Case Study 1: Estimating Click Probabilities

Tackling an Unknown Number of Features with Sketching

Machine Learning for Big Data
CSE547/STAT548, University of Washington
Emily Fox
January 16th, 2014

Problem 1: Complexity of Update Rules for Logistic Regression

- Logistic regression update: stoch. grad. asc.

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta_t \left\{ -\lambda w_i^{(t)} + x_i^{(t)} [y^{(t)} - P(Y = 1 | \mathbf{x}^{(t)}, \mathbf{w}^{(t)})] \right\}$$

- Complexity of updates:
  - Constant in number of data points ✓
  - In number of features? O(d)
    - Problem both in terms of computational complexity and sample complexity

What if we have 1B features??

- What can we with very high dimensional feature spaces?
  - Kernels not always appropriate, or scalable ← "kernel trick"
  - What else?

Problem 2: Unknown Number of Features

- For example, bag-of-words features for text data: 'Obamacare'
  - "Mary had a little lamb, little lamb…"

X: | 1 | 1 | 1 | 2 | 3 | 1 |

'Mary' 'had' 'a' 'little' 'lamb'

- What's the dimensionality of **x**? size of vocabulary … millions
- What if we see new word that was not in our vocabulary?
  - Obamacare
  - Theoretically, just keep going in your learning, and initialize $\mathbf{w}_{\text{Obamacare}} = 0$
  - In practice, need to re-allocate memory, fix indices,… A big problem for Big Data

Bloom Filter: Multiple Hash Tables

- Single hash table -> Many false positives
- Multiple hash tables with independent hash functions
  - Apply $h_1(i),\ldots, h_k(i)$, set all bits to 1

$h_1(\text{'Mary'})=7$ $h_1(\text{'Obamacare'})=7$

$h_2(\text{'Mary'})=4$ $h_2(\text{'Obamacare'})=9$

- Query Q(i)?

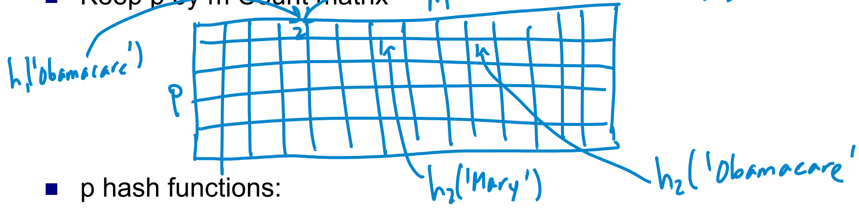
'Mary' + 'Obamacare' collide in h_1 but not h_2

if $\forall_j\ h_j(i) = 1$
$Q(i)$ = very probably yes
else $Q(i)$ = no

- Significantly decrease probability of false positives

Count-Min Sketch: general case

- Keep p by m Count matrix



- p hash functions:
  - Just like in Bloom Filter, decrease errors with multiple hashes
  - Every time see string *i*:

row j^{th} hash fcn   input

$$\forall j \in \{1,\ldots,p\} : Count[j, h_j(i)] \leftarrow Count[j, h_j(i)] + 1$$

Finally, Sketching for LR

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta_t \left\{ -\lambda w_i^{(t)} + x_i^{(t)} [y^{(t)} - P(Y=1|\mathbf{x}^{(t)}, \mathbf{w}^{(t)})] \right\}$$

- Never need to know size of vocabulary!
- At every iteration, update Count-Min matrix:

$\forall j,k \quad Count[j,k] = (1-\eta_t \lambda)\, count[j,k]$

$\forall x_i^{(t)} \neq 0$

$\quad \forall j \quad Count[j, h_j(i)] \mathrel{+}= x_i^{(t)} \cdot const \leftarrow \eta_t (y^{(t)} - P(Y=1|\ldots))$

- Making a prediction:

Remember our est. of $w_i^{(t)}$: $\operatorname{median}_j Count[j, h_j(i)]$

Make pred:

$-\log odds = w_0^{(t)} + \sum_{i: x_i \neq 0} \operatorname{median}_j count[j, h_j(i)]\, x_i^{(t)}$

- Scales to huge problems, great practical implications…

Hash Kernels

- Count-Min sketch not designed for negative updates
- Biased estimates of dot products
- **Hash Kernels**: Very simple, but powerful idea to remove bias
- Pick 2 hash functions:
  - h : Just like in Count-Min hashing $h: X \to \{1, \dots, m\}$
  - ξ : Sign hash function $\xi: X \to \{+1, -1\}$
    - Removes the bias found in Count-Min hashing (see homework)
- Define a "kernel", a projection ϕ for **x**:

can think of as random projection of X

For each non-zero element of X, add to bin $h(j)$: $\xi(j)X_j$

$\phi(x) =$

$\phi_i(x) = \sum_{j:h(j)=i} \xi(j) X_j$

If $X_j = 7$
$h(j) = 4$
$\xi(j) = -1$
add -7 to bin 4

Hash Kernels Preserve Dot Products

$$\phi_i(\mathbf{x}) = \sum_{j:h(j)=i} \xi(j)\mathbf{x}_j$$

- Hash kernels provide unbiased estimate of dot-products!

$E_{h,\xi}[\phi(x) \cdot \phi(y)] = x \cdot y$ Pf: by homework

- Variance decreases as O(1/*m*) gets better w/ more dims
- Choosing *m*? For ε>0, if

$$m = \mathcal{O}\left(\frac{\log \frac{N}{\delta}}{\epsilon^2}\right)$$

log in data size

  - Under certain conditions…
  - Then, with probability at least 1-δ:

$$(1-\epsilon)||\mathbf{x}-\mathbf{x}'||_2^2 \leq ||\phi(\mathbf{x})-\phi(\mathbf{x}')||_2^2 \leq (1+\epsilon)||\mathbf{x}-\mathbf{x}'||_2^2$$

Learning With Hash Kernels

- Given hash kernel of dimension *m*, specified by *h* and ξ
  - Learn *m* dimensional weight vector
- Observe data point **x**
  - Dimension does not need to be specified a priori!
- Compute ϕ(**x**):
  - Initialize ϕ(**x**)
  - For non-zero entries *j* of $\mathbf{x}_j$:
- Use normal update as if observation were ϕ(**x**), e.g., for LR using SGD:

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta_t \left\{ -\lambda w_i^{(t)} + \phi_i(\mathbf{x}^{(t)})[y^{(t)} - P(Y=1|\phi(\mathbf{x}^{(t)}), \mathbf{w}^{(t)})] \right\}$$

Interesting Application of Hash Kernels: Multi-Task Learning

- Personalized click estimation for many users:
  - One global click prediction vector **w**:
    - But…
  - A click prediction vector $\mathbf{w}_u$ per user *u*:
    - But…
- Multi-task learning: Simultaneously solve multiple learning related problems:
  - Use information from one learning problem to inform the others
- In our simple example, learn both a global **w** and one $\mathbf{w}_u$ per user:
  - Prediction for user *u*:
  - If we know little about user *u*:
  - After a lot of data from user *u*:

Problems with Simple Multi-Task Learning

- Dealing with new user is annoying, just like dealing with new words in vocabulary

- Dimensionality of joint parameter space is HUGE, e.g. personalized email spam classification from Weinberger et al.:
  - 3.2M emails
  - 40M unique tokens in vocabulary
  - 430K users
  - 16T parameters needed for personalized classification!

