Trees

CS 189

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Fall 2015

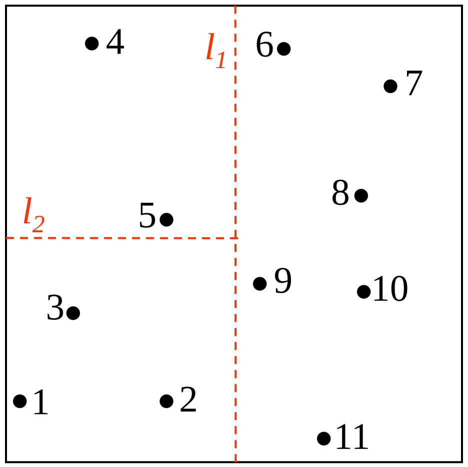
Nearest Neighbors: Reducing Computational Cost

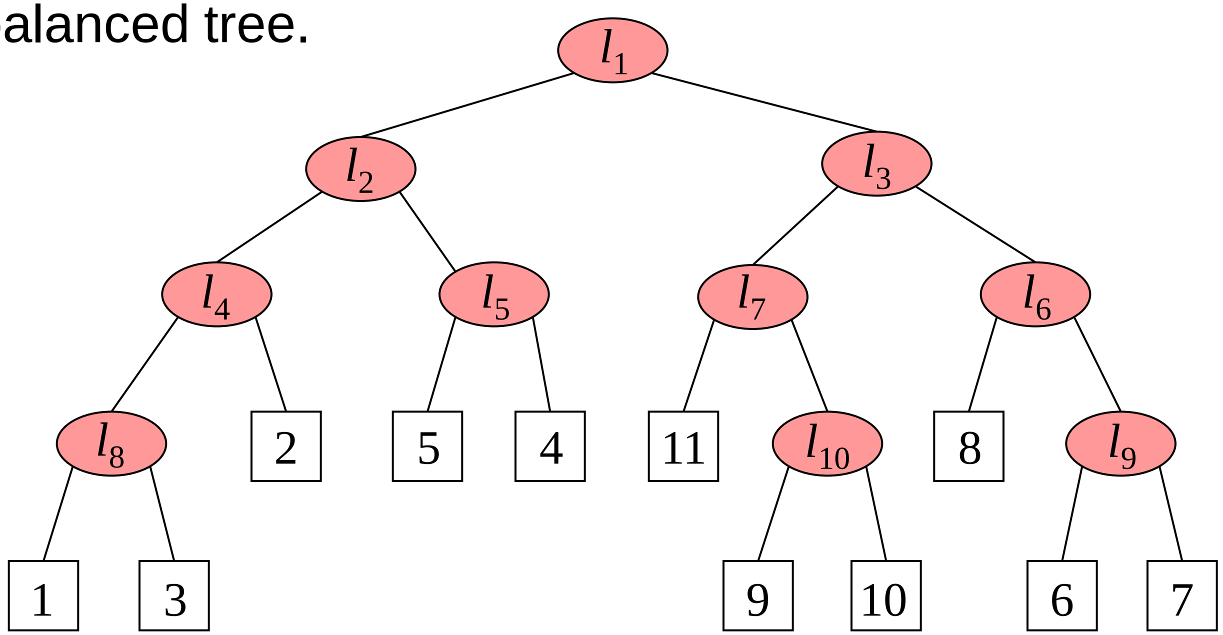
- Nearest-neighbors has O(N) complexity
  - Infeasible for large datasets

- Can we speed it up?
  - Think of guessing a number between 1 and 10…

K-d tree

- K-d tree is a binary tree data structure for organizing a set of points in a K-dimensional space.
- Each internal node is associated with an axis aligned hyper-plane splitting its associated points into two sub-trees.
- Dimensions with high variance are chosen first.
- Position of the splitting hyper-plane is chosen as the mean/median of the projected points – balanced tree.

