Decision tree learning

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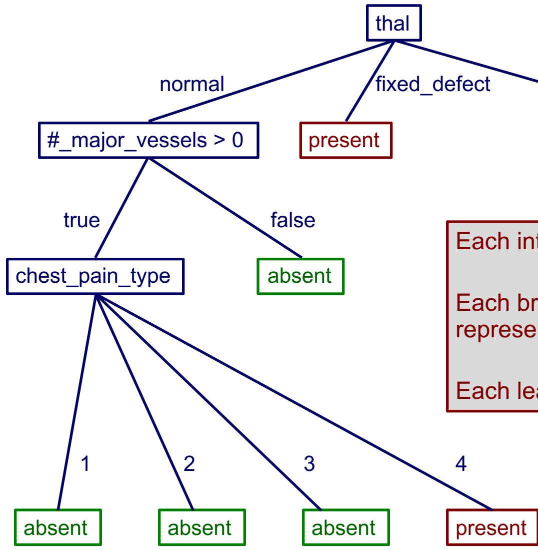
Goals for the lecture

you should understand the following concepts

- the decision tree representation
- the standard top-down approach to learning a tree
- Occam's razor
- entropy and information gain
- types of decision-tree splits
- test sets and unbiased estimates of accuracy
- overfitting
- early stopping and pruning
- tuning (validation) sets
- regression trees
- probability estimation trees
- m-of-n splits
- using lookahead in decision tree search

A decision tree to predict heart disease



Each internal node tests one feature x_i

Each branch from an internal node represents one outcome of the test

Each leaf predicts y or $P(y \mid \boldsymbol{x})$

Decision tree exercise

Suppose $X_1 \ldots X_5$ are Boolean features, and Y is also Boolean

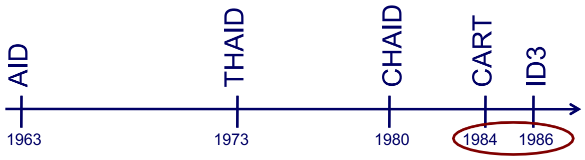
How would you represent the following with decision trees?

$$Y = X_2 X_5 \quad \text{(i.e. } Y = X_2 \wedge X_5\text{)}$$

$$Y = X_2 \vee X_5$$

$$Y = X_2 X_5 \vee X_3 \neg X_1$$

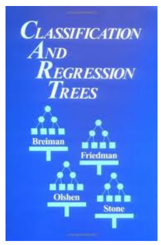
History of decision tree learning



many DT variants have been developed since CART and ID3

dates of seminal publications: work on these 2 was contemporaneous

CART developed by Leo Breiman, Jerome Friedman, Charles Olshen, R.A. Stone



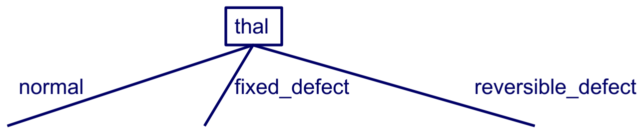
ID3, C4.5, C5.0 developed by Ross Quinlan

Top-down decision tree learning

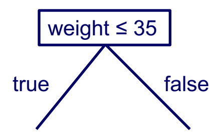
MakeSubtree(set of training instances D)
- C = DetermineCandidateSplits(D)
- if stopping criteria met
  - make a leaf node N
  - determine class label/probabilities for N
- else
  - make an internal node N
  - S = FindBestSplit(D, C)
  - for each outcome k of S
    - D_k = subset of instances that have outcome k
    - k^{th} child of N = MakeSubtree(D_k)
- return subtree rooted at N

Candidate splits in ID3, C4.5

- splits on nominal features have one branch per value



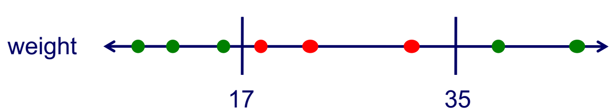
- splits on numeric features use a threshold

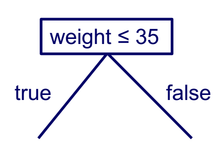


Candidate splits on numeric features

given a set of training instances D and a specific feature X_i

- sort the values of X_i in D
- evaluate split thresholds in intervals between instances of different classes





