Einführung in Web- und Data-Science

Prof. Dr. Ralf Möller

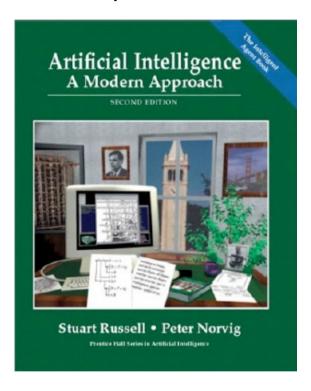
Universität zu Lübeck Institut für Informationssysteme

Tanya Braun (Übungen)



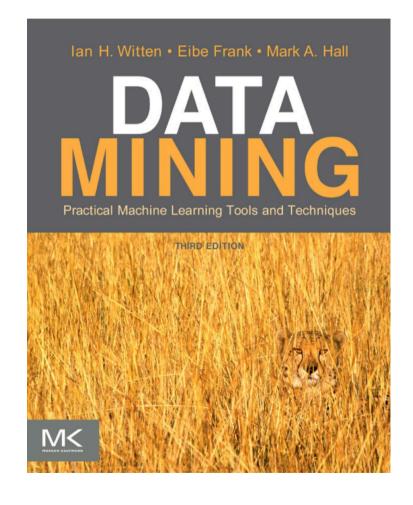
Inductive Learning

Chapter 18/19



Material adopted from Yun Peng, Chuck Dyer, Gregory Piatetsky-Shapiro & Gary Parker

Chapters 3 and 4





Card Example: Guess a Concept

- Given a set of examples
 - Positive: e.g., 4♣ 7♣ 2♠
 - Negative: e.g., 5♥ j♠
- What cards are accepted?
 - What concept lays behind it?



Card Example: Guess a Concept

$$(r=1) \vee ... \vee (r=10) \vee (r=J) \vee (r=Q) \vee (r=K) \Leftrightarrow ANY-RANK(r)$$

 $(r=1) \vee ... \vee (r=10) \Leftrightarrow NUM(r)$
 $(r=J) \vee (r=Q) \vee (r=K) \Leftrightarrow FACE(r)$
 $(s=\clubsuit) \vee (s=\clubsuit) \otimes BLACK(s)$
 $(s=\spadesuit) \vee (s=\clubsuit) \Leftrightarrow RED(s)$

A hypothesis is any sentence of the form:

 $R(r) \wedge S(s)$

where:

- R(r) is ANY-RANK(r), NUM(r), FACE(r), or (r=x)
- S(s) is ANY-SUIT(s), BLACK(s), RED(s), or (s=y)



Simplified Representation

For simplicity, we represent a concept by rs, with:

- $r \in \{a, n, f, 1, ..., 10, j, q, k\}$
- $s \in \{a, b, r, \clubsuit, \spadesuit, \blacklozenge, \heartsuit\}$

For example:

- n♠ represents:
 NUM(r) ∧ (s=♠)
- aa represents:
 ANY-RANK(r) ∧ ANY-SUIT(s)



Extension of a Hypothesis

The extension of a hypothesis h is the set of objects that satisfies h

Examples:

- The extension of $f \spadesuit is: \{j \spadesuit, q \spadesuit, k \spadesuit\}$
- The extension of aa is the set of all cards



More General/Specific Relation

- Let h₁ and h₂ be two hypotheses in H
- h₁ is more general than h₂ iff the extension of h₁ is a proper superset of the extension of h₂

Examples:

- aa is more general than f
- f♥ is more general than q♥
- fr and nr are not comparable

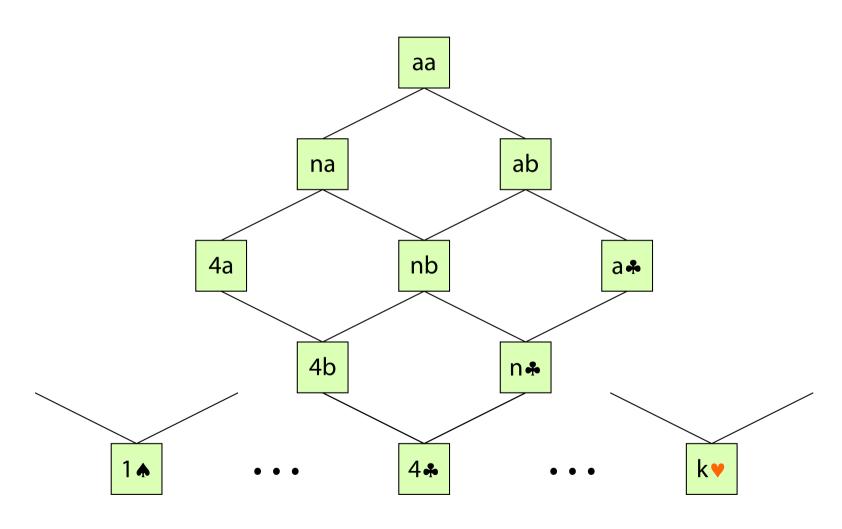


More General/Specific Relation

- Let h₁ and h₂ be two hypotheses in H
- h₁ is more general than h₂ iff the extension of h₁ is a proper superset of the extension of h₂
- The inverse of the "more general" relation is the "more specific" relation
- The "more general" relation defines a partial ordering on the hypotheses in H



Example: Subset of Partial Order





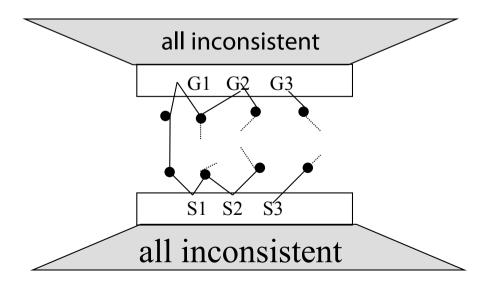
G-Boundary / S-Boundary of V

- A hypothesis in V is most general iff no hypothesis in V is more general
- G-boundary G of V: Set of most general hypotheses in V

