Decision Trees

(slides from McGill COMP-551 course)

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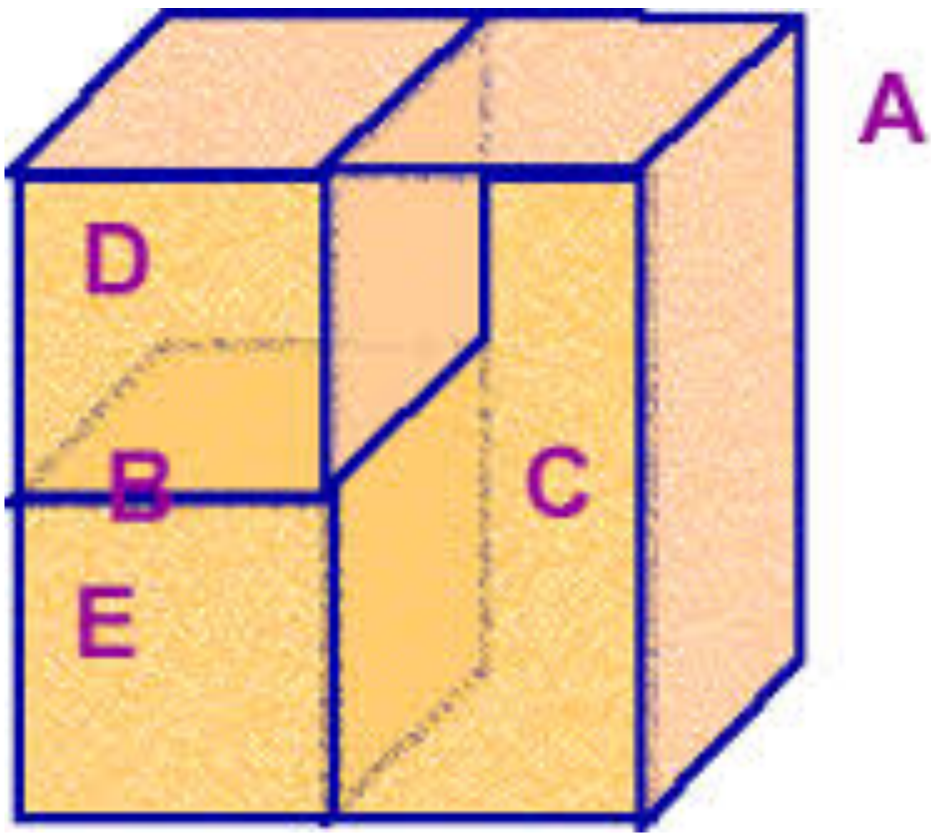
Back to machine learning: A quick recap

- Linear regression: Fit a linear function from input data to output.
- Linear classification: Find a **linear** hyper-plane separating classes.
- Many problems require more sophisticated models!

Richer partitioning of the input space



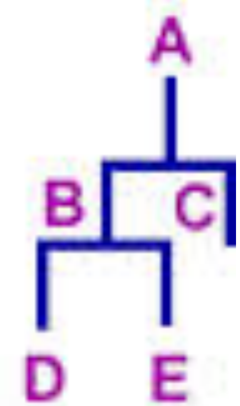


Image from *http://www.euclideanspace.com*

Example: Cancer Outcome Prediction

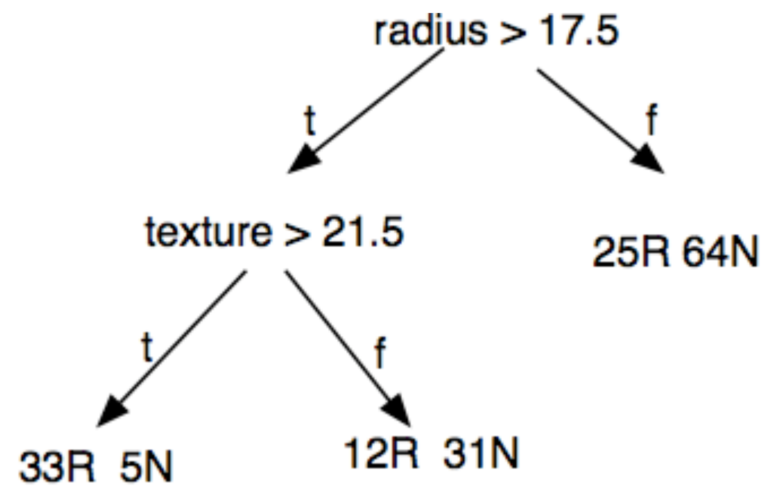
- Researchers computed 30 different features (or attributes) of the cancer cells' nuclei
  - Features relate to radius, texture, perimeter, smoothness, concavity, etc. of the nuclei
  - For each image, mean, standard error, and max of these properties across nuclei
- Vectors in the form ($(x_1, x_2, x_3, \ldots\ldots)$, y) = (**X** **,** y)
- Data set **D** in the form of a data table:

tumor size	texture	perimeter	...	outcome
18.02	27.6	117.5		N
17.99	10.38	122.8		N
20.29	14.34	135.1		R
...				

Decision tree example

- What does a node represent?
  - A partitioning of the input space.

- Internal nodes are tests on the values of different features.
  - Don't need to be binary test.



R = recurrence
N = no recurrence

Decision tree example

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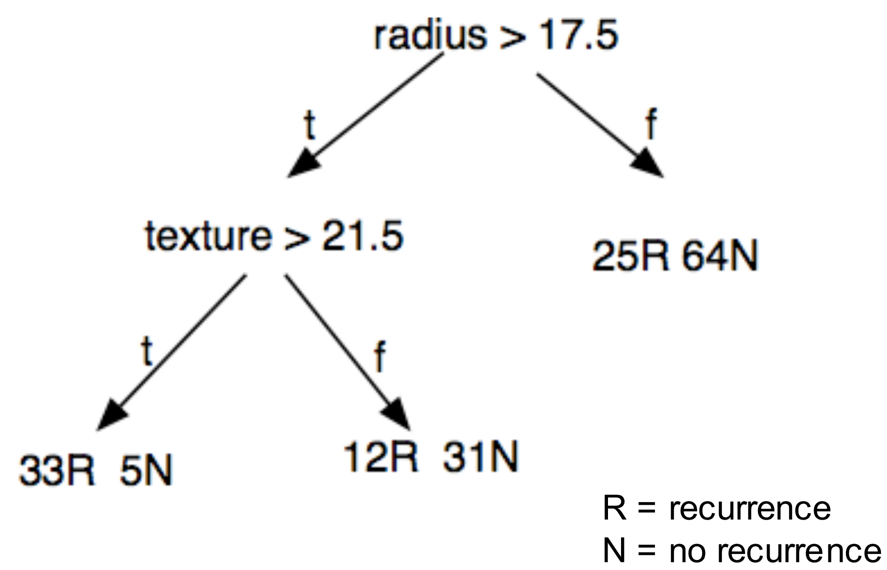


- Internal nodes are tests on the values of different features.
  - Don't need to be binary test.