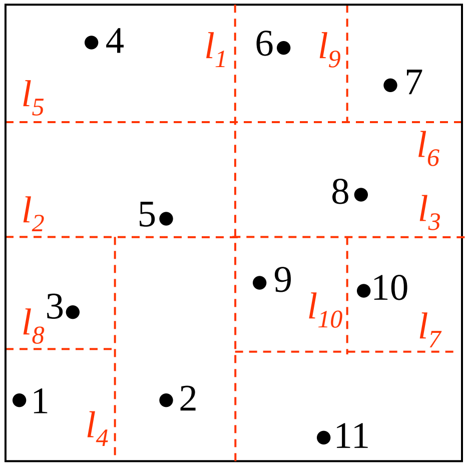


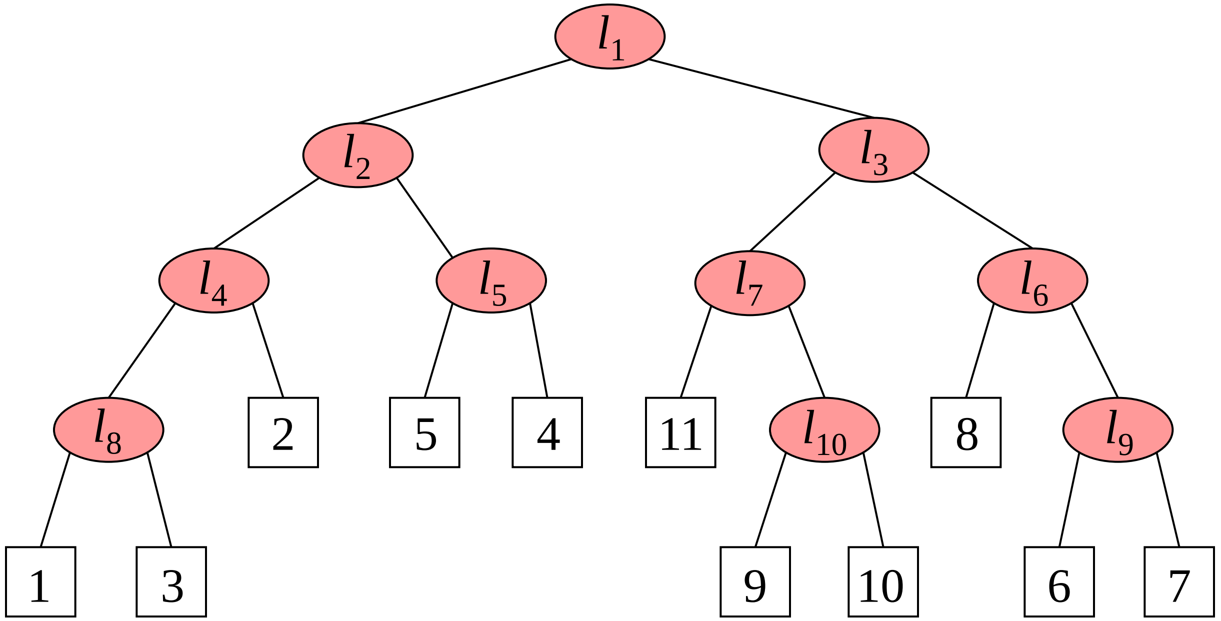


Images: Anna Atramentov

K-d tree construction

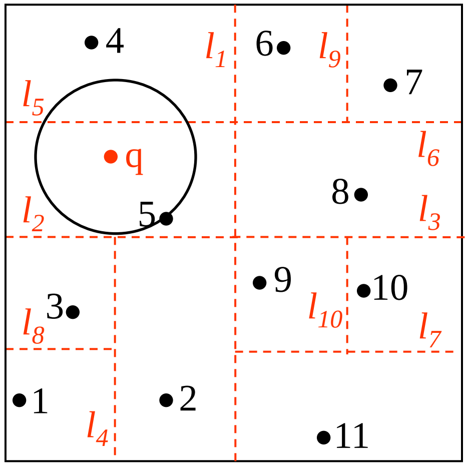
Simple 2D example

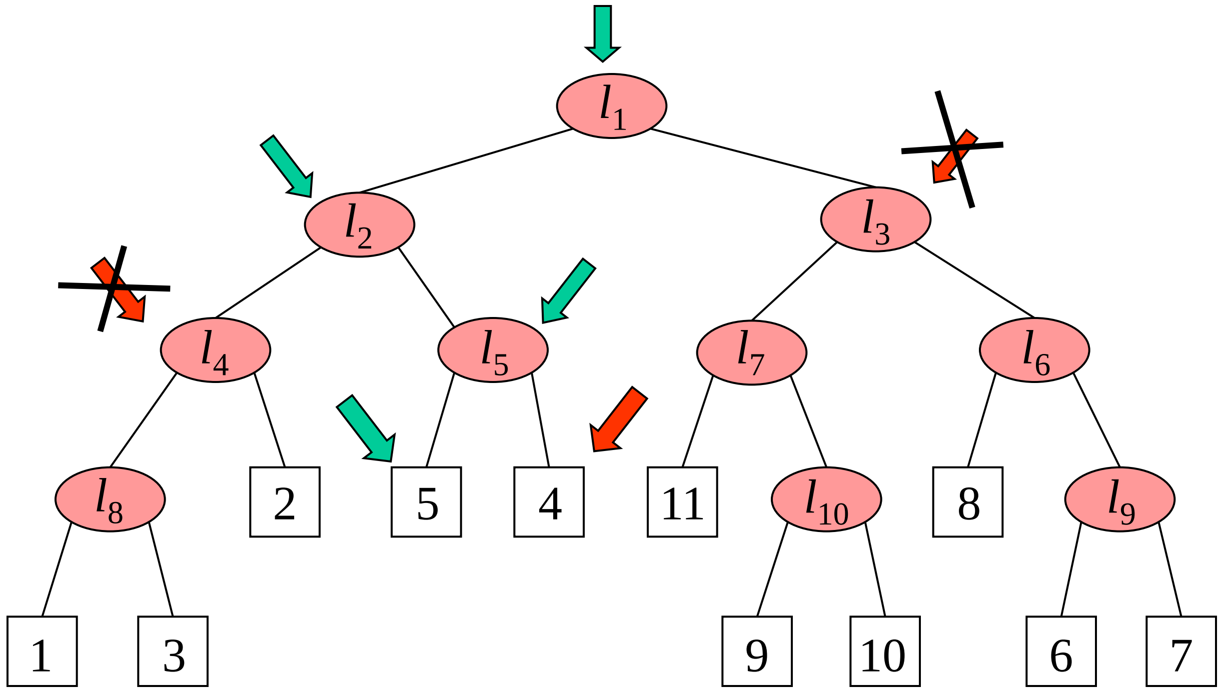




Slide credit: Anna Atramentov

K-d tree query





Slide credit: Anna Atramentov

K-d tree: Backtracking

- Backtracking is necessary as the true nearest neighbor may not lie in the query cell.
- But
  be i

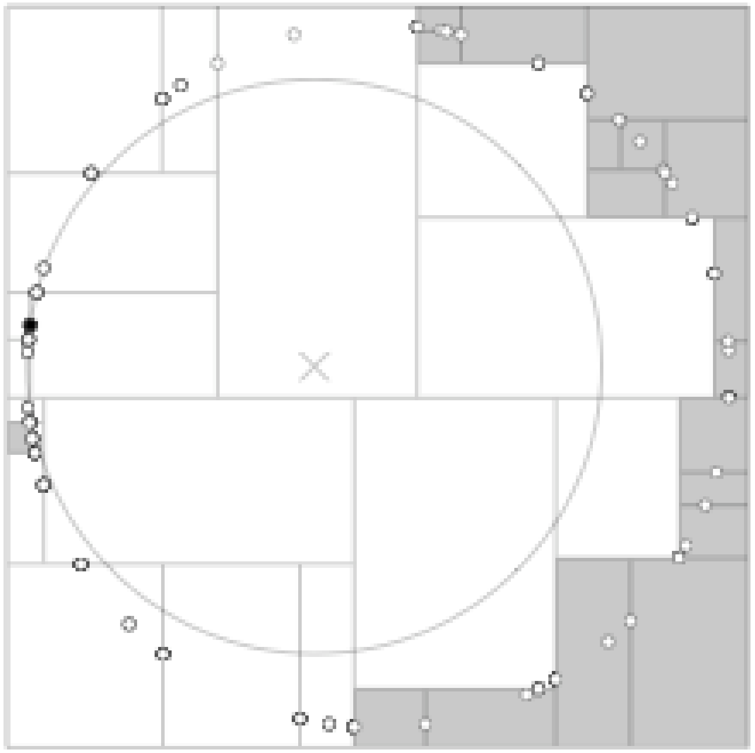


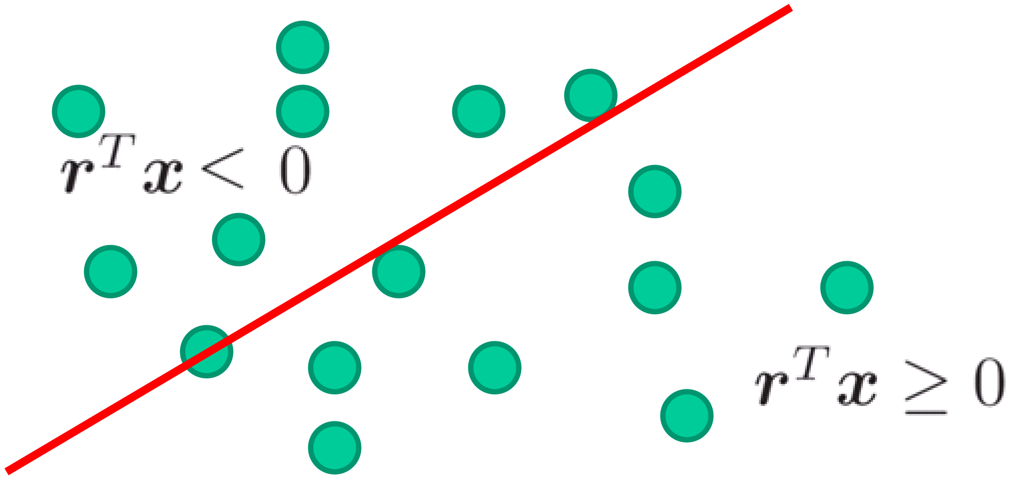
Figure 6.6

A bad distribution which forces almost all nodes to be inspected.

Figure: A. Moore

Do we need axis-aligned hyperplanes?

Normal unit vector *r* defines is a hyperplane separating the space

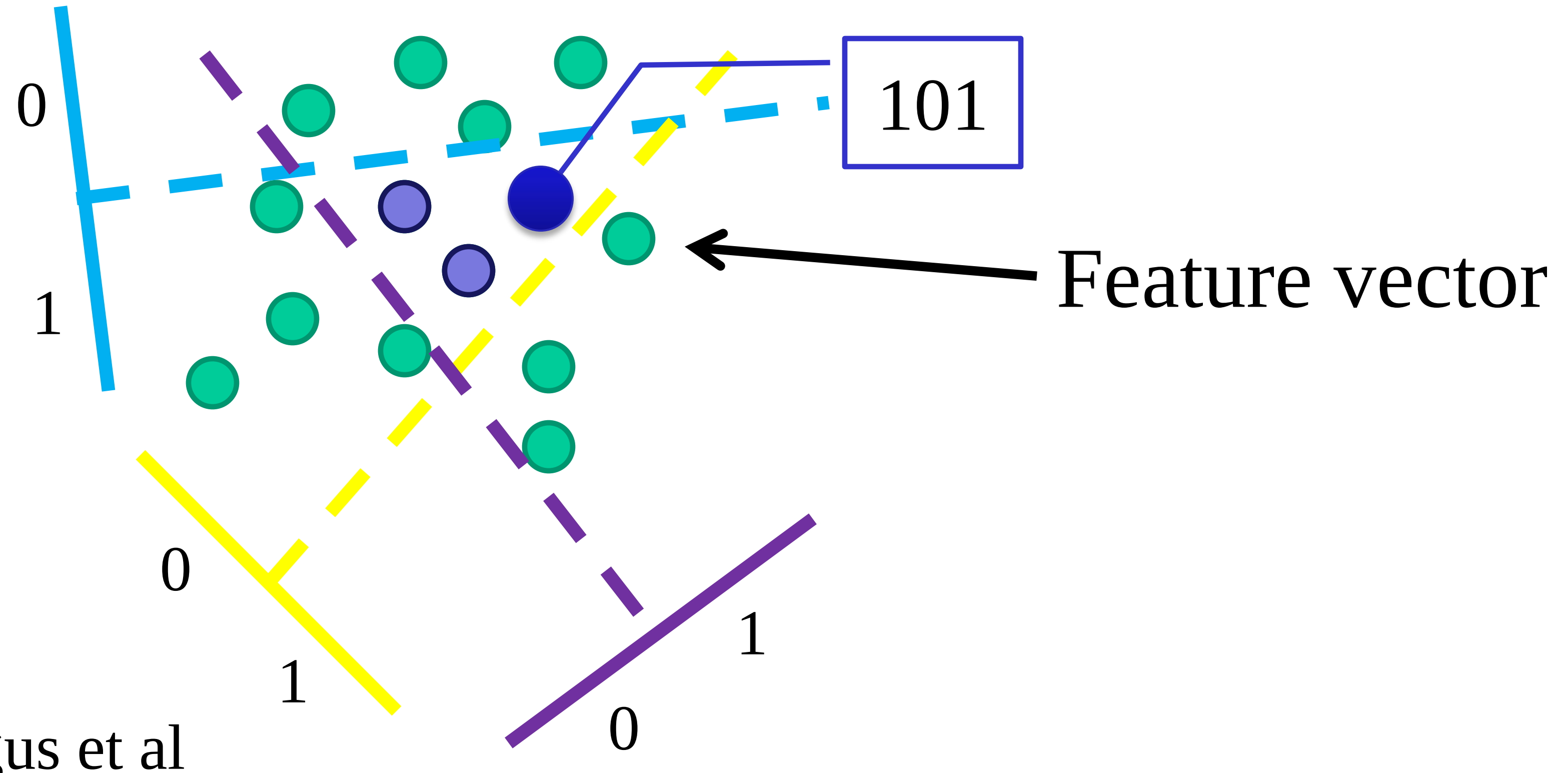

$\boldsymbol{r}^T\boldsymbol{x} < 0$
$\boldsymbol{r}^T\boldsymbol{x} \geq 0$

For any point x, define:

$$h_{\boldsymbol{r}}(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \boldsymbol{r}^T\boldsymbol{x} \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

