Lecture outline

• Nearest-neighbor search in low dimensions
  – kd-trees

• Nearest-neighbor search in high dimensions
  – LSH

• Applications to data mining
Definition

• Given: a set \( X \) of \( n \) points in \( \mathbb{R}^d \)
• Nearest neighbor: for any query point \( q \in \mathbb{R}^d \) return the point \( x \in X \) minimizing \( D(x,q) \)

• **Intuition:** Find the point in \( X \) that is the closest to \( q \)
Motivation

• **Learning**: Nearest neighbor rule
• **Databases**: Retrieval
• **Data mining**: Clustering
• Donald Knuth in vol.3 of *The Art of Computer Programming* called it the post-office problem, referring to the application of assigning a resident to the nearest–post office
Nearest-neighbor rule
MNIST dataset “2”
Methods for computing NN

• **Linear scan**: $O(nd)$ time

• This is pretty much all what is known for exact algorithms with theoretical guarantees

• In practice:
  – *kd-trees* work “well” in “low-medium” dimensions
2–dimensional kd–trees

• A data structure to support range queries in $\mathbb{R}^2$
  – Not the most efficient solution in theory
  – Everyone uses it in practice

• Preprocessing time: $O(n \log n)$
• Space complexity: $O(n)$
• Query time: $O(n^{1/2} + k)$
2-dimensional kd-trees

• Algorithm:
  – Choose $x$ or $y$ coordinate (alternate)
  – Choose the median of the coordinate; this defines a horizontal or vertical line
  – Recurse on both sides

• We get a binary tree:
  – Size $O(n)$
  – Depth $O(\log n)$
  – Construction time $O(n \log n)$
Construction of kd-trees
Construction of kd-trees
Construction of kd-trees
Construction of kd-trees
Construction of kd-trees
The complete kd-tree
Region of node $v$

Region($v$) : the subtree rooted at $v$ stores the points in black dots
Searching in kd–trees

• Range–searching in 2–d
  – Given a set of \( n \) points, build a data structure that for any query rectangle \( R \) reports all points in \( R \)
kd-tree: range queries

- Recursive procedure starting from $v = \text{root}$

- **Search** $(v, R)$
  - If $v$ is a leaf, then report the point stored in $v$ if it lies in $R$
  - Otherwise, if $\text{Reg}(v)$ is contained in $R$, report all points in the $\text{subtree}(v)$
  - Otherwise:
    - If $\text{Reg}(\text{left}(v))$ intersects $R$, then $\text{Search}(\text{left}(v), R)$
    - If $\text{Reg}(\text{right}(v))$ intersects $R$, then
Query time analysis

• We will show that **Search** takes at most $O(n^{1/2} + P)$ time, where $P$ is the number of reported points
  
  - The total time needed to report all points in all sub-trees is $O(P)$
  
  - We just need to bound the number of nodes $v$ such that $\text{region}(v)$ intersects $R$ but is not contained in $R$ (i.e., boundary of $R$ intersects the boundary of $\text{region}(v)$)

  - **gross overestimation**: bound the number of $\text{region}(v)$ which are crossed by any of the 4 horizontal/vertical lines
Query time (Cont’d)

- **Q(n):** max number of regions in an n-point kd-tree intersecting a (say, vertical) line.

  - If \( \ell \) intersects region\((v)\) (due to vertical line splitting), then after two levels it intersects 2 regions (due to 2 vertical splitting lines).
  
  - The number of regions intersecting \( \ell \) is \( Q(n)=2+2Q(n/4) \) \( \Rightarrow \) \( Q(n)=(n^{1/2}) \)
d-dimensional kd-trees

- A data structure to support range queries in $\mathbb{R}^d$
- Preprocessing time: $O(n \log n)$
- Space complexity: $O(n)$
- Query time: $O(n^{1-1/d} + k)$
Construction of the $d$-dimensional kd-trees

