Machine Learning

10-701/15-781, Spring 2008

Decision Trees

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Lecture 6, February 4, 2008

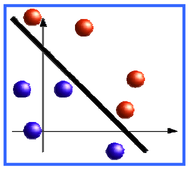
Reading: Chap. 1.6, CB & Chap 3, TM

Learning non-linear functions

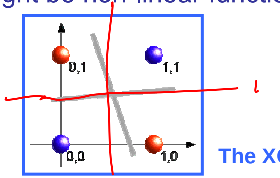
f: X → Y

- X (vector of) continuous and/or discrete vars
- Y discrete vars

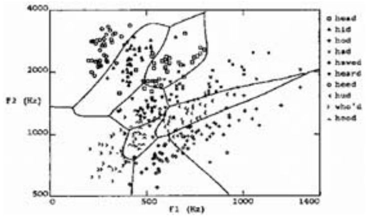
- Linear separator



- f might be non-linear function



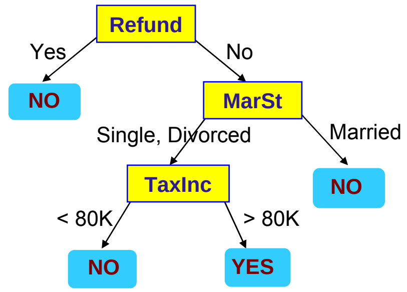
The XOR gate



Speech recognition

A hypothesis for *TaxFraud*

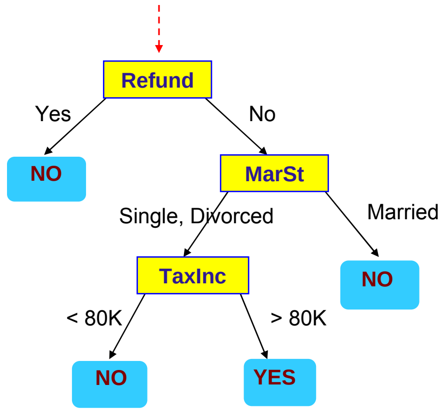
- Input: a vector of attributes
  - X=[Refund,MarSt,TaxInc]
- Output:
  - Y= Cheating or Not
- *H* as a procedure:



- Each internal node: test one attribute X_i
- Each branch from a node: selects one value for X_i
- Each leaf node: predict Y

Apply Model to Query Data

Start from the root of tree.



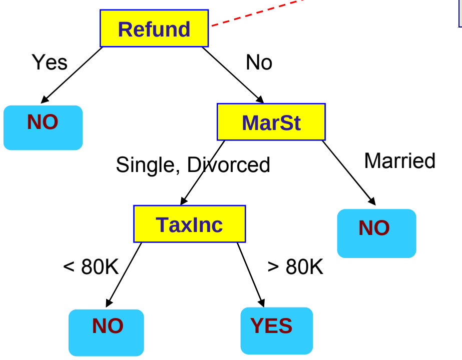
Query Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Query Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Apply Model to Test Data

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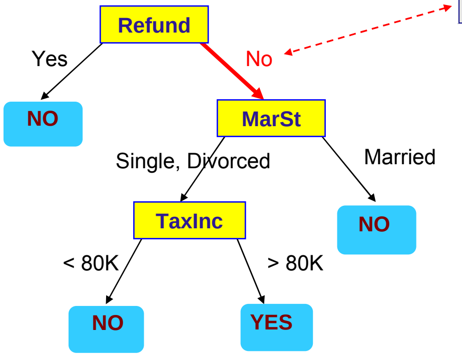

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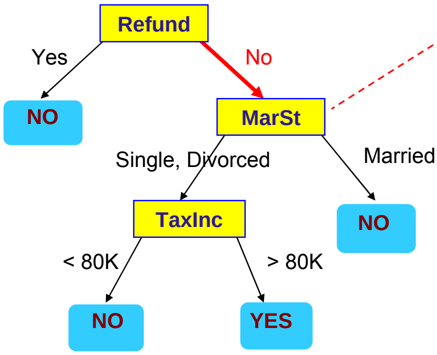

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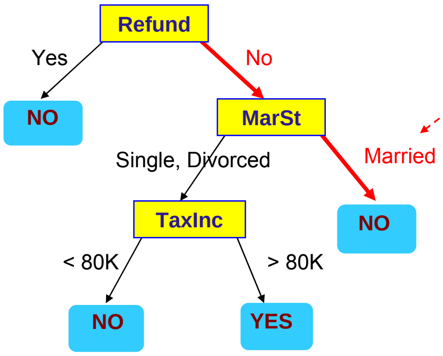

Apply Model to Test Data

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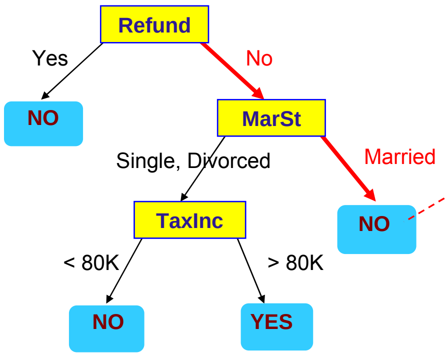


