Case Study 2: Document Retrieval

Task Description: Finding Similar Documents

or Images

Machine Learning for Big Data
CSE547/STAT548, University of Washington
Sham Kakade
April 11, 2017

Announcements:

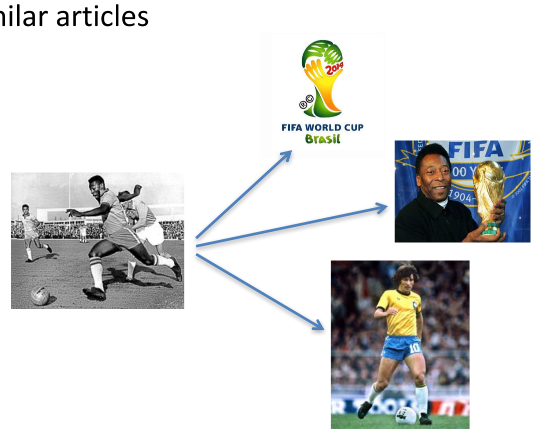
- HW1 due
- Project Milestones
  - Start early
  - Lit. review (>= 3 papers read carefully)
  - First rounds of experiments
- Today:
  - Review: Hash kernels
  - Today: similarity search, k-NNs, KD-trees

Document Retrieval

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

Task 1: Find Similar Documents

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



Document Representation

- Bag of words model

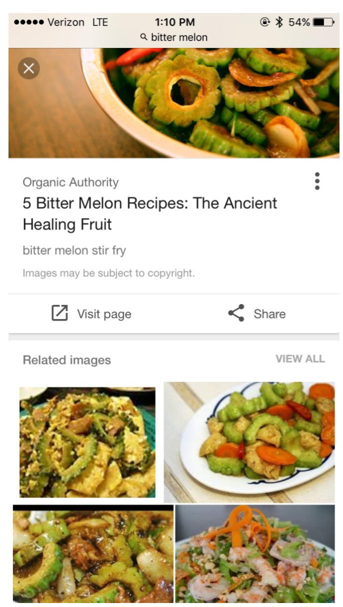
$$X = \begin{bmatrix} wc_1 \\ \vdots \\ wc_d \end{bmatrix} \in \mathbb{R}^d$$

"Bag of words" wc_i - word count of word i

ignore word order.

©Sham Kakade 2017 5

Image Search…



6

1-Nearest Neighbor

- Articles = $\mathcal{X} = \{x^1 \ldots x^N\}$
  $x^i \in \mathbb{R}^d$
- Query:
  x
- 1-NN
  - Goal: find $x \in \mathcal{X} \setminus x$ "closest" to x.
    query
  - Formulation:
    $$x^{NN} \in \underset{x^i \in \mathcal{X} \setminus x}{\arg\min} \; d(x^i, x)$$

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: find k closest items in $\mathcal{X}$ to x
  - 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,

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

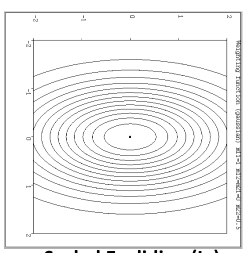
where $$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & \ldots & \sigma_d^2 \end{bmatrix}$$

Other Metrics…

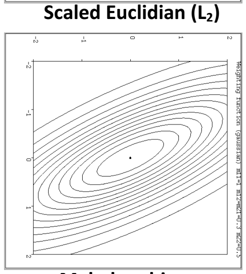
- Mahalanobis, Rank-based, Correlation-based, cosine similarity…

9

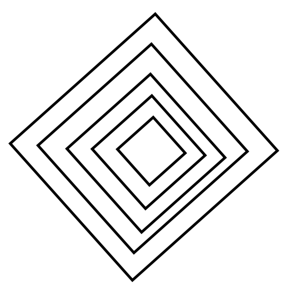
Notable Distance Metrics
(and their level sets)



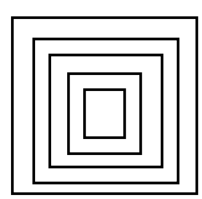
Scaled Euclidian (L_2)



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

    $u \leftarrow \alpha u$

  - What happens to measure of similarity?