Hash Kernels for Multi-Task Learning

- Simple, pretty solution with hash kernels:
  - Very multi-task learning as (sparse) learning problem with (huge) joint data point **z** for point **x** and user *u*:

- Estimating click probability as desired:

- Address huge dimensionality, new words, and new users using hash kernels:

  - Desired effect achieved if *j* includes both
    - just word (for global **w**)
    - word,user (for personalized $\mathbf{w}_u$)

Simple Trick for Forming Projection $\phi(\mathbf{x},u)$

- Observe data point $\mathbf{x}$ for user u
  - Dimension does not need to be specified a priori and user can be unknown!
- Compute $\phi(\mathbf{x},u)$:
  - Initialize $\phi(\mathbf{x},u)$
  - For non-zero entries j of $\mathbf{x}_j$:
    - E.g., j='Obamacare'
    - Need two contributions to ϕ:
      - Global contribution
      - Personalized Contribution
    - Simply:
- Learn as usual using $\phi(\mathbf{x},u)$ instead of $\phi(\mathbf{x})$ in update function

Results from Weinberger et al. on Spam Classification: Effect of *m*

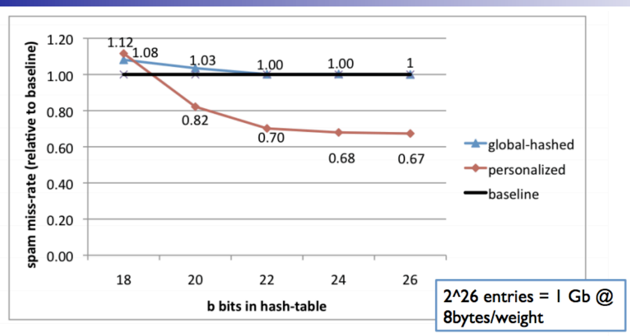


Figure 2. The decrease of uncaught spam over the baseline classifier averaged over all users. The classification threshold was chosen to keep the not-spam misclassification fixed at 1%. The hashed global classifier (*global-hashed*) converges relatively soon, showing that the distortion error ϵ_d vanishes. The personalized classifier results in an average improvement of up to 30%.

Results from Weinberger et al. on Spam Classification: Illustrating Multi-Task Effect

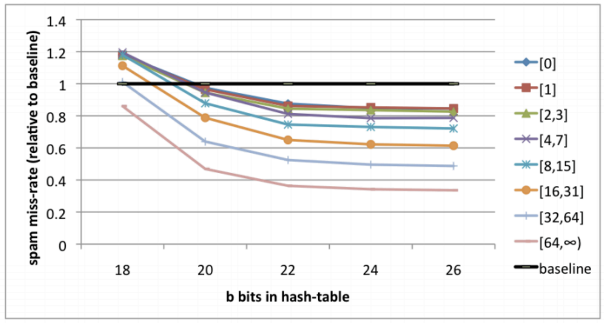


Figure 3. Results for users clustered by training emails. For example, the bucket $[8, 15]$ consists of all users with eight to fifteen training emails. Although users in buckets with large amounts of training data do benefit more from the personalized classifier (up-to 65% reduction in spam), even users that did not contribute to the training corpus at all obtain almost 20% spam-reduction.

What you need to know

- Hash functions
- Bloom filter
  - Test membership with some false positives, but very small number of bits per element
- Count-Min sketch
  - Positive counts: upper bound with nice rates of convergence
  - General case
- Application to logistic regression
- Hash kernels:
  - Sparse representation for feature vectors
  - Very simple, use two hash function (Can use one hash function…take least significant bit to define ξ)
  - Quickly generate projection $\phi(\mathbf{x})$
  - Learn in projected space
- Multi-task learning:
  - Solve many related learning problems simultaneously
  - Very easy to implement with hash kernels
  - Significantly improve accuracy in some problems (if there is enough data from individual users)

Case Study 2: Document Retrieval

Task Description: Finding Similar Documents

Machine Learning for Big Data
CSE547/STAT548, University of Washington
Emily Fox
January 16th, 2014