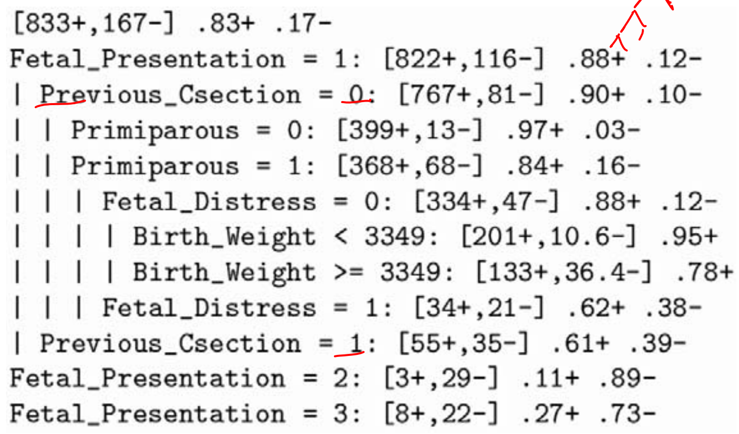
Assign Cheat to “No”

A Tree to Predict C-Section Risk

- Learned from medical records of 1000 wonman

  Negative examples are C-sections

Fe

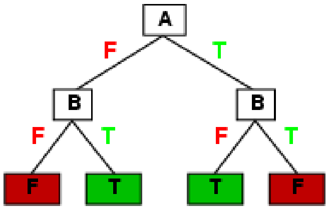


```
[833+,167-] .83+ .17-
Fetal_Presentation = 1: [822+,116-] .88+ .12-
| Previous_Csection = 0: [767+,81-] .90+ .10-
| | Primiparous = 0: [399+,13-] .97+ .03-
| | Primiparous = 1: [368+,68-] .84+ .16-
| | | Fetal_Distress = 0: [334+,47-] .88+ .12-
| | | | Birth_Weight < 3349: [201+,10.6-] .95+
| | | | Birth_Weight >= 3349: [133+,36.4-] .78+
| | | Fetal_Distress = 1: [34+,21-] .62+ .38-
| Previous_Csection = 1: [55+,35-] .61+ .39-
Fetal_Presentation = 2: [3+,29-] .11+ .89-
Fetal_Presentation = 3: [8+,22-] .27+ .73-
```

Expressiveness

- Decision trees can express any function of the input attributes.
- E.g., for Boolean functions, truth table row → path to leaf:

A	B	C	A xor B
F	F	T	F
F	T	T	T
T	F	T	T
T	T	T	F
?	?	F	?



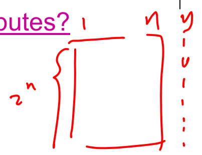
- Trivially, there is a consistent decision tree for any training set with one path to leaf for each example (unless *f* nondeterministic in *x*) but it probably won't generalize to new examples
- Prefer to find more compact decision trees

Hypothesis spaces

How many distinct decision trees with *n* Boolean attributes?

= number of Boolean functions

= number of distinct truth tables with 2^n rows = 2^{2^n}



- E.g., with 6 Boolean attributes, there are 18,446,744,073,709,551,616 trees

Hypothesis spaces

How many distinct decision trees with *n* Boolean attributes?

= number of Boolean functions

= number of distinct truth tables with 2^n rows = 2^{2^n}

- E.g., with 6 Boolean attributes, there are 18,446,744,073,709,551,616 trees

How many purely conjunctive hypotheses (e.g., *Hungry* $\wedge$ $\neg$*Rain*)?

- Each attribute can be in (positive), in (negative), or out

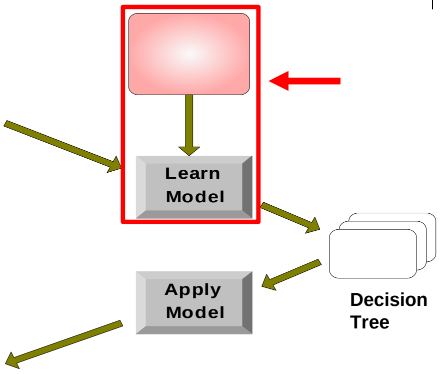
  $\Rightarrow$ 3^n distinct conjunctive hypotheses

- More expressive hypothesis space
  - increases chance that target function can be expressed
  - increases number of hypotheses consistent with training set

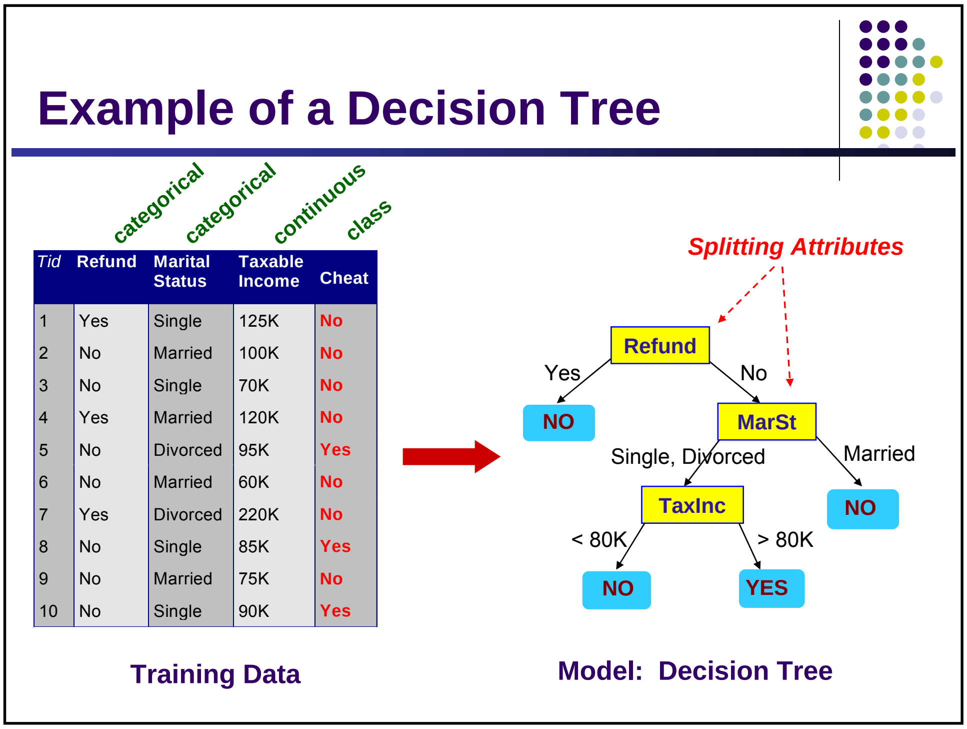
    $\Rightarrow$ may get worse predictions

