Case Study 2: Document Retrieval

Task Description: Finding Similar Documents

Machine Learning for Big Data
CSE547/STAT548, University of Washington
Sham Kakade

April 11, 2017

 1

Document Retrieval

- **Goal:** Retrieve documents of interest
- **Challenges:**
  - Tons of articles out there
  - How should we measure similarity?

 2

Task 1: Find Similar Documents

- **To begin…**
  - **Input:** Query article
  - **Output:** Set of *k* similar articles

Document Representation

- Bag of words model

1-Nearest Neighbor

- Articles
- Query:
- 1-NN
  - Goal:
  - Formulation:

k-Nearest Neighbor

- Articles $X = \{x^1, \ldots, x^N\}, \quad x^i \in \mathbb{R}^d$
- Query: $x \in \mathbb{R}^d$
- *k*-NN
  - Goal:
  - Formulation:

Distance Metrics – Euclidean

$$d(u,v) = \sqrt{\sum_{i=1}^{d} (u_i - v_i)^2}$$

Or, more generally, $$d(u,v) = \sqrt{\sum_{i=1}^{d} \sigma_i^2 (u_i - v_i)^2}$$

Equivalently,

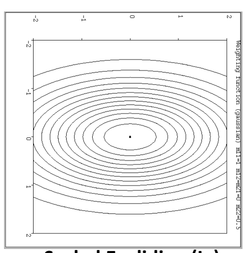
$$d(u,v) = \sqrt{(u-v)'\Sigma(u-v)}$$

where $$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & \ldots & \sigma_d^2 \end{bmatrix}$$

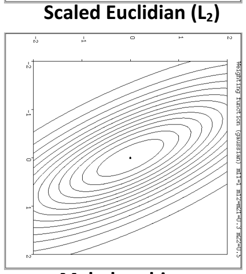
Other Metrics…

- Mahalanobis, Rank-based, Correlation-based, cosine similarity…

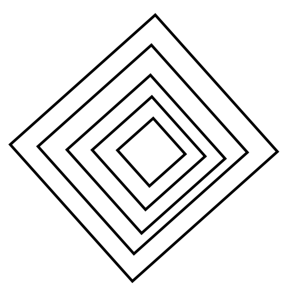
Notable Distance Metrics
(and their level sets)



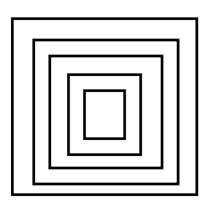
Scaled Euclidian (L_2)



Mahalanobis
(Σ is general sym pos def matrix, on previous slide = diagonal)



L_1 norm (absolute)



L_∞ *(max)* norm

Euclidean Distance + Document Retrieval

- Recall distance metric

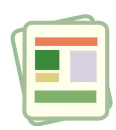
$$d(u,v) = \sqrt{\sum_{i=1}^{d}(u_i - v_i)^2}$$

- What if each document were α times longer?
  - Scale word count vectors
  - What happens to measure of similarity?
- Good to normalize vectors

9

Issues with Document Representation

- Words counts are ***bad*** for standard similarity metrics



- Term Frequency – Inverse Document Frequency (tf-idf)
  - Increase importance of rare words

TF-IDF

- Term frequency:

$$\mathrm{tf}(t,d) =$$

  - Could also use $\{0,1\}, 1+\log f(t,d), \ldots$
- Inverse document frequency:

$$\mathrm{idf}(t,D) =$$

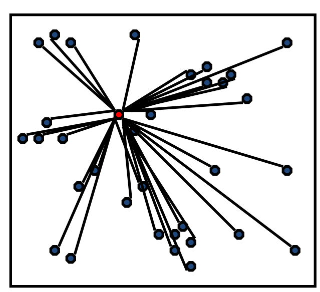
- tf-idf:

$$\mathrm{tfidf}(t,d,D) =$$

  - High for document d with high frequency of term t (high "term frequency") and few documents containing term t in the corpus (high "inverse doc frequency")

Issues with Search Techniques

- Naïve approach:
  Brute force search
  - Given a query point x
  - Scan through each point x^i
  - O(*N*) distance computations per 1-NN query!
  - O(*N*log*k*) per *k*-NN query!