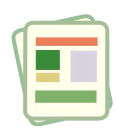
when $\alpha = \frac{1}{\|u\|}$

- Good to normalize vectors

11

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:

$$\mathrm{tf}(t, d) = \# \text{ occurrences of } t \in d.$$

term, d

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

$$\mathrm{idf}(t, \cancel{D}X) = \log \frac{|X|}{1 + |\{d \in X : t \in d\}|}$$

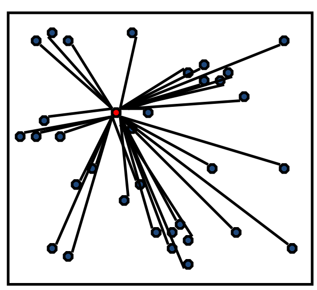
- tf-idf:

$$\mathrm{tfidf}(t, d, D) = \mathrm{tf}(t, d) \times \mathrm{idf}(t, X)$$

  - 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?

→ # of web pages

N → # of images

- How fast do we desire to do recall?

Intuition (?): NN in 1D and Sorting

- How do we do 1-NN searches in 1 dim?

or How do we sort?

approx.

- Pre-processing time:

$O(N)$ bins

sorting $O(N \log N)$

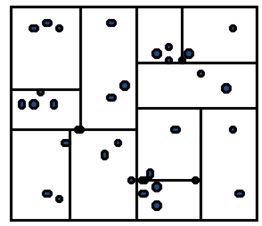
- Query time:

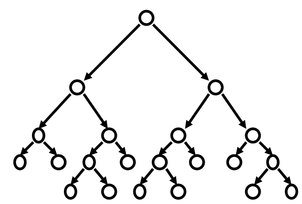
$O(1)$

$O(\log N)$

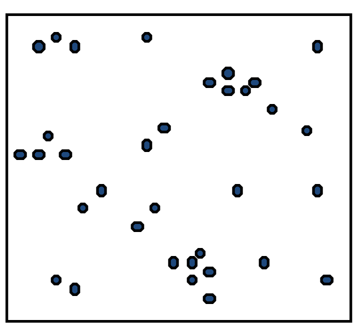
KD-Trees

- 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…





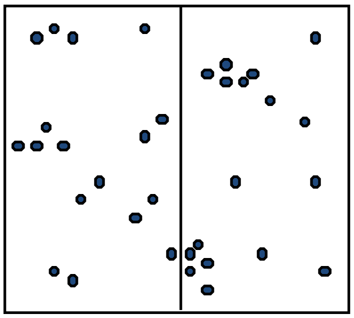
KD-Tree Construction



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



X>.5

NO

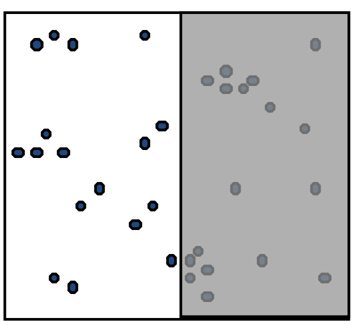
Pt	X	Y
1	0.00	0.00
3	0.13	2.85
…	…	…

YES

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



X>.5

NO

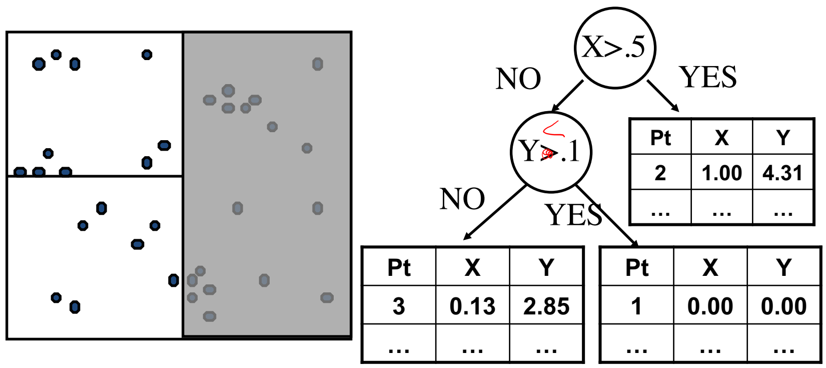
Pt	X	Y
1	0.00	0.00
3	0.13	2.85
…	…	…

YES

Pt	X	Y
2	1.00	4.31
…	…	…

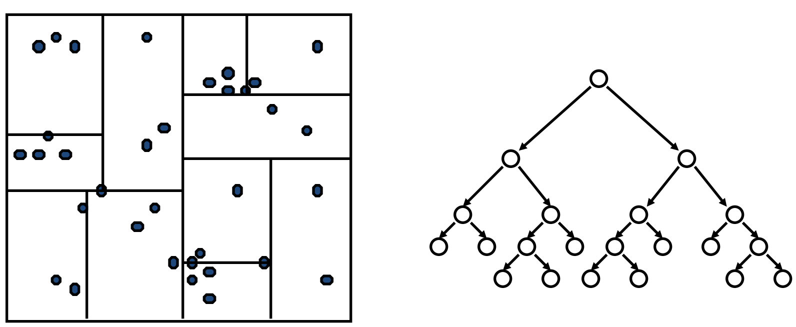
- Consider each group separately and possibly split again (along same/different dimension).
  - Stopping criterion to be discussed…

KD-Tree Construction



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

KD-Tree Construction

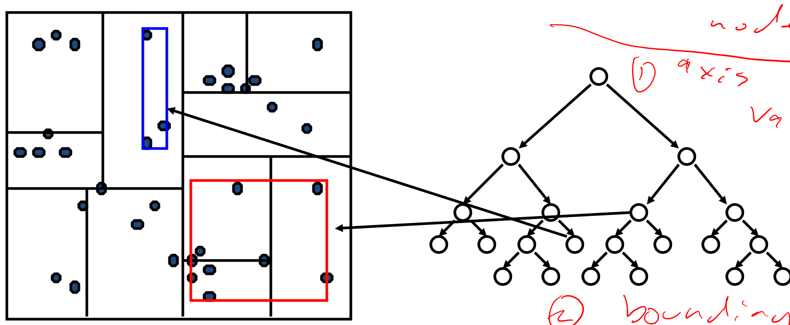


- Continue splitting points in each set
  - creates a binary tree structure
- Each leaf node contains a list of points

KD-Tree Construction

maintain at all nodes

(1) axis & value



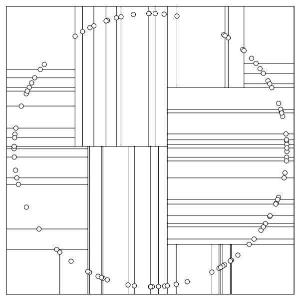
(2) bounding box

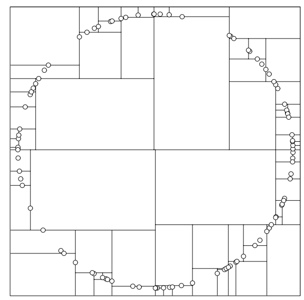
- Keep one additional piece of information at each node:
  - The (tight) bounds of the points at or below this node.

KD-Tree Construction

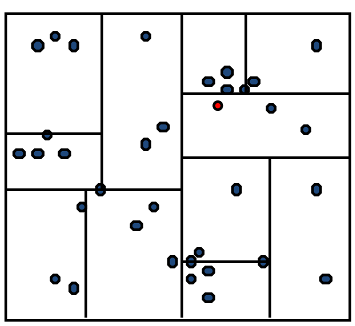
- Use heuristics to make splitting decisions:
- Which dimension do we split along?
- Which value do we split at?
- When do we stop?