Decision Tree Learning

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes



Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

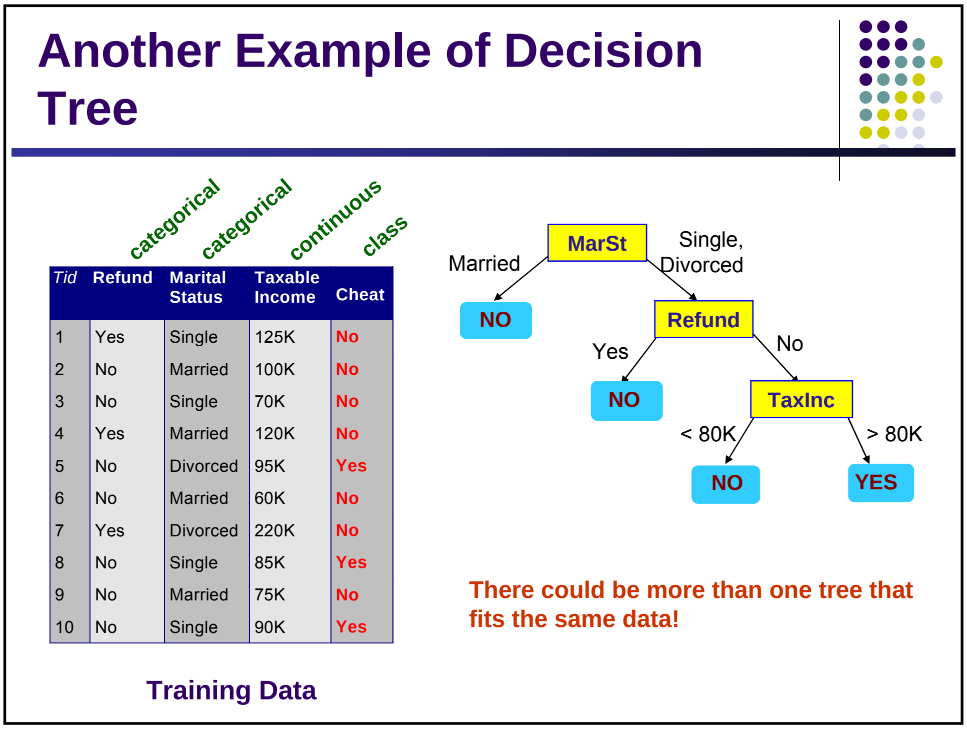


Example of a Decision Tree

	categorical	categorical	continuous	class
Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data

Model: Decision Tree



Another Example of Decision Tree

	categorical	categorical	continuous	class
Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
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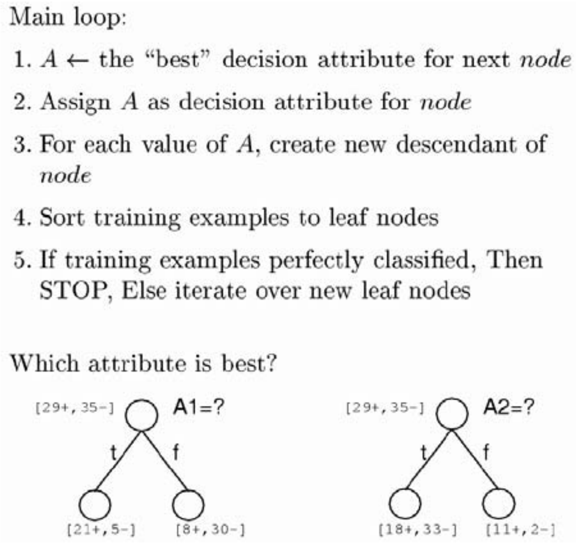
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

There could be more than one tree that fits the same data!

Training Data

Top-Down Induction of DT

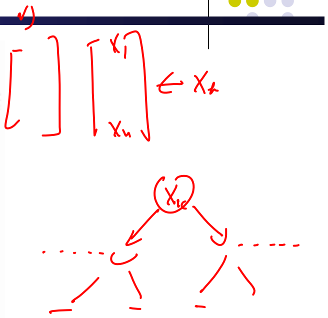


Main loop:

1. $A \leftarrow$ the "best" decision attribute for next *node*
2. Assign A as decision attribute for *node*
3. For each value of A, create new descendant of *node*
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes

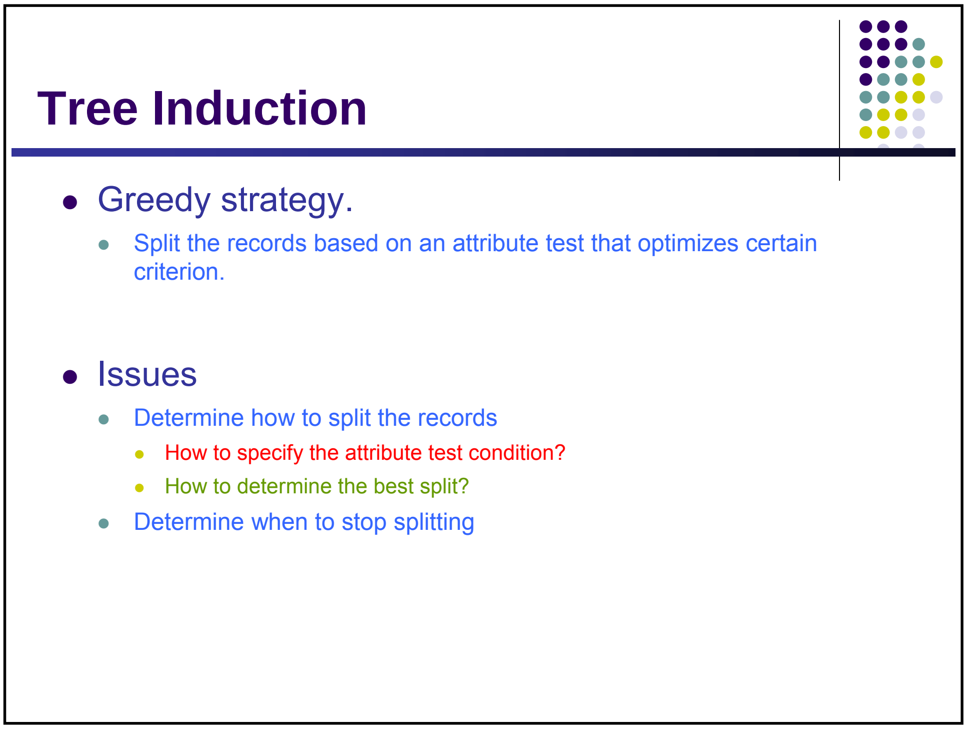
Which attribute is best?

[29+, 35-]
A1=?
t
f
[21+, 5-]
[8+, 30-]
[29+, 35-]
A2=?
t
f
[18+, 33-]
[11+, 2-]



Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting



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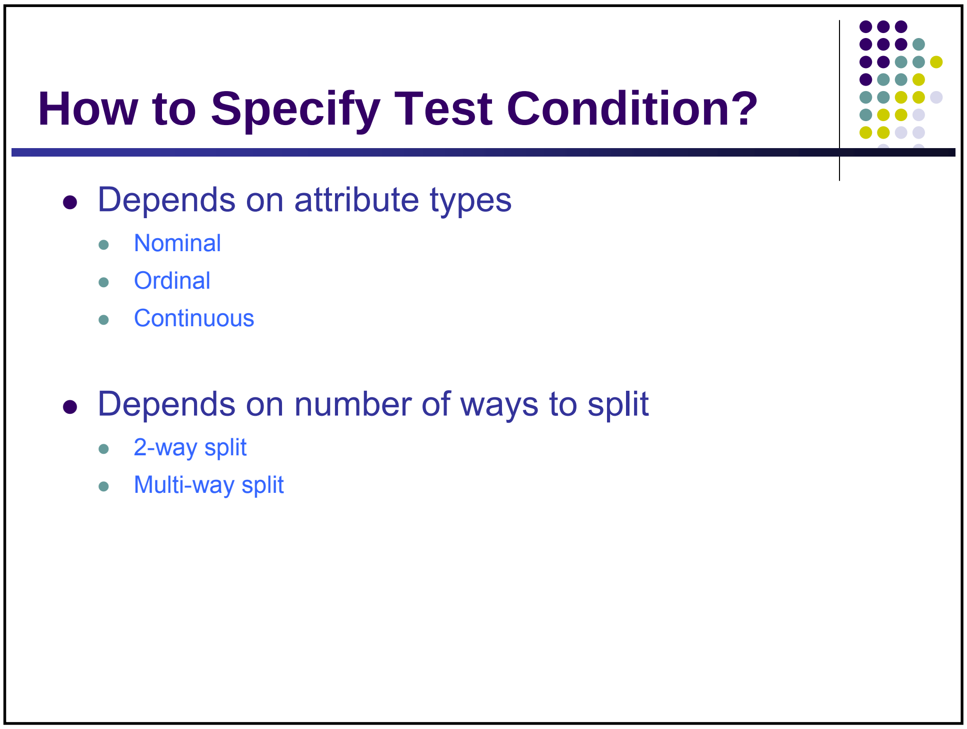
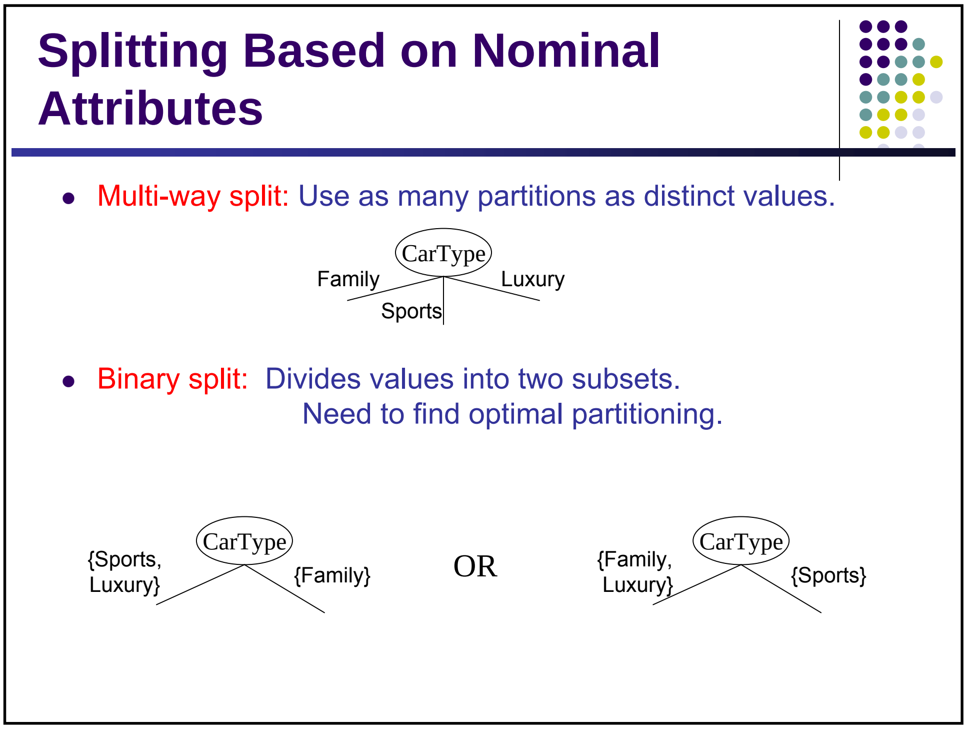