33 Distance Computations

- What if *N* is huge??? (and many queries)

Think about Web Search/Image Search

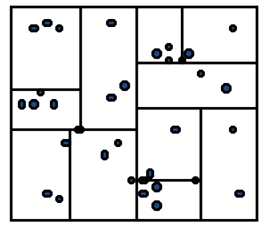
- How big is N?
- How fast do we desire to do recall?

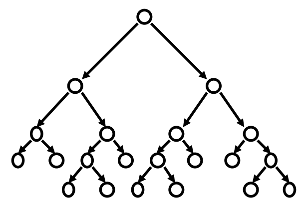
Intuition (?): NN in 1D and Sorting

- How do we do 1-NN searches in 1 dim?
- Pre-processing time:
- Query time:

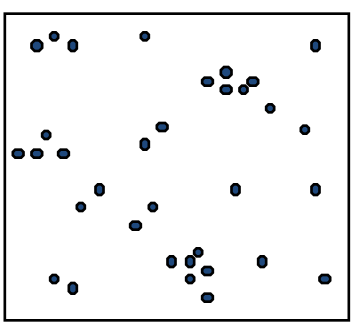
KD-Trees

- Smarter approach: ***kd-trees***
  - Structured organization of documents
    - Recursively partitions points into axis aligned boxes.
  - Enables more efficient pruning of search space
    - Examine nearby points first.
    - Ignore any points that are further than the nearest point found so far.
- ***kd-trees*** work “well” in “low-medium” dimensions
  - We’ll get back to this…





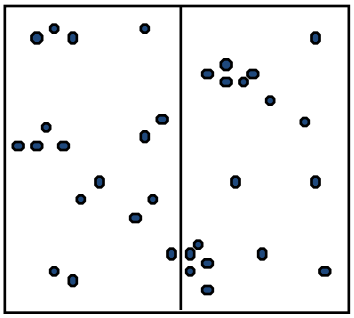
KD-Tree Construction

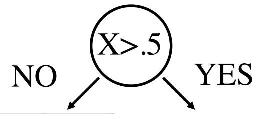


Pt	X	Y
1	0.00	0.00
2	1.00	4.31
3	0.13	2.85
…	…	…

- Start with a list of *d*-dimensional points.

KD-Tree Construction



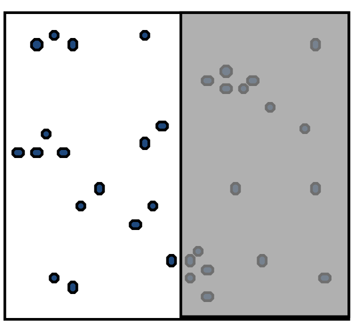


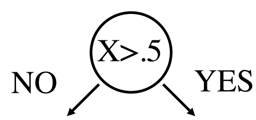
Pt	X	Y
1	0.00	0.00
3	0.13	2.85
…	…	…

Pt	X	Y
2	1.00	4.31
…	…	…

- Split the points into 2 groups by:
  - Choosing dimension d_j and value V (methods to be discussed…)
  - Separating the points into $x^i_{d_j}$ > V and $x^i_{d_j}$ <= V.