Hashing by Random Projections

- Take random projections of data $\boldsymbol{r}^T\boldsymbol{x}$
- Quantize each projection with few bits



Fergus et al

Locality Sensitive Hashing

- The basic idea behind LSH is to project the data into a low-dimensional binary (Hamming) space; that is, each data point is mapped to a b-bit vector, called the *hash key*.
- Unlike normal hashing, here we <u>want</u> our hashes to cluster – create collisions
- Each hash function h must satisfy the locality sensitive hashing property:

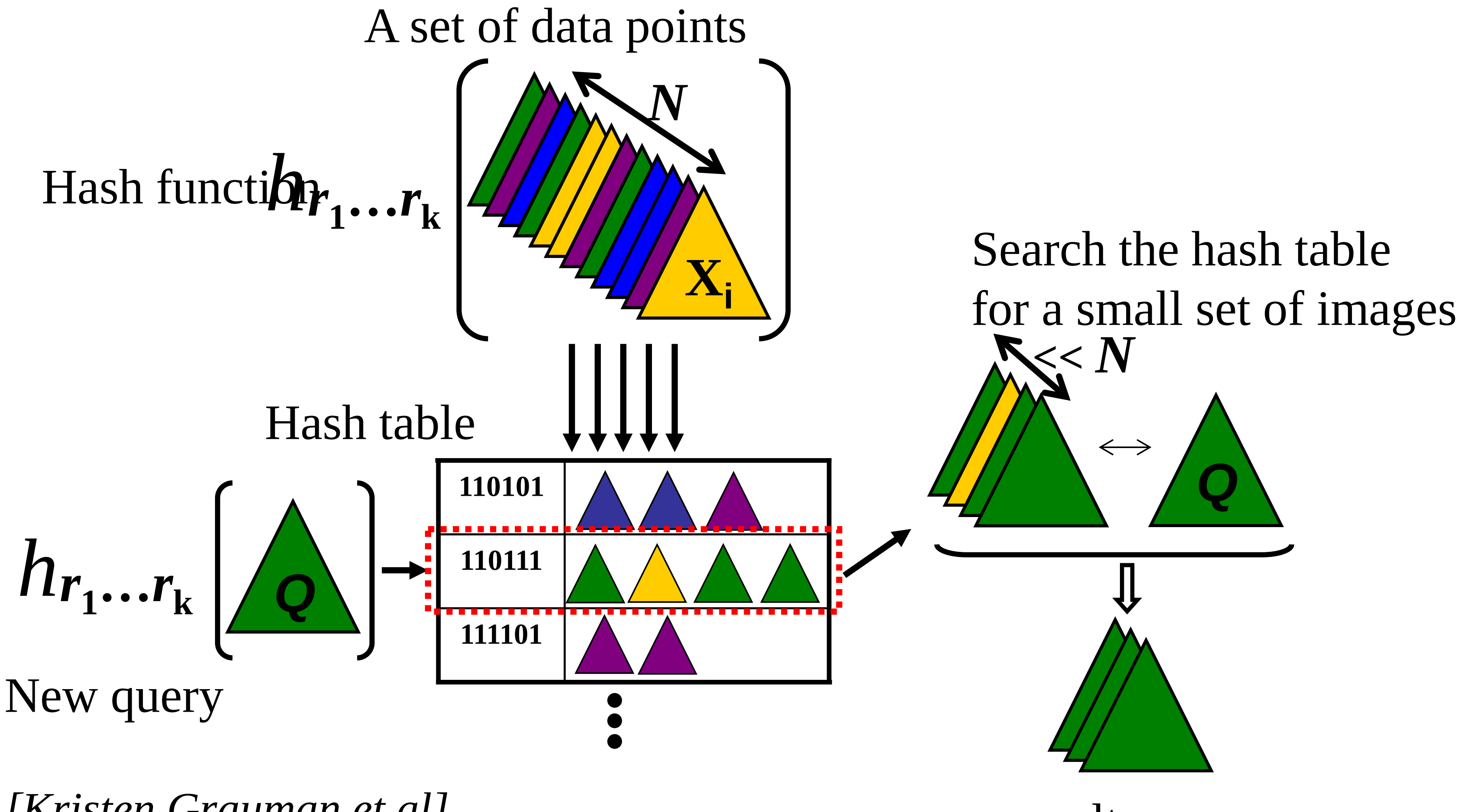
$$\Pr[h(\boldsymbol{x}_i) = h(\boldsymbol{x}_j)] = \mathrm{sim}(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

  – Where $\mathrm{sim}(\boldsymbol{x}_i, \boldsymbol{x}_j)$ ∈ [0, 1] is the similarity function. In our case: $Pr[h(u) = h(v)] = 1 - \frac{\theta(u,v)}{\pi}$

Kristen Grauman et al

Datar, N. Immorlica, P. Indyk, and V. Mirrokni. Locality-Sensitive Hashing Scheme Based on p-

Approximate Nearest-Neighbor Search



[Kristen Grauman et al]

Decision Trees

Nearest Neighbors

+ Nonlinear: arbitrary complex decision boundary possible

+ Non-parametric: can absorb unlimited amounts of data

+ / - Can decide on classes/labels at run-time

- This makes it dead slow!
- Even in kd-tree / LSH, we looked at the data *x*, but not the labels *y*

– Easily confused by irrelevant features

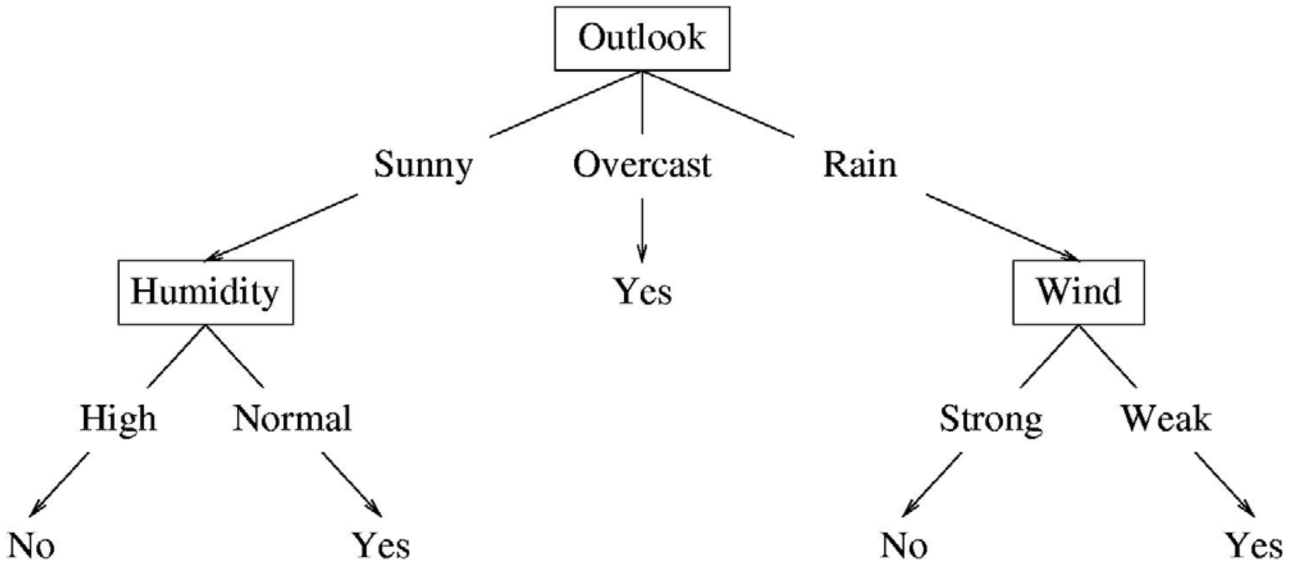
Decision Trees

- Let’s bring back labels!
  - Keep most benefits
  - but much more efficient

Let’s make a decision tree!