How to Specify Test Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous
- Depends on number of ways to split
  - 2-way split
  - Multi-way split



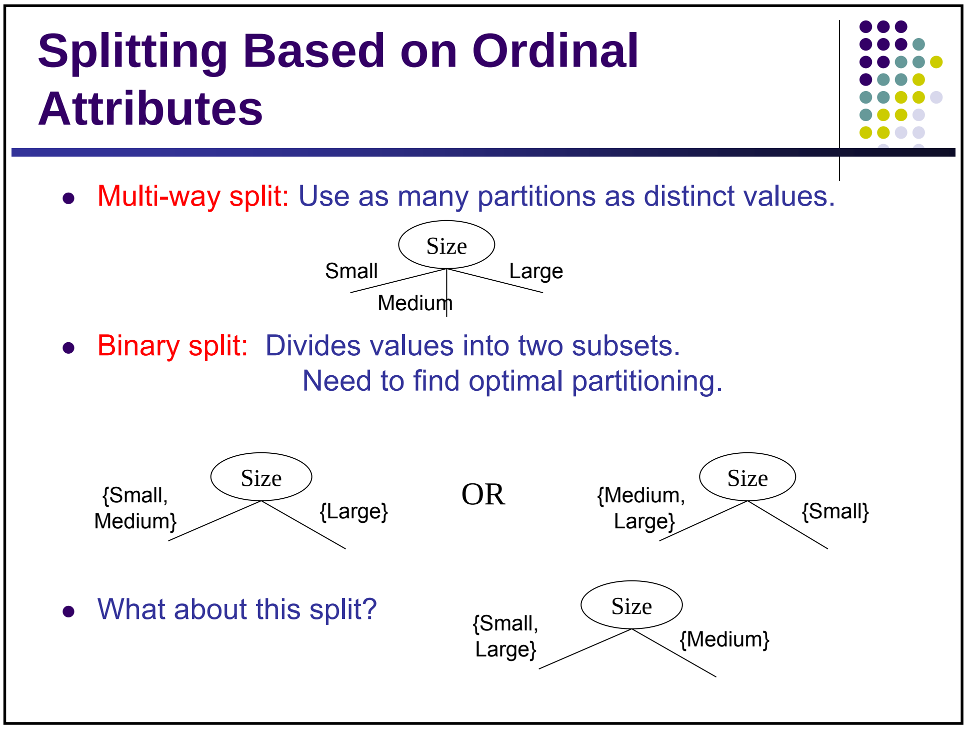
Splitting Based on Nominal Attributes

- Multi-way split: Use as many partitions as distinct values.

CarType
Family
Sports
Luxury

- Binary split: Divides values into two subsets.
  Need to find optimal partitioning.

CarType
{Sports, Luxury}
{Family}
OR
CarType
{Family, Luxury}
{Sports}



Splitting Based on Ordinal Attributes

- Multi-way split: Use as many partitions as distinct values.

Size
Small
Medium
Large

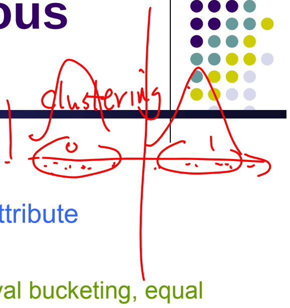
- Binary split: Divides values into two subsets.
  Need to find optimal partitioning.

Size
{Small, Medium}
{Large}
OR
Size
{Medium, Large}
{Small}

- What about this split?