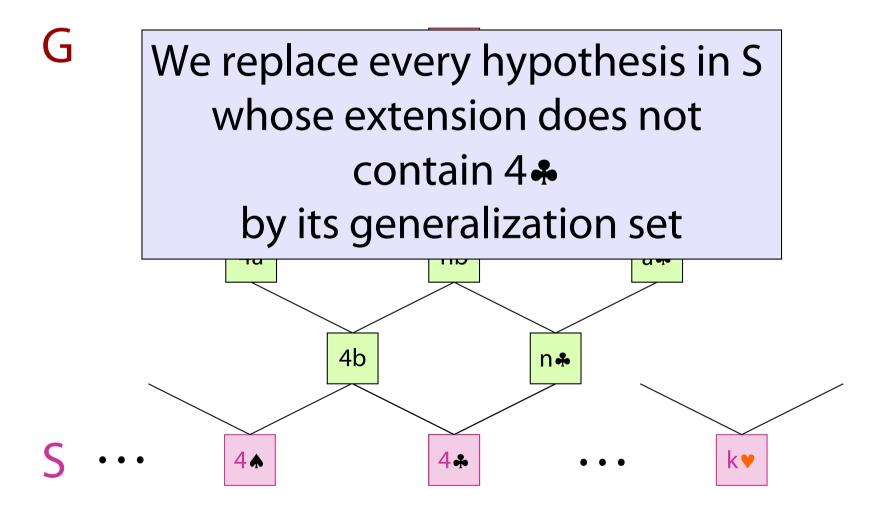


G-Boundary / S-Boundary of V

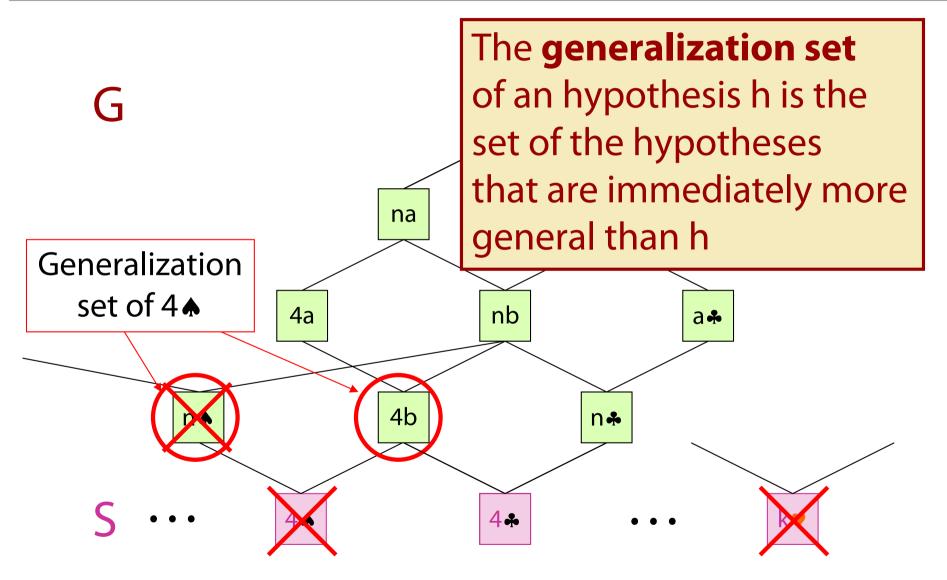
- A hypothesis in V is most general iff no hypothesis in V is more general
- G-boundary G of V: Set of most general hypotheses in V
- A hypothesis in V is most specific iff no hypothesis in V is more specific
- S-boundary S of V: Set of most specific hypotheses in V







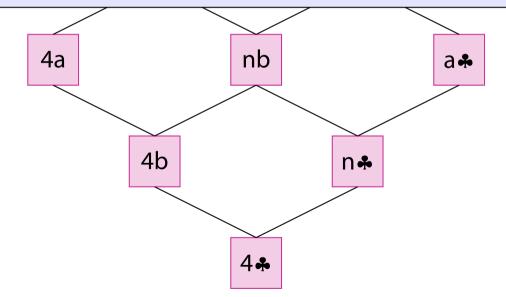






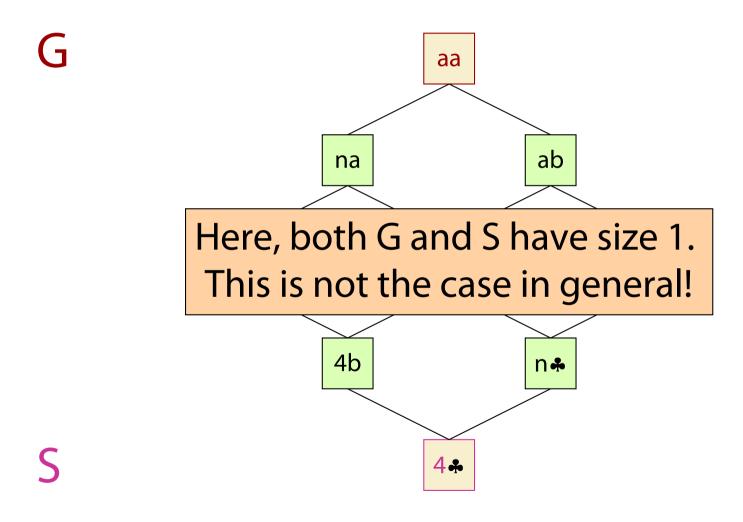
G

We remove every hypothesis in S that is more general than another hypothesis in G