- The construction algorithm is similar as in 2-d
- At the root we split the set of points into two subsets of same size by a hyperplane vertical to $x_1$-axis
- At the children of the root, the partition is based on the second coordinate: $x_2$-coordinate
- At depth $d$, we start all over again by partitioning on the first coordinate
- The recursion stops until there is only one
Locality-sensitive hashing (LSH)

• **Idea:** Construct hash functions \( h: \mathbb{R}^d \rightarrow U \) such that for any pair of points \( p, q \):
  – If \( D(p, q) \leq r \), then \( \Pr[h(p) = h(q)] \) is high
  – If \( D(p, q) \geq cr \), then \( \Pr[h(p) = h(q)] \) is small

Then, we can solve the “approximate NN” problem by hashing

• LSH is a general framework; for a given \( D \) we need to find the right \( h \)
Approximate Nearest Neighbor

- Given a set of points $X$ in $\mathbb{R}^d$ and query point $q \in \mathbb{R}^d$
- $c$-Approximate $r$-Nearest Neighbor search returns:
  - Returns $p \in P$, $D(p,q) \leq r$
  - Returns NO if there is no $p' \in X$, $D(p',q) \leq cr$
Locality-Sensitive Hashing (LSH)

- A family $H$ of functions $h: \mathbb{R}^d \rightarrow U$ is called $(P_1, P_2, r, cr)$-sensitive if for any $p, q$:
  - if $D(p, q) \leq r$, then $\Pr[h(p) = h(q)] \geq P_1$
  - if $D(p, q) \geq cr$, then $\Pr[h(p) = h(q)] \leq P_2$

- $P_1 > P_2$

- Example: Hamming distance
  - LSH functions: $h(p) = p_i$, i.e., the $i$-th bit of $p$
  - Probabilities: $\Pr[h(p) = h(q)] = 1 - D(p, q)/d$
Algorithm -- preprocessing

• $g(p) = <h_1(p), h_2(p), ..., h_k(p)>$

• Preprocessing
  – Select $g_1, g_2, ..., g_L$
  – For all $p \in X$ hash $p$ to buckets $g_1(p), ..., g_L(p)$
  – Since the number of possible buckets might be large we only maintain the non empty ones

• Running time?
Algorithm -- query

• Query $q$:
  – Retrieve the points from buckets $g_1(q), g_2(q), \ldots, g_L(q)$ and let points retrieved be $x_1, \ldots, x_L$
    • If $D(x_i, q) \leq r$ report it
    • Otherwise report that there does not exist such a NN
  – Answer the query based on the retrieved points
  – Time $O(dL)$
Applications of LSH in data mining

• Numerous…. 
Applications

• Find pages with similar sets of words (for clustering or classification)

• Find users in Netflix data that watch similar movies

• Find movies with similar sets of users

• Find images of related things
How would you do it?

• Finding very similar items might be computationally demanding task

• We can relax our requirement to finding somewhat similar items
Running example: comparing documents

• Documents have common text, but no common topic

• Easy special cases:
  – Identical documents
  – Fully contained documents (letter by letter)

• General case:
  – Many small pieces of one document appear out of order in another. What do we do then?
Finding similar documents

• Given a collection of documents, find pairs of documents that have lots of text in common
  – Identify mirror sites or web pages
  – Plagiarism
  – Similar news articles
Key steps

• **Shingling**: convert documents (news articles, emails, etc) to sets

• **LSH**: convert large sets to small signatures, while preserving the similarity

• Compare the signatures instead of the actual documents
Shingles

• A k–shingle (or k–gram) is a sequence of k characters that appears in a document

• If doc = abcab and k=3, then 2–singles: {ab, bc, ca}

• Represent a document by a set of k–shingles
Assumption

• Documents that have similar sets of $k$-shingles are similar: same text appears in the two documents; the position of the text does not matter

• What should be the value of $k$?
  – What would large or small $k$ mean?
Data model: sets

• Data points are represented as sets (i.e., sets of shingles)

• Similar data points have large intersections in their sets
  – Think of documents and shingles
  – Customers and products
  – Users and movies
Similarity measures for sets

- Now we have a set representation of the data

- Jaccard coefficient

- \( A, B \) sets (subsets of some, large, universe \( U \))

\[
sim(A, B) = \frac{|A \cap B|}{|A \cup B|}
\]
Find similar objects using the Jaccard similarity

• Naïve method?