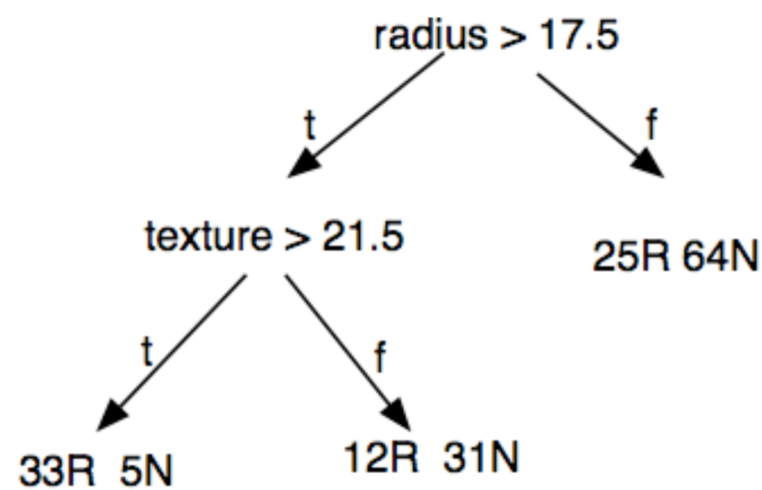
- Leaf nodes include the set of training examples that satisfy the tests along the branch.
  - Each training example falls in precisely one leaf.
  - Each leaf typical contains more than one example.

Using decision trees for classification

- Suppose we get a new instance:

  radius=18, texture=12, …

  How do we classify it?



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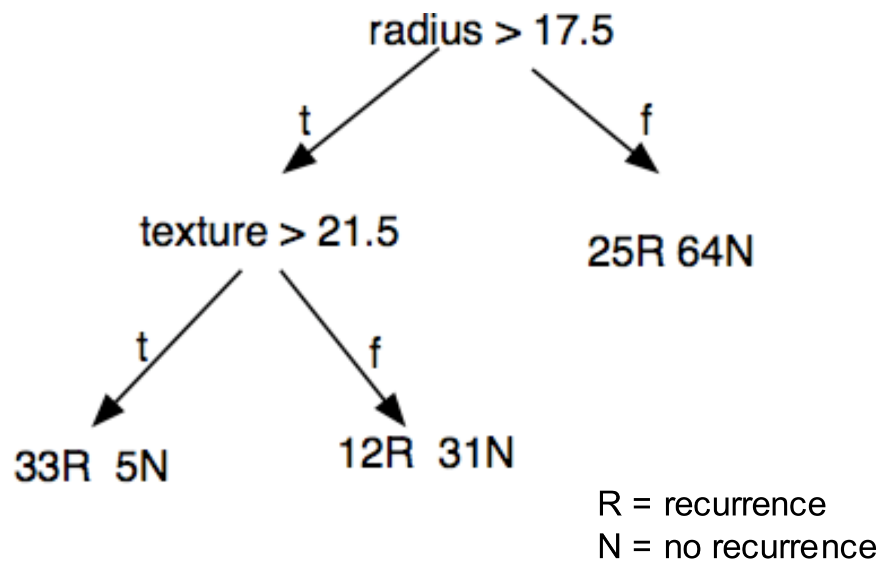
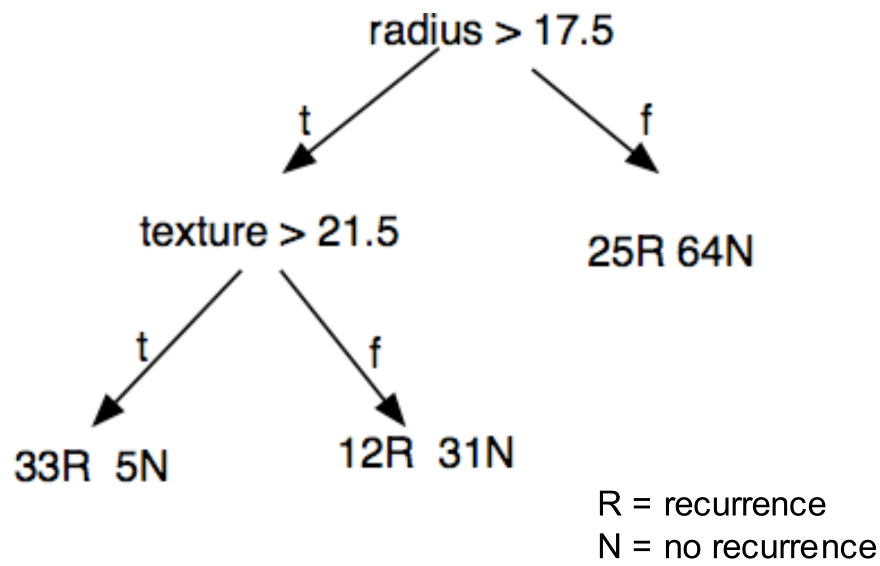


- Simple procedure:
  - At every node, test the corresponding attribute
  - Follow the appropriate branch of the tree
  - At a leaf, either predict the class of the majority of the examples for that leaf, or sample from the probabilities of the two classes.

Interpreting decision trees

Can always convert a decision tree into equivalent set of if-then rules.

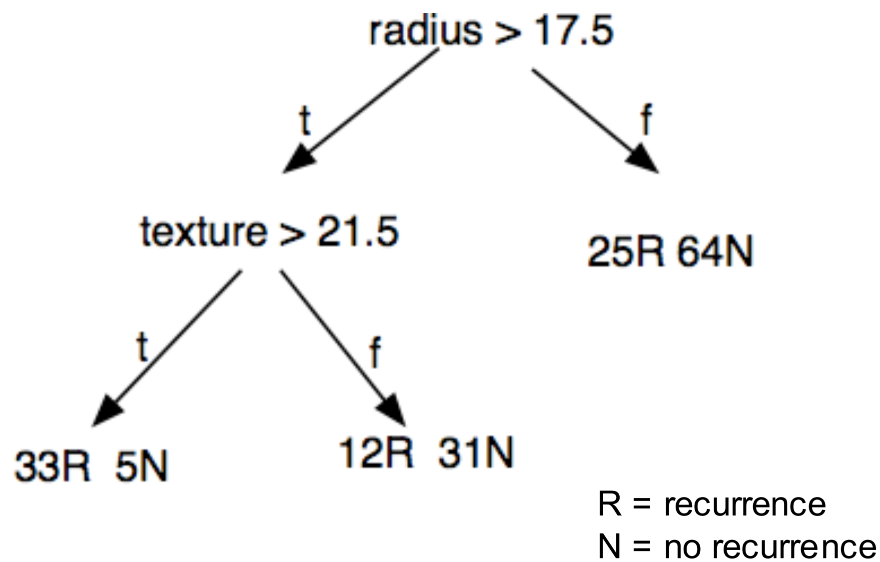


IF	THEN most likely class is
radius>17.5 AND texture>21.5	R
radius>17.5 AND texture≤21.5	N
radius≤17.5	N

Interpreting decision trees

Can always convert a decision tree into equivalent set of if-then rules.