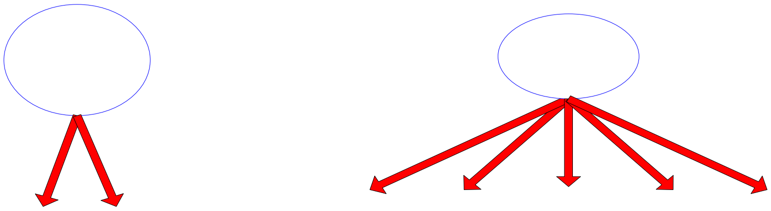
Size
{Small, Large}
{Medium}

Splitting Based on Continuous Attributes



- Different ways of handling
  - Discretization to form an ordinal categorical attribute
    - Static – discretize once at the beginning
    - Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - Binary Decision: (A < v) or (A ≥ v)
    - consider all possible splits and finds the best cut
    - can be more compute intensive

Splitting Based on Continuous Attributes



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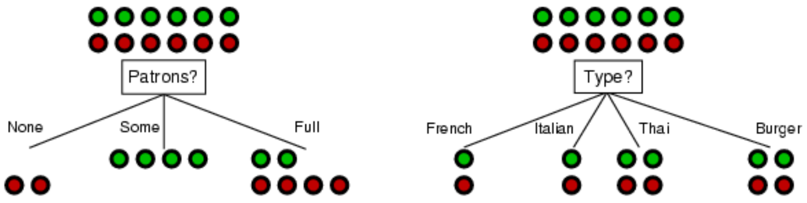
How to determine the Best Split

- Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"



Homogeneous,
Low degree of impurity

Non-homogeneous,
High degree of impurity

- Greedy approach:
  - Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

How to compare attribute?

- Entropy
  - Entropy *H(X)* of a random variable *X*

$$\boxed{H(X) = -\sum_{i=1}^{N} P(x=i)\log_2 P(x=i)}$$

1. – –

  - *H(X)* is the expected number of bits needed to encode a randomly drawn value of *X* (under most efficient code)
  - Why?

100 110 111 1.

1. 10 100 1000 10^4 . . . . 10^8

99999

Information theory:

Most efficient code assigns $-\log_2 P(X=i)$ bits to encode the message *X=I*,
So, expected number of bits to code one random *X* is:

$$-\sum_{i=1}^{N} P(x=i)\log_2 P(x=i)$$

How to compare attribute?

- Conditional Entropy
  - Specific conditional entropy *H(X|Y=v)* of *X* given *Y=v* :

$$H(X|y=j) = -\sum_{i=1}^{N} P(x=i|y=j)\log_2 P(x=i|y=j)$$

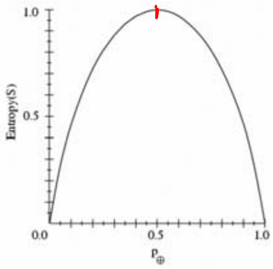
  - Conditional entropy *H(X|Y)* of *X* given *Y* :

$$H(X|Y) = -\sum_{j\in Val(y)} P(y=j)\log_2 H(X|y=j)$$

  - Mututal information (aka information gain) of *X* and *Y* :

$$\begin{aligned} I(X;Y) &= H(X) - H(X|Y) = H(Y) - H(Y|X) \\ &= H(X) + H(Y) - H(X,Y) \end{aligned}$$

Sample Entropy



- S is a sample of training examples
- p_+ is the proportion of positive examples in S
- p_- is the proportion of negative examples in S
- Entropy measure the impurity of S

$$H(S) \equiv -p_+ \log_2 \underline{p_+} - p_- \log_2 \underline{p_-}$$

Examples for computing Entropy

$$\boxed{H(X) = -\sum_{i=1}^{N} P(x=i) \log_2 P(x=i)}$$

C1	**0**
C2	**6**

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1

Entropy = – 0 log 0 – 1 log 1 = – 0 – 0 = 0

C1	**1**
C2	**5**

P(C1) = 1/6 P(C2) = 5/6

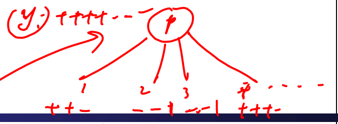
Entropy = – (1/6) $\log_2$ (1/6) – (5/6) $\log_2$ (1/6) = 0.65

C1	**2**
C2	**4**

P(C1) = 2/6 P(C2) = 4/6

Entropy = – (2/6) $\log_2$ (2/6) – (4/6) $\log_2$ (4/6) = 0.92

Information Gain

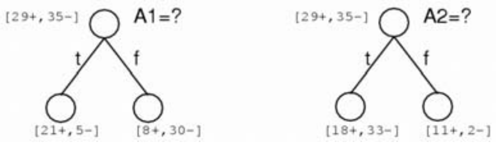


- Information Gain:

$$GAIN_{split} = Entropy(p) - \left(\sum_{i=1}^{k} \frac{n_i}{n} Entropy(i) \right)$$

Parent Node, p is split into k partitions; n_i is number of records in partition i

- Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)
- Used in ID3 and C4.5
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.



Gain(S,A) = mutual information between A and target class variable over sample S

Splitting Based on INFO...