Decision Tree Hypothesis Space

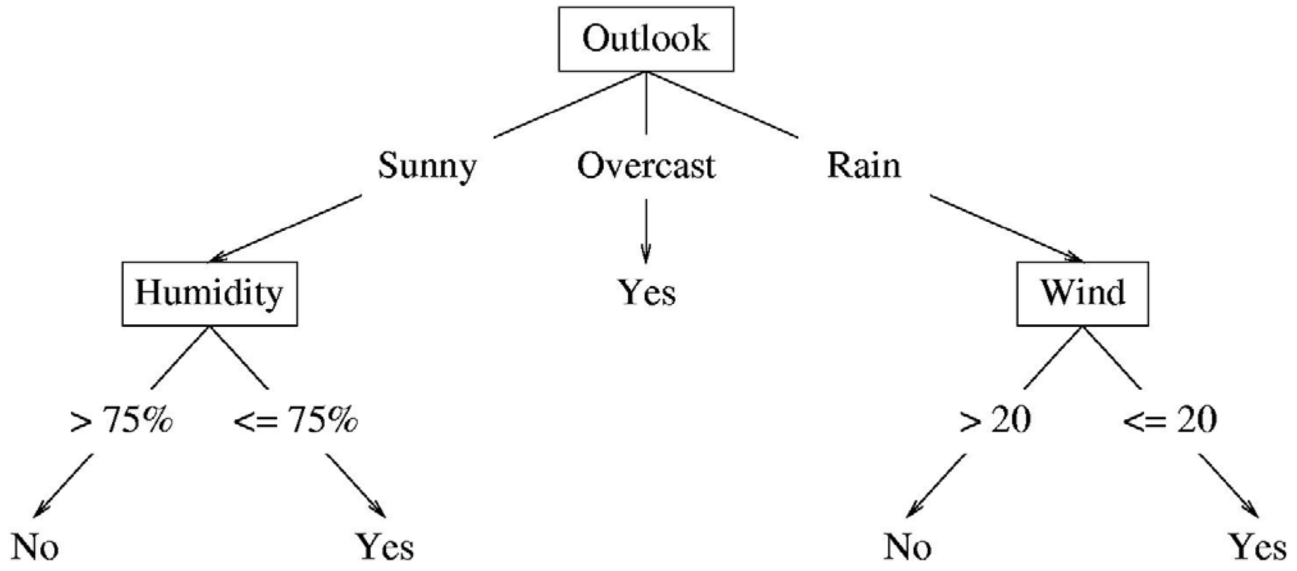
- **Internal nodes** test the value of particular features x_j and branch according to the results of the test.
- **Leaf nodes** specify the class $h(\mathbf{x})$.



Suppose the features are **Outlook** (x_1), **Temperature** (x_2), **Humidity** (x_3), and **Wind** (x_4). Then the feature vector $\mathbf{x} = (Sunny, Hot, High, Strong)$ will be classified as **No**. The **Temperature** feature is irrelevant.

Decision Tree Hypothesis Space

If the features are continuous, internal nodes may test the value of a feature against a threshold.

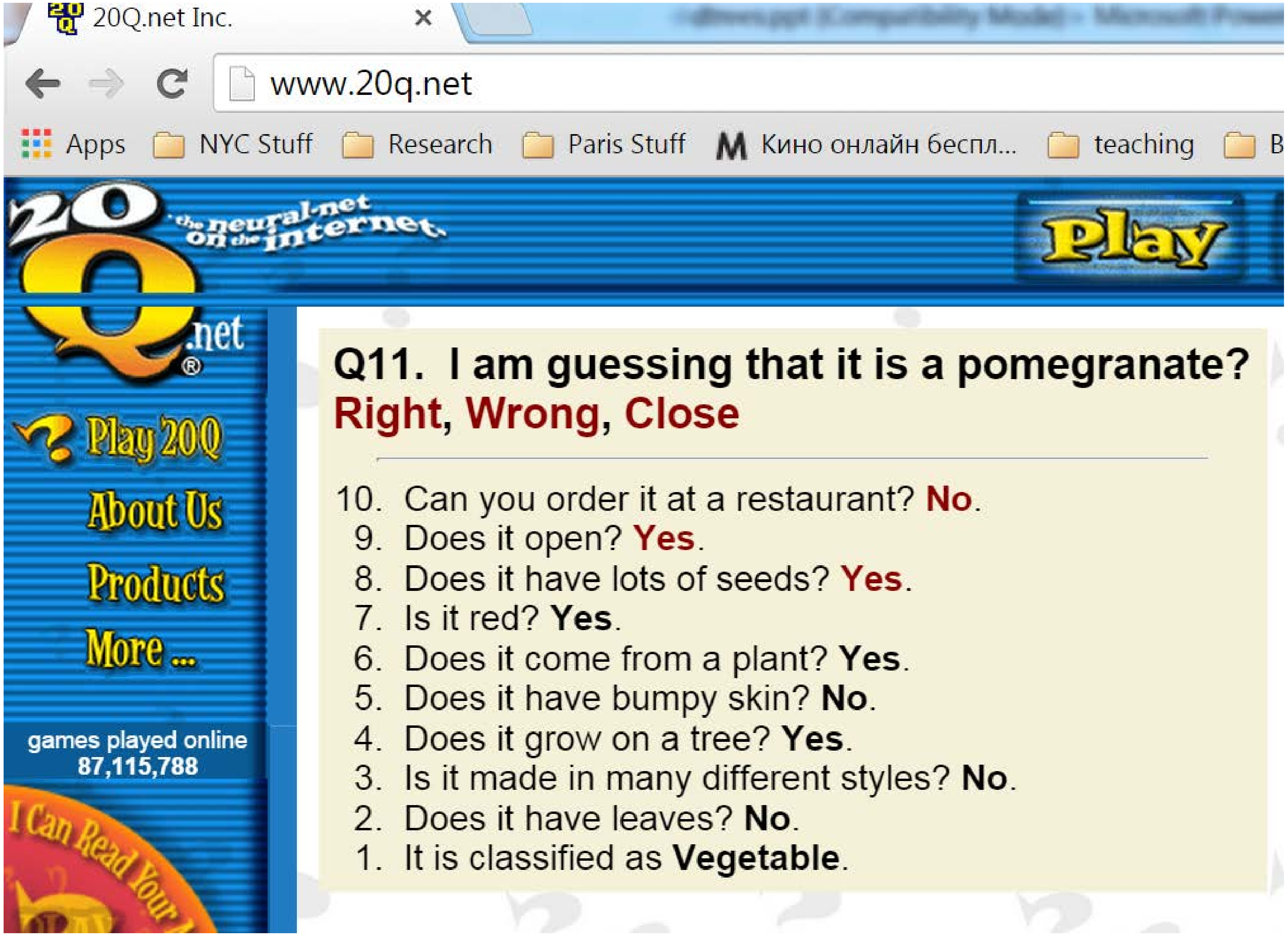


Benefits of Decision Trees

- works well with categorical features
- interpretable result
- Performs feature selection

- What would the decision regions look like?

20 Questions Game



Q11. I am guessing that it is a pomegranate?
Right, Wrong, Close

10. Can you order it at a restaurant? **No**.
9. Does it open? **Yes**.
8. Does it have lots of seeds? **Yes**.
7. Is it red? **Yes**.
6. Does it come from a plant? **Yes**.
5. Does it have bumpy skin? **No**.
4. Does it grow on a tree? **Yes**.
3. Is it made in many different styles? **No**.
2. Does it have leaves? **No**.
1. It is classified as **Vegetable**.

Building a Decision Tree

1. Decide on the best attribute on which to split the data
2. Long live recursion!!!

Learning Algorithm for Decision Trees

The same basic learning algorithm has been discovered by many people independently:

```
GrowTree($S$)
if ($y = 0$ for all $\langle \mathbf{x}, y \rangle \in S$) return new leaf(0)
else if ($y = 1$ for all $\langle \mathbf{x}, y \rangle \in S$) return new leaf(1)
else
    choose best attribute $x_j$
    $S_0 =$ all $\langle \mathbf{x}, y \rangle \in S$ with $x_j = 0$;
    $S_1 =$ all $\langle \mathbf{x}, y \rangle \in S$ with $x_j = 1$;
    return new node($x_j$, GrowTree($S_0$), GrowTree($S_1$))
```

Decision trees for Classification

- Training time = find good set of “questions”
  - Construct the tree, i.e. pick the questions at each node of the tree. Typically done so as to make each of the child nodes “purer” (lower entropy). Each leaf node will be associated with a set of training examples
- Test time
  - Evaluate the tree by sequentially evaluating questions, starting from the root node. Once a particular leaf node is reached, we predict the class to be the one with the most examples (from training set) at this node.