Can also calculate an estimated probability of recurrence.



IF	THEN P(R) is
radius>17.5 AND texture>21.5	$\frac{33}{33+5}$
radius>17.5 AND texture≤21.5	$\frac{12}{12+31}$
radius≤17.5	$\frac{25}{25+64}$

More Formally : Tests

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  - For discrete features, we typically branch on all possibilities
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  - Test typically depends on only on feature.
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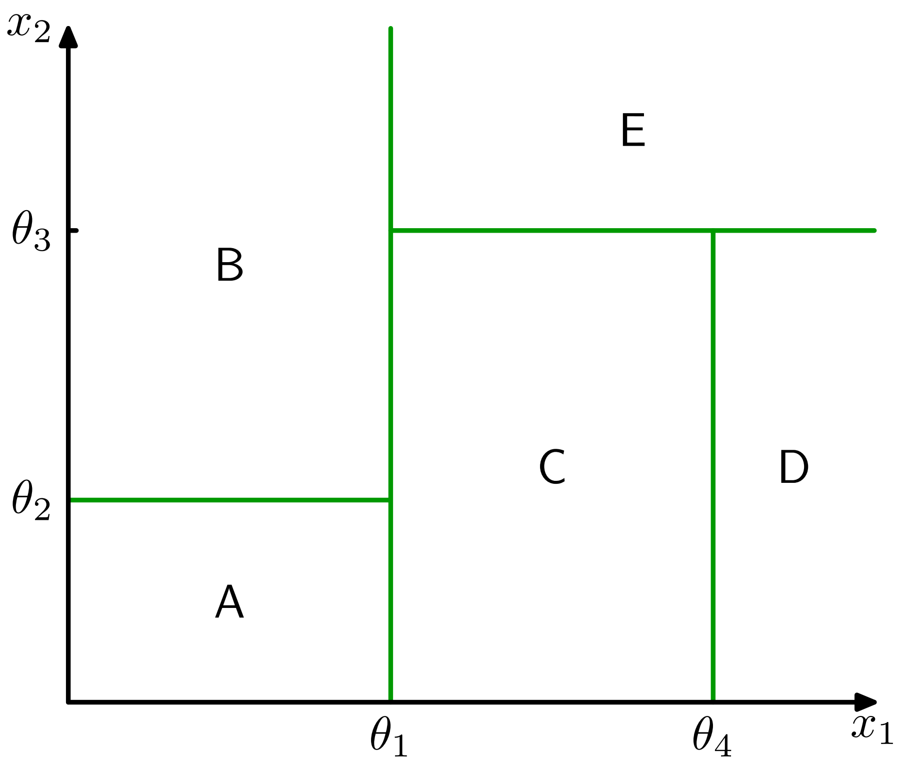
  - For real features, we typically branch on a threshold value
- Test returns a discrete outcome, e.g.
  - radius > 17.5
  - radius $\in [12, 18]$
  - grade is $\{A, B, C, D, F\}$
  - grade is $\geq B$
  - color is RED
  - 2$*$radius$-$3$*$texture > 16
- Learning = choosing tests at every node and shape of the tree.
  - A finite set of candidate tests is chosen before learning the tree.

Example



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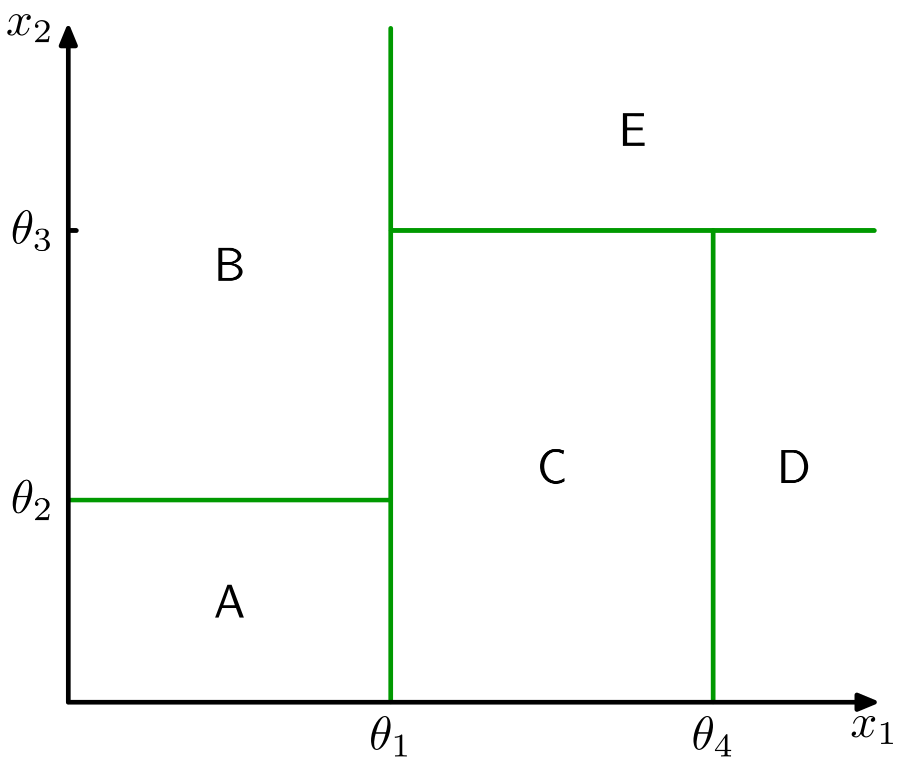
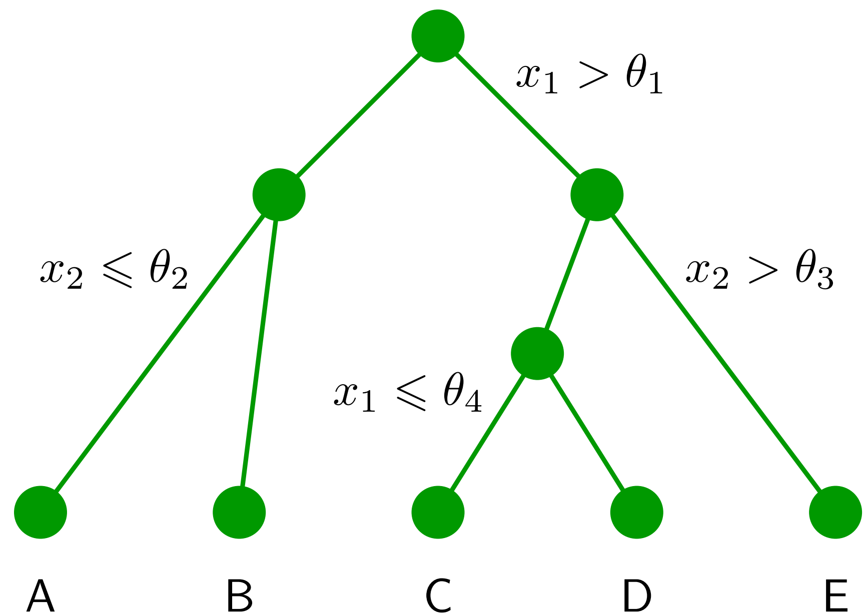