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

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,

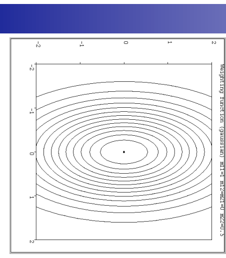
$$d(u,v) = \sqrt{(u-v)'\Sigma(u-v)}$$

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

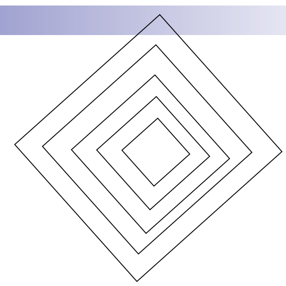
Other Metrics…

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

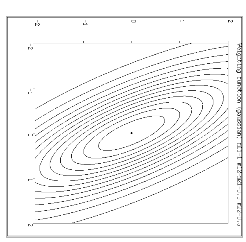
Notable Distance Metrics (and their level sets)



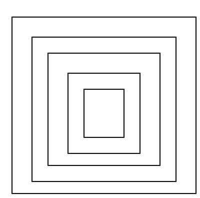
Scaled Euclidian (L_2)



L_1 norm (absolute)



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



L1 *(max) norm*

Euclidean Distance + Document Retrieval

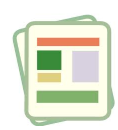
- Recall distance metric

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

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

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:

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

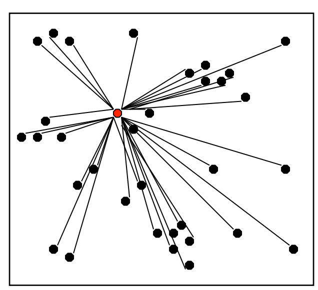
- tf-idf:

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

  - 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(Nlog$k$) per k-NN query!

