Approximate Nearest Neighbor in High Dimension

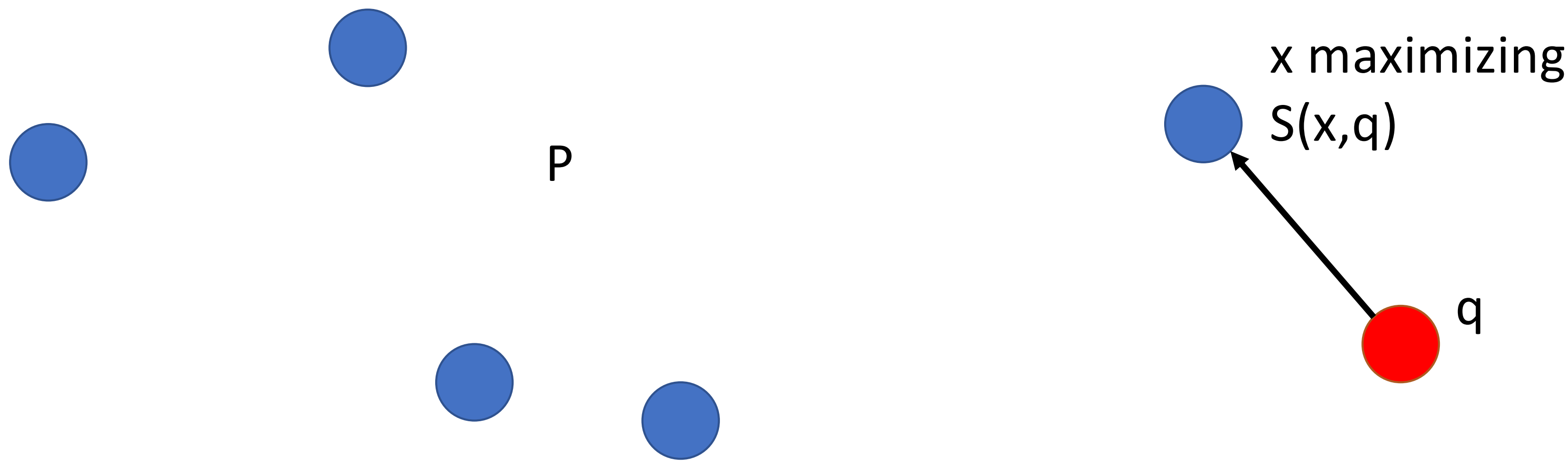
PPT by Brandon Fain

Outline

- Nearest Neighbor Problem in Low Dimension
- High Dimension Application: Classifying Articles in the Bag of Words Model
- Locality Sensitive Hashing

Nearest Neighbor Problem

- Given n points P, a similarity measure S(), and a query point q, find x in P that maximizes S(x, q). Call this $NN_S(q)$.
- Equivalently, given…distance measure D()…that minimizes D(x, q).



Similarity Measures for Geometric Data

- Suppose that our data is geometric: each point x in P is a point in d-dimensional Euclidean space.
- Euclidean:

$$S(x, y) = -\sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}$$

- Cosine:

$$S(x, y) = \cos\theta_{xy} = \frac{x \cdot y}{\|x\|_2 \|y\|_2} = \frac{\sum_{i=1}^{d} x_i y_i}{\sqrt{\left(\sum_{i=1}^{d} x_i^2\right)\left(\sum_{i=1}^{d} y_i^2\right)}}$$

Nearest Neighbor Problem

- Of course, we can always trivially answer $NN_S(q)$ in $O(n)$ time by scanning over all of P. So why is this interesting?

- Consider a live application where you want to answer these queries in time that scales *sublinearly* with n. Can we preprocess the data so that this is possible?