• Problems with the naïve method?
  – There are too many objects
  – Each object consists of too many sets
Speeding up the naïve method

• Represent every object by a signature (summary of the object)
• Examine pairs of signatures rather than pairs of objects
• Find all similar pairs of signatures
• **Check point:** check that objects with similar signatures are actually similar
Still problems

• Comparing large number of signatures with each other may take too much time (although it takes less space)

• The method can produce pairs of objects that might not be similar (false positives). The check point needs to be enforced
Creating signatures

• For object $x$, signature of $x$ ($\text{sign}(x)$) is much smaller (in space) than $x$

• For objects $x, y$ it should hold that $\text{sim}(x,y)$ is almost the same as $\text{sim}(\text{sign}(x), \text{sign}(y))$
Intuition behind Jaccard similarity

- Consider two objects: $x, y$

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- $a$: # of rows of form same as $a$
- $\text{sim}(x,y) = \frac{a}{(a+b+c)}$
A type of signatures -- minhashes

- Randomly **permute** the rows

\[-\]

- \( h(x) \): first row (in permuted data) in which column \( x \) has an \( 1 \)

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- Use several (e.g., 100) independent hash functions to design a signature

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“Surprising” property

• The probability (over all permutations of rows) that $h(x) = h(y)$ is the same as $\text{sim}(x,y)$

• Both of them are $a/(a+b+c)$

• So?
  
  – The similarity of signatures is the fraction of the hash functions on which they agree
Minhash algorithm

• Pick $k$ (e.g., 100) permutations of the rows

• Think of $\text{sign}(x)$ as a new vector

• Let $\text{sign}(x)[i]$: in the $i$–th permutation, the index of the first row that has 1 for object $x$
Example of minhash signatures

- **Input matrix**

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Example of minhash signatures

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Is it now feasible?

• Assume a billion rows
• Hard to pick a random permutation of 1…billion
• Even representing a random permutation requires 1 billion entries!!!
• How about accessing rows in permuted order?
• 😞
Being more practical

- Approximating row permutations: pick \( k=100 \) hash functions \((h_1, \ldots, h_k)\)

\[
\begin{align*}
\text{for each row } r \\
\quad \text{for each column } c \\
\quad \quad \text{if } c \text{ has 1 in row } r \\
\quad \quad \quad \text{for each hash function } h_i \text{ do} \\
\quad \quad \quad \quad \text{if } h_i(r) \text{ is a smaller value than } M(i,c) \\
\quad \quad \quad \quad \text{then} \\
\quad \quad \quad \quad \quad M(i,c) = h_i(r); \\
\end{align*}
\]
Being more practical

• Approximating row permutations: pick \( k=100 \) hash functions \((h_1, \ldots, h_k)\).

For each row \( r \)
  
  For each column \( c \)
    
    If \( c \) has 1 in row \( r \)
      
      For each hash function \( h \)
        
        If \( h(r) \) is a smaller value than \( M(i,c) \)
          
          Then
            
            \[ M(i,c) = h_i(r); \]

\( M(i,c) \) will become the smallest value of \( h_i(r) \) for which column \( c \) has 1 in row \( r \); i.e., \( h_i(r) \) gives order of rows for \( i \)-th permutation.
Example of minhash signatures

• Input matrix

\[
\begin{array}{c|cc}
   & \text{x1} & \text{x2} \\
\hline
1 & 1 & 0 \\
2 & 0 & 1 \\
3 & 1 & 1 \\
4 & 1 & 0 \\
5 & 0 & 1 \\
\end{array}
\]

\[
\begin{array}{c|cc}
   & \text{x1} & \text{x2} \\
\hline
1 & 0 & 1 \\
2 & 2 & 0 \\
\end{array}
\]

\[
h(r) = r + 1 \mod 5 \\
g(r) = 2r + 1 \mod 5
\]