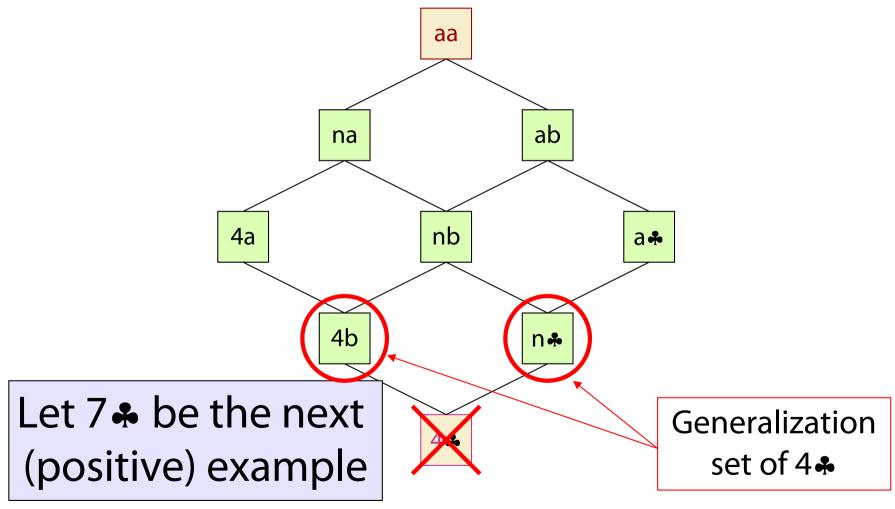


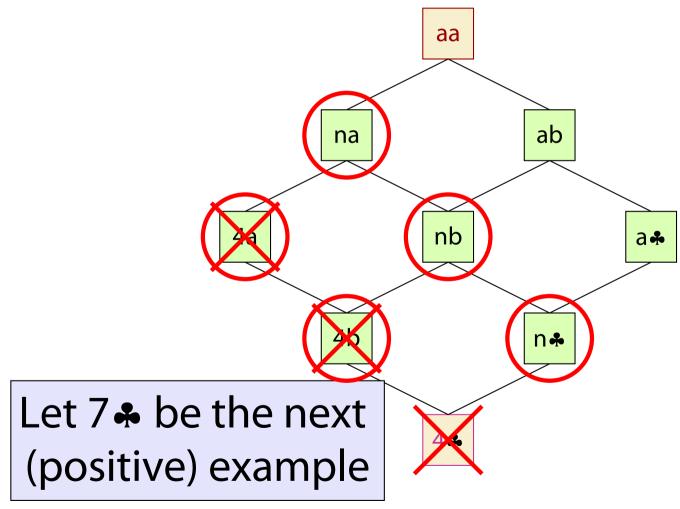
S

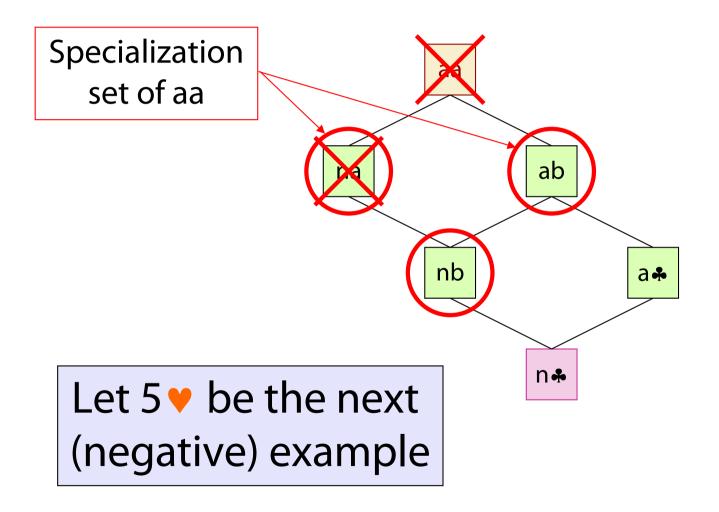






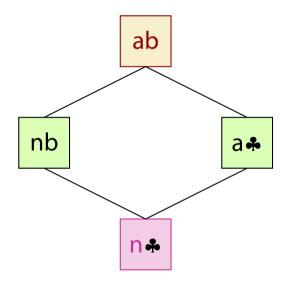






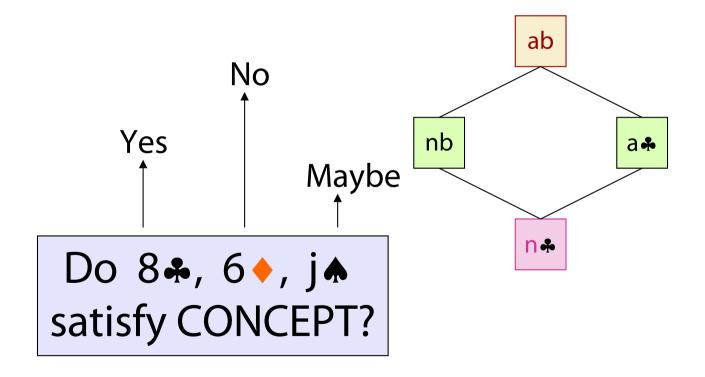


G and S, and all hypotheses in between form exactly the version space

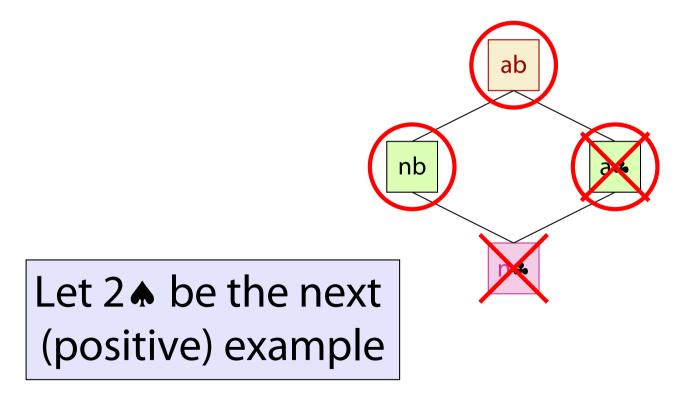


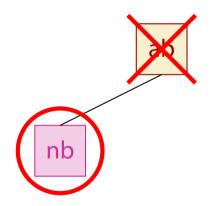


At this stage ...









Let j♠ be the next (negative) example



nb

 $NUM(r) \land BLACK(s)$



Let us return to the version space and let 8. be the next ab (negative) example nb a .* The only most specific hypothesis disagrees with n this example, so no hypothesis in Hagrees with

all examples

ab

n

a .*

nb

Let us return to the version space ...

... and let j♥ be the next (positive) example

The only most general hypothesis disagrees with this example, so no hypothesis in H agrees with all examples

Example-Selection Strategy

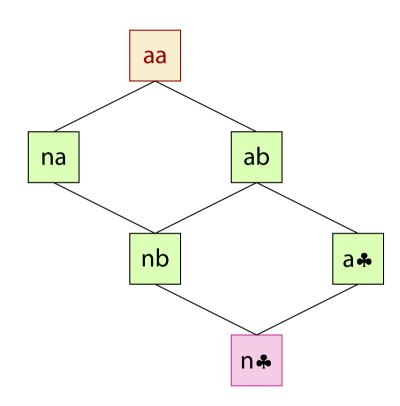
- Suppose that at each step the learning procedure has the possibility to select the object (card) of the next example
- Let it pick the object such that, whether the example is positive or not, it will eliminate one-half of the remaining hypotheses
- Then a single hypothesis will be isolated in O(log |H|) steps



Example



- •j**∀**? •j**♣**?





Example-Selection Strategy

- Suppose that at each step the learning procedure has the possibility to select the object (card) of the next example
- Let it pick the object such that, whether the example is positive or not, it will eliminate one-half of the remaining hypotheses
- Then a single hypothesis will be isolated in O(log |H|) steps
- But picking the object that eliminates half the version space may be expensive



Noise

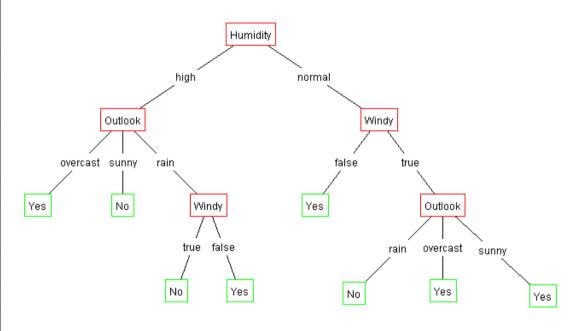
- If some examples are misclassified, the version space may collapse
- Possible solution:

Maintain several G- and S-boundaries, e.g., consistent with all examples, all examples but one, etc...