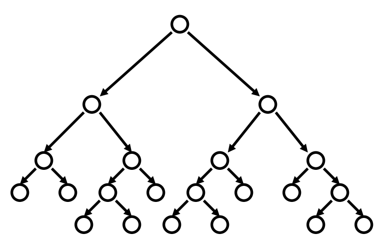
Many heuristics…


median heuristic


center-of-range heuristic

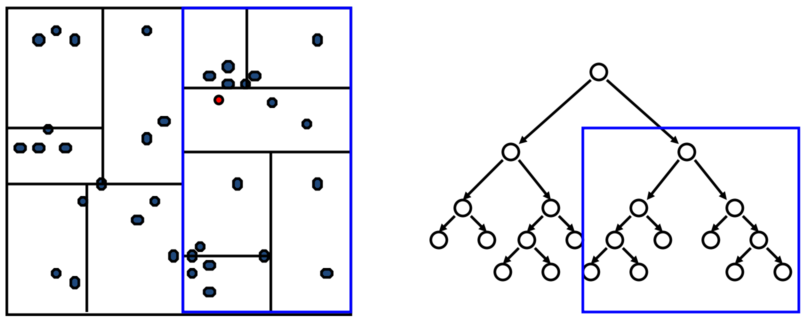
Nearest Neighbor with KD Trees





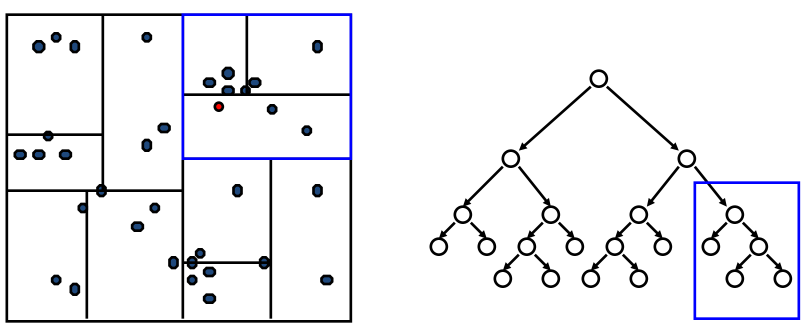
- Traverse the tree looking for the nearest neighbor of the query point.

Nearest Neighbor with KD Trees



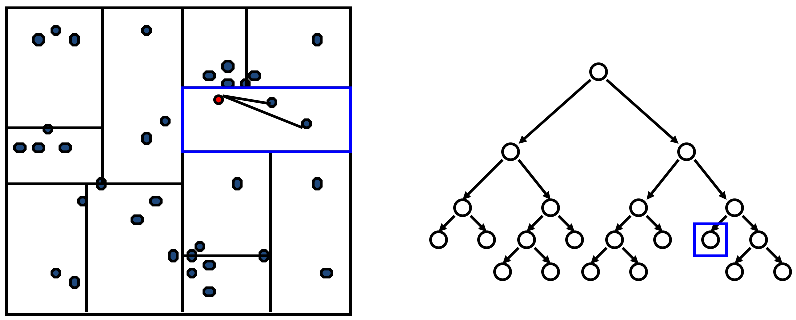
- Examine nearby points first:
  - Explore branch of tree closest to the query point first.

Nearest Neighbor with KD Trees



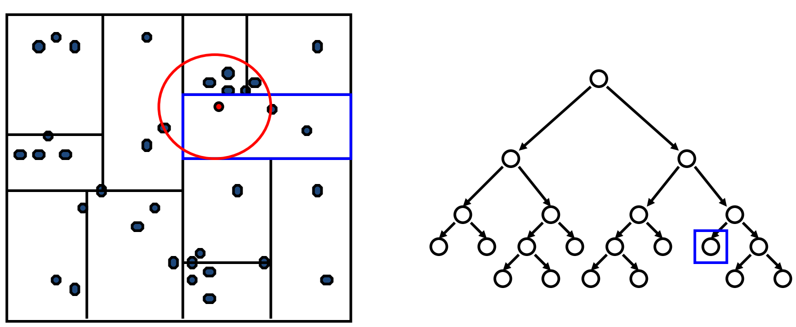
- Examine nearby points first:
  - Explore branch of tree closest to the query point first.

