Announcements

Recitation sessions:
- Review of linear algebra:
  - Tuesday, April 2, 3:30-5pm CSE2 G01
- Review of “big data tricks” (e.g. vectorization):
  - Thursday, April 4, 3:30-5pm CSE2 G04

For office hours – please check our website

More Spark tutorials? Revisit recitation and check out our next homework questions. If you want to know more, you’ll need to take a focused course.
Please give us feedback 😊

Finding Similar Items: Locality Sensitive Hashing

CSE547 Machine Learning for Big Data
Tim Althoff

PAUL G. ALLEN SCHOOL OF COMPUTER SCIENCE & ENGINEERING
New thread: High dim. data

High dim. data
- Locality sensitive hashing
- Clustering
- Dimensionality reduction

Graph data
- PageRank, SimRank
- Network Analysis
- Spam Detection

Infinite data
- Sampling data streams
- Filtering data streams
- Queries on streams

Machine learning
- SVM
- Decision Trees
- Perceptron, kNN

Apps
- Recommender systems
- Association Rules
- Duplicate document detection
Pinterest Visual Search

Given a query image patch, find similar images
Collect billions of images
- Determine feature vector for each image (4k dim)
- Given a query Q, find nearest neighbors FAST
How does it work?

Nearest neighbor query in the embedding space
Application: Visual Search

Visually similar results

- Nike
- "zizi repetto"
- kris van assche sneakers
- This COS top from the men's section kicks all the right...
- stan smith outfits - Buscar con Google
- Glorious Ladies

Tags:
- shoes
- sneakers
- nike
- adidas
- fashion
- light up shoes
- style
- air force
A Common Metaphor

- Many problems can be expressed as finding “similar” sets:
  - Find near-neighbors in high-dimensional space

- Examples:
  - Pages with similar words
    - For duplicate detection, classification by topic
  - Customers who purchased similar products
    - Products with similar customer sets
  - Images with similar features
    - Image completion
  - Recommendations and search
Problem for today’s lecture

- **Given:** High dimensional data points $x_1, x_2, ...$
  - **For example:**
    - An image is a long vector of pixel colors
    - A documents might be a bag-of-words or set of shingles
- **And some distance function** $d(x_1, x_2)$
  - which quantifies the “distance” between $x_1$ and $x_2$
- **Goal:** Find **all pairs of data points** $(x_i, x_j)$ that are within distance threshold $d(x_i, x_j) \leq s$
- **Note:** Naïve solution would take $O(N^2)$
  where $N$ is the number of data points
- **MAGIC:** This can be done in $O(N)$!! How??

LSH: Locality Sensitive Hashing

- LSH is really a family of related techniques
- In general, one throws items into buckets using several different “hash functions”
- You examine only those pairs of items that share a bucket for at least one of these hash functions
- **Upside:** Designed correctly, only a small fraction of pairs are ever examined
- **Downside:** There are *false negatives* – pairs of similar items that never even get considered
Motivating Application: Finding Similar Documents
Motivation for Min-Hash/LSH

- Suppose we need to find near-duplicate documents among $N = 1$ million documents
  - Naïvely, we would have to compute pairwise similarities for every pair of docs
    - $N(N - 1)/2 \approx 5 \times 10^{11}$ comparisons
    - At $10^5$ secs/day and $10^6$ comparisons/sec, it would take 5 days
  - For $N = 10$ million, it takes more than a year...

- Similarly, we have a dataset of 10m images, quickly find the most similar to query image $Q$
3 Essential Steps for Similar Docs

1. *Shingling*: Converts a document into a set representation (Boolean vector)

2. *Min-Hashing*: Convert large sets to short signatures, while preserving similarity

3. *Locality-Sensitive Hashing*: Focus on pairs of signatures likely to be from similar documents
   - Candidate pairs!
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
Step 1: **Shingling**
Convert a document into a set

The set of strings of length $k$ that appear in the document.
Documents as High-Dim Data

Step 1: **Shingling**: Converts a document into a set

- A *k*-shingle (or *k*-gram) for a document is a sequence of *k* tokens that appears in the doc
  - Tokens can be characters, words or something else, depending on the application
  - Assume tokens = characters for lecture examples
- To **compress long shingles**, we can hash them to (say) 4 bytes
- **Represent a document by the set of hash values of its *k*-shingles**
Compressing Shingles