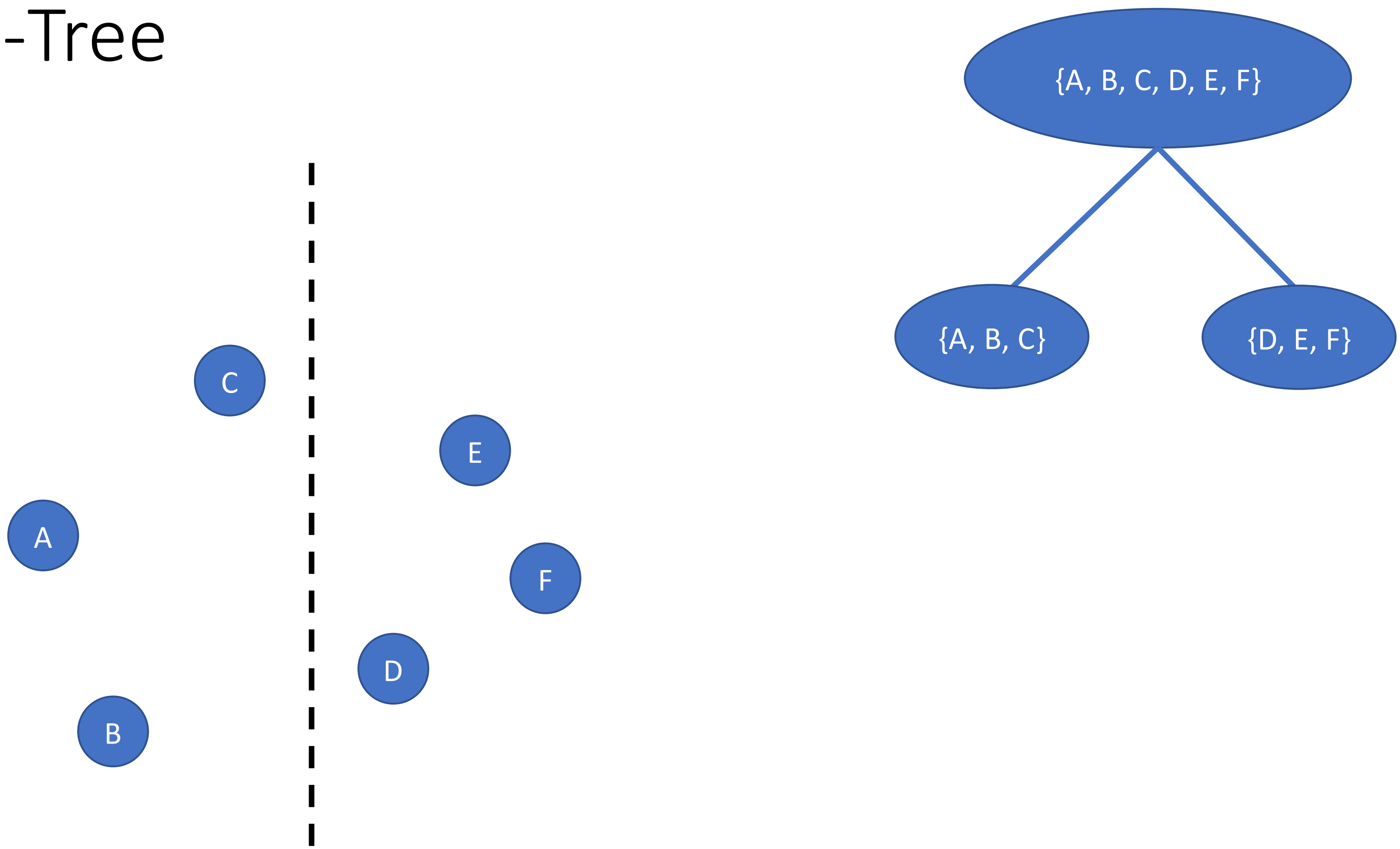
- Example: suppose P is one dimensional. Can you preprocess to get log(n) query time?

Nearest Neighbor Problem

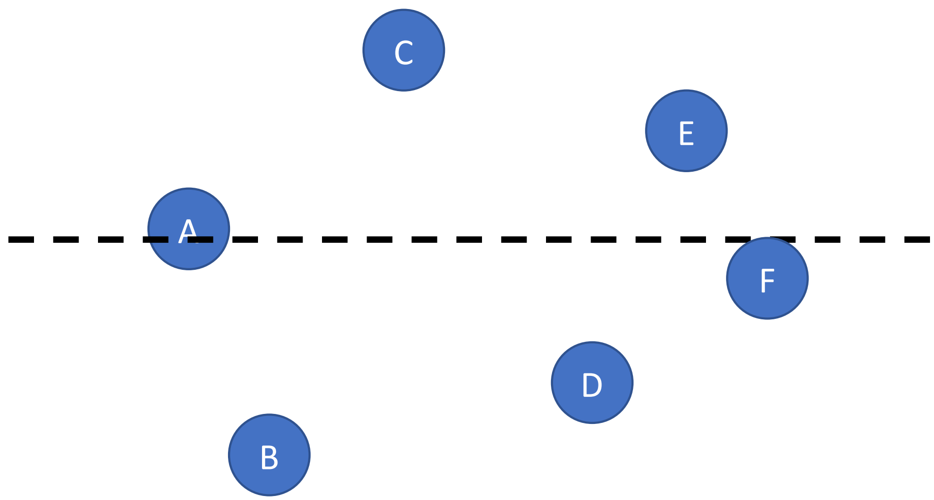
- So there is hope! What if our points are 2-dimensional?