- could use midpoint of each considered interval as the threshold
- C4.5 instead picks the largest value of X_i in the entire training set that does not exceed the midpoint

Candidate splits on numeric features (in more detail)

// Run this subroutine for each numeric feature at each node of DT induction

DetermineCandidateNumericSplits(set of training instances D, feature X_i)

$C = \{\}$ // initialize set of candidate splits for feature X_i

S = partition instances in D into sets $s_1 \ldots s_V$ where the instances in each set have the same value for X_i

let v_j denote the value of X_i for set s_j

sort the sets in S using v_j as the key for each s_j

for each pair of adjacent sets s_j, s_{j+1} in sorted S

if s_j and s_{j+1} contain a pair of instances with different class labels

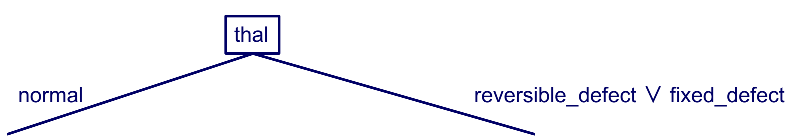
// assume we're using midpoints for splits

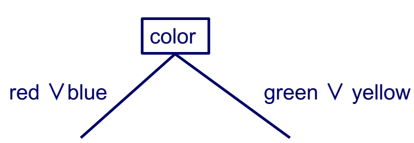
add candidate split $X_i \leq (v_j + v_{j+1})/2$ to C

return C

Candidate splits

- instead of using k-way splits for k-valued features, could require binary splits on all discrete features (CART does this)





- Breiman et al. proved for the 2-class case, the optimal binary partition can be found considering only $O(k)$ possibilities instead of $O(2^k)$

Finding the best split

- How should we select the best feature to split on at each step?
- Key hypothesis: the simplest tree that classifies the training instances accurately will work well on previously unseen instances

Occam's razor

- attributed to 14th century William of Ockham
- "Nunquam ponenda est pluralitis sin necesitate"
- "Entities should not be multiplied beyond necessity"
- "when you have two competing theories that make exactly the same predictions, the simpler one is the better"

Occam's razor and decision trees

Why is Occam's razor a reasonable heuristic for decision tree learning?

- there are fewer short models (i.e. small trees) than long ones
- a short model is unlikely to fit the training data well by chance
- a long model is more likely to fit the training data well coincidentally

Finding the best splits

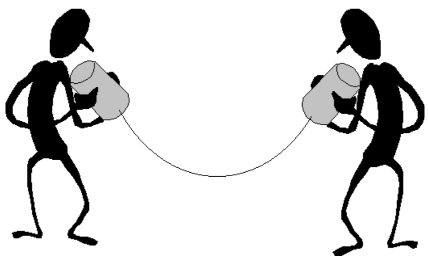
- Can we find and return the smallest possible decision tree that accurately classifies the training set?

  NO! This is an NP-hard problem
  [Hyafil & Rivest, *Information Processing Letters, 1976]*

- Instead, we'll use an information-theoretic heuristic to greedily choose splits

Information theory background

- consider a problem in which you are using a code to communicate information to a receiver
- example: as bikes go past, you are communicating the manufacturer of each bike



Information theory background

- suppose there are only four types of bikes
- we could use the following code

type	code
Trek	11
Specialized	10
Cervelo	01
Serrota	00

- expected number of bits we have to communicate: 2 bits/bike

Information theory background

- we can do better if the bike types aren't equiprobable
- optimal code uses $-\log_2 P(y)$ bits for event with probability $P(y)$

Type/probability	# bits	code
$P(\text{Trek}) = 0.5$	1	1
$P(\text{Specialized}) = 0.25$	2	01
$P(\text{Cervelo}) = 0.125$	3	001
$P(\text{Serrota}) = 0.125$	3	000

- expected number of bits we have to communicate: 1.75 bits/bike

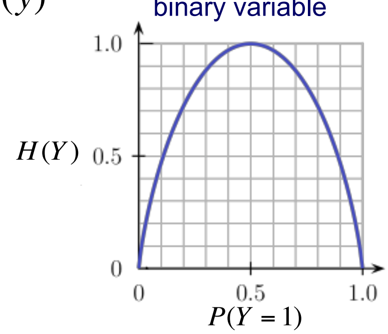
$$-\sum_{y \in \text{values}(Y)} P(y) \log_2 P(y)$$