Decision Trees

Outlook	Temperature	Humidity	Windy	Play?
sunny	hot	high	false	No
sunny	hot	high	true	No
overcast	hot	high	false	Yes
rain	mild	high	false	Yes
rain	cool	normal	false	Yes
rain	cool	normal	true	No
overcast	cool	normal	true	Yes
sunny	mild	high	false	No
sunny	cool	normal	false	Yes
rain	mild	normal	false	Yes
sunny	mild	normal	true	Yes
overcast	mild	high	true	Yes
overcast	hot	normal	false	Yes
rain	mild	high	true	No





Decision trees

- An internal node is a test on an attribute.
- A branch represents an outcome of the test, e.g.,
 Color=red.
- A leaf node represents a class label or class label distribution.
- At each node, one attribute is chosen to split training examples into distinct classes as much as possible
- A new case is classified by following a matching path to a leaf node.

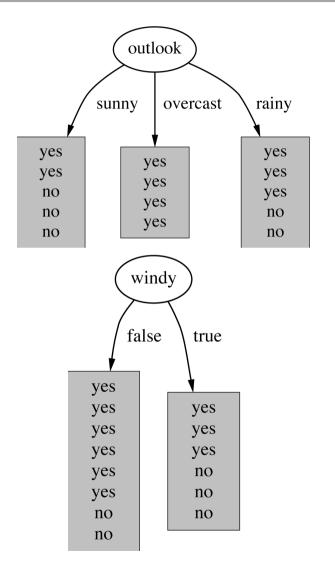


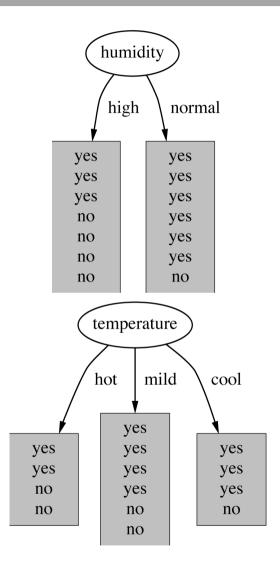
Building Decision Trees

- Top-down tree construction
 - At start, all training examples are at the root.
 - Partition the examples recursively by choosing one attribute each time.
- Bottom-up tree pruning
 - Remove subtrees or branches, in a bottom-up manner, to improve the estimated accuracy on new cases.



Which attribute to select?







Choosing the Best Attribute

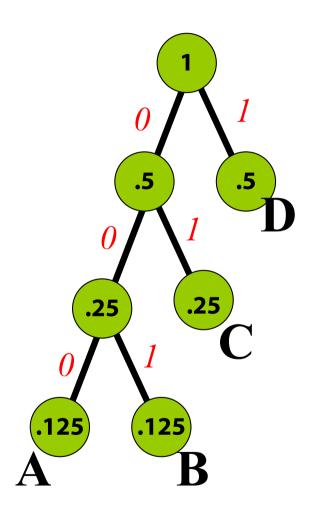
- The key problem is choosing which attribute to split a given set of examples.
- Some possibilities are:
 - Random: Select any attribute at random
 - Least-Values: Choose the attribute with the smallest number of possible values
 - Most-Values: Choose the attribute with the largest number of possible values
 - Information gain: Choose the attribute that has the largest expected information gain, i.e. select attribute that will result in the smallest expected size of the subtrees rooted at its children.

Information Theory

- Assume you can bet 1\$ for a coin flip (10000 bets), if your bet is right, you
 get back 2\$ otherwise you get nothing
- You know that the coin used is rigged and comes up heads with probability 0.99, so you bet heads - obviously (but find somebody arranging this bet :)
- The expected value for the bet is 1.98\$
- How much will you be willing to pay for the advance information about the actual outcome of the flip? What the value of the advance information?
- Less than 0.02\$!
- If the coin were fair, your expected value would 1\$ and you would be willing to pay up to 1\$
- The less you know, the more valuable the information
- Information theory does not measure the value of information in \$ but the information content of a message in bits.



Huffman code example



M	code length		prob	
A	000	3	0,125	0,375
В	001	3	0,125	0,375
C	01	2	0,250	0,500
D	1	1	0,500	0,500
averag	1,750			

If we need to send many messages (A,B,C or D) and they have this probability distribution and we use this code, then over time, the average bits/message should approach 1.75



Information Theory Background

- If there are n equally probable possible messages, then the probability p
 of each is 1/n
- Information conveyed by a message is log(n) = -log(p)
- Eg, if there are 16 messages, then log(16) = 4 and we need 4 bits to identify/send each message.
- In general, if we are given a probability distribution P = (p1, p2, ..., pn)
- the information conveyed by distribution (aka entropy of P) is:

$$I(P) = -(p1*log(p1) + p2*log(p2) + .. + pn*log(pn))$$

= - $\sum_{i} pi*log(pi)$



Information Theory Background

Information conveyed by distribution (aka entropy of P) is:

$$I(P) = -(p1*log(p1) + p2*log(p2) + .. + pn*log(pn))$$

- Examples:
 - if P is (0.5, 0.5) then I(P) is 1
 - if P is (0.67, 0.33) then I(P) is 0.92,
 - if P is (1, 0) or (0,1) then I(P) is 0.
- The more uniform is the probability distribution, the greater is its information.
- The entropy is the average number of bits/message needed to represent a stream of messages.



Example: attribute "Outlook", 1

Outlook	Temperature	Humidity	Windy	Play?
sunny	hot	high	false	No
sunny	hot	high	true	No
overcast	hot	high	false	Yes
rain	mild	high	false	Yes
rain	cool	normal	false	Yes
rain	cool	normal	true	No
overcast	cool	normal	true	Yes
sunny	mild	high	false	No
sunny	cool	normal	false	Yes
rain	mild	normal	false	Yes
sunny	mild	normal	true	Yes
overcast	mild	high	true	Yes
overcast	hot	normal	false	Yes
rain	mild	high	true	No



Example: attribute "Outlook", 2

"Outlook" = "Sunny":

$$\inf([2,3]) = \exp(2/5,3/5) = -2/5\log(2/5) - 3/5\log(3/5) = 0.971 \text{ bits}$$

"Outlook" = "Overcast":

Note: log(0) is not defined, but we evaluate 0*log(0) as zero

info([4,0]) = entropy(1,0) = $-1\log(1) - 0\log(0) = 0$ bits • "Outlook" = "Rainy":

$$\inf([3,2]) = \exp(3/5,2/5) = -3/5\log(3/5) - 2/5\log(2/5) = 0.971 \text{ bits}$$

Expected information for attribute:

info([3,2],[4,0],[3,2]) =
$$(5/14) \times 0.971 + (4/14) \times 0 + (5/14) \times 0.971$$

= 0.693 bits



Computing the information gain

• Information gain:

(information before split) – (information after split)



Computing the information gain

• Information gain:

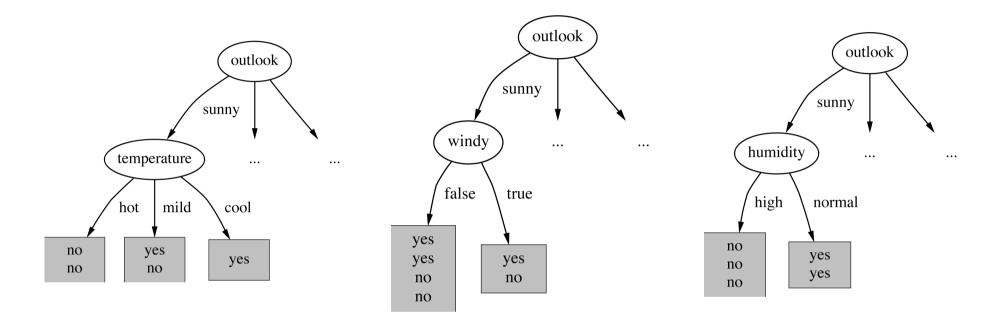
(information before split) – (information after split)

Information gain for attributes from weather data:

gain("Outlook") = 0.247 bits gain("Temperature") = 0.029 bits gain("Humidity") = 0.152 bits gain("Windy") = 0.048 bits



Continuing to split



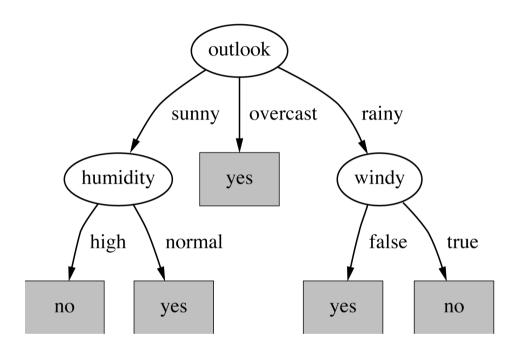
gain("Humidity") = 0.971 bits

gain("Temperature") = 0.571 bits

gain("Windy") = 0.020 bits



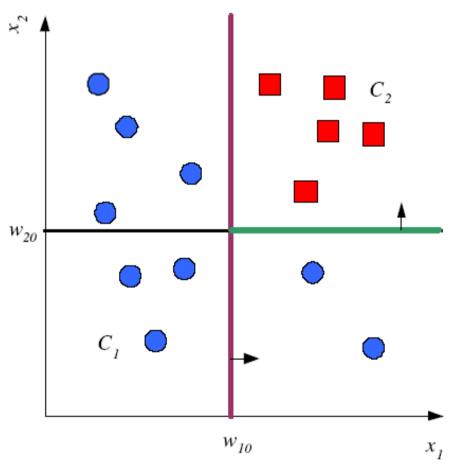
The final decision tree

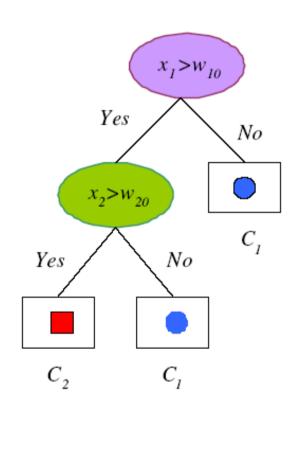


- Note: not all leaves need to be pure; sometimes identical instances have different classes
 - ⇒ Splitting stops when data can't be split any further



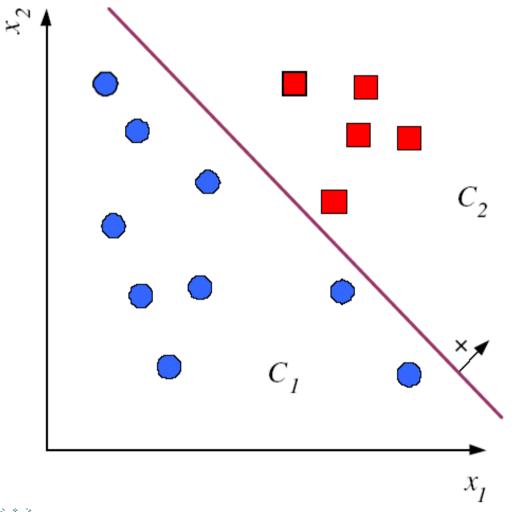
Univariate Splits

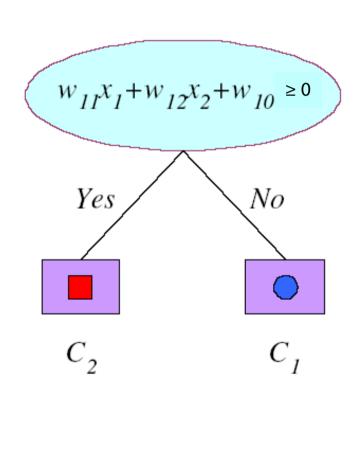






Multivariate Splits







1R – Simplicity First!

Given: Table with data

Goal: Learn decision function

- Based on rules that all test one particular attribute
- One branch for each value
- Each branch assigns most frequent class
- Error rate: proportion of instances that don't belong to the majority class of their corresponding branch
- Choose attribute with lowest error rate

(Assumes nominal attributes)

Classification

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

Evaluating the Weather Attributes

Classification

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

Attribute	Rules	Errors	Total errors
Outlook	$Sunny \to No$	2/5	4/14
	$Overcast \to Yes$	0/4	
	Rainy → Yes	2/5	
Temp	$Hot \to No^*$	2/4	5/14
	$Mild \rightarrow Yes$	2/6	
	Cool o Yes	1/4	
Humidity	High o No	3/7	4/14
	$Normal \to Yes$	1/7	
Windy	False → Yes	2/8	5/14
	True → No*	3/6	

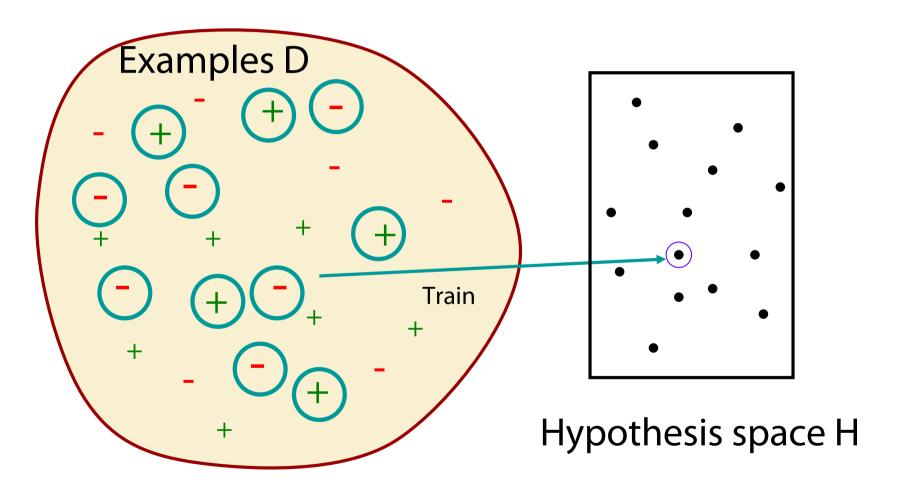
* indicates a tie

Assessing Performance of a Learning Algorithm

- Take out some of the training set
 - Train on the remaining training set
 - Test on the excluded instances
 - Cross-validation