x_2
θ_3
θ_2
θ_1
θ_4
x_1
E
B
C
D
A



$x_1 > \theta_1$
$x_2 \leqslant \theta_2$
$x_2 > \theta_3$
$x_1 \leqslant \theta_4$
A
B
C
D
E

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  - Each entry in truth table could be one path (very inefficient!)
  - Most boolean functions can be encoded more compactly.
- Some functions are harder to encode
  - Parity Function = Returns 1 iff an even number of inputs are 1
    - An exponentially big decision tree $O(2^M)$ would be needed
  - Majority Function = Returns 1 if more than half the inputs are 1

Expressivity of decision trees

What kind of function can be encoded via a decision tree?

- Every Boolean Function can be **fully** expressed
- Many other functions can be approximated by a Boolean function.
- With real-valued features, decision trees are good at problems in which the class label is constant in large connected axis-orthogonal regions of the input space.

Learning Decision trees

- We could enumerate all possible trees (assuming the number of possible tests is finite)
  - Each tree could be evaluated using the training set or, better yet, a test set
  - There are many possible trees!   We'd probably overfit the data.

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- Usually, decision trees are constructed in two phases:
  1. A recursive, top-down procedure "grows" a tree (possibly until the training data is completely fit)
  2. The tree is "pruned" back to avoid overfitting

Top-down (recursive) induction of decision trees

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3. Split the training set according to the value of the outcome of the test.
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How do we pick the **best test**?

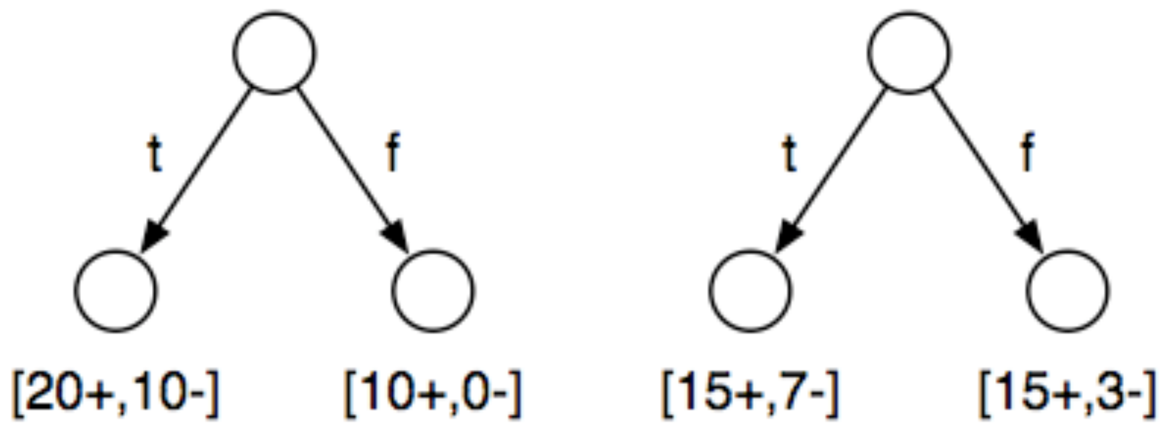
What is a good Test?

- The test should provide **information** about the class label.

  E.g. You are given 40 examples: 30 positive, 10 negative

  Consider two tests that would split the examples as follows:

  Which is best?



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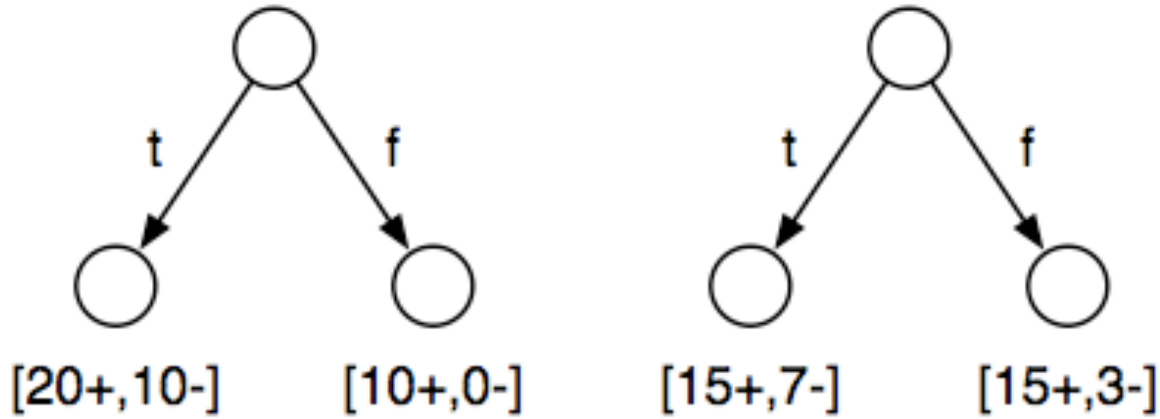

- Intuitively, we prefer an attribute that separates the training instances as well as possible. How do we quantify this (mathematically)?

What is information?

- Consider three cases:
  - You are about to observe the outcome of a dice roll
  - You are about to observe the outcome of a coin flip
  - You are about to observe the outcome of a biased coin flip

- Intuitively, in each situation, you have a different amount of uncertainty as to what outcome / message you will observe.

Information content

- Let E be an event that occurs with probability $P(E)$. If we are told that E has occurred with certainty, then we received $I(E)$ **bits of information**.

$$I(E) = \log_2 \frac{1}{P(E)}$$

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- You can also think of information as the amount of "surprise" in the outcome (e.g., consider $P(E) = 1$, then $I(E) \approx 0$)

  E.g.