Entropy

- entropy is a measure of uncertainty associated with a random variable
- defined as the expected number of bits required to communicate the value of the variable

$$H(Y) = -\sum_{y \in \text{values}(Y)} P(y) \log_2 P(y)$$

entropy function for binary variable



Conditional entropy

- What's the entropy of Y if we condition on some other variable X?

$$H(Y \mid X) = \sum_{x \in \text{values}(X)} P(X = x)\, H(Y \mid X = x)$$

where

$$H(Y \mid X = x) = -\sum_{y \in \text{values}(Y)} P(Y = y \mid X = x)\, \log_2 P(Y = y \mid X = x)$$

Information gain (a.k.a. mutual information)

- choosing splits in ID3: select the split S that most reduces the conditional entropy of Y for training set D

$$\text{InfoGain}(D,S) = H_D(Y) - H_D(Y \mid S)$$

D indicates that we're calculating probabilities using the specific sample D

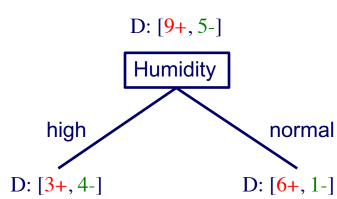
Information gain example

PlayTennis: training examples

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Information gain example

- What's the information gain of splitting on Humidity?



$$H_D(Y) = -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right) = 0.940$$

$$H_D(Y \mid \text{high}) = -\frac{3}{7}\log_2\left(\frac{3}{7}\right) - \frac{4}{7}\log_2\left(\frac{4}{7}\right) = 0.985$$

$$H_D(Y \mid \text{normal}) = -\frac{6}{7}\log_2\left(\frac{6}{7}\right) - \frac{1}{7}\log_2\left(\frac{1}{7}\right) = 0.592$$

$$\begin{aligned}\text{InfoGain}(D,\text{Humidity}) &= H_D(Y) - H_D(Y \mid \text{Humidity}) \\ &= 0.940 - \left[\frac{7}{14}(0.985) + \frac{7}{14}(0.592)\right] \\ &= 0.151\end{aligned}$$

Information gain example

- Is it better to split on Humidity or Wind?

$H_D(Y \mid \text{weak}) = 0.811$ $\quad$ $H_D(Y \mid \text{strong}) = 1.0$

✔ $$\text{InfoGain}(D, \text{Humidity}) = 0.940 - \left[\frac{7}{14}(0.985) + \frac{7}{14}(0.592)\right]$$
$$= 0.151$$

$$\text{InfoGain}(D, \text{Wind}) = 0.940 - \left[\frac{8}{14}(0.811) + \frac{6}{14}(1.0)\right]$$
$$= 0.048$$

One limitation of information gain

- information gain is biased towards tests with many outcomes
- e.g. consider a feature that uniquely identifies each training instance
  - splitting on this feature would result in many branches, each of which is “pure” (has instances of only one class)
  - maximal information gain!

Gain ratio

- To address this limitation, C4.5 uses a splitting criterion called *gain ratio*
- gain ratio normalizes the information gain by the entropy of the split being considered

$$\text{GainRatio}(D,S) = \frac{\text{InfoGain}(D,S)}{H_D(S)} = \frac{H_D(Y) - H_D(Y \mid S)}{H_D(S)}$$

Stopping criteria

We should form a leaf when

- all of the given subset of instances are of the same class
- we've exhausted all of the candidate splits

Is there a reason to stop earlier, or to prune back the tree?

How can we assess the accuracy of a tree?

- Can we just calculate the fraction of training instances that are correctly classified?