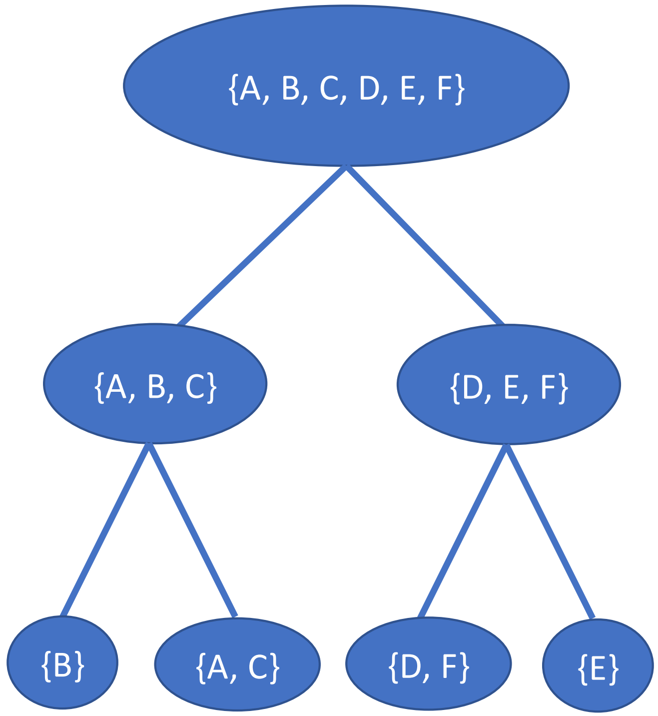
- Solution: kd-trees. This is a form of hierarchical clustering. We won’t go through the full construction today, but here is the idea in pictures.