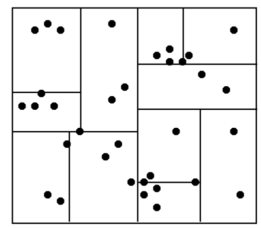


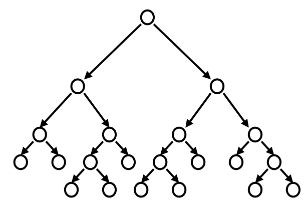
33 Distance Computations

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

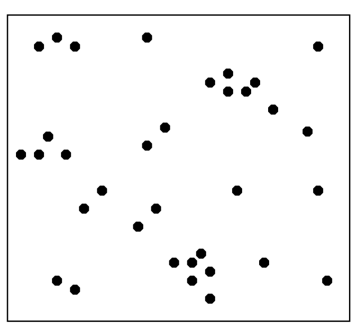
KD-Trees

- 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…





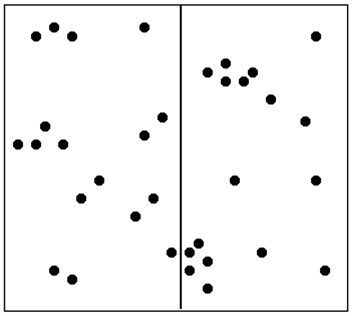
KD-Tree Construction



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

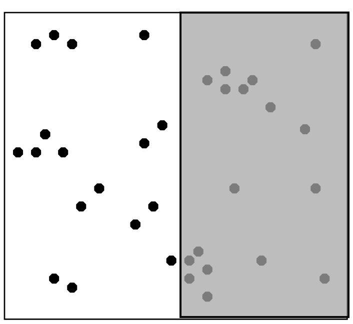
Pt	X	Y
1	0.00	0.00
3	0.13	2.85
…	…	…

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

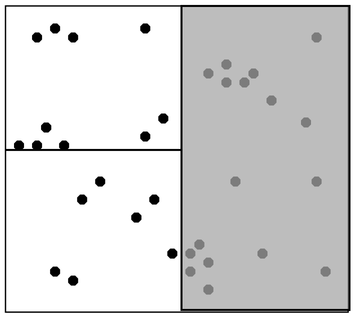
Pt	X	Y
1	0.00	0.00
3	0.13	2.85
…	…	…

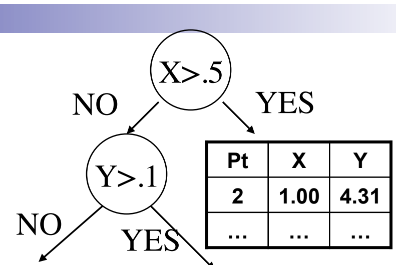
YES

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





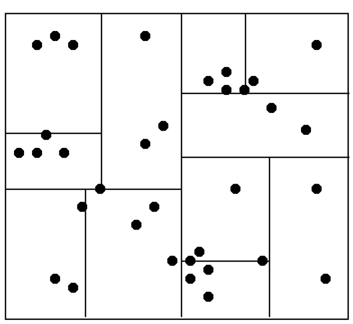
Pt	X	Y
2	1.00	4.31
…	…	…

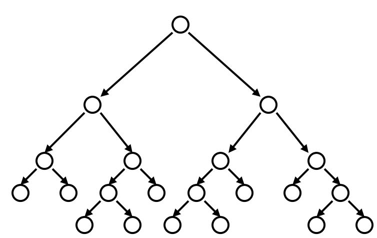
Pt	X	Y
3	0.13	2.85
…	…	…

Pt	X	Y
1	0.00	0.00
…	…	…

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

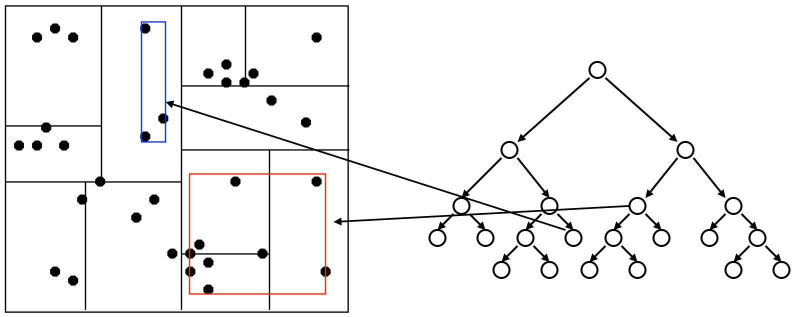
KD-Tree Construction





- 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.

©Emily Fox 2014

35

KD-Tree Construction

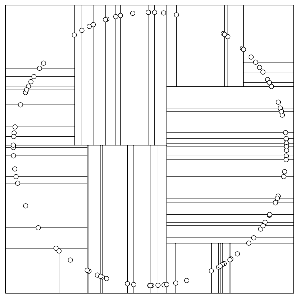
Use heuristics to make splitting decisions:

- Which dimension do we split along?
- Which value do we split at?
- When do we stop?