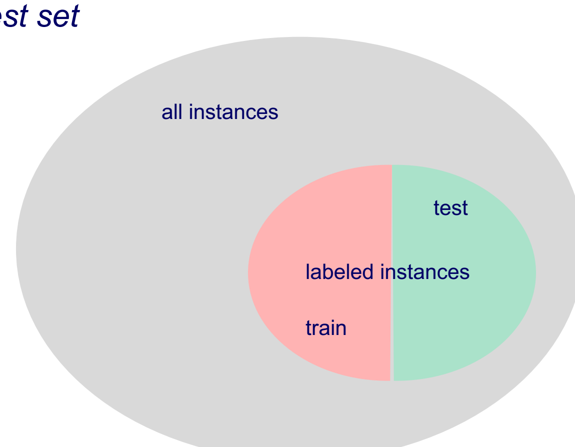
- Consider a problem domain in which instances are assigned labels at random with $P(Y = \mathrm{t}) = 0.5$

  - How accurate would a learned decision tree be on previously unseen instances?

  - How accurate would it be on its training set?

How can we assess the accuracy of a tree?

- to get an unbiased estimate of a learned model's accuracy, we must use a set of instances that are held-aside during learning
- this is called a *test set*



Overfitting

- consider error of model h over
  - training data: $error_{D}(h)$
  - entire distribution of data: $error_{\mathcal{D}}(h)$

- model $h \in H$ *overfits* the training data if there is an alternative model $h' \in H$ such that

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

$$error_{D}(h) < error_{D}(h')$$

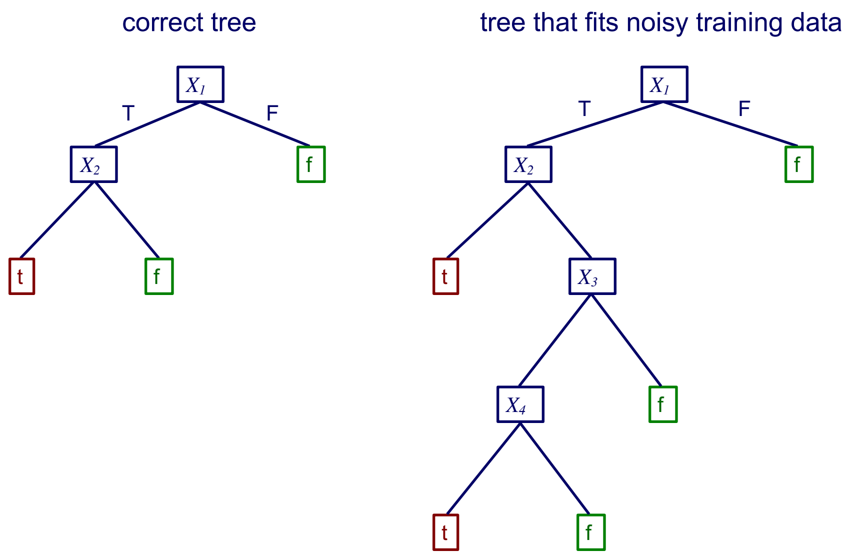
Overfitting with noisy data

suppose
- the target concept is $Y = X_1 \wedge X_2$
- there is noise in some feature values
- we're given the following training set

X_1	X_2	X_3	X_4	X_5	…	Y
t	t	t	t	t	…	t
t	t	f	f	t	…	t
t	f	t	t	f	…	t
t	f	f	t	f	…	f
t	f	t	f	f	…	f
f	t	t	f	t	…	f

noisy value

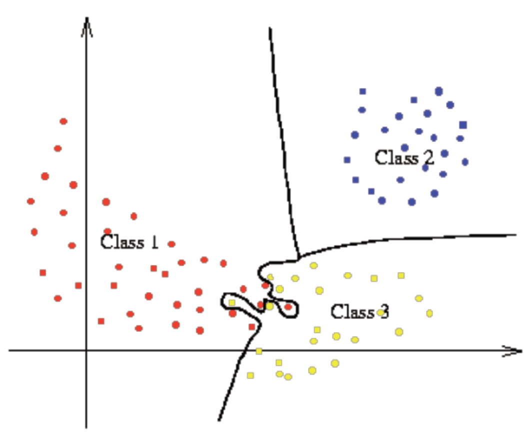
Overfitting with noisy data



Overfitting visualized

consider a problem with

- 2 continuous features
- 3 classes
- some noisy training instances



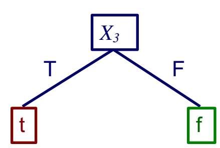
Overfitting with noise-free data

suppose

- the target concept is $Y = X_1 \wedge X_2$
- $P(X_3 = t)$ = 0.5 for both classes
- $P(Y = t)$ = 0.67
- we're given the following training set