Building a Decision Tree

1. Decide on the best attribute on which to split the data
2. Long live recursion!!!

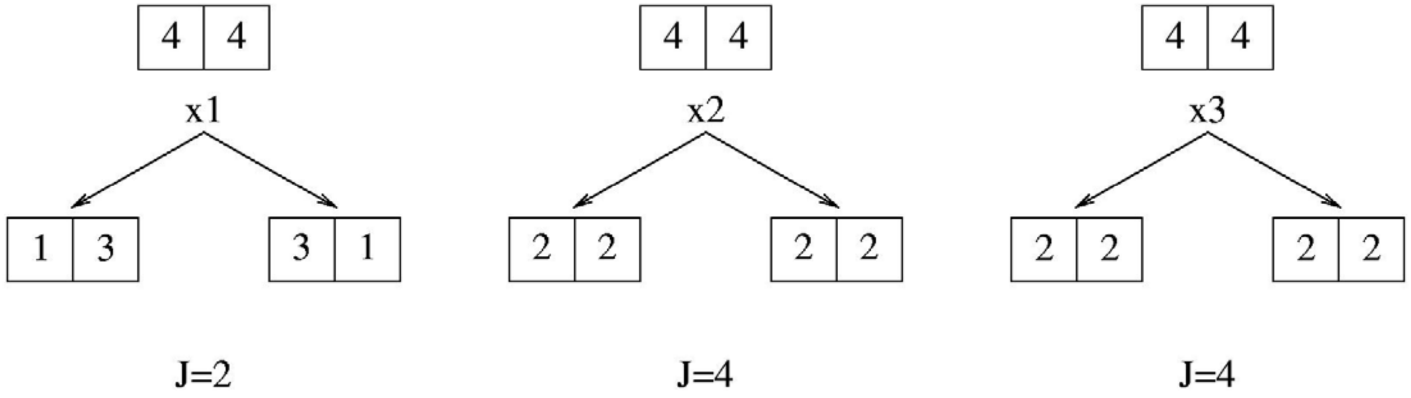
Choosing the Best Attribute

One way to choose the best attribute is to perform a 1-step lookahead search and choose the attribute that gives the lowest error rate on the training data.

```
ChooseBestAttribute(S)
choose $j$ to minimize $J_j$, computed as follows:
    $S_0 =$ all $\langle \mathbf{x}, y \rangle \in S$ with $x_j = 0$;
    $S_1 =$ all $\langle \mathbf{x}, y \rangle \in S$ with $x_j = 1$;
    $y_0 =$ the most common value of $y$ in $S_0$
    $y_1 =$ the most common value of $y$ in $S_1$
    $J_0 =$ number of examples $\langle \mathbf{x}, y \rangle \in S_0$ with $y \neq y_0$
    $J_1 =$ number of examples $\langle \mathbf{x}, y \rangle \in S_1$ with $y \neq y_1$
    $J_j = J_0 + J_1$ (total errors if we split on this feature)
return $j$
```

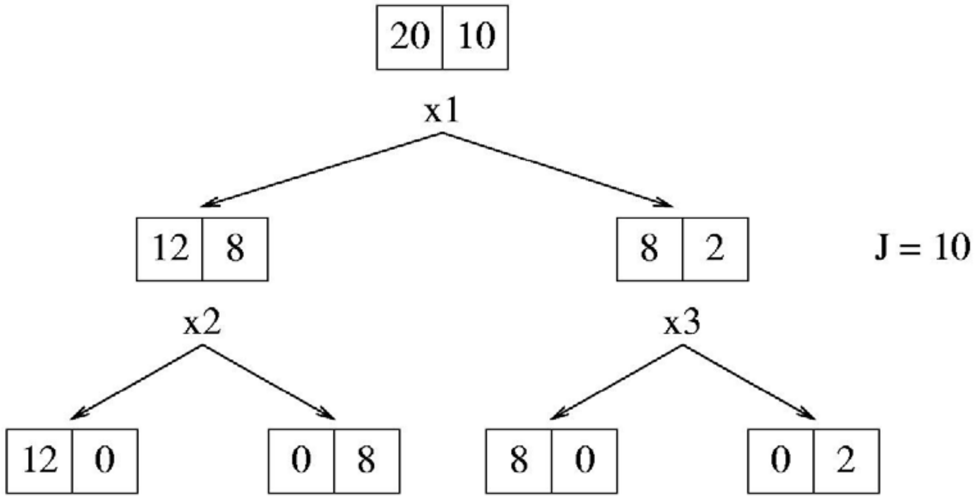
Choosing the Best Attribute—An Example

x_1	x_2	x_3	y
0	0	0	1
0	0	1	0
0	1	0	1
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	0
1	1	1	0



Choosing the Best Attribute (3)

Unfortunately, this measure does not always work well, because it does not detect cases where we are making "progress" toward a good tree.



Need a way to measure if we are "gaining information" even if error is not yet reduced.

A Better Heuristic From Information Theory

Let V be a random variable with the following probability distribution:

$P(V = 0)$	$P(V = 1)$
0.2	0.8

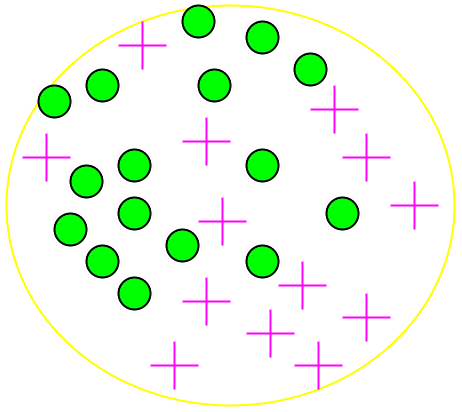
The ***surprise***, $S(V = v)$ of each value of V is defined to be

$$S(V = v) = -\lg P(V = v).$$

An event with probability 1 gives us zero surprise.
An event with probability 0 gives us infinite surprise!
It turns out that the surprise is equal to the number of bits of information that need to be transmitted to a recipient who knows the probabilities of the results.
This is also called the ***description length*** of $V = v$.
Fractional bits only make sense if they are part of a longer message (e.g., describe a whole sequence of coin tosses).

Entropy: Average Surprise

- Entropy H = $\sum_i - p_i \log_2 p_i$



p_i is the probability of class i

(compute it as the proportion of class *i* in the set)

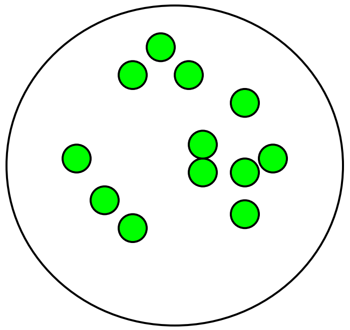
Entropy measures the (im)purity of collection of examples

in 2-Class case:

- What is the entropy of a group in which all examples belong to the same class?
  - entropy = - 1 $\log_2 1$ = 0

We are done!

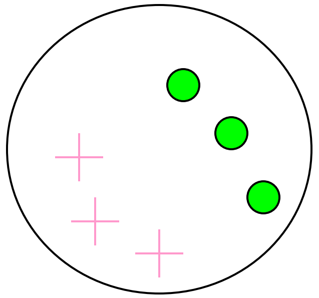
Minimum entropy



- What is the entropy of a group with 50% in either class?
  - entropy = -0.5 $\log_2 0.5$ – 0.5 $\log_2 0.5$ =1