- **Example:** k=2; document $D_1 = \text{abcbab}$
  - Set of 2-shingles: $S(D_1) = \{ab, bc, ca\}$
  - Hash the shingles: $h(D_1) = \{1, 5, 7\}$
- $k = 8, 9, \text{ or } 10$ is often used in practice

- **Benefits of shingles:**
  - Documents that are intuitively similar will have many shingles in common
  - Changing a word only affects k-shingles within distance $k-1$ from the word
Similarity Metric for Shingles

- **Document** $D_1$ **is represented by a set of its k-shingles** $C_1 = S(D_1)$
- **A natural similarity measure is the Jaccard similarity:**

  $$\text{sim}(D_1, D_2) = \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|}$$

  **Jaccard distance:**

  $$d(C_1, C_2) = 1 - \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|}$$

  3 in intersection.
  8 in union.
  Jaccard similarity
  $= 3/8$
Encode sets using 0/1 (bit, Boolean) vectors

- **Rows** = elements (shingles)
- **Columns** = sets (documents)
  - 1 in row \( e \) and column \( s \) if and only if \( e \) is a member of \( s \)
  - Column similarity is the Jaccard similarity of the corresponding sets (rows with value 1)
- **Typical matrix is sparse!**
- **Each document is a column:**
  - Example: \( \text{sim}(C_1, C_2) = ? \)
    - Size of intersection = 3; size of union = 6, Jaccard similarity (not distance) = 3/6
    - \( d(C_1, C_2) = 1 - \text{(Jaccard similarity)} = 3/6 \)

We don’t really construct the matrix; just imagine it exists
Outline: Finding Similar Columns

- **So far:**
  - Documents to Sets of shingles
  - Represent sets as Boolean vectors in a matrix

- **Next goal:** Find similar columns while computing small signatures
  - Similarity of columns == similarity of signatures

- **Warnings:**
  - Comparing all pairs takes too much time: **Job for LSH**
    - These methods can produce false negatives, and even false positives (if the optional check is not made)
Step 2: **Min-Hashing**: Convert large sets to short signatures, while preserving similarity.
Hashing Columns (Signatures)

- **Key idea:** “hash” each column $C$ to a small signature $h(C)$, such that:
  - $\text{sim}(C_1, C_2)$ is the same as the “similarity” of signatures $h(C_1)$ and $h(C_2)$

- **Goal:** Find a hash function $h(\cdot)$ such that:
  - If $\text{sim}(C_1, C_2)$ is high, then with high prob. $h(C_1) = h(C_2)$
  - If $\text{sim}(C_1, C_2)$ is low, then with high prob. $h(C_1) \neq h(C_2)$

- **Idea:** Hash docs into buckets. Expect that “most” pairs of near duplicate docs hash into the same bucket!
Min-Hashing: Goal

- **Goal:** Find a hash function $h(\cdot)$ such that:
  - if $\text{sim}(C_1, C_2)$ is high, then with high prob. $h(C_1) = h(C_2)$
  - if $\text{sim}(C_1, C_2)$ is low, then with high prob. $h(C_1) \neq h(C_2)$

- Clearly, the hash function depends on the similarity metric:
  - Not all similarity metrics have a suitable hash function

- There is a suitable hash function for the Jaccard similarity: It is called **Min-Hashing**
Min-Hashing: Overview

- Permute the rows of the Boolean matrix using some permutation $\pi$
  - Thought experiment – not actually materialized

- Define **minhash function** for this permutation $\pi$, $h_\pi(C) =$ the number of the first (in the permuted order) row in which column $C$ has value 1.
  - Denoted this as: $h_\pi(C) = \min_\pi \pi(C)$

- Apply, to all columns, several randomly chosen permutations $\pi$ to create a **signature** for each column

- **Result is a signature matrix**: Columns = sets, Rows = minhash values for each permutation $\pi$
Min-Hashing Example

Input matrix
(Shingles x Documents)

Permutation $\pi$

$h_\pi(C) = \min_\pi \pi(C)$

Signature matrix $M$
Min-Hashing Example

Input matrix
(Shingles x Documents)

Permutation $\pi$

$ h_{\pi}(C) = \min_{\pi} \pi(C) $ 

Signature matrix $M$
Min-Hashing Example

Input matrix (Shingles x Documents)