KD-Tree Construction



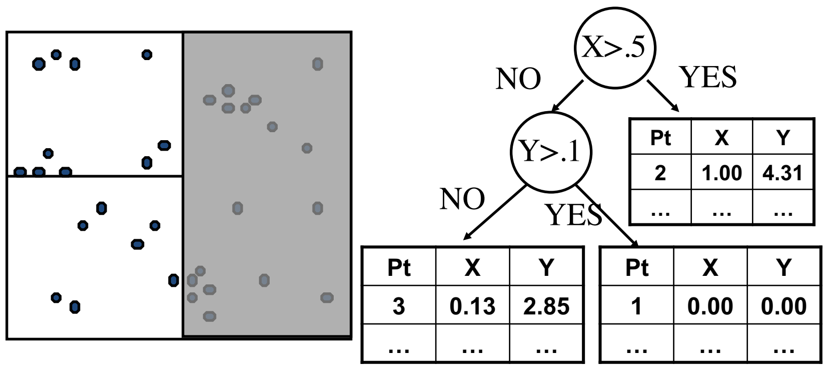


Pt	X	Y
1	0.00	0.00
3	0.13	2.85
…	…	…

Pt	X	Y
2	1.00	4.31
…	…	…

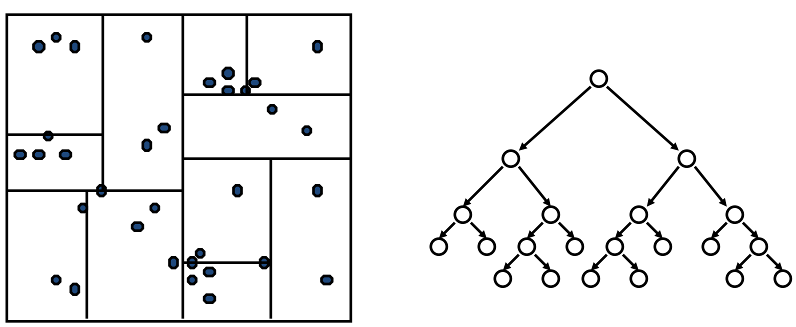
- Consider each group separately and possibly split again (along same/different dimension).
  - Stopping criterion to be discussed…

KD-Tree Construction



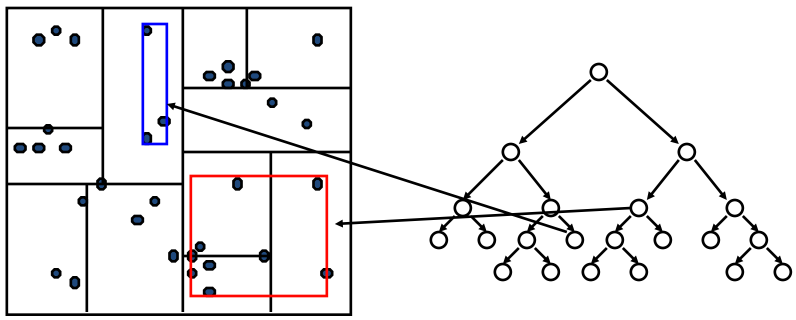
- Consider each group separately and possibly split again (along same/different dimension).
  - Stopping criterion to be discussed…

KD-Tree Construction



- Continue splitting points in each set
  - creates a binary tree structure
- Each leaf node contains a list of points

KD-Tree Construction

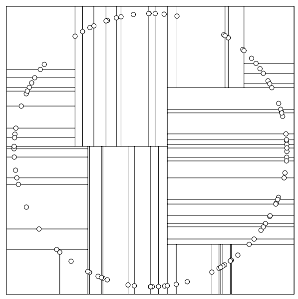


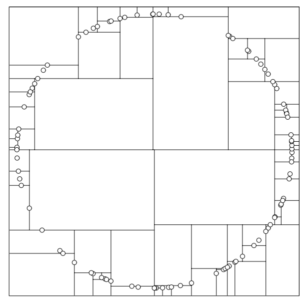
- Keep one additional piece of information at each node:
  - The (tight) bounds of the points at or below this node.