Better start splitting

Maximum entropy

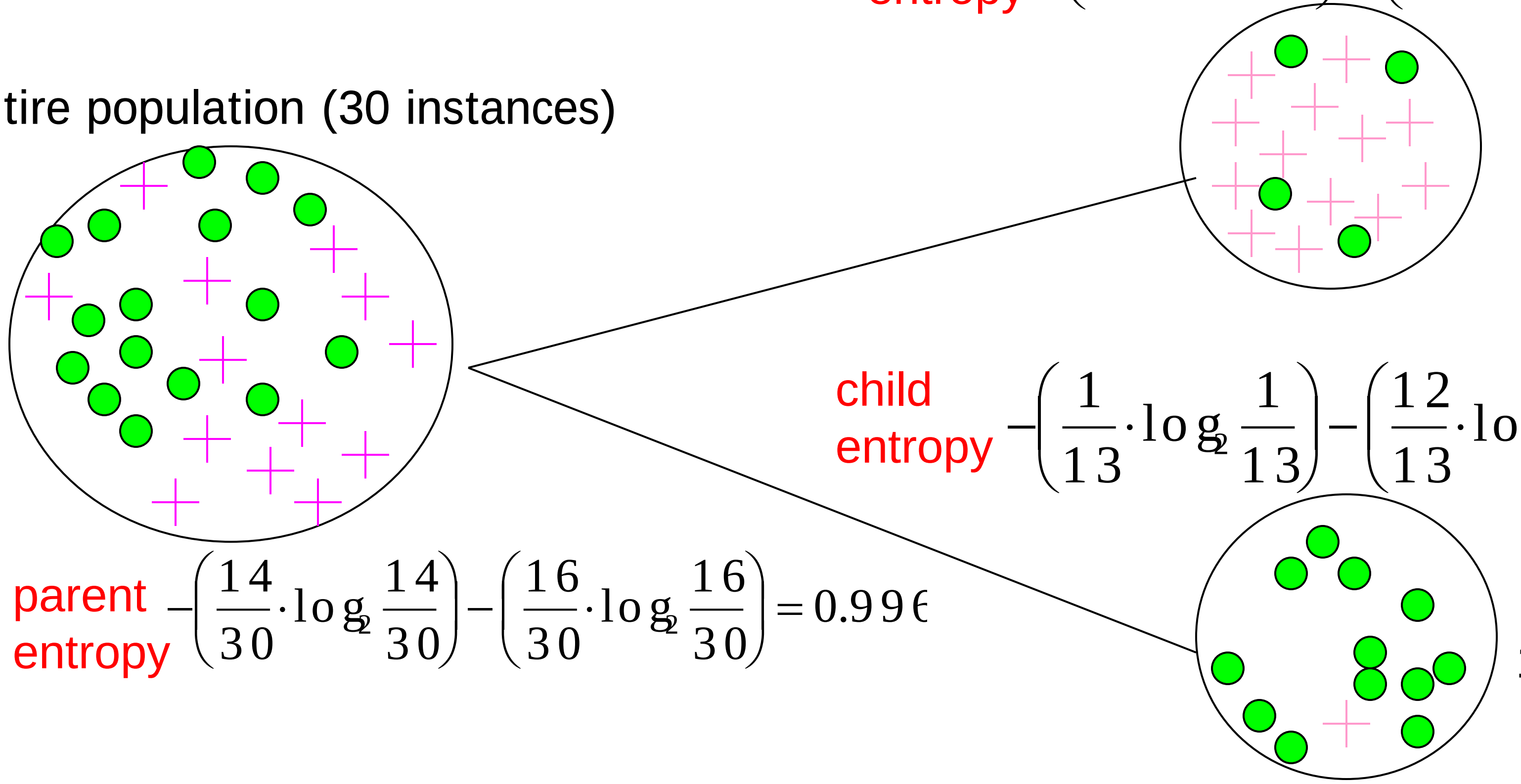


How much can we gain from splitting?

Information Gain = entropy(parent) – [average entropy(children)]

child entropy $-\left(\frac{13}{17}\cdot\log_2\frac{13}{17}\right)-\left(\frac{4}{17}\cdot\log_2\frac{4}{17}\right)=0.787$

Entire population (30 instances)



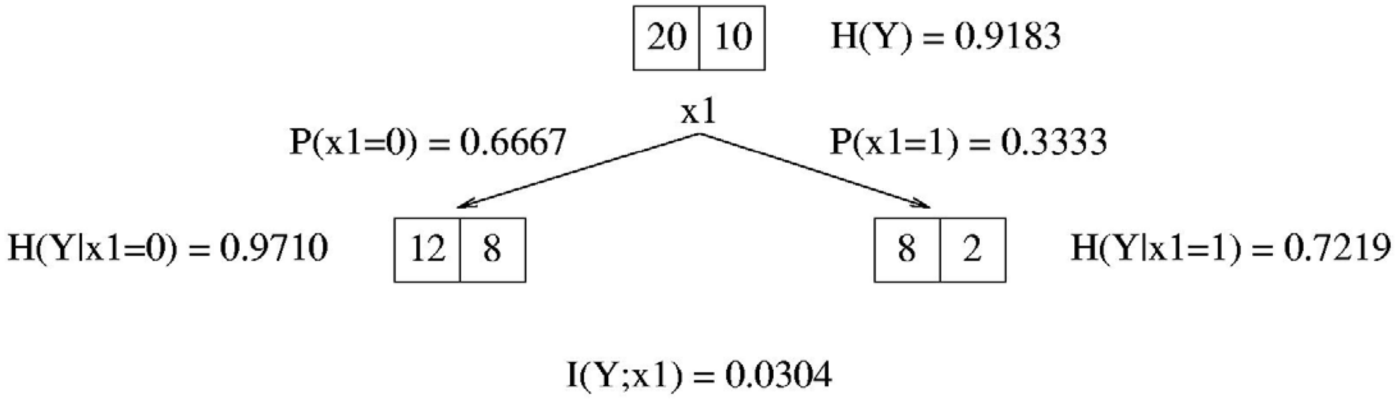
child entropy $-\left(\frac{1}{13}\cdot\log_2\frac{1}{13}\right)-\left(\frac{12}{13}\cdot\log_2\frac{12}{13}\right)=0.391$

parent entropy $-\left(\frac{14}{30}\cdot\log_2\frac{14}{30}\right)-\left(\frac{16}{30}\cdot\log_2\frac{16}{30}\right)=0.996$

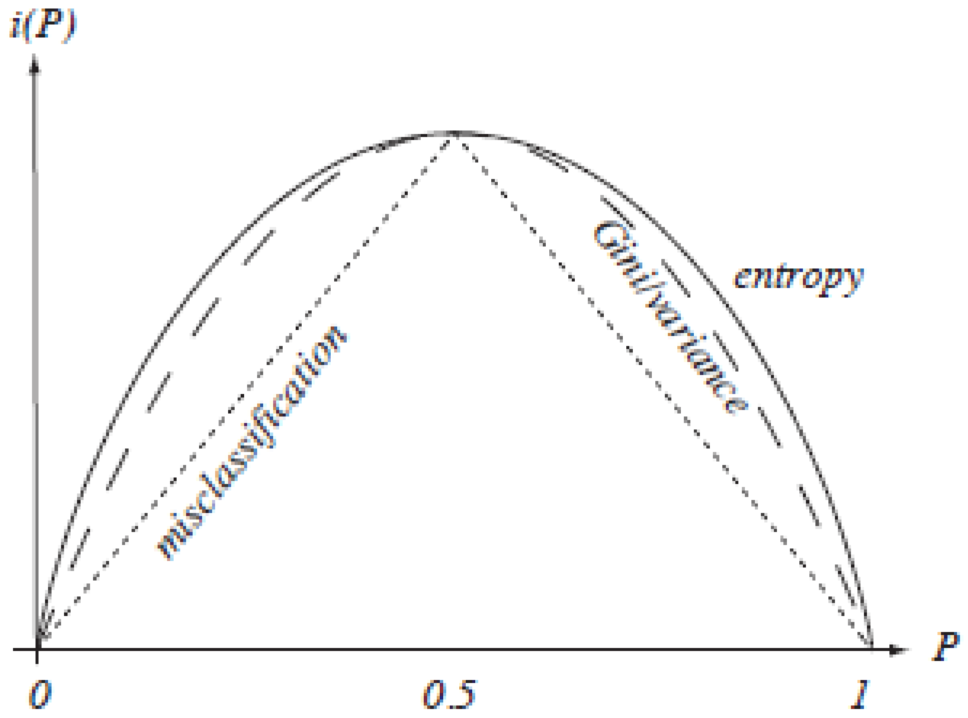
(Weighted) Average Entropy of Children = $\left(\frac{17}{30}\cdot 0.787\right)+\left(\frac{13}{30}\cdot 0.391\right)=0.615$

Information Gain = 0.996 - 0.615 = 0.38

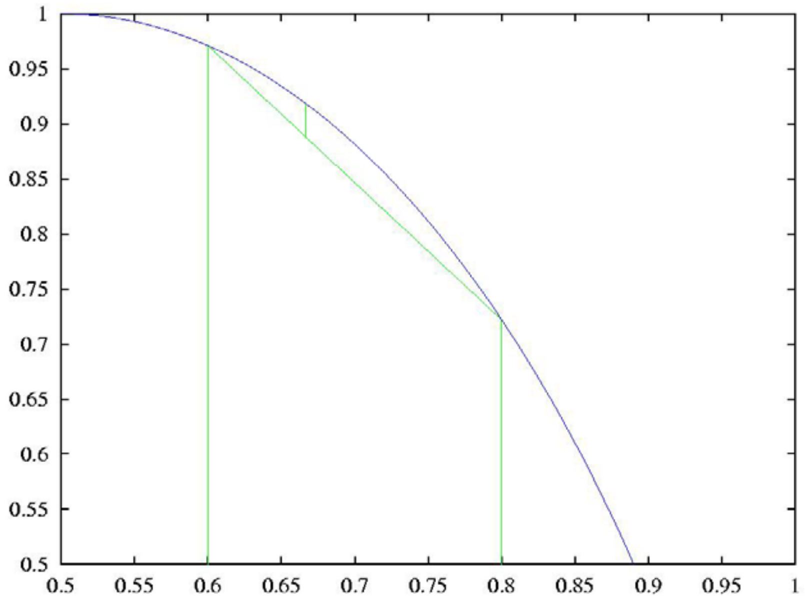
Information Gain can tell when we are making progress