Permutation $\pi$

$h_\pi(C) = \min_\pi \pi(C)$

Signature matrix $M$
A Subtle Point

- Students sometimes ask whether the minhash value should be the original number of the row, or the number in the permuted order (as we did in our example)

**Answer:** it doesn’t matter

- We only need to be consistent, and assure that two columns get the same value if and only if their first 1’s in the permuted order are in the same row
The Min-Hash Property

- Choose a random permutation $\pi$
- **Claim:** $\Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
- **Why?**
  - Let $X$ be a doc (set of shingles), $z \in X$ is a shingle
  - **Then:** $\Pr[\pi(z) = \min(\pi(X))] = 1/|X|$
    - It is equally likely that any $z \in X$ is mapped to the $\min$ element
  - Let $y$ be s.t. $\pi(y) = \min(\pi(C_1 \cup C_2))$
  - **Then either:** $\pi(y) = \min(\pi(C_1))$ if $y \in C_1$, or $\pi(y) = \min(\pi(C_2))$ if $y \in C_2$
  - So the prob. that both are true is the prob. $y \in C_1 \cap C_2$
  - $\Pr[\min(\pi(C_1))=\min(\pi(C_2))] = \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|} = sim(C_1, C_2)$
Four Types of Rows

- Given cols $C_1$ and $C_2$, rows are classified as:

<table>
<thead>
<tr>
<th></th>
<th>$C_1$</th>
<th>$C_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>B</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>D</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Define: $a = \# \text{ rows of type } A$, etc.

- Note: $\text{sim}(C_1, C_2) = \frac{a}{a + b + c}$

- Then: $\text{Pr}[h(C_1) = h(C_2)] = Sim(C_1, C_2)$

  - Look down the permuted cols $C_1$ and $C_2$ until we see a 1
  - If it’s a type-A row, then $h(C_1) = h(C_2)$
  - If a type-B or type-C row, then not
Similarity for Signatures

- We know: $\Pr[h_{\pi}(C_1) = h_{\pi}(C_2)] = sim(C_1, C_2)$
- Now generalize to multiple hash functions

- The *similarity of two signatures* is the fraction of the hash functions in which they agree

- Thus, the expected similarity of two signatures equals the Jaccard similarity of the columns or sets that the signatures represent
  - And the longer the signatures, the smaller will be the expected error
Min-Hashing Example

Permutation $\pi$

<table>
<thead>
<tr>
<th>2</th>
<th>4</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>7</td>
<td>1</td>
<td>7</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>7</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

Input matrix (Shingles x Documents)

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td></td>
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<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

Signature matrix $M$

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>4</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

Similarities:

<table>
<thead>
<tr>
<th></th>
<th>1-3</th>
<th>2-4</th>
<th>1-2</th>
<th>3-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Col/Col</td>
<td>0.75</td>
<td>0.75</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sig/Sig</td>
<td>0.67</td>
<td>1.00</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Implementation Trick

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

How to pick a random hash function $h(x)$?
Universal hashing:
\[ h_{a,b}(x) = ((a \cdot x + b) \mod p) \mod N \]
where:
\[ a, b \ldots \text{random integers} \]
\[ p \ldots \text{prime number (} p > N \text{)} \]
for each row \( r \) do begin
for each hash function \( h_i \) do
compute \( h_i(r) \);
for each column \( c \) if \( c \) has 1 in row \( r \)
for each hash function \( h_i \) do
if \( h_i(r) < M(i, c) \) then
\[ M(i, c) := h_i(r); \]
end;
## Example Implementation

The functions are defined as follows:

- \( h(x) = x \mod 5 \)
- \( g(x) = (2x+1) \mod 5 \)

### Permutation $h(x)$ and $g(x)$

<table>
<thead>
<tr>
<th>Row</th>
<th>C₁</th>
<th>C₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

### Signature Matrix $M$:

\[
\begin{align*}
M(i, C₁) & \quad M(i, C₂) \\
1 \quad & \quad 1 \quad \infty \\
3 \quad & \quad 3 \quad \infty \\
2 \quad & \quad 1 \quad 2 \\
0 \quad & \quad 3 \quad 0 \\
4 \quad & \quad 1 \quad 2 \\
4 \quad & \quad 2 \quad 0 \\
0 \quad & \quad 1 \quad 0 \\
2 \quad & \quad 2 \quad 0 \\
4 \quad & \quad 1 \quad 0 \\
0 \quad & \quad 2 \quad 0 \\
\end{align*}
\]
Step 3: **Locality Sensitive Hashing:**
Focus on pairs of signatures likely to be from similar documents