kd-Tree

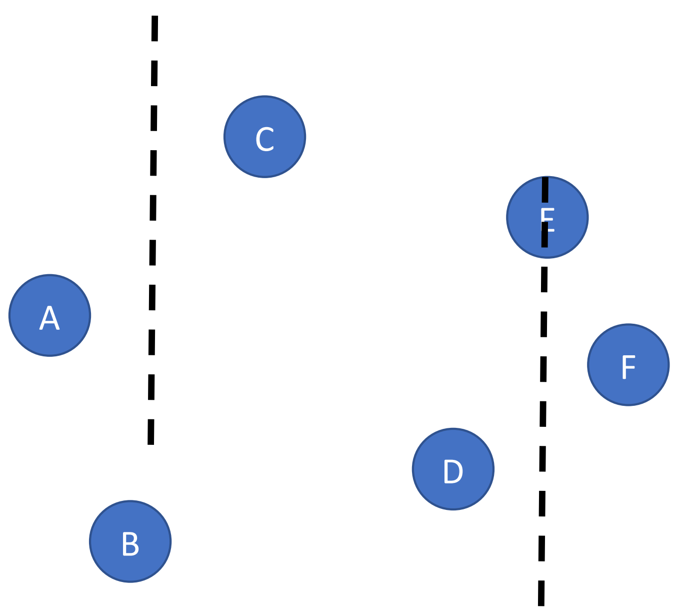


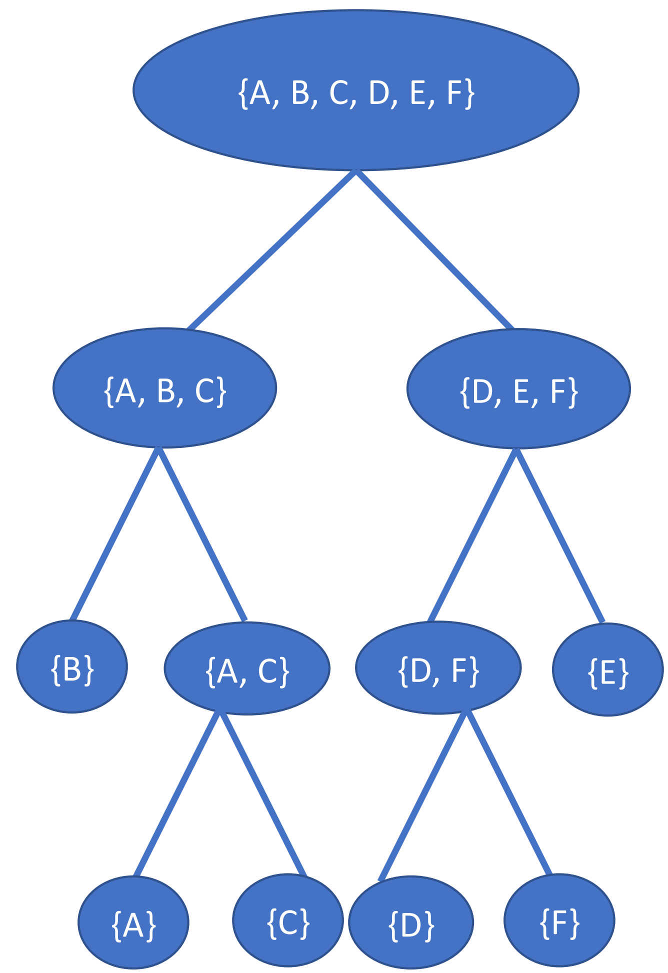
kd-Tree





kd-Tree





Curse of Dimensionality

- We will leave as an exercise figuring out how to use the kd-tree to get an O(log(n)) algorithm for the nearest neighbor problem.
- This solution suffers from the *curse of dimensionality*. That is to say, it does not scale well with the dimensionality of the data.
- Instead, we want a nearest neighbor algorithm that still runs quickly in high dimension, perhaps at the cost of accuracy.
- Why would we care about this?

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Application: Classifying Articles, Bag of Words

- Suppose we have n news articles, of m basic types (e.g., politics, sports, etc). As input, we are told the type of each of these n articles.
- We want to build a *classifier* from news articles to basic types, i.e., a function that given a new article, predicts what type it is.
- Option 1: Natural Language Processing.
  - (Not in this course)

Application: Classifying Articles, Bag of Words

- Option 2: We will use nearest neighbor classification in the bag of words model.

- Suppose there are d “important” words used across all n articles (so not including articles, prepositions, etc.)

- Represent each article as a vector $x \in \mathbb{R}^d$ where that x_i is the number of times that word i appears in that article.
  - We are simplifying our data by *entirely ignoring the order in which the words occur*.
  - Note that d is large, likely on the order of 100,000!

Application: Classifying Articles, Bag of Words

- Now, our classifier using the nearest neighbor problem is incredibly simple.

- Let $S(x, y) = \cos\theta_{xy} = \frac{x \cdot y}{\|x\|_2 \|y\|_2}$; we will use cosine similarity.

- To classify a new article with bag of words representation y, let x = NN_S(y). Output the type of x.

- Thus, if we can efficiently solve the nearest neighbor problem in high dimension in sublinear time, we can do efficient classification of high dimensional data.

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Locality Sensitive Hash in General

- Recall the standard universal hashing assumption: for any $x \neq y, \Pr[h(x) = h(y)] \leq \frac{1}{n}$, for a hash table of size n. Such hash functions try to *obscure* how similar x and y are.

- Could we define a hash function with the *opposite* sort of property? One for which the probability of a collision depends on how similar x and y are?

- If so, maybe we can approximately solve the nearest neighbor problem by hashing with multiple trials, as we have seen in the count min sketch!

Locality Sensitive Hash for Cosine Similarity

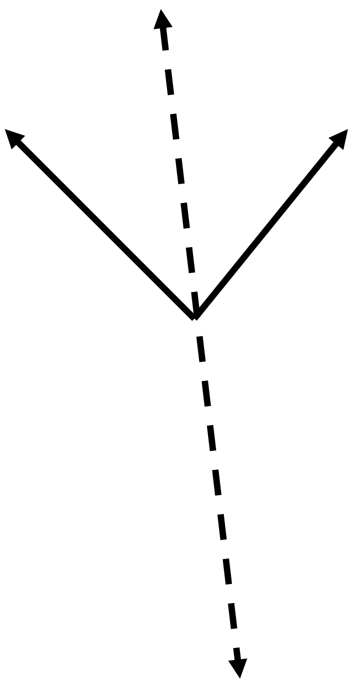
- For cosine similarity, recall that $S(x, y) = \cos\theta_{xy} = \frac{x \cdot y}{\|x\|_2 \|y\|_2}$, which varies between -1 and 1.