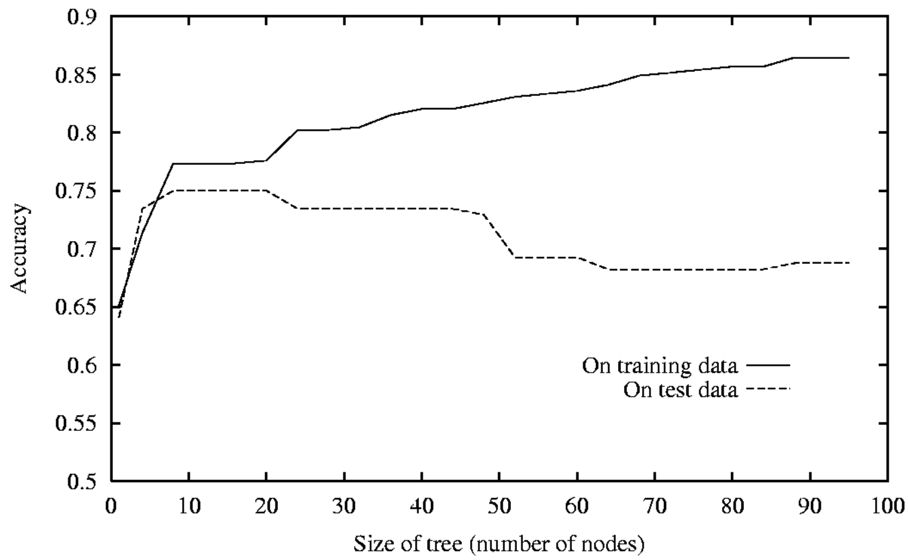
X_1	X_2	X_3	X_4	X_5	…	Y
t	t	t	t	t	…	t
t	t	t	f	t	…	t
t	t	t	t	f	…	t
t	f	f	t	f	…	f
f	t	f	f	t	…	f

Overfitting with noise-free data

	training set accuracy	test set accuracy
	100%	50%
t	66%	66%

- because the training set is a limited sample, there might be (combinations of) features that are correlated with the target concept by chance

Overfitting in decision trees



Avoiding overfitting in DT learning

two general strategies to avoid overfitting

1. *early stopping*: stop if further splitting not justified by a statistical test
   - Quinlan's original approach in ID3

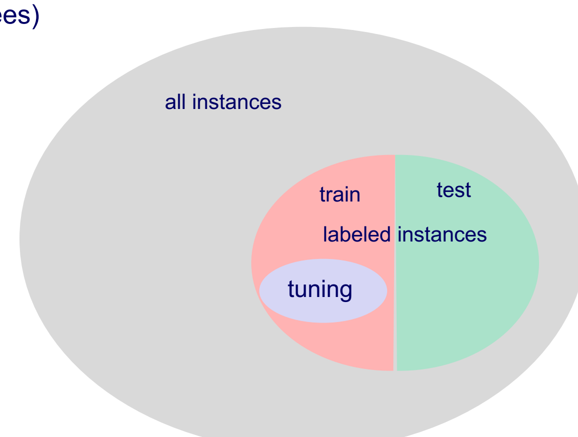
2. *post-pruning*: grow a large tree, then prune back some nodes
   - more robust to myopia of greedy tree learning

Pruning in C4.5

1. split given data into training and *tuning* (*validation*) sets
2. grow a complete tree
3. do until further pruning is harmful
   - evaluate impact on tuning-set accuracy of pruning each node
   - greedily remove the one that most improves tuning-set accuracy