  - fair coin flip provides $\log_2 2 = 1$ bit of information
  - fair dice roll provides $\log_2 6 \approx 2.58$ bits of information

Entropy

- Given an information source *S* which emits symbols from an alphabet $\{s_1, \ldots s_k\}$ with probabilities $\{p_1, \ldots p_k\}$.
- Each emission is independent of the others. What is the **average amount of information** we expect from the output of *S*?

$$H(S) = \sum_i p_i I(s_i) = \sum_i p_i \log \frac{1}{p_i} = -\sum_i p_i \log p_i$$

H(S) is the **entropy** of *S.*

- Note that this depends only on the probability distribution, and not on the actual alphabet. So we can write *H(P).*

Entropy

$$H(P) = \sum_i p_i \log \frac{1}{p_i}$$

- Several ways to think about entropy:
  - Average amount of information per symbol.
  - Average amount of surprise when observing the symbol.
  - Uncertainty the observer has before seeing the symbol.
  - Average number of bits needed to communicate the symbol.

Binary Classification

- We try to classify sample data using a decision tree.
- Suppose we have *p* positive samples and *n* negative samples.
- What is the entropy of this data set?

$$H(D) = -\frac{p}{p+n} log_2 \frac{p}{p+n} - \frac{n}{p+n} log_2 \frac{n}{p+n}$$

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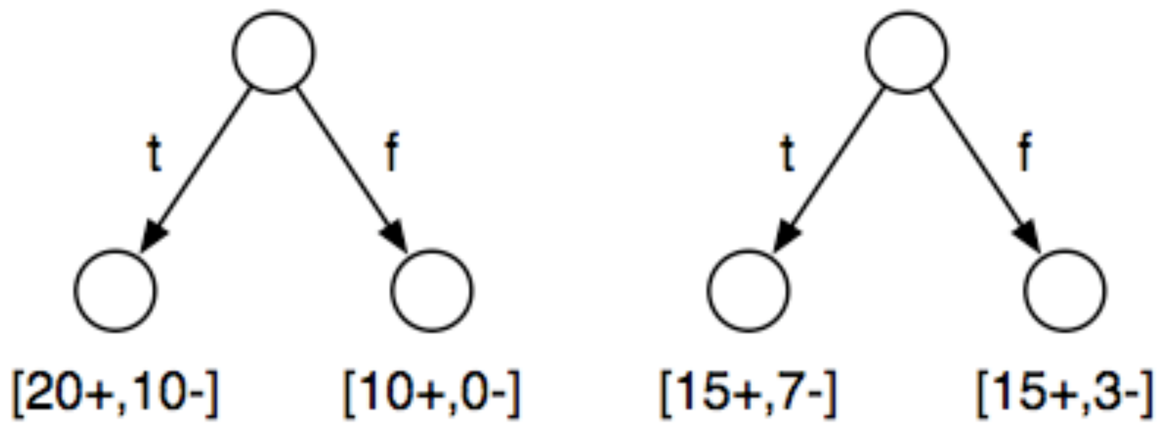

$H(D) = -(3/4)\log_2(3/4)-(1/4)\log_2(1/4) = 0.811$

Conditional entropy

- The conditional entropy, *H(y|x)*, is the average specific conditional entropy of y given the values of *x*:

$$H(y|x) = \sum_v P(x=v) H(y|x=v)$$

- **Interpretation**: the expected number of bits needed to transmit y if both the emitter and receiver know the possible values of *x* (but before they are told *x*'s specific value.)

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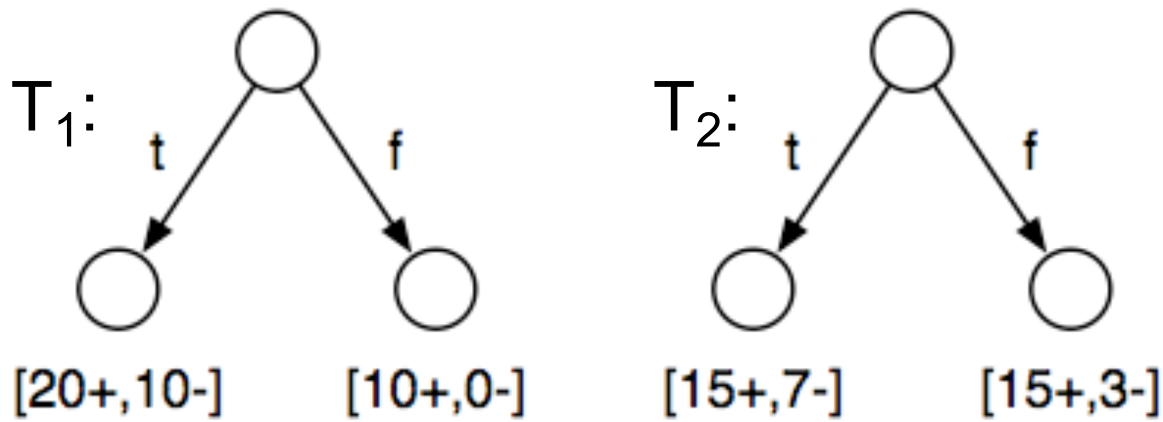

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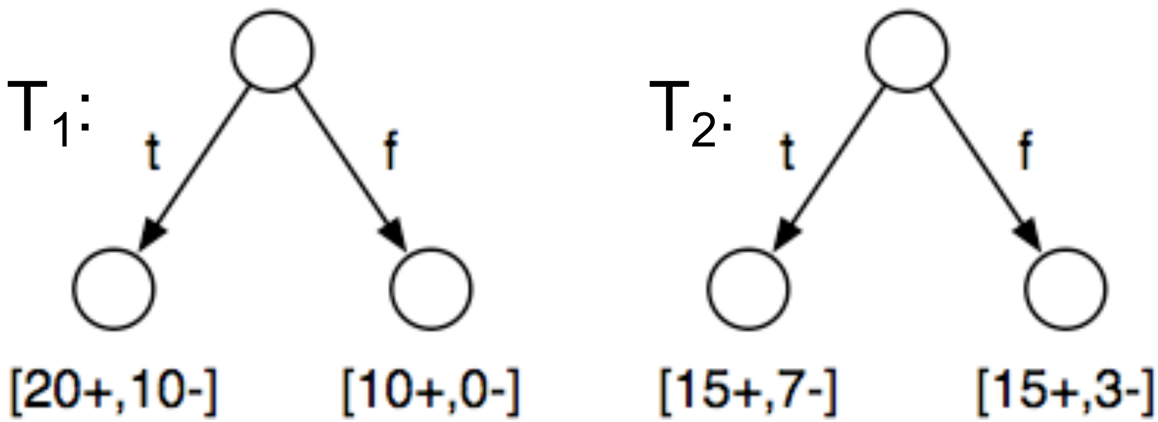

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$H(D|T_1) = (30/40)[-(20/30)\log_2(20/30)-(10/30)\log_2(10/30)]+(10/40)[0] = 0.688$

$H(D|T_2) = (22/40)[-(15/22)\log_2(15/22)-(7/22)\log_2(7/22)]$

$\quad + (18/40)[-(15/18)\log_2(15/18)-(3/18)\log_2(3/18)] = 0.788$

Information gain

- The reduction in entropy that would be obtained by knowing *x* :

$$IG(x) = H(D) - H(D|x)$$

- Equivalently, suppose one has to transmit y. How many bits (on average) would it save if both the transmitter and emitter knew *x*?