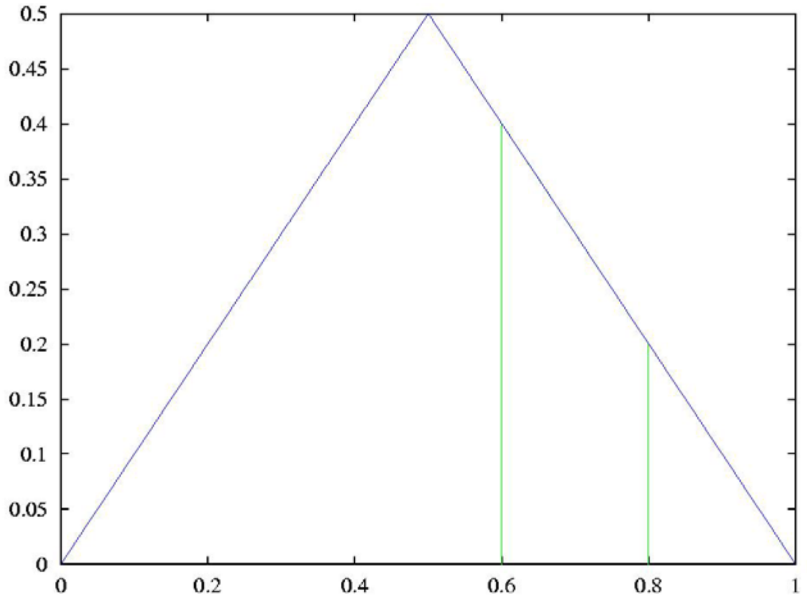
Misclassification Error vs. Entropy



Visualizing Heuristics



Entropy



Absolute Error

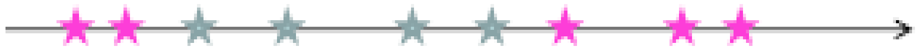
Mutual information works because it is a convex measure.

Non-binary Features

- Features with multiple discrete values
  - Multiway split
    - Need to normalize Information Gain, else it will always prefer multiway splits. See Information Gain Ratio
  - One-vs-all split
    - Makes a cascade of binary splits
  - Group values into two disjoint subsets
    - Loop over all possible pairs of subsets and pick the one with best Information Gain

Dealing with Continuous Features

- Test against a threshold
- How to compute the best threshold θ_j for X_j?
  - Sort the examples according to X_j.
  - Move the threshold θ from the smallest to the largest value
  - Select θ that gives the best information gain
  - Trick: only need to compute information gain when class label changes

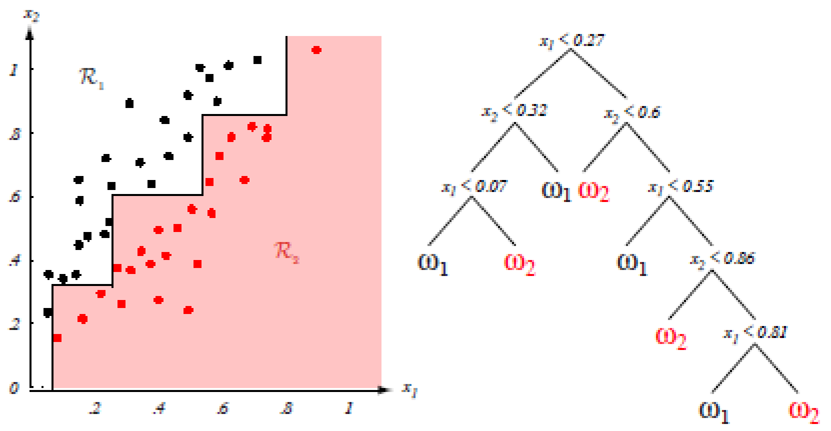


- Note that continuous features can be tested for multiple times in a DT

Considering both discrete and continuous features

- If a data set contains both types of features, do we need special handling?
- No, we simply consider all possibly splits in every step of the decision tree building process, and choose the one that gives the highest information gain
  - This include all possible (meaningful) thresholds

Multivariate Splits



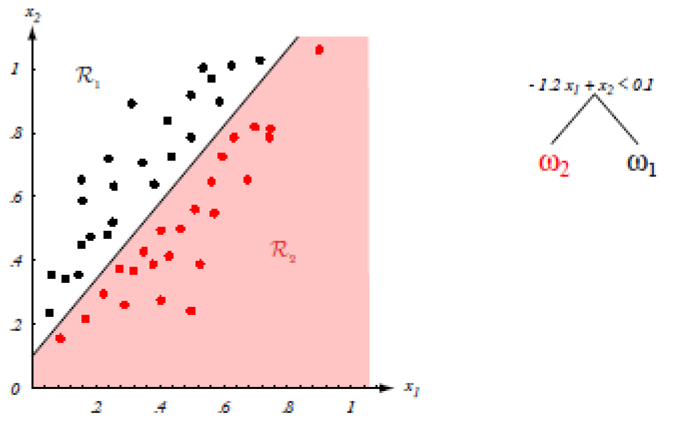


Figure 8.5: If the class of node decisions does not match the form of the training data, a very complicated decision tree will result, as shown at the top. Here decisions are parallel to the axes while in fact the data is better split by boundaries along another direction. If however "proper" decision forms are used (here, linear combinations of the features), the tree can be quite simple, as shown at the bottom.

Unknown Attribute Values

What if some examples are missing values of A?

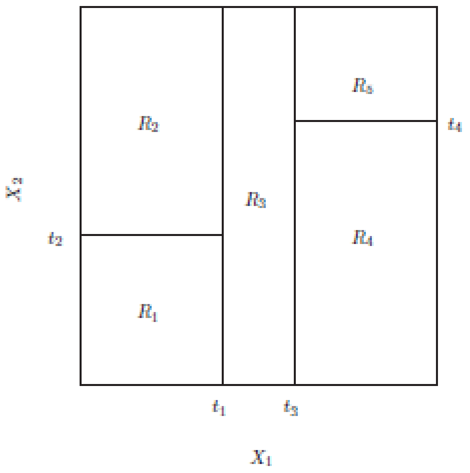
Use training example anyway, sort through tree

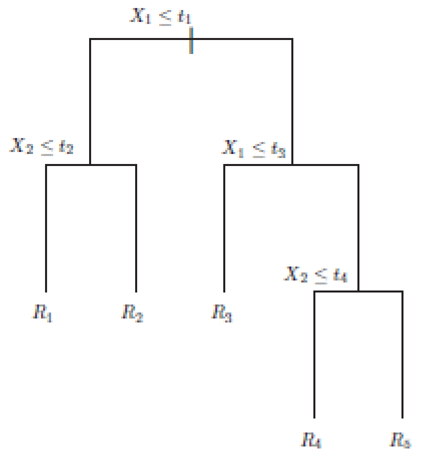
- If node n tests A, assign most common value of A among other examples sorted to node n
- Assign most common value of A among other examples with same target value
- Assign probability p_i to each possible value v_i of A
  Assign fraction p_i of example to each descendant in tree

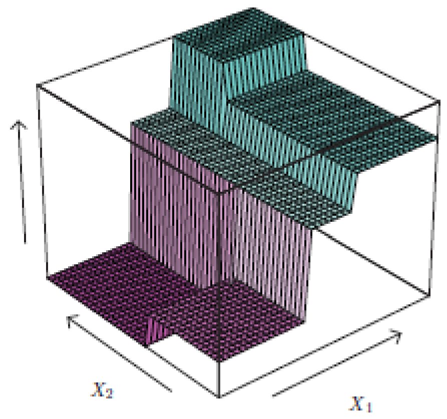
Classify new examples in same fashion

Classification vs. Regression Trees

- Classification tree: $x \rightarrow \{0,1\}$
- Regression tree: $x \rightarrow y \in R$