KD-Tree Construction

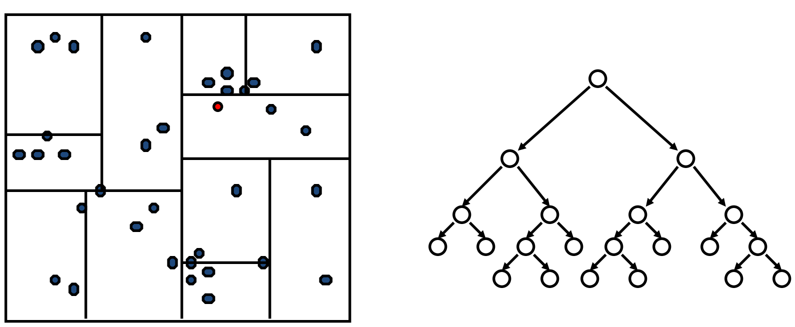
- Use heuristics to make splitting decisions:
- Which dimension do we split along?
- Which value do we split at?
- When do we stop?

Many heuristics…


median heuristic

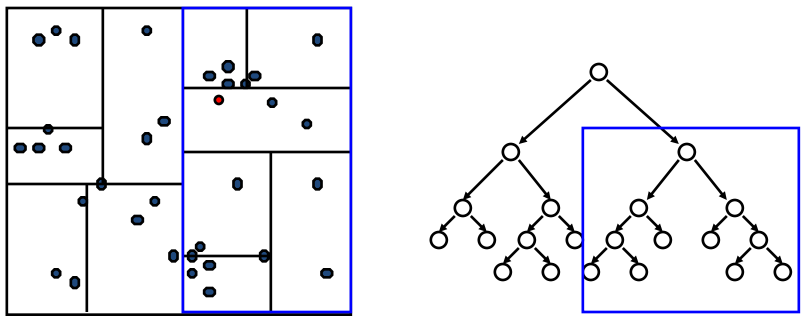

center-of-range heuristic

Nearest Neighbor with KD Trees



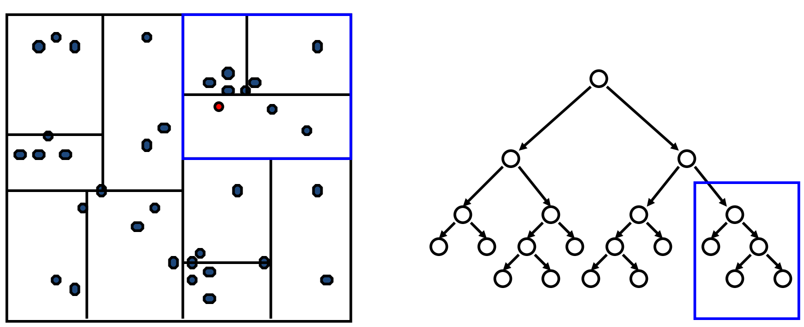
- Traverse the tree looking for the nearest neighbor of the query point.

Nearest Neighbor with KD Trees



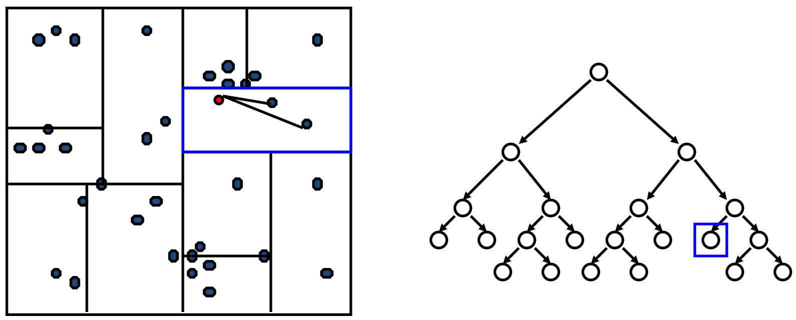
- Examine nearby points first:
  - Explore branch of tree closest to the query point first.