- Gain Ratio:

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO} \qquad SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent Node, p is split into k partitions

n_i is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5
- Designed to overcome the disadvantage of Information Gain

Exercise

	categorical	categorical	continuous	class
Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	**No**
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Stopping Criteria for Tree Induction

- Stop expanding a node when all the records belong to the same class
- Stop expanding a node when all the records have similar attribute values
- Early termination (to be discussed later)

Decision Tree Based Classification

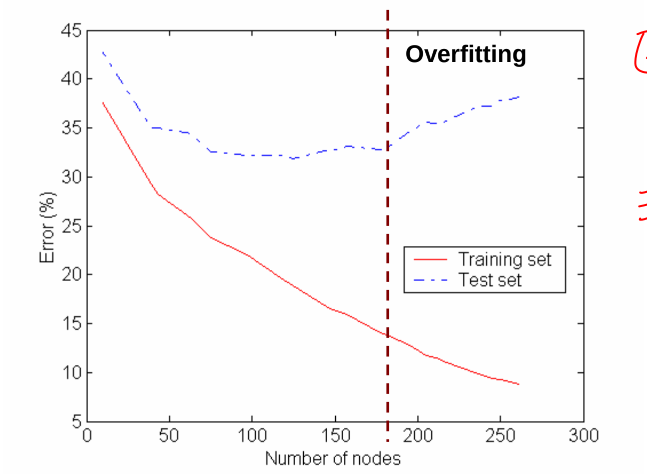
- Advantages:
  - Inexpensive to construct
  - Extremely fast at classifying unknown records
  - Easy to interpret for small-sized trees
  - Accuracy is comparable to other classification techniques for many simple data sets
- Example: C4.5
  - Simple depth-first construction.
  - Uses Information Gain
  - Sorts Continuous Attributes at each node.
  - Needs entire data to fit in memory.
  - Unsuitable for Large Datasets.
    - Needs out-of-core sorting.
  - You can download the software from: http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz

Practical Issues of Classification

- Underfitting and Overfitting
- Missing Values
- Costs of Classification

  -- Later lectures

Underfitting and Overfitting



$E_t(h_t^*) \le E_t(h')$

$h' \in H$.

$\exists\ h'' \in H$

$E_{Test}(h'') < E_{Test}(h^*)$

Underfitting: when model is too simple, both training and test errors are large

Notes on Overfitting

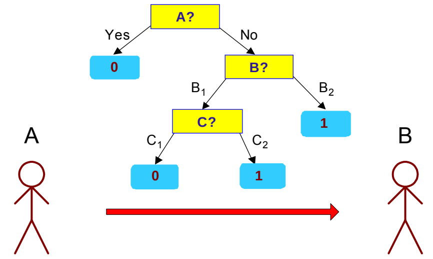
- Overfitting results in decision trees that are more complex than necessary
- Training error no longer provides a good estimate of how well the tree will perform on previously unseen records
- **Which Tree Should We Output?**
  - Occam’s razor: prefer the simplest hypothesis that fits the data

Occam’s Razor

- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
- For complex models, there is a greater chance that it was fitted accidentally by errors in data
- Therefore, one should include model complexity when evaluating a model

Minimum Description Length (MDL)

X	y
X_1	1
X_2	0
X_3	0
X_4	1
…	…
X_n	1



X	y
X_1	?
X_2	?
X_3	?
X_4	?
…	…
X_n	?

- Cost(Model,Data) = Cost(Data|Model) + Cost(Model)
  - Cost is the number of bits needed for encoding.
  - Search for the least costly model.
- Cost(Data|Model) encodes the misclassification errors.
- Cost(Model) uses node encoding (number of children) plus splitting condition encoding.

How to Address Overfitting

- Pre-Pruning (Early Stopping Rule)
  - Stop the algorithm before it becomes a fully-grown tree
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - More restrictive conditions:
    - Stop if number of instances is less than some user-specified threshold
    - Stop if class distribution of instances are independent of the available features (e.g., using χ^2 test)
    - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).

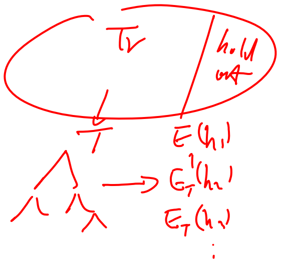
How to Address Overfitting…

- Post-pruning
  - Grow decision tree to its entirety
  - Trim the nodes of the decision tree in a bottom-up fashion
  - If generalization error improves after trimming, replace sub-tree by a leaf node.
  - Class label of leaf node is determined from majority class of instances in the sub-tree
  - Can use MDL for post-pruning