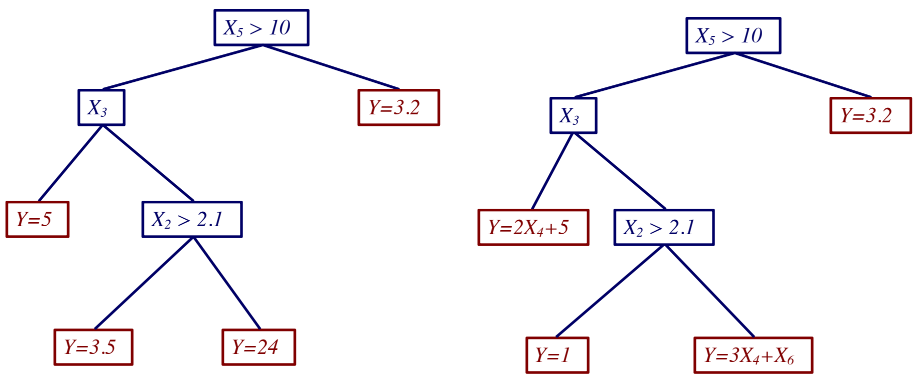
Tuning sets

- a *tuning set* (a.k.a. *validation set*) is a subset of the training set that is held aside
  - not used for primary training process (e.g. tree growing)
  - but used to select among models (e.g. trees pruned to varying degrees)



Regression trees

- in a regression tree, leaves have functions that predict numeric values instead of class labels
- the form of these functions depends on the method
  - CART uses constants
  - some methods use linear functions



Regression trees in CART

- CART does *least squares regression* which tries to minimize

$$\sum_{i=1}^{|D|} \left(y^{(i)} - \hat{y}^{(i)} \right)^2$$

target value for i^{th} training instance

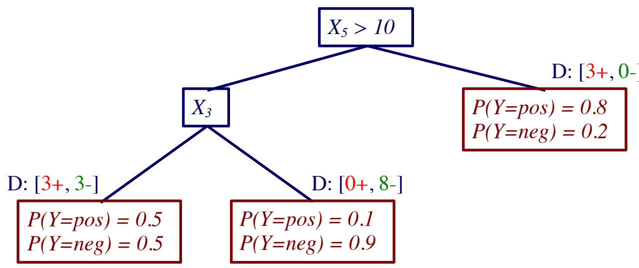
value predicted by tree for i^{th} training instance (average value of y for training instances reaching the leaf)

$$= \sum_{L \in \text{leaves}} \sum_{i \in L} \left(y^{(i)} - \hat{y}^{(i)} \right)^2$$

- at each internal node, CART chooses the split that most reduces this quantity

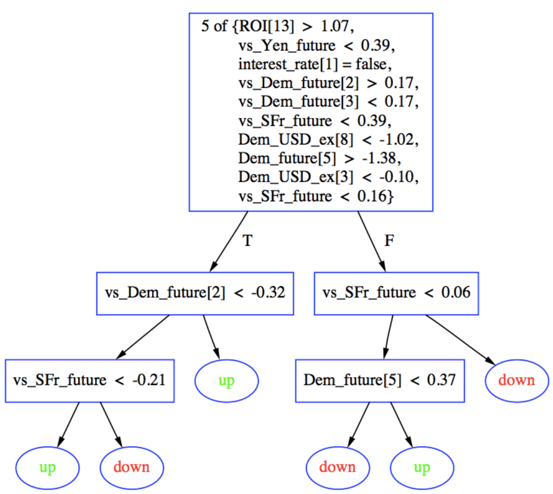
Probability estimation trees

- in a PE tree, leaves estimate the probability of each class
- could simply use training instances at a leaf to estimate probabilities, but…
- *smoothing* is used to make estimates less extreme (we'll revisit this topic when we cover Bayes nets)



m-of-*n* splits

- a few DT algorithms have used *m*-of-*n* splits [Murphy & Pazzani '91]
- each split is constructed using a heuristic search process
- this can result in smaller, easier to comprehend trees



test is satisfied if 5 of 10 conditions are true

tree for exchange rate prediction [Craven & Shavlik, 1997]