Recursive learning of decision trees

Given a set of labeled training instances:

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How do we pick the **best test**?

For **classification**: choose the test with highest information gain.

For **regression**: choose the test with lowest mean-squared error.

Caveats on tests with multiple values

- If the outcome of a test is not binary, the number of possible values influences the information gain.
  - The more possible values, the higher the gain!
  - Nonetheless, the attribute could be irrelevant
- Could transform attribute in one (or many) binary attributes.

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- C4.5 (the most popular decision tree construction algorithm in ML community) uses only binary tests:
  - Attribute =Value (discrete) or Attribute<Value (continuous)
- Other approaches consider smarter metrics which account for the number of possible outcomes.

Tests for real-valued features

- Suppose feature j is real-valued
- How do we choose a finite set of possible thresholds, for tests of the form $x_j > \tau$?

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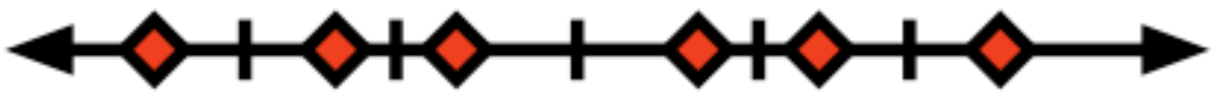
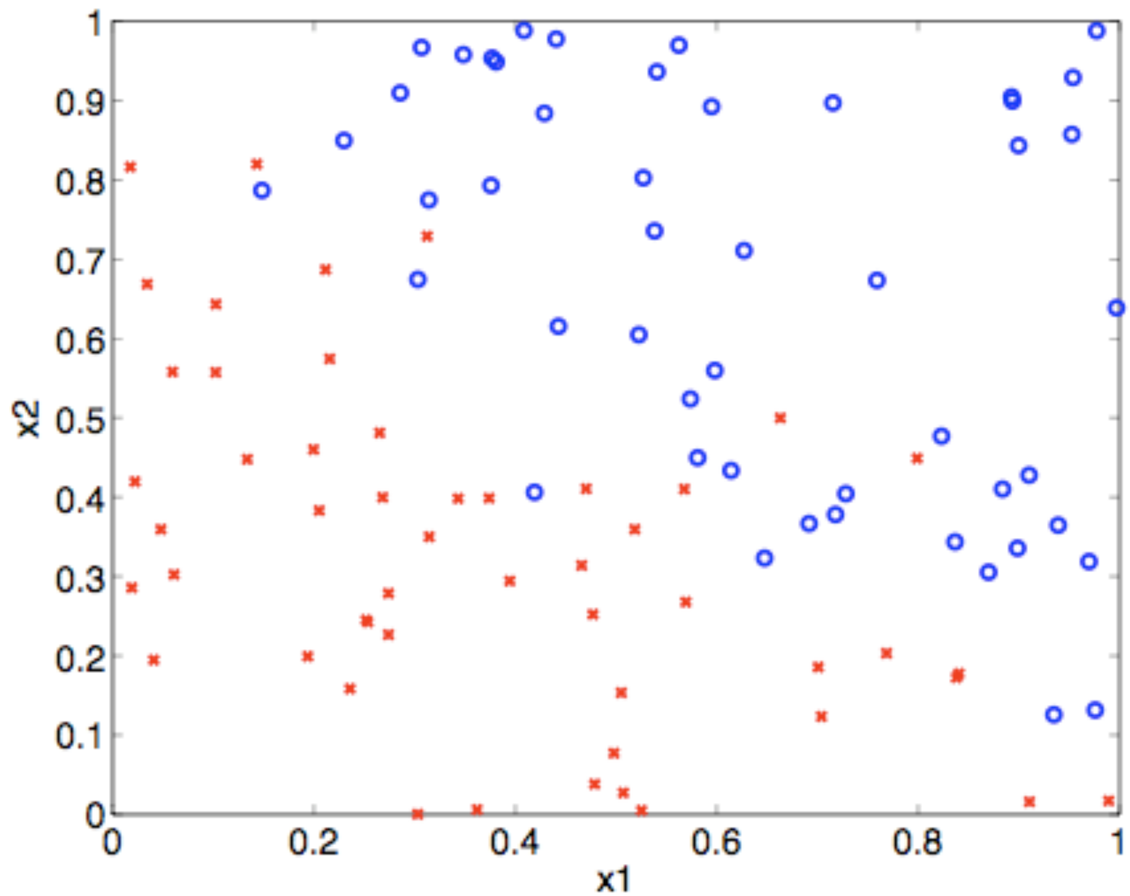
- Suppose feature j is real-valued
- How do we choose a finite set of possible thresholds, for tests of the form $x_j > \tau$?
- Choose midpoints of the observed data values, $x_{1,j}, \ldots, x_{m,j}$