**Shingling**
The set of strings of length $k$ that appear in the document

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

**Locality-Sensitive Hashing**
Candidate pairs: those pairs of signatures that we need to test for similarity
Goal: Find documents with Jaccard similarity at least $s$ (for some similarity threshold, e.g., $s=0.8$)

LSH – General idea: Use a hash function 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
LSH: Overview

- 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
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

$\begin{array}{cccc} 
2 & 1 & 4 & 1 \\
1 & 2 & 1 & 2 \\
2 & 1 & 2 & 1 
\end{array}$

Signature matrix $M$

$b$ bands

$r$ rows per band

One signature
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

Columns 2 and 6 are probably identical (candidate pair)

Columns 6 and 7 are surely different.
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.
Assume the following case:

- Suppose 100,000 columns of $M$ (100k docs)
- Signatures of 100 integers (rows)
- Therefore, signatures take 40MB
- **Goal:** Find pairs of documents that are at least $s = 0.8$ similar
- Choose $b = 20$ bands of $r = 5$ integers/band
C₁, C₂ are 80% Similar

- Find pairs of $s \geq 0.8$ 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 identical 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
C₁, C₂ are 30% Similar

- **Find pairs of \( \geq s = 0.8 \) similarity, set \( b = 20, r = 5 \)
- **Assume**: \( \text{sim}(C₁, C₂) = 0.3 \)
  - Since \( \text{sim}(C₁, C₂) < s \) we want \( C₁, C₂ \) to hash to **NO common buckets** (all bands should be different)
- **Probability** \( C₁, C₂ \) identical in one particular band: \( (0.3)^5 = 0.00243 \)
- Probability \( C₁, C₂ \) 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 0.3 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 \( s \)
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
    - Note, $M=b*r$

- **Example:** If we had only 10 bands of 10 rows, how would FP/FN change?

- **Answer:** The number of false positives would go down, but the number of false negatives would go up (it’s harder to become a candidate pair in a bucket now).
Analysis of LSH – What We Want

Probability of sharing a bucket

Similarity threshold \( s \)

Probability = 1 if \( t > s \)

No chance if \( t < s \)

Similarity \( t = \text{sim}(C_1, C_2) \) of two sets

Say “yes” if you are below the red line.
What 1 Band of 1 Row Gives You

Remember:
Probability of equal hash-values = similarity

Similarity $t = \text{sim}(C_1, C_2)$ of two sets
What 1 Band of 1 Row Gives You

Similarity $t = \text{sim}(C_1, C_2)$ of two sets

Probability of sharing a bucket

False positives

False negatives

Say “yes” if you are below the line.
$b$ bands, $r$ rows/band

- Say 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

Similarity $t = \text{sim}(C_1, C_2)$ of two sets

1: All rows of a band are equal
2: Some row of a band is unequal
3: No bands are identical
4: At least one band is identical

Probability of sharing at least one bucket

$1 - (1 - t^r)^b$
Example: \( b = 20; r = 5 \)

- **Similarity threshold** \( s \)
- **Prob. that at least 1 band is identical:**

<table>
<thead>
<tr>
<th>( s )</th>
<th>( 1-(1-s^r)^b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.006</td>
</tr>
<tr>
<td>0.3</td>
<td>0.047</td>
</tr>
<tr>
<td>0.4</td>
<td>0.186</td>
</tr>
<tr>
<td>0.5</td>
<td>0.470</td>
</tr>
<tr>
<td>0.6</td>
<td>0.802</td>
</tr>
<tr>
<td>0.7</td>
<td>0.975</td>
</tr>
<tr>
<td>0.8</td>
<td>0.9996</td>
</tr>
</tbody>
</table>
Picking $r$ and $b$: The S-curve

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

Yellow area: False Negative rate
Blue 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 set representation
  - 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 $\Pr[h_{\pi}(C_1) = h_{\pi}(C_2)] = sim(C_1, C_2)$
  - 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 $\geq s$
Please give us feedback 😊