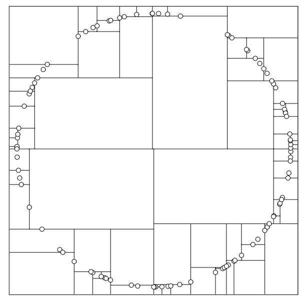
©Emily Fox 2014

36

Many heuristics…

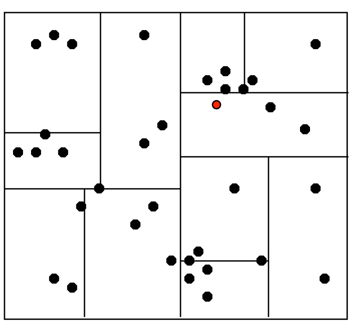


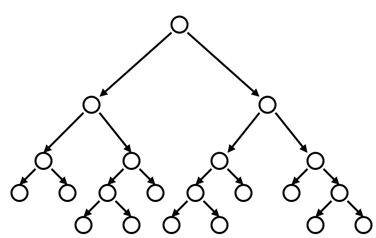
median heuristic



center-of-range heuristic

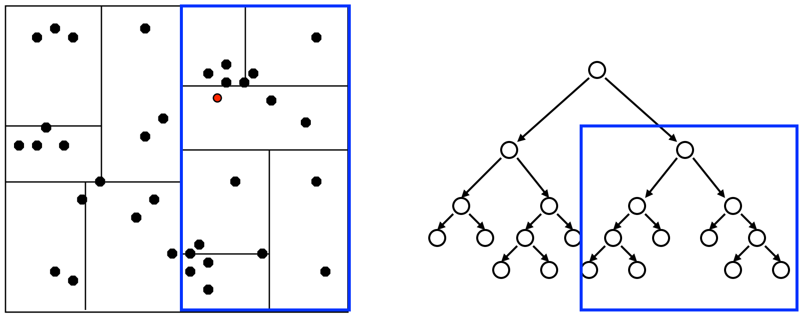
Nearest Neighbor with KD Trees





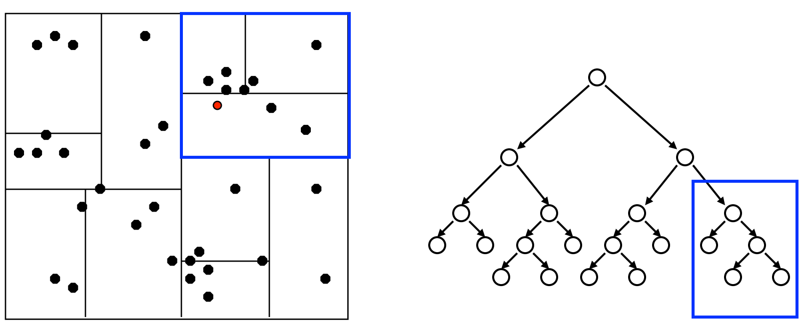
- Traverse the tree looking for the nearest neighbor of the query point.

Nearest Neighbor with KD Trees



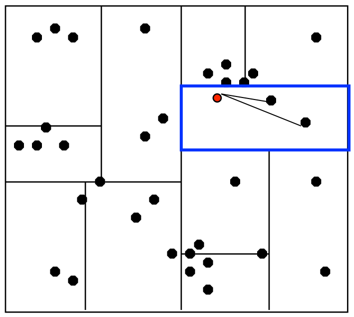
- Examine nearby points first:
  - Explore branch of tree closest to the query point first.

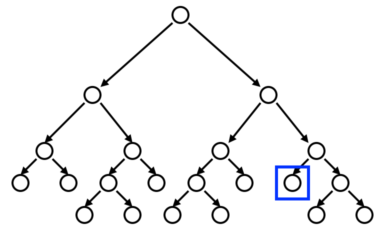
Nearest Neighbor with KD Trees



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

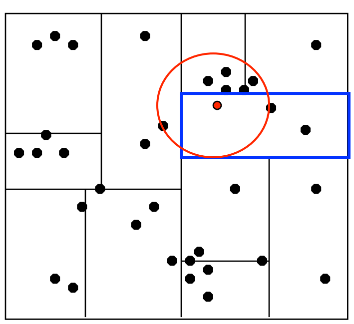
Nearest Neighbor with KD Trees

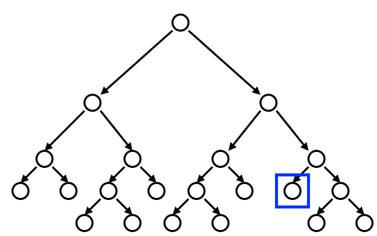




- When we reach a leaf node:
  - Compute the distance to each point in the node.