Nearest Neighbor with KD Trees



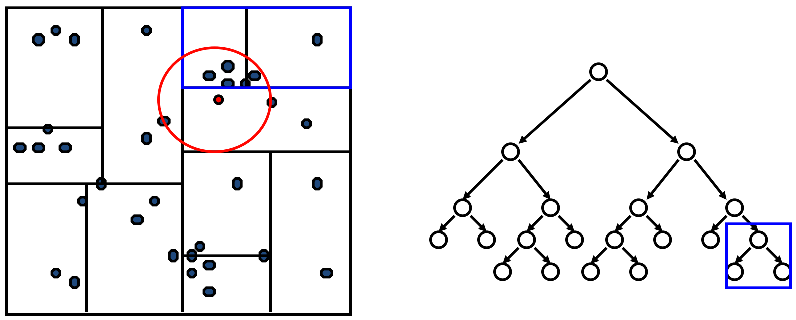
- When we reach a leaf node:
  - Compute the distance to each point in the node.

Nearest Neighbor with KD Trees



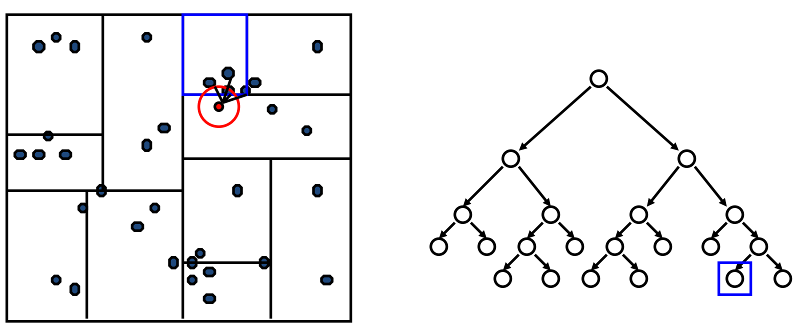
- When we reach a leaf node:
  - Compute the distance to each point in the node.

Nearest Neighbor with KD Trees



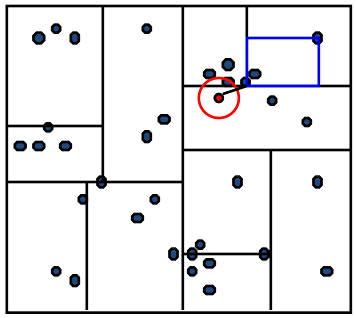
- Then backtrack and try the other branch at each node visited

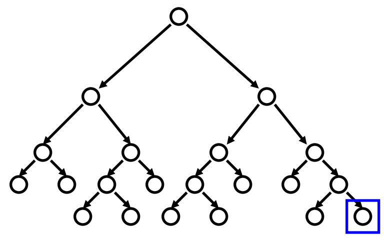
Nearest Neighbor with KD Trees



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

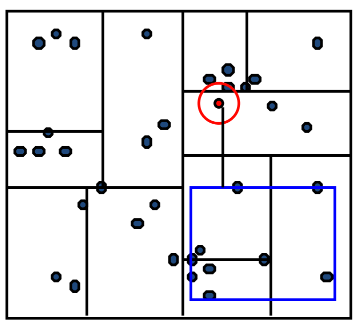
Nearest Neighbor with KD Trees

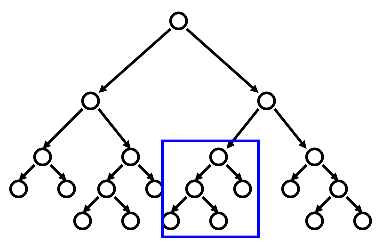




- Using the distance bound and bounding box of each node:
  - Prune parts of the tree that could NOT include the nearest neighbor