- We want a *locality sensitive hash function h* such that $\Pr[h(x) = h(y)] \approx \frac{1+S(x,y)}{2}$, where the randomness will (as usual) come from the random draw of *h* from a family.

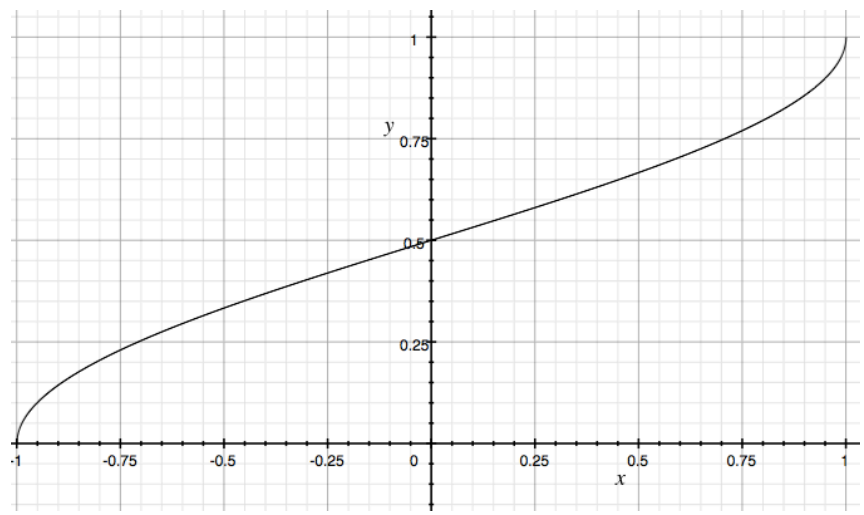
- Solution: Draw a random unit vector $r \in \mathbb{R}^d$, say by taking $r_i \sim N(0,1)$ for every coordinate and normalizing. Now let $h_r(x) = Sign(x \cdot r)$, that is, +1 if the inner product is nonnegative, and -1 otherwise.

Locality Sensitive Hash for Cosine Similarity

$$\Pr[h_r(x) = h_r(y)] = \Pr[Sign(x \cdot r) = Sign(y \cdot r)]$$



$$= 1 - \frac{\theta_{xy}}{\pi} = 1 - \frac{\cos^{-1} S(x,y)}{\pi} \approx \frac{1 + S(x,y)}{2}$$



Algorithm for Nearest Neighbor Problem

At a high level, we want to use our locality sensitive hash h() to

1. hash all of our data
2. answer nearest neighbor queries by hashing the query point and only searching over the colliding data points.

- **Problem.** The hash we developed only maps to -1 or +1, so this could still require us to search over roughly half of the points at each step.
- **Solution.** Create a new hash function H() by drawing k independent hash functions $h_1, \ldots, h_k$ and letting $H(x) = (h_1(x), \ldots, h_k(x))$.

Algorithm for Nearest Neighbor Problem

- **Solution.** Create a new hash function H() by drawing k independent hash functions $h_1()$, …, $h_k()$ and letting $H(x) = (h_1(x), …, h_k(x))$.
  - Recall that each $h_i()$ is defined by drawing a random unit vector in $\mathbb{R}^d$.
  - Also note that the hash function H() maps to 2^k possible buckets, since it is a length *k* bit string.
- Now, $\Pr[H(x) = H(y)] = \left(1 - \frac{\theta_{xy}}{\pi}\right)^k$, so we can substantially cut down the number of other points we have to scan over.
- **Problem.** Since we look at fewer points, our error is likely to increase.
- **Solution.** Draw *l* independent hash functions $H_1()$, …, $H_l()$, and search over collisions on any of these

Algorithm for Nearest Neighbor Problem

Altogether then, here is our algorithm. We have n articles, each represented as a vector $x \in \mathbb{R}^d$. We have parameters *k* and *l*.