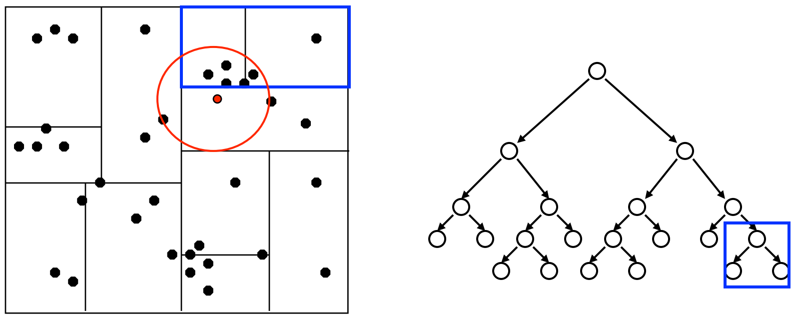
Nearest Neighbor with KD Trees





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

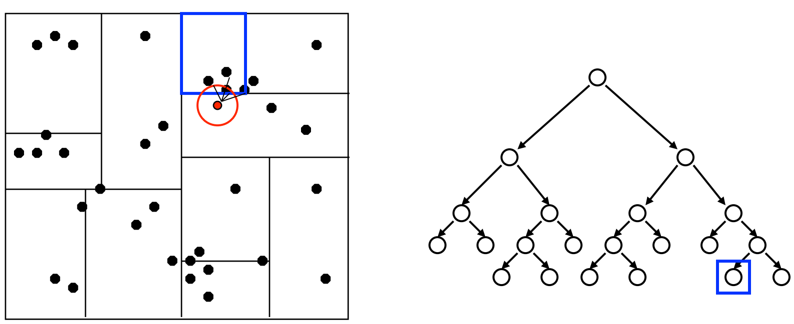
Nearest Neighbor with KD Trees



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

©Emily Fox 2014 43

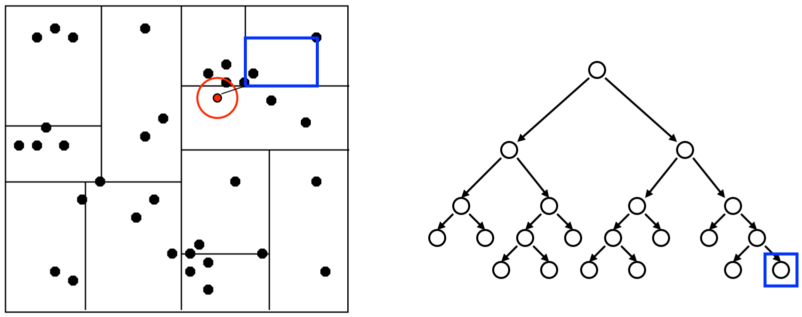
Nearest Neighbor with KD Trees



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

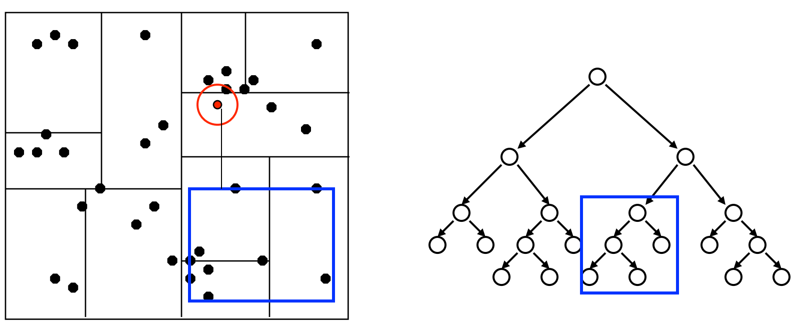
©Emily Fox 2014 44

Nearest Neighbor with KD Trees



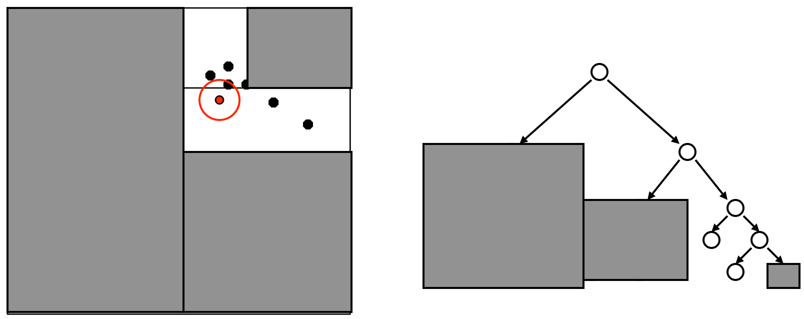
- Using the distance bound and bounding box of each node:
  - Prune parts of the tree that could NOT include the nearest neighbor

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

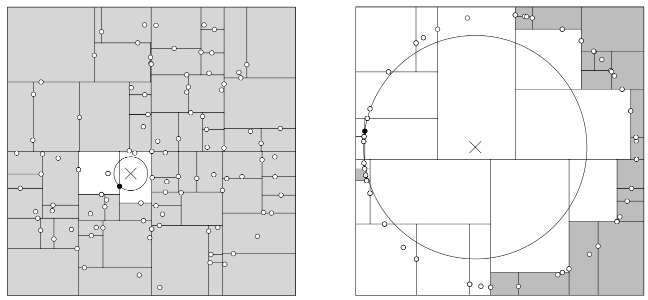


- Using the distance bound and bounding box of each node:
  - Prune parts of the tree that could NOT include the nearest neighbor

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)

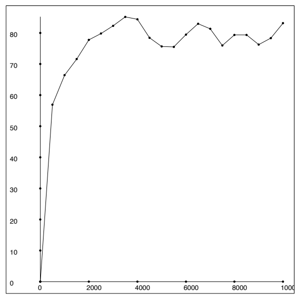
Complexity

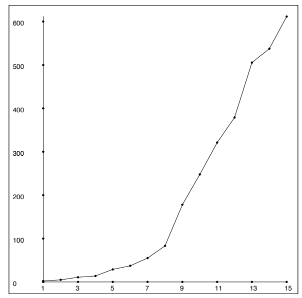


Complexity for N Queries

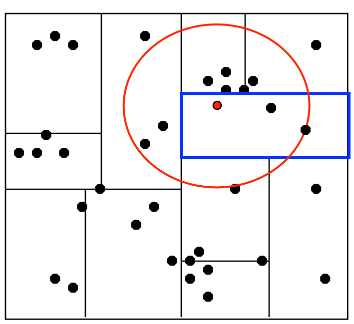
- Ask for nearest neighbor to each document
- Brute force 1-NN:
- kd-trees:

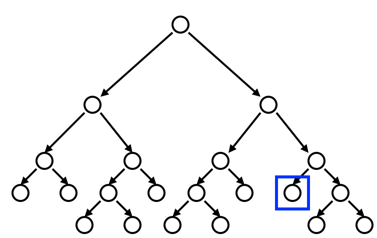
Inspections vs. *N* and *d*





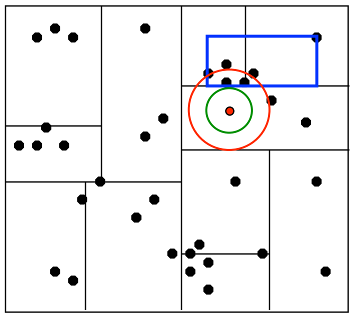
K-NN with KD Trees

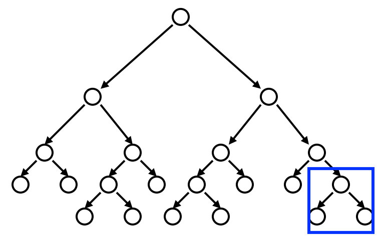




- Exactly the same algorithm, but maintain distance as distance to furthest of current *k* nearest neighbors
- Complexity is:

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.

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., 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