Nearest Neighbor with KD Trees



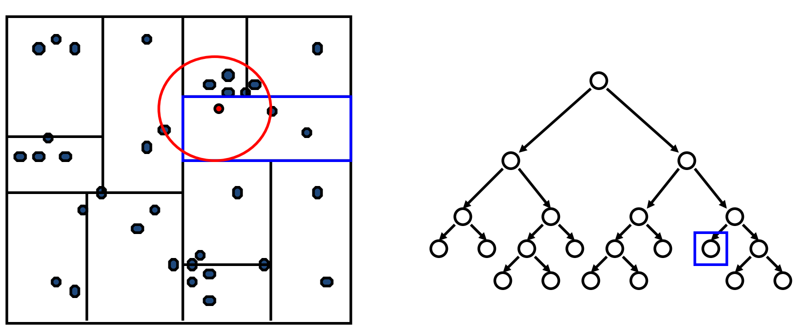
- Examine nearby points first:
  - Explore branch of tree closest to the query point first.

Nearest Neighbor with KD Trees



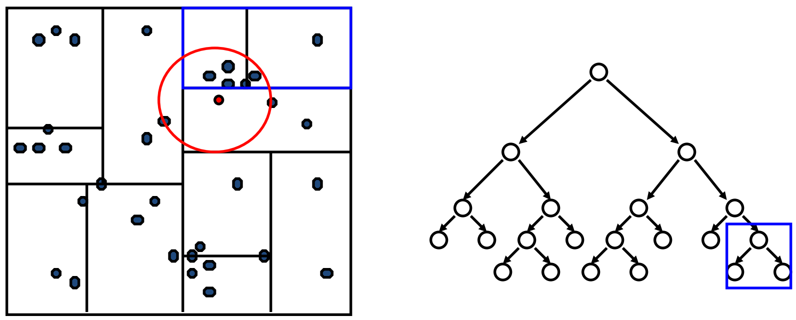
- When we reach a leaf node:
  - Compute the distance to each point in the node.

Nearest Neighbor with KD Trees



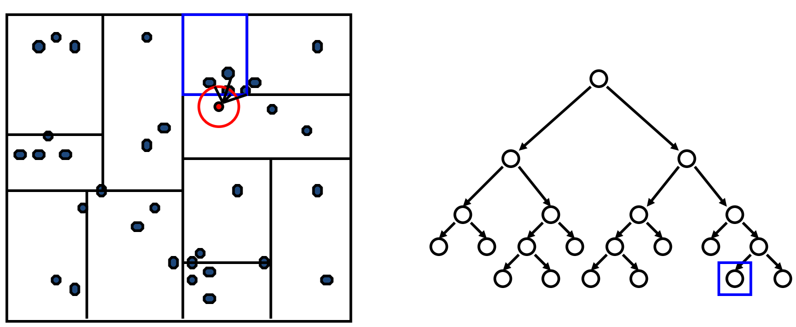
- When we reach a leaf node:
  - Compute the distance to each point in the node.

Nearest Neighbor with KD Trees



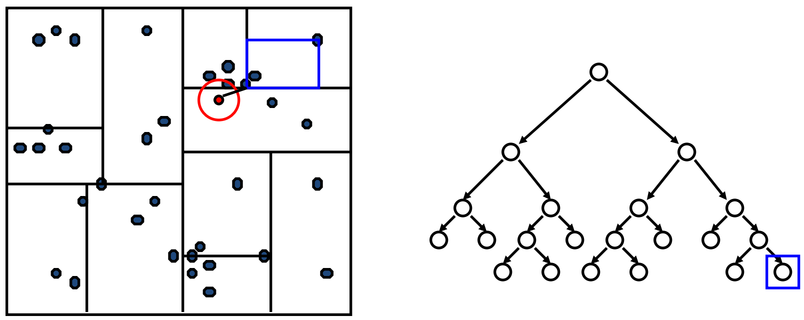
- Then backtrack and try the other branch at each node visited