- Choose midpoints of data values with different y values

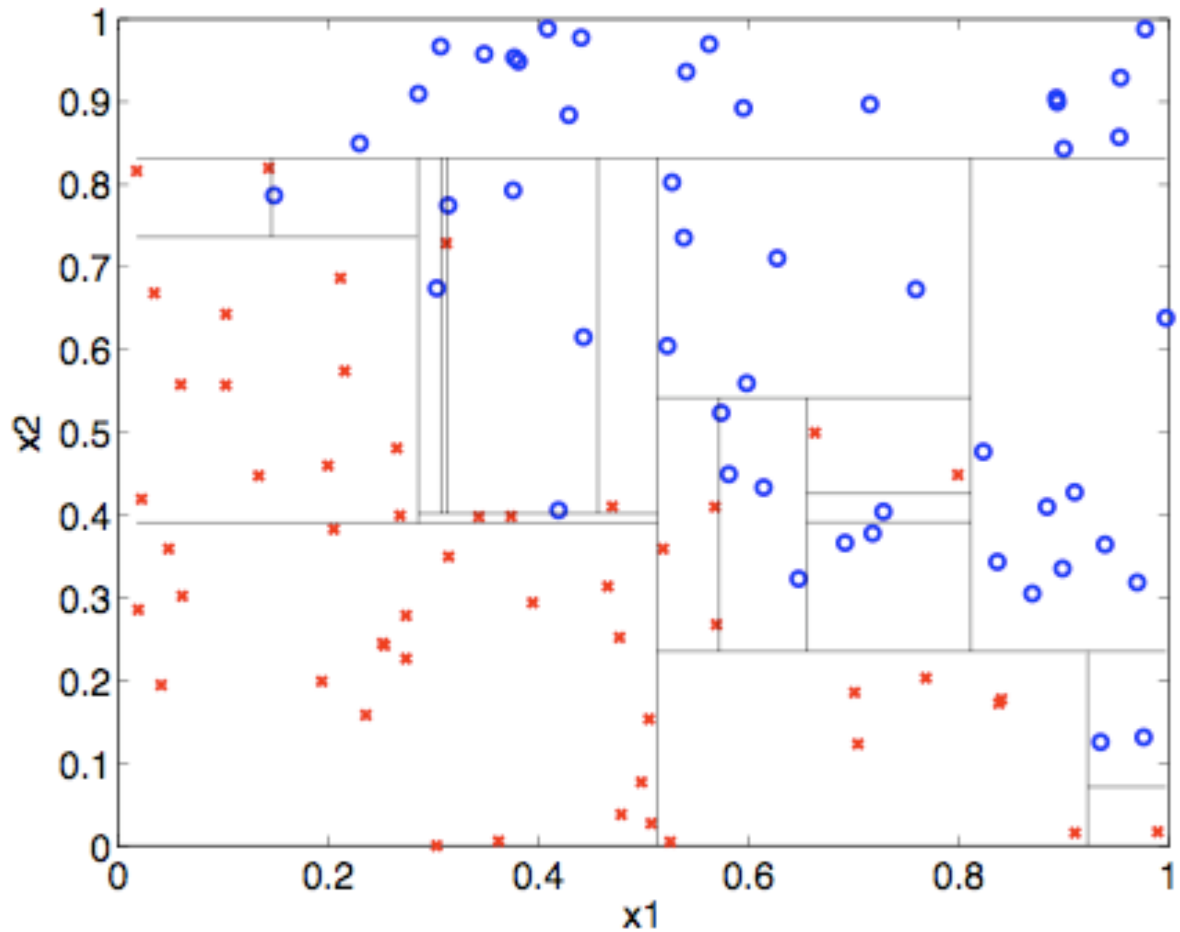
A complete (artificial) example

- An artificial binary classification problem with two real-valued input features:



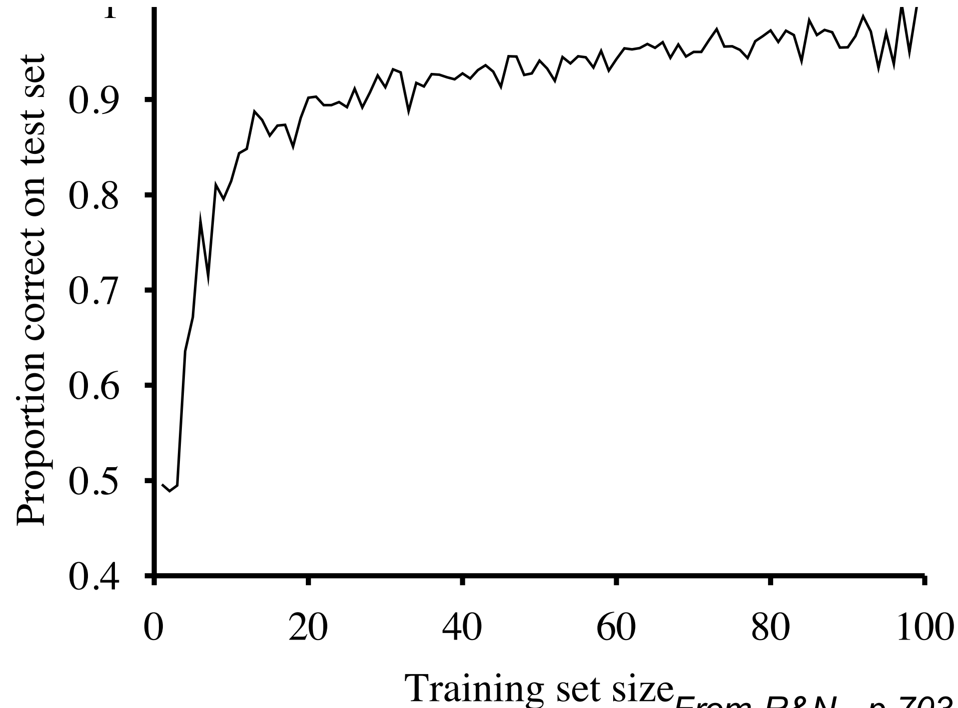
A complete (artificial) example

- The decision tree, graphically:



Assessing Performance

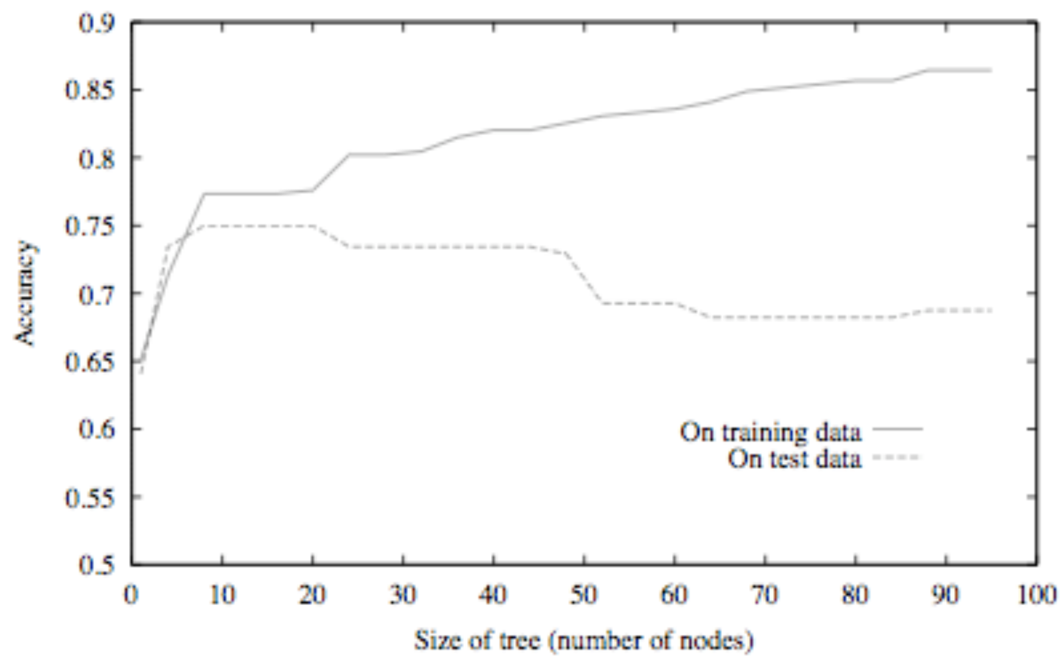
- Split data into a **training set** and a **validation set**
- Apply learning algorithm to training set.
- Measure error with the validation set.