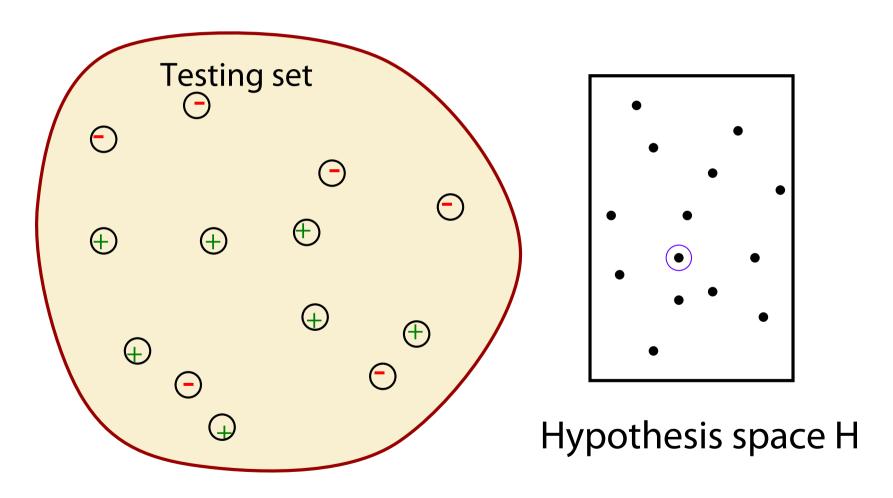


• Split original set of examples, train



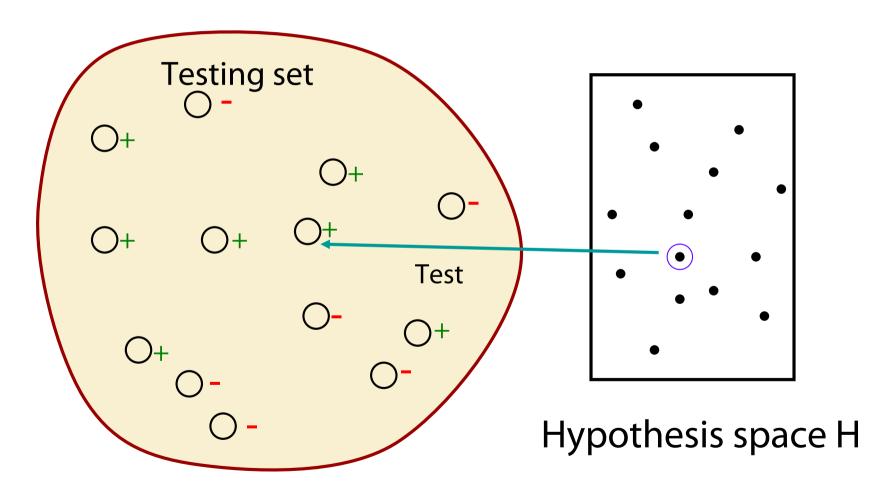


• Evaluate hypothesis on testing set

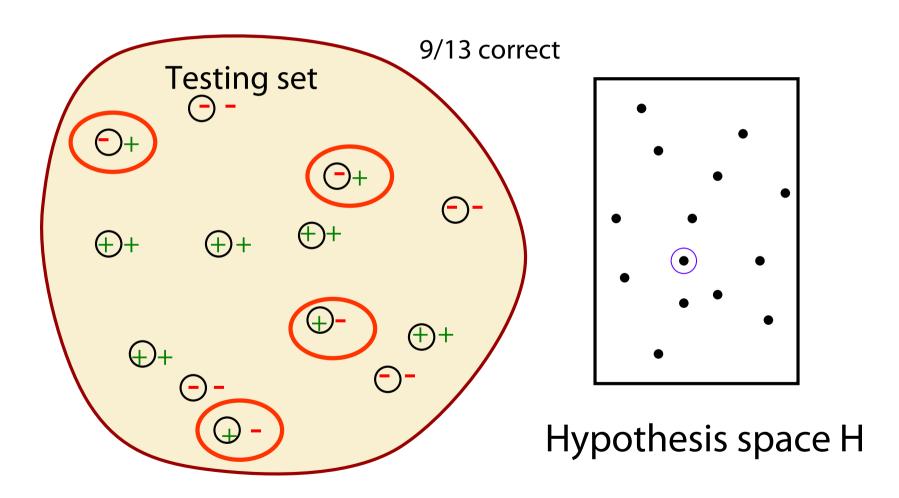




• Evaluate hypothesis on testing set



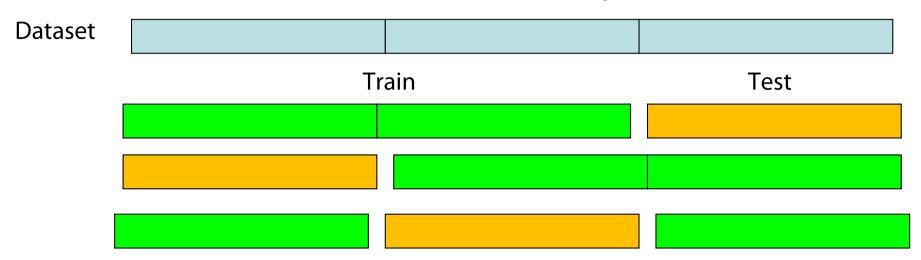
Compare true concept against prediction





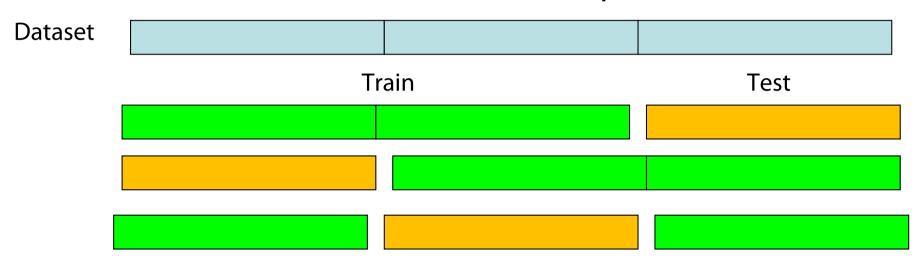
Common Splitting Strategies

k-fold cross-validation: k random partitions



Common Splitting Strategies

k-fold cross-validation: k random partitions



Leave-p-out: all possible combinations of p instances



Discussion of 1R

- 1R was described in a paper by Holte (1993)
 - Contains an experimental evaluation on 16 datasets (using cross-validation so that results were representative of performance on future data)
 - Minimum number of instances was set to 6 after some experimentation
 - 1R's simple rules performed not much worse than much more complex classifiers
- Simplicity first pays off!