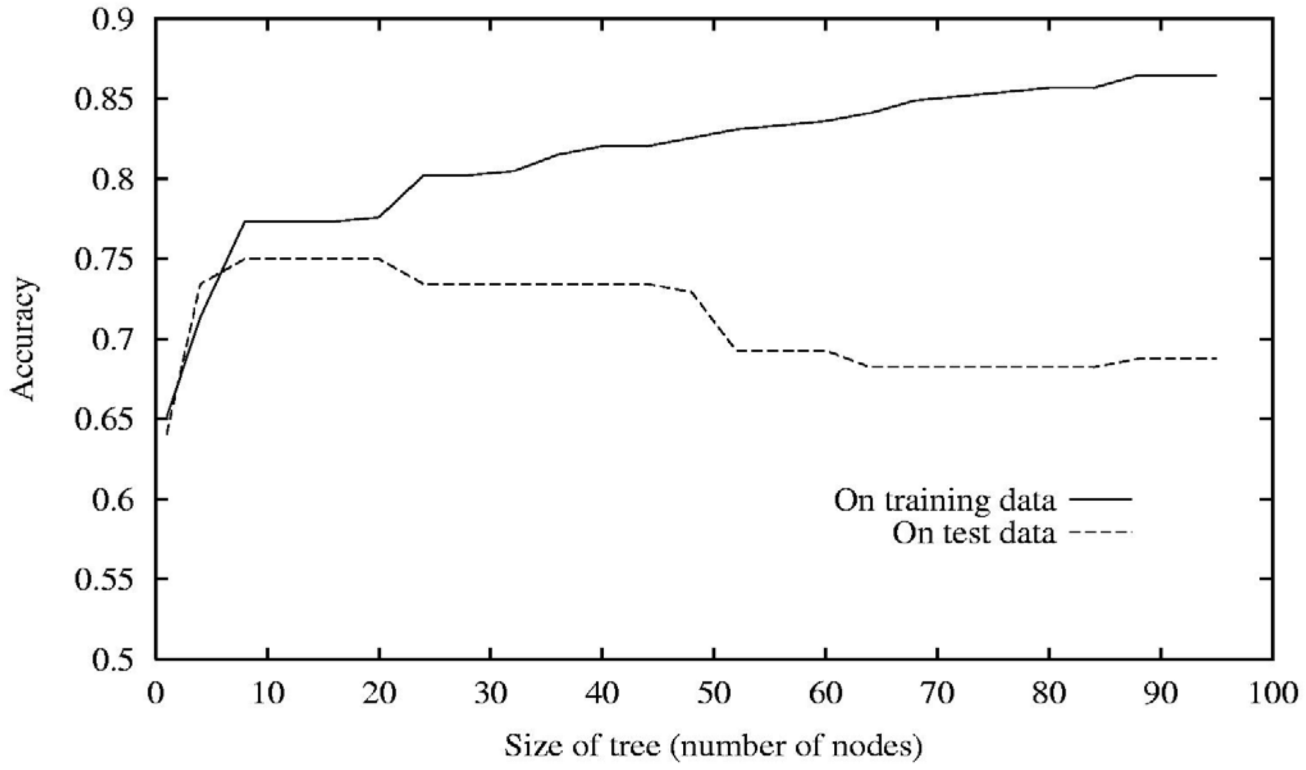
- *f(x)* is the average *y* of the training points at the leaf
- Instead of minimizing entropy, we minimize sum of variances after the split:

$$\sum_{i:\, x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:\, x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

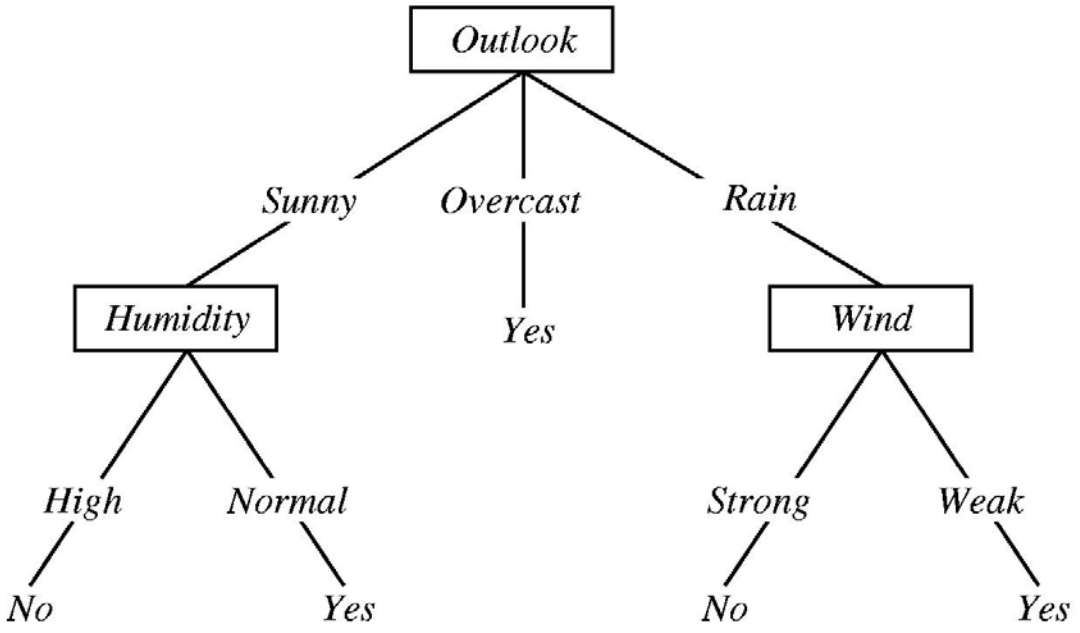
Limiting Tree Size

- Shouldn't wait until absolute purity:
  - It might never happen (label noise)
  - Data-starvation: as tree becomes deeper, each branch gets very few data points
  - Deep trees are slow and huge
- We can stop splitting earlier and make leaf node:
  - Average of *y*'s at the leaf (for regression trees)
  - Majority class or posterior distribution at the leaf (for classification trees)

Overfitting in Decision Tree Learning



Overfitting in Decision Trees



Consider adding a noisy training example:

Sunny, Hot, Normal, Strong, No!

What effect on tree?

How do we know when to stop growing?

- Stopping criteria:
  - Max tree depth
  - Min # of points at a node
  - Tree complexity penalty
  - Validation error monitoring

- Problem: “horizon effect”
  - Biases trees to be “early deciders”

Tree Pruning

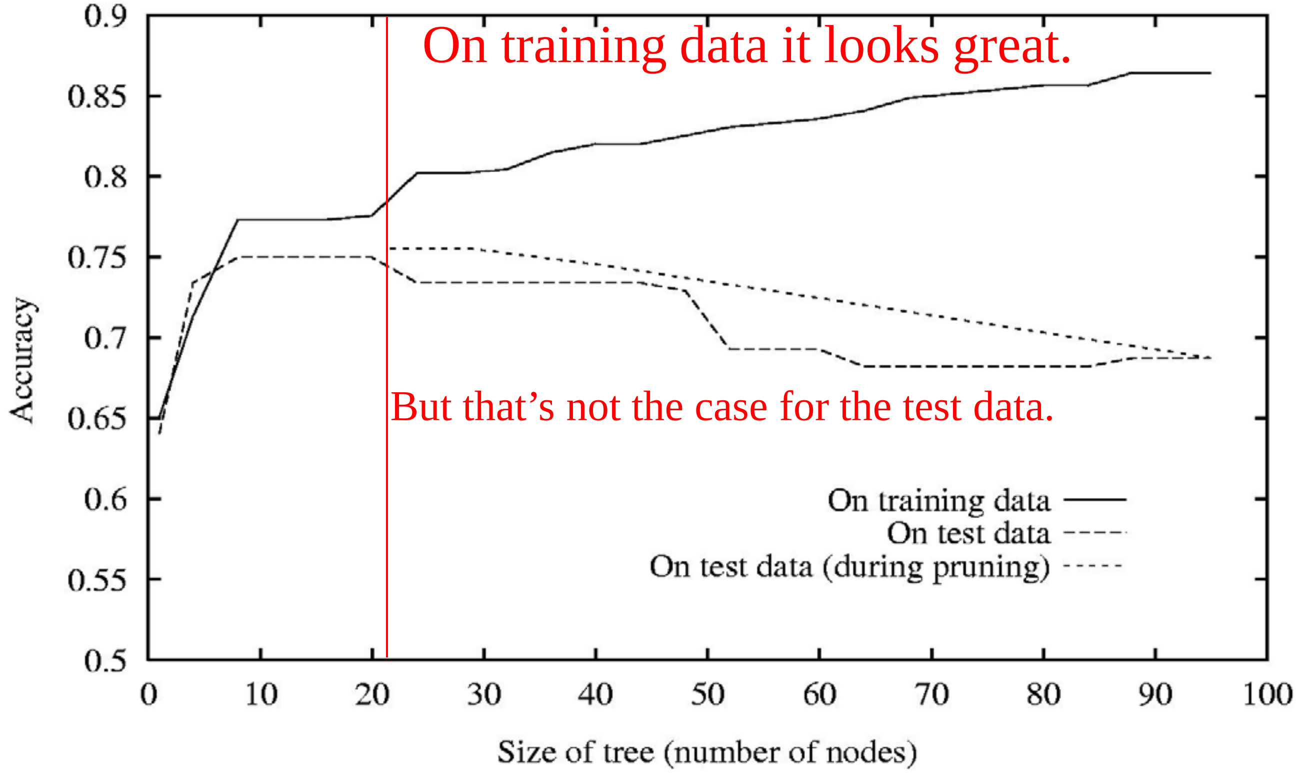
(post-pruning, reduced-error pruning)

Split data into *training* and *validation* set

Do until further pruning is harmful:

1. Evaluate impact on *validation* set of pruning each possible node (plus those below it)
2. Greedily remove the one that most improves *validation* set accuracy

Effect of Reduced-Error Pruning



The tree is pruned back to the red line where it gives more accurate results on the test data.