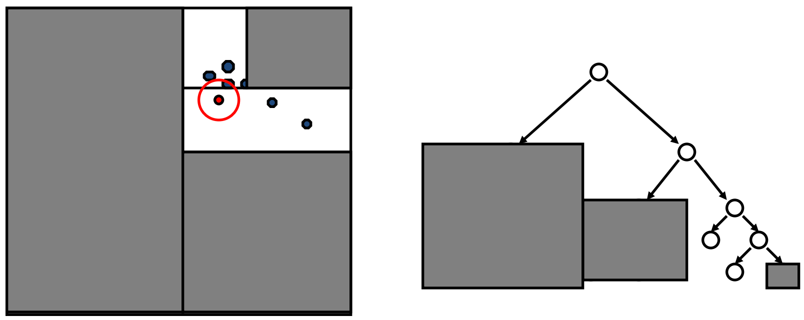
Nearest Neighbor with KD Trees





- 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

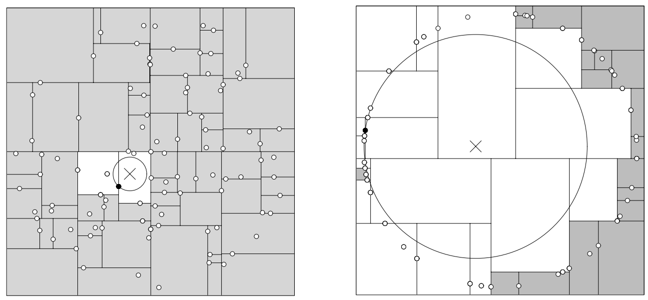


- Using the distance bound and bounding box of each node:
  - Prune parts of the tree that could NOT include the nearest neighbor

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)

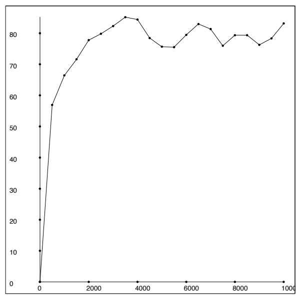
Complexity

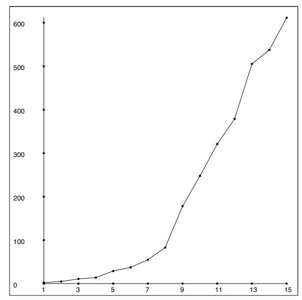


Complexity for *N* Queries

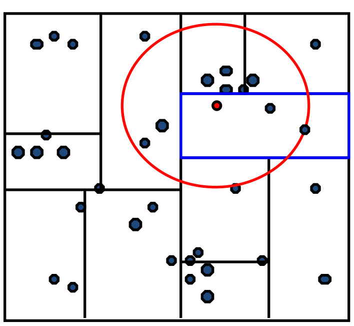
- Ask for nearest neighbor to each document
- Brute force 1-NN:
- kd-trees:

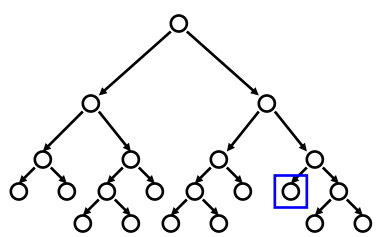
Inspections vs. *N* and *d*





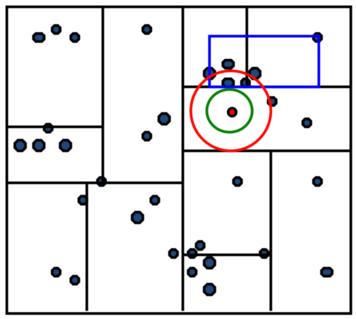
K-NN with KD Trees

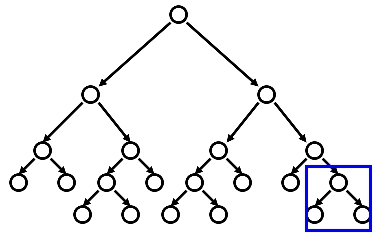




- Exactly the same algorithm, but maintain distance as distance to furthest of current *k* nearest neighbors
- Complexity is:

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