From R&N , p.703

Overfitting in decision trees

- Decision tree construction proceeds until all leaves are "pure" , i.e. all examples are from the same class.
- As the tree grows, the generalization performance can start to degrade, because the algorithm is including irrelevant attributes/tests/outliers.
- How can we avoid this?



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- Post pruning: Grow a full tree, then prune the tree by eliminating lower nodes that have low information gain on the validation set.

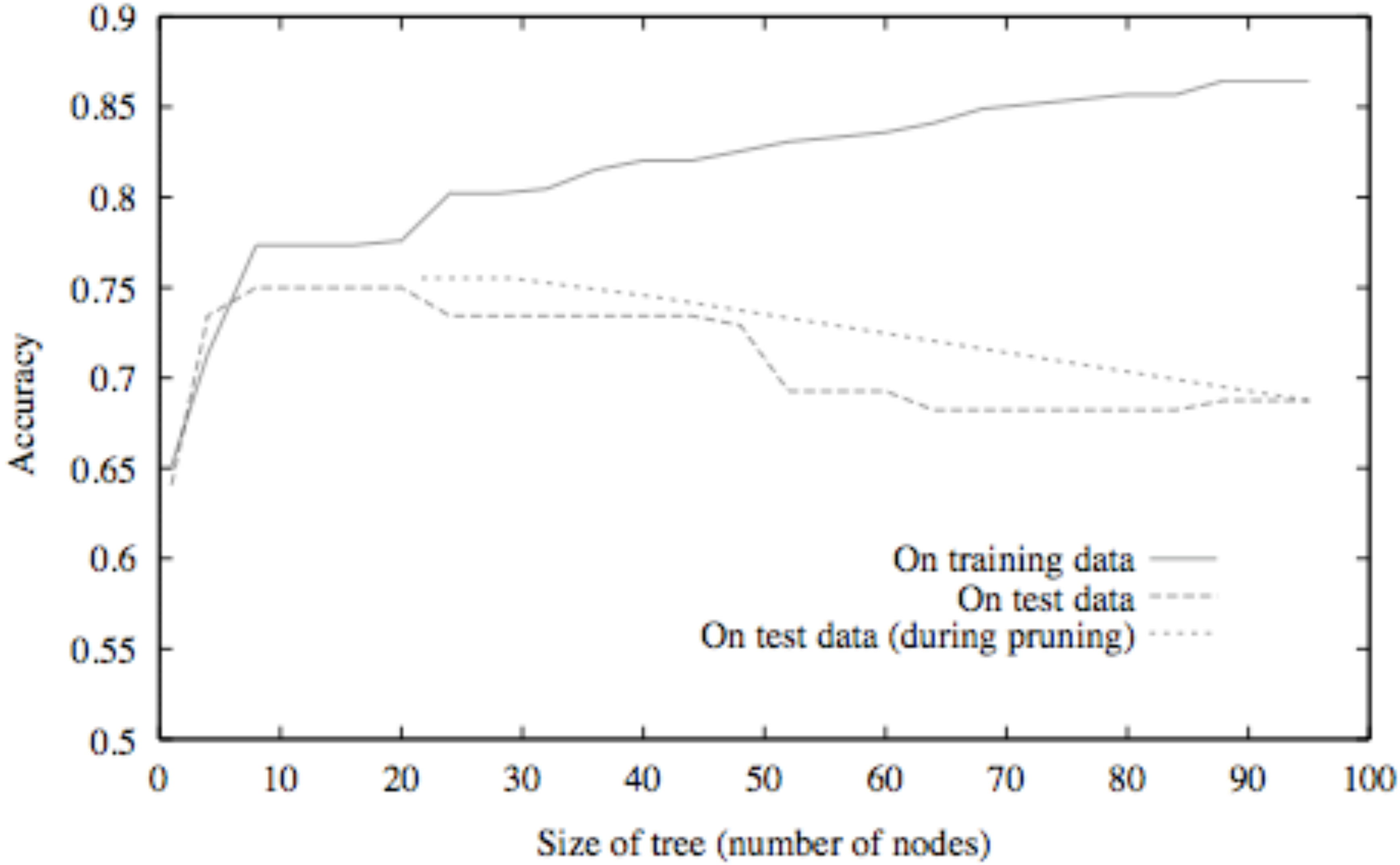
Avoiding Overfitting

- Objective: Remove some nodes to get better generalization.
- Early stopping: Stop growing the tree when further splitting the data does not improve information gain of the validation set.
- Post pruning: Grow a full tree, then prune the tree by eliminating lower nodes that have low information gain on the validation set.
- In general, post pruning is better. It allows you to deal with cases where a single attribute is not informative, but a combination of attributes is informative.

Reduced-error pruning (aka post pruning)

- Split the data set into a training set and a validation set
- Grow a large tree (e.g. until each leaf is pure)
- For each node:
  - Evaluate the validation set accuracy of pruning the subtree rooted at the node
  - Greedily remove the node that most improves validation set accuracy, with its corresponding subtree
  - Replace the removed node by a leaf with the majority class of the corresponding examples
- Stop when pruning starts hurting the accuracy on validation set.

Example: Effect of reduced-error pruning



Advantages of decision trees

- Provide a general representation of classification rules
  - Scaling / normalization not needed, as we use no notion of "distance" between examples.
- The learned function, $y = h(x)$, is easy to interpret.
- Fast learning algorithms (e.g. C4.5, CART).
- Good accuracy in practice – many applications in industry!

Limitations

- Sensitivity:
  - Exact tree output may be sensitive to small changes in data
  - With many features, tests may not be meaningful
- Good for learning (nonlinear) piecewise axis-orthogonal decision boundaries, but not for learning functions with smooth, curvilinear boundaries.
  - Some extensions use non-linear tests in internal nodes.

What you should know

- How to use a decision tree to classify a new example.
- How to build a decision tree using an information-theoretic approach.
- How to detect (and fix) overfitting in decision trees.
- How to handle both discrete and continuous attributes and outputs.