From ID3 to C4.5: History

- ID3 (Quinlan) 1960s
- CHAID (CHi-squared Automatic Interaction Detector) 1960s
- CART (Classification And Regression Tree)
 - Uses another split heuristics (Gini impurity measure)
- C4.5 innovations (Quinlan):
 - Permit numeric attributes
 - Deal with missing values
 - Pruning to deal with noisy data
- C4.5 one of best-known and most widely-used learning algorithms
 - Last research version: C4.8, implemented in Weka as J4.8 (Java)
 - Commercial successor: C5.0 (available from Rulequest)



Dealing with Numeric (Metric) Attributes

Outlook	Temperature	Humidity	Windy	Play	
Sunny	85.3	85	False	No	
Sunny	80.2	90	True	No	
Overcast	83.8	86	False	Yes	
Rainy	75.2	80	False	Yes	

64 65 68 69 70 71 72 72 75 75 80 81 83 85

- Discretize numeric attributes
- Divide each attribute's range into intervals
 - Sort instances according to attribute's values
 - Place breakpoints where the class changes
 This minimizes the total error



The problem of Overfitting

- This procedure is very sensitive to noise
 - One instance with an incorrect class label will probably produce a separate interval
- Also: time stamp attribute will have zero errors
- Simple solution: enforce minimum number of instances in majority class per interval



Discretization Example

• Example (with min = 3):



Same decision for both intervals

Final result for temperature attribute

```
64 65 68 69 70 71 72 72 75 75 80 81 83 85

Yes No Yes Yes Yes Yes Yes Yes No Yes Yes No
```



With Overfitting Avoidance

Resulting rule set:

Attribute	Rules	Errors	Total errors
Outlook	Sunny → No	2/5	4/14
	Overcast → Yes	0/4	
	Rainy → Yes	2/5	
Temperature	\leq 77.5 \rightarrow Yes	3/10	5/14
	> 77.5 → No*	2/4	
Humidity	\leq 82.5 \rightarrow Yes	1/7	3/14
	> 82.5 and \leq 95.5 \rightarrow No	2/6	
	> 95.5 → Yes	0/1	
Windy	False → Yes	2/8	5/14
	True → No*	3/6	



Numeric Attributes – Advanced

- Standard method: binary splits
 - E.g. temp < 45
- Unlike nominal attributes, every attribute has many possible split points
- Solution is straightforward extension:
 - Evaluate info gain (or other measure)
 for every possible split point of attribute
 - Choose "best" split point
 - Info gain for best split point is info gain for attribute
- Computationally more demanding



Example

Split on temperature attribute:

- E.g. temperature < 71.5: yes/4, no/2 temperature ≥ 71.5: yes/5, no/3
- Info([4,2],[5,3])= 6/14 info([4,2]) + 8/14 info([5,3])= 0.939 bits
- Place split points halfway between values
- Can evaluate all split points in one pass!



Missing as a Separate Value

- Missing value denoted "?" in C4.X (Null value)
- Simple idea: treat missing as a separate value
- Q: When is this not appropriate?
- A: When values are missing due to different reasons
 - Example 1: blood sugar value could be missing when it is very high or very low
 - Example 2: field **IsPregnant** missing for a male patient should be treated differently (no) than for a female patient of age 25 (unknown)



Missing Values – Advanced

Questions:

- How should tests on attributes with different unknown values be handled?
- How should the partitioning be done in case of examples with unknown values?
- How should an unseen case with missing values be handled?



Missing Values – Advanced

- Info gain with unknown values during learning
 - Let T be the training set and X a test on an attribute with unknown values and F be the fraction of examples where the value is known.
 - Rewrite the gain:

```
Gain(X) = probability that A is known * (info(T) – info<sub>X</sub>(T))+
probability that A is unknown * 0
= F * (info(T) - info<sub>X</sub>(T))
```

- Consider instances w/o missing values
- Split w.r.t. those instances
- Distribute instances with missing values proportionally



Pruning

- Goal: Prevent overfitting to noise in the data
- Two strategies for "pruning" the decision tree:
 - Postpruning take a fully-grown decision tree and discard unreliable parts
 - Prepruning stop growing a branch when information becomes unreliable
- Postpruning preferred in practice—prepruning can "stop too early"



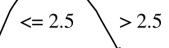
Post-pruning

- First, build full tree
- Then, prune it
 - Fully-grown tree shows all attribute interactions
- Two pruning operations:
 - 1. Subtree replacement
 - 2. Subtree raising



Subtree replacement

wage increase 1st year



bad

statutory holidays

> 10

- Bottom-up
- Consider replacing a tree

only after considering all its subtrees wage increase 1st y

<= 2.5

good

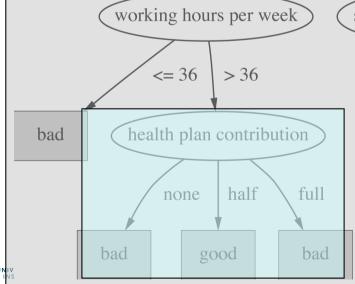
wage increase 1st year

<= 10



bad

good



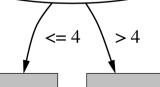
statutory holidays

> 2.5



good

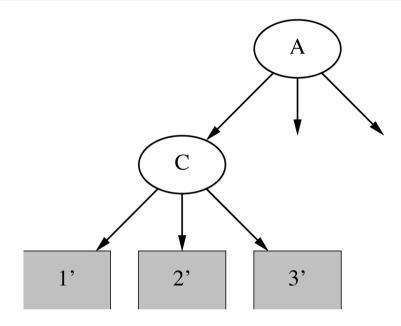
wage increase 1st year



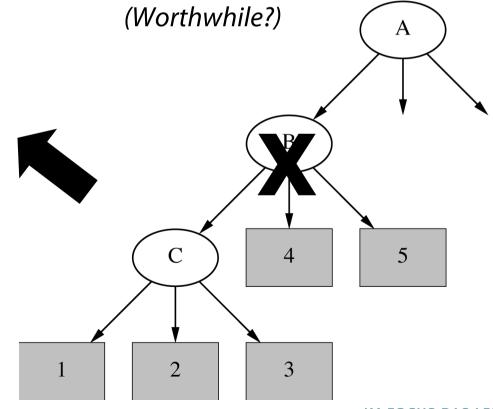
bad

good

*Subtree raising



- Delete node
- Redistribute instances
- Slower than subtree replacement





Post-pruning

- First, build full tree
- Then, prune it
 - Fully-grown tree shows all attribute interactions
- → Expected Error Pruning



Estimating Error Rates

- Prune only if it reduces the estimated error
- Error on the training data is NOT a useful estimator
 - Q: Why would it result in very little pruning?
- Use hold-out set for pruning ("reduced-error pruning")



Expected Error Pruning

- Approximate expected error assuming that we prune at a particular node.
- Approximate backed-up error from children assuming we did not prune.
- If expected error is less than backed-up error, prune.