- There are *l* hash tables, T_1, …, T_l, each with 2^k buckets
- To define the hash functions, draw *l* matrices M_1, …, M_l, each of dimension $k \times d$, where every entry is drawn independently from a standard normal distribution $N(0,1)$.
  - Normalize every row of every matrix to be a unit vector.
- The i'th hash of some x is $Sign(M_i x)$. Store x in T_i.
  - Note that this is a vector of *k* values in {-1,+1}, which you will have to map to the 2^k table T_i somehow.

Example

Suppose we have l = k = 2, and we are tracking d = 5 words in our bag of words model (this is a toy example).

We draw 2 random 2 by 5 matrices where every row is a unit vector:

M_1 =

0.70	-0.27	-0.04	0.65	-0.14
0.71	-0.38	-0.26	0.36	-0.39

M_2 =

-0.11	0.07	-0.63	-0.73	0.23
-0.64	0.68	-0.22	-0.19	0.22

To hash the inputs x = (5, 1, 0, 2, 0), we compute: M_1x = (4.53, 3.89) and M_2x = (-1.95, -2.89). We take the sign to get the hash values (1, 1) and (-1, -1). Then we store x the corresponding tables.

(-1, -1)	(-1, 1)	(1, -1)	(1, 1)
			(5,1,0,2,0)

(-1, -1)	(-1, 1)	(1, -1)	(1, 1)
(5,1,0,2,0)			

Algorithm for Nearest Neighbor Problem

- To compute the nearest neighbor of an article, also represented in the bag of words model as some $y \in \mathbb{R}^d$:
  - Scan over all x hashed to the same bucket in at least one of the *l* hash tables.
  - Among all such, x, return the one with maximum similarity to y.

- If we then want to solve the classification problem using nearest neighbor classification, simply classify the query point y as the same class as the x returned as the nearest neighbor.

- **Question.** How do we decide how to set *l* and *k*?

Reasoning About the Parameters

- The greater the value of k, the *lower* the probability that a collision happens on any given hash table.
- So as we increase k, we expect to have to scan over *fewer* points looking for a nearest neighbor.
- = faster query time, but less accurate results.
- The greater l is, the more independent hashes we compute for each data point.
- Since we compare any points that collide on *at least one* hash, as we increase l, we expect to increase the probability that we find a good nearest neighbor.
- = more accurate results, but slower query time.

Formal Guarantees

- You may have noticed that we have been extremely loose with our guarantees, for example:
  - What is the big-O runtime?
  - What is our approximation or probability of correctness?

- We can formulate the problem more formally as follows. The **approximate nearest neighbor problem** asks a query $NN(y, r, c)$, with $r \geq 0, c \geq 1$. We want to give an algorithm that, with constant probability (say 1/3):
  - If there is an x^* with $S(x^*, y) \geq r$, returns some x such that $S(x, y) \geq r/c$.
  - If there is no x^* with $S(x^*, y) \geq r/c$, reports failure
  - Else, reports failure or returns some x such that $S(x, y) \geq r/c$.

Formal Guarantees

- This parameterized version of the problem is easier to work with in theory, although what we have already described in the more practical version.

- Using the techniques we have already seen, one can prove that it is sufficient to set $k \approx \frac{1}{cr}\log(n)$ and $l = n^{1/c}$ to solve this problem with probability at least 1/3.

- To get an error probability of, say, 1%, just run the algorithm $\lceil \log_3 100 \rceil = 5$ times and take the best (most similar) result.

Formal Guarantees

- One can show that the expected total number of similarity comparisons you have to make during a query with these parameters is $O\left(\frac{n^{1/c}}{cr}\log(n)\right)$.

- So, for example, if we take r=1 and c=2, we get an expected query time of $O(\sqrt{n}\log(n))$. That's a lot better than $O(n)$!

- See [MunagalaLectureNotes] for these details (also linked under optional reading for this lab).

Practical Guarantees

- That said, you might be left wondering: how well does nearest neighbor classification work in practice for our news article classification problem?

- Lucky for you, you will implement and test this on just such a data set in lab homework 3.

Summary

- We described the nearest neighbor problem in computational geometry; where the key idea is to trade off space and preprocessing to get sublinear query time.
- For low dimensional data, kd-trees are very effective solutions. The curse of dimensionality makes them impractical in high dimension.
- We care about high dimensional data for applications like classification of documents in the bag of words models.
- We can use locality sensitive hashing to approximately solve the nearest neighbor problem for high dimensional data.