Nearest Neighbor with KD Trees



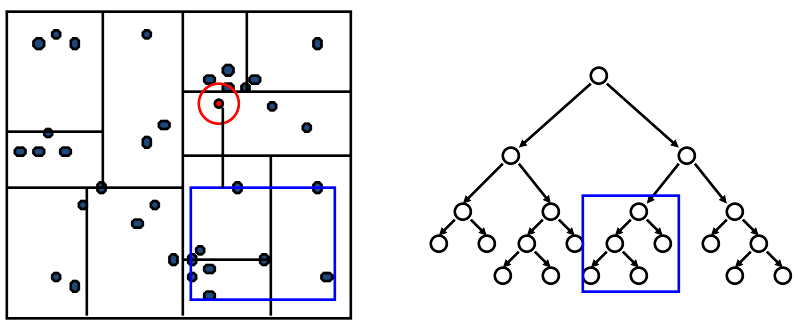
- Each time a new closest node is found, update the distance bound

Nearest Neighbor with KD Trees



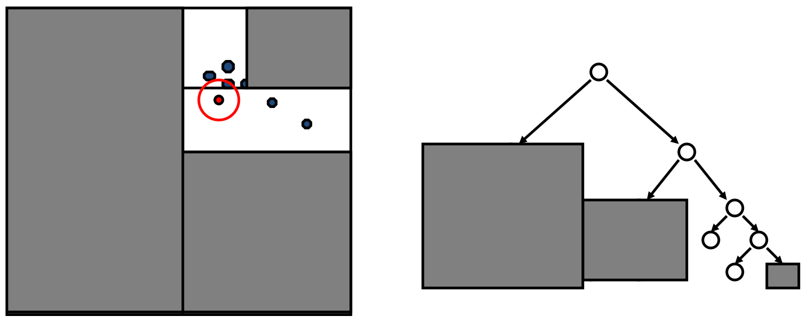
- Using the distance bound and bounding box of each node:
  - Prune parts of the tree that could NOT include the nearest neighbor

Nearest Neighbor with KD Trees



- Using the distance bound and bounding box of each node:
  - Prune parts of the tree that could NOT include the nearest neighbor

Nearest Neighbor with KD Trees



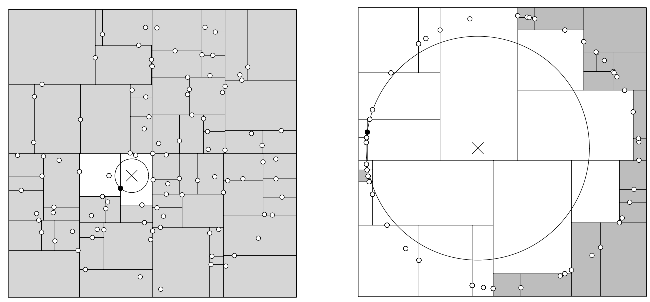
- Using the distance bound and bounding box of each node:
  - Prune parts of the tree that could NOT include the nearest neighbor

Complexity

- For (nearly) balanced, binary trees...
- Construction
  - Size:
  - Depth:
  - Median + send points left right:
  - Construction time:
- 1-NN query
  - Traverse down tree to starting point:
  - Maximum backtrack and traverse:
  - Complexity range:

- Under some assumptions on distribution of points, we get O(log$N$) but exponential in d (see citations in reading)