Static Expected Error

- If we prune a node, it becomes a leaf labeled C
- What will be the expected classification error at this leaf?

$$E(S) = \frac{N - n + k - 1}{N + k}$$

S is the set of examples in a node

k is the number of classes

N examples in S

C the majority class in S

n out of N examples in S belong to C

Laplace error estimate – based on the assumption that the distribution of probabilities that examples will belong to different classes is uniform.



Backed-up Error

- For a non-leaf node Node
- Let children of Node be Node₁, Node₂, etc.
 - Probabilities can be estimated by relative frequencies of attribute values in sets of examples that fall into child nodes

$$BackedUpError(Node) = \sum_{i} P_{i} \times Error(Node_{i})$$

$$Error(Node) = min(E(Node), BackedUpError(Node))$$

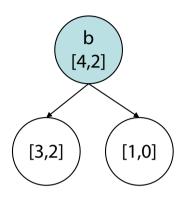


Example Calculation

Error Calculation for Pruning Example

• Left child of b has class frequencies [3, 2]

$$E = \frac{N - n + k - 1}{N + k} = \frac{5 - 3 + 2 - 1}{5 + 2} = 0.429$$



- Right child has error of 0.333, calculated in the same way
- Static error estimate E(b) is 0.375, again calculated using the Laplace error estimate formula, with N=6, n=4, and k=2.
- · Backed-up error is:

$$BackedUpError(b) = (5/6) \times 0.429 + (1/6) \times 0.333 = 0.413$$

(5/6 and 1/6 because there are 4+2=6 examples handled by node b, of which 3+2=5 go to the left subtree and 1 to the right subtree.

 Since backed-up estimate of 0.413 is greater than static estimate of 0.375, we prune the tree and use the static error of 0.375

Example Calculation

Static Expected Error of b

$$E([4,2]) = \frac{N-n+k}{N+k}$$

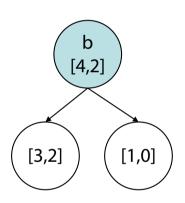
0,375

Left child of b

$$E([3,2]) = \frac{5-3+2-1}{5+2} = 0,429$$

Right child of b

$$E([1,0]) = \frac{1-1+2-1}{1+2} = 0.333$$

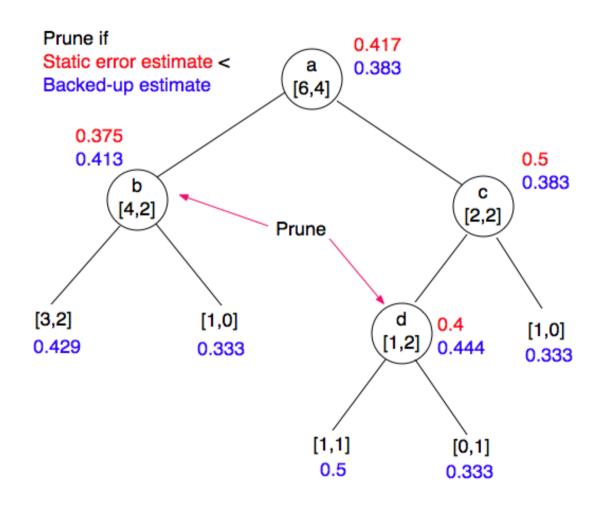


Backed Up Error of b

$$BackedUpError(b) = \frac{5}{6}E([3,2]) + \frac{1}{6}E([1,0]) = 0,413$$

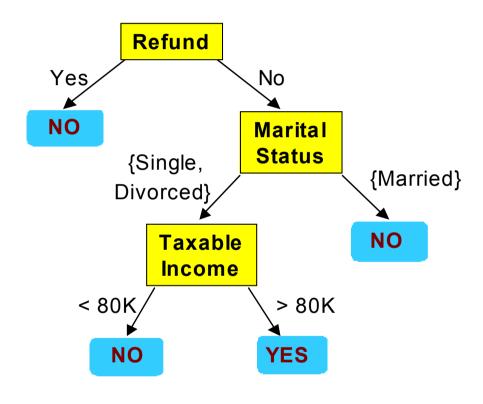
• $0,375 < 0,413 \rightarrow Prune tree.$

Example





From Decision Trees To Rules



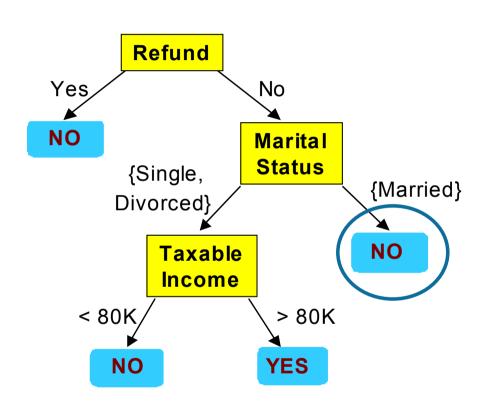
- Refund = Yes \rightarrow No
- Refund = No ∧ Marital
 Status = {Single, Divorced}
 ∧ Taxable Income < 80k
 → No
- Refund = No ∧ Marital
 Status = {Single, Divorced}
 ∧ Taxable Income > 80k
 → Yes
- Refund = No ∧ Marital
 Status = Married → No

From Decision Trees to Rules

- Derive a rule set from a decision tree:
 Write a rule for each path from the root to a leaf.
 - The left-hand side is easily built from the label of the nodes and the labels of the arcs.
- Rules are mutually exclusive and exhaustive.
- Rule set contains as much information as the tree



Rules Can Be Simplified



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

Initial Rule: (Refund=N

 $(Refund=No) \land (Status=Married) \rightarrow No$



Rules Can Be Simplified

- The resulting rules set can be simplified:
 - Let LHS be the left hand side of a rule.
 - Let LHS' be obtained from LHS by eliminating some conditions.
 - We can certainly replace LHS by LHS' in this rule if the subsets of the training set that satisfy respectively LHS and LHS' are equal.
 - A rule may be eliminated by using meta-conditions such as "if no other rule applies".



VSL vs DTL

- Decision tree learning (DTL) is more efficient if all examples are given in advance; else, it may produce successive hypotheses, each poorly related to the previous one
- Version space learning (VSL) is incremental
- DTL can produce simplified hypotheses that do not agree with all examples
- DTL has been more widely used in practice