Searching for m-of-n splits

m-of-n splits are found via a hill-climbing search

- initial state: best 1-of-1 (ordinary) binary split
- evaluation function: information gain
- operators:

m-of-n ➔ m-of-$(n+1)$

1 of { X_1=t, X_3=f } ➔ 1 of { X_1=t, X_3=f, X_7=t }

m-of-n ➔ $(m+1)$-of-$(n+1)$

1 of { X_1=t, X_3=f } ➔ 2 of { X_1=t, X_3=f, X_7=t }

Lookahead

- most DT learning methods use a hill-climbing search
- a limitation of this approach is myopia: an important feature may not appear to be informative until used in conjunction with other features
- can potentially alleviate this limitation by using a *lookahead* search [Norton '89; Murphy & Salzberg '95]
- empirically, often doesn't improve accuracy or tree size

Choosing best split in ordinary DT learning

OrdinaryFindBestSplit(set of training instances D, set of candidate splits C)

$maxgain = -\infty$

for each split S in C

$gain$ = InfoGain(D, S)

if $gain > maxgain$

$maxgain = gain$

$S_{best} = S$

return S_{best}

Choosing best split with lookahead (part 1)

LookaheadFindBestSplit(set of training instances D, set of candidate splits C)

$maxgain = -\infty$

for each split S in C

$gain$ = EvaluateSplit(D, C, S)

if $gain > maxgain$

$maxgain = gain$

$S_{best} = S$

return S_{best}

Choosing best split with lookahead (part 2)

EvaluateSplit(D, C, S)

if a split on S separates instances by class (i.e. $H_D(Y \mid S) = 0$)

// no need to split further

return $H_D(Y) - H_D(Y \mid S)$

else

for each outcome k of S

// see what the splits at the next level would be

D_k = subset of instances that have outcome k

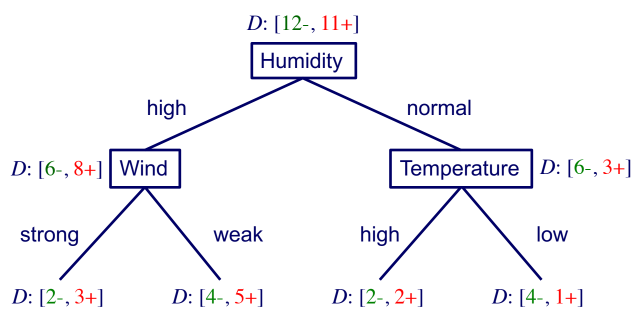
S_k = OrdinaryFindBestSplit(D_k, $C - S$)

// return information gain that would result from this 2-level subtree

return $$H_D(Y) - \left(\sum_k \frac{|D_k|}{|D|} H_{D_k}(Y \mid S = k, S_k \right)$$

Calculating information gain with lookahead

Suppose that when considering Humidity as a split, we find that Wind and Temperature are the best features to split on at the next level



We can assess value of choosing Humidity as our split by

$$H_D(Y) - \left(\frac{14}{23} H_D(Y \mid \text{Humidity} = \text{high}, \text{Wind}) + \frac{9}{23} H_D(Y \mid \text{Humidity} = \text{low}, \text{Temperature}) \right)$$

Calculating information gain with lookahead

Using the tree from the previous slide:

$$\frac{14}{23}H_D(Y \mid \text{Humidity}=\text{high},\text{Wind})+\frac{9}{23}H_D(Y \mid \text{Humidity}=\text{low},\text{Temperature})$$

$$=\frac{5}{23}H_D(Y \mid \text{Humidity}=\text{high},\text{Wind}=\text{strong})+$$

$$\frac{9}{23}H_D(Y \mid \text{Humidity}=\text{high},\text{Wind}=\text{weak})+$$

$$\frac{4}{23}H_D(Y \mid \text{Humidity}=\text{low},\text{Temperature}=\text{high})+$$

$$\frac{5}{23}H_D(Y \mid \text{Humidity}=\text{low},\text{Temperature}=\text{low})$$

$$H_D(Y \mid \text{Humidity}=\text{high},\text{Wind}=\text{strong}) = -\frac{2}{5}\log\left(\frac{2}{5}\right)-\frac{3}{5}\log\left(\frac{3}{5}\right)$$

$$\vdots$$

Comments on decision tree learning

- widely used approach
- many variations
- provides humanly comprehensible models when trees not too big
- insensitive to monotone transformations of numeric features
- standard methods learn axis-parallel hypotheses*
- standard methods not suited to on-line setting*
- usually not among most accurate learning methods

* although variants exist that are exceptions to this