N-1 . 1

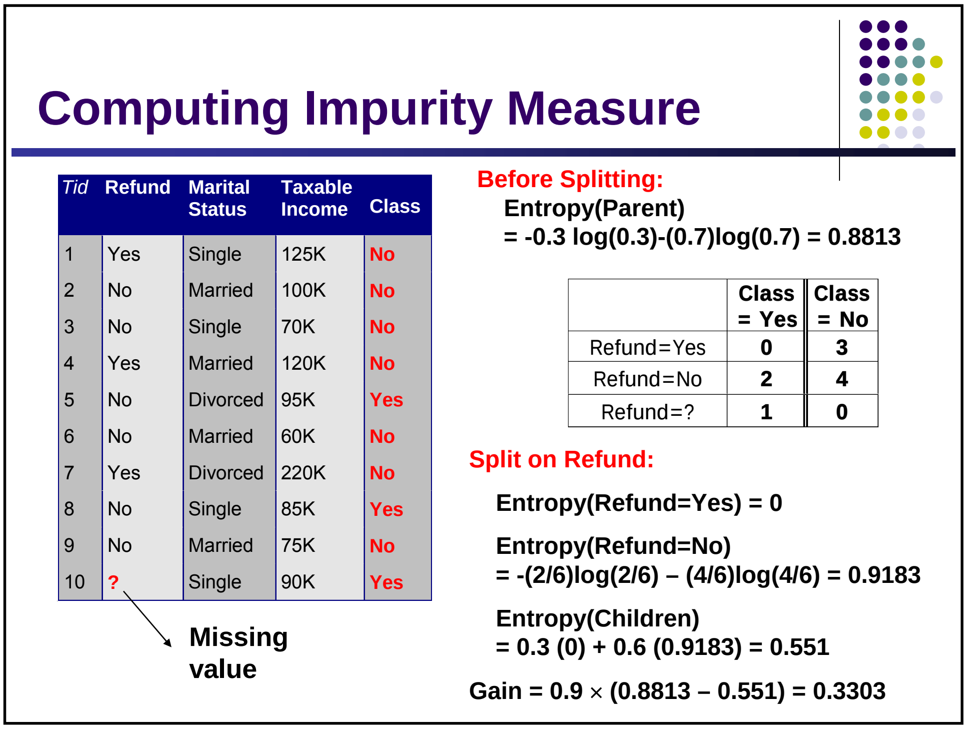
Leve-one-out-CV

k-fold - CV



Handling Missing Attribute Values

- Missing values affect decision tree construction in three different ways:
  - Affects how impurity measures are computed
  - Affects how to distribute instance with missing value to child nodes
  - Affects how a test instance with missing value is classified



Computing Impurity Measure

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	?	Single	90K	Yes

Missing value

Before Splitting:

Entropy(Parent)
= -0.3 log(0.3)-(0.7)log(0.7) = 0.8813

	Class = Yes	Class = No
Refund=Yes	0	3
Refund=No	2	4
Refund=?	1	0

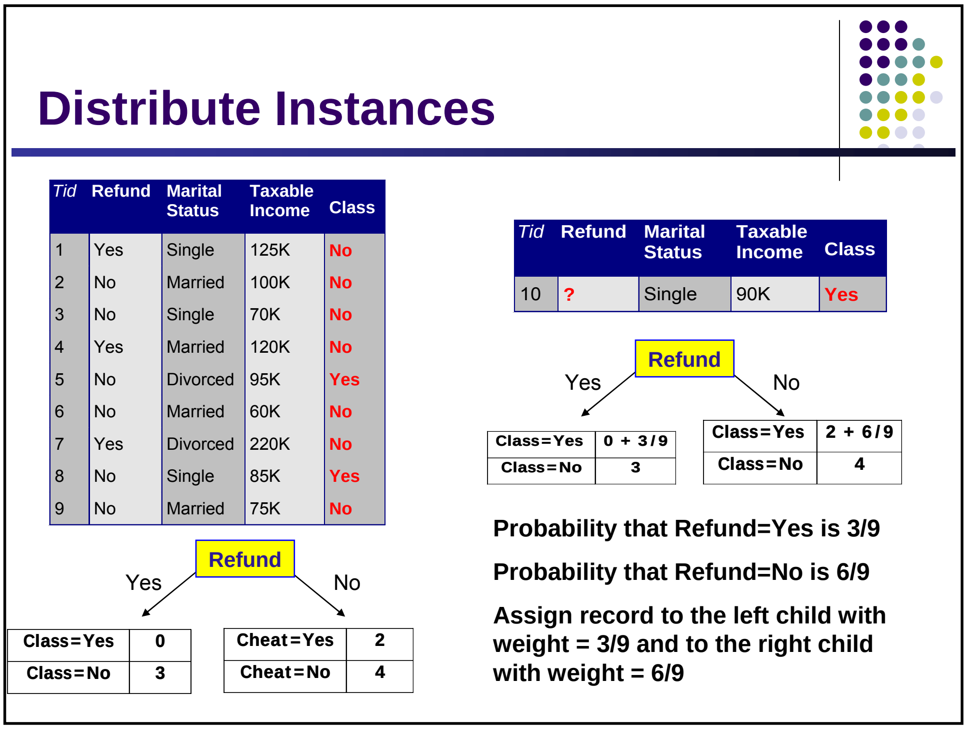
Split on Refund:

Entropy(Refund=Yes) = 0

Entropy(Refund=No)
= -(2/6)log(2/6) – (4/6)log(4/6) = 0.9183

Entropy(Children)
= 0.3 (0) + 0.6 (0.9183) = 0.551

Gain = 0.9 × (0.8813 – 0.551) = 0.3303



Distribute Instances

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No

Refund

Yes

Class=Yes	0
Class=No	3

No

Cheat=Yes	2
Cheat=No	4

Tid	Refund	Marital Status	Taxable Income	Class
10	?	Single	90K	Yes

Refund

Yes

Class=Yes	0 + 3/9
Class=No	3

No

Class=Yes	2 + 6/9
Class=No	4

Probability that Refund=Yes is 3/9

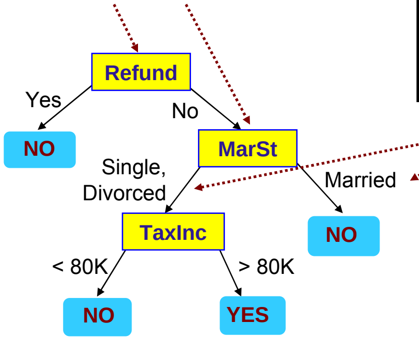
Probability that Refund=No is 6/9

Assign record to the left child with weight = 3/9 and to the right child with weight = 6/9

Classify Instances

New record:

Tid	Refund	Marital Status	Taxable Income	Class
11	No	?	85K	?



	Married	Single	Divorced	Total
Class=No	3	1	0	4
Class=Yes	6/9	1	1	2.67
Total	3.67	2	1	6.67

Probability that Marital Status = Married is 3.67/6.67

Probability that Marital Status ={Single,Divorced} is 3/6.67