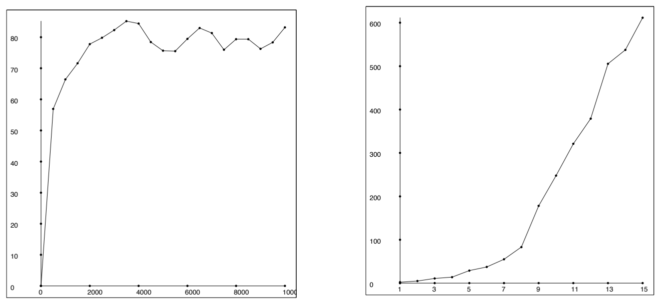
Complexity



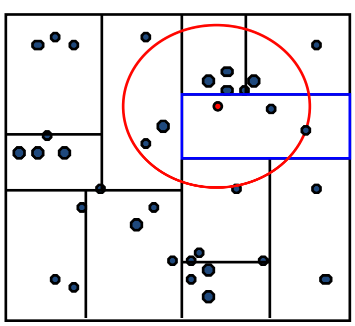
Complexity for *N* Queries

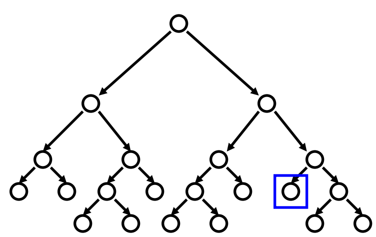
- Ask for nearest neighbor to each document
- Brute force 1-NN:
- kd-trees:

Inspections vs. *N* and *d*



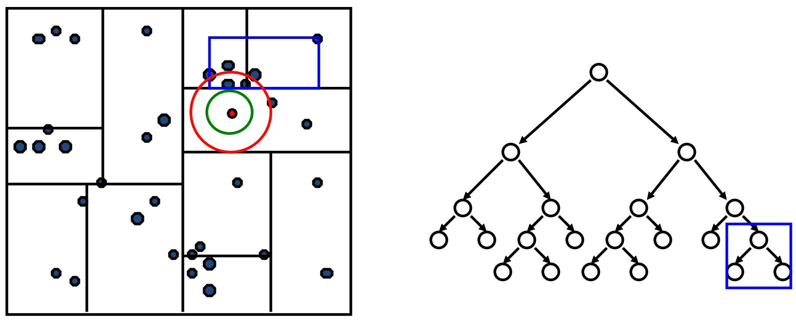
K-NN with KD Trees





- Exactly the same algorithm, but maintain distance as distance to furthest of current *k* nearest neighbors
- Complexity is:

Approximate K-NN with KD Trees



- **Before:** Prune when distance to bounding box >
- **Now:** Prune when distance to bounding box >
- Will prune more than allowed, but can guarantee that if we return a neighbor at distance r, then there is no neighbor closer than r/α.
- In practice this bound is loose…Can be closer to optimal.
- Saves lots of search time at little cost in quality of nearest neighbor.

Cover trees (+ ball trees)

- What about exact NNs searches in high dimensions?
- Idea: utilize triangle inequality of metric (so allow for arbitrary metric)
- cover-tree guarantees:

Cover trees: what does the triangle inequality imply?

Cover trees: data structure

Wrapping Up – Important Points

kd-trees

- Tons of variants
  - On construction of trees (heuristics for splitting, stopping, representing branches…)
  - Other representational data structures for fast NN search (e.g.,cover trees, ball trees,…)

Nearest Neighbor Search

- Distance metric and data representation are crucial to answer returned

For both…

- High dimensional spaces are hard!
  - Number of kd-tree searches can be exponential in dimension
    - Rule of thumb… $N >> 2^d$… Typically useless.
  - Distances are sensitive to irrelevant features
    - Most dimensions are just noise → Everything equidistant (i.e., everything is far away)
    - Need technique to learn what features are important for your task

What you need to know

- Document retrieval task
  - Document representation (bag of words)
  - tf-idf
- Nearest neighbor search
  - Formulation
  - Different distance metrics and sensitivity to choice
  - Challenges with large N
- kd-trees for nearest neighbor search
  - Construction of tree
  - NN search algorithm using tree
  - Complexity of construction and query
  - Challenges with large d

Acknowledgment

- This lecture contains some material from Andrew Moore's excellent collection of ML tutorials:
  - http://www.cs.cmu.edu/~awm/tutorials
- In particular, see:
  - http://grist.caltech.edu/sc4devo/.../files/sc4devo_scalable_datamining.ppt