8, .8, .2)-sensitive family into a (.2, .8, .9999996, .0008715)-sensitive family

Note this family uses 256 (=4*4*4*4) of the original hash functions
For each AND-OR S-curve $1-(1-s^r)^b$, there is a threshold $t$, for which $1-(1-t^r)^b = t$

Above $t$, high probabilities are increased; below $t$, low probabilities are decreased

You improve the sensitivity as long as the low probability is less than $t$, and the high probability is greater than $t$

- Iterate as you like

Similar observation for the OR-AND type of S-curve: $(1-(1-s)^b)^r$
Pick any two distances \( d_1 < d_2 \)

Start with a \((d_1, d_2, (1- d_1), (1- d_2))\)-sensitive family

Apply constructions to amplify \((d_1, d_2, p_1, p_2)\)-sensitive family, where \( p_1 \) is almost 1 and \( p_2 \) is almost 0

The closer to 0 and 1 we get, the more hash functions must be used!
LSH for other distance metrics
LSH methods for other distance metrics:
- **Cosine distance:** Random hyperplanes
- **Euclidean distance:** Project on lines

Design a \((d_1, d_2, p_1, p_2)\)-sensitive family of hash functions (for that particular distance metric)

Depends on the distance function used

**Signatures:** short integer signatures that reflect their similarity

**Locality-sensitive Hashing**

**Candidate pairs:** those pairs of signatures that we need to test for similarity

Amplify the family using \textbf{AND} and \textbf{OR} constructions
**Summary of what we will learn**

- **Data**: Input data
- **Hash func.**: Map data to signatures
- **Signatures**: Short integer signatures that reflect their similarity
- **Locality-sensitive Hashing**: Select candidate pairs for similarity testing

**Candidate pairs**: Pairs of signatures that need to be tested for similarity

**Documents**

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**Data points**

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**MinHash**

- 1 5 1 5
- 2 3 1 3
- 6 4 6 4

**Random Hyperplanes**

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**“Bands” technique**

- Candidate pairs
LSH for Cosine Distance
**Cosine Distance**

- **Cosine distance** = angle between vectors from the origin to the points in question

\[ d(A, B) = \theta = \arccos\left(\frac{A \cdot B}{\|A\| \cdot \|B\|}\right) \]

- Has range \([0, \pi]\) (equivalently \([0,180^\circ]\))
- Can divide \(\theta\) by \(\pi\) to have distance in range \([0,1]\)

- **Cosine similarity** = \(1 - d(A,B)\)

- But often defined as **cosine sim**: \(\cos(\theta) = \frac{A \cdot B}{\|A\| \cdot \|B\|}\)
  - Has range -1...1 for general vectors
  - Range 0..1 for non-negative vectors (angles up to 90°)
For cosine distance, there is a technique called Random Hyperplanes

- Technique similar to Min-Hashing

Random Hyperplanes method is a \((d_1, d_2, (1-d_1/\pi), (1-d_2/\pi))\)-sensitive family for any \(d_1\) and \(d_2\)

- Reminder: \((d_1, d_2, p_1, p_2)\)-sensitive
  1. If \(d(x,y) \leq d_1\), then prob. that \(h(x) = h(y)\) is at least \(p_1\)
  2. If \(d(x,y) \geq d_2\), then prob. that \(h(x) = h(y)\) is at most \(p_2\)
Each vector $\mathbf{v}$ determines a hash function $h_{\mathbf{v}}$ with two buckets

- $h_{\mathbf{v}}(x) = +1$ if $\mathbf{v} \cdot x \geq 0$; $= -1$ if $\mathbf{v} \cdot x < 0$

- LS-family $H = \text{set of all functions derived from any vector}$

- **Claim:** For points $\mathbf{x}$ and $\mathbf{y}$,
  \[
  \Pr[h(\mathbf{x}) = h(\mathbf{y})] = 1 - \frac{d(\mathbf{x},\mathbf{y})}{\pi}
  \]
Proof of Claim

Look in the plane of \( x \) and \( y \).

Hyperplane normal to \( v \).
Here \( h(x) = h(y) \)

Hyperplane normal to \( v' \).
Here \( h(x) \neq h(y) \)

Note: what is important is that hyperplane is outside the angle, not that the vector is inside.
Proof of Claim

So: \( \text{Prob[Red case]} = \frac{\theta}{\pi} \)

So: \( P[h(x)=h(y)] = 1 - \frac{\theta}{\pi} = 1 - \frac{d(x,y)}{\pi} \)
Pick some number of random vectors, and hash your data for each vector

The result is a signature (sketch) of +1’s and −1’s for each data point

Can be used for LSH like we used the Min-Hash signatures for Jaccard distance

Amplify using AND/OR constructions
Expensive to pick a random vector in $M$ dimensions for large $M$
- Would have to generate $M$ random numbers

A more efficient approach
- It suffices to consider only vectors $v$ consisting of $+1$ and $-1$ components
  - **Why?** Assuming data is random, then vectors of $+/-1$ cover the entire space evenly (and does not bias in any way)
LSH for Euclidean Distance
Idea: Hash functions correspond to lines

Partition the line into buckets of size \( a \)

Hash each point to the bucket containing its projection onto the line

- An element of the “Signature” is a bucket id for that given projection line

Nearby points are always close; distant points are rarely in same bucket
“Lucky” case:
- Points that are close hash in the same bucket
- Distant points end up in different buckets

Two “unlucky” cases:
- **Top**: unlucky quantization
- **Bottom**: unlucky projection
Multiple Projections
Points at distance $d$

If $d << a$, then the chance the points are in the same bucket is at least $1 - \frac{d}{a}$. 

Randomly chosen line

Bucket width $a$
If $d \gg a$, $\theta$ must be close to $90^\circ$ for there to be any chance points go to the same bucket.
If points are distance $d \leq a/2$, prob. they are in same bucket $\geq 1 - d/a = \frac{1}{2}$

If points are distance $d > 2a$ apart, then they can be in the same bucket only if $d \cos \theta \leq a$

- $\cos \theta \leq \frac{1}{2}$
- $60 \leq \theta \leq 90$, i.e., at most $1/3$ probability

Yields a $(a/2, 2a, 1/2, 1/3)$-sensitive family of hash functions for any $a$

Amplify using AND-OR cascades
**Summary**

Data $\rightarrow$ Hash func. $\rightarrow$ **Signatures:** short integer signatures that reflect their similarity $\rightarrow$ Localy-sensitive Hashing

**Candidate pairs:** those pairs of signatures that we need to test for similarity

- Design a $(d_1, d_2, p_1, p_2)$-sensitive family of hash functions (for that particular distance metric)

- Amplify the family using AND and OR constructions

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**MinHash**

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1 5 1 5
2 3 1 3
6 4 6 4
```

**Candidate pairs**

**Data points**

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**Random Hyperplanes**

```
-1 +1 -1 -1
+1 +1 -1 -1
-1 -1 -1 -1
```

**Candidate pairs**
Two Important Points

- Property $P(h(C_1)=h(C_2))=\text{sim}(C_1,C_2)$ of hash function $h$ is the essential part of LSH, without which we can’t do anything.

- LS-hash functions transform data to signatures so that the bands technique (AND, OR constructions) can then be applied.