# Einführung in Web- und Data-Science

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Tanya Braun (Übungen)



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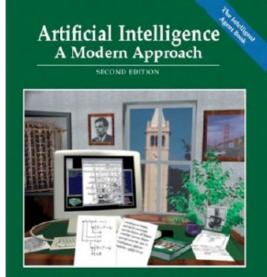
# Übersicht

- Einführung, Klassifikation vs. Regression, parametrisches und nicht-parametrisches überwachtes Lernen
- Neuronale Netze und Support-Vektor-Maschinen
- Häufungsanalysen, Warenkorbanalyse, Empfehlungen
- Statistische Grundlagen: Stichproben, Schätzer, Verteilung, Dichte, kumulative Verteilung, Skalen: Nominal-, Ordinal-, Intervall- und Verhältnisskala, Hypothesentests, Konfidenzintervalle, Reliabilität, Interne Konsistenz, Cronbach Alpha, Trennschärfe
- Bayessche Statistik, Bayessche Netze zur Spezifikation von diskreten Verteilungen, Anfragen, Anfragebeantwortung, Lernverfahren für Bayessche Netze bei vollständigen Daten
- Induktives Lernen: Versionsraum, Informationstheorie, Entscheidungsbäume, Lernen von Regeln
- Ensemble-Methoden, Bagging, Boosting, Random Forests
- Clusterbildung, K-Means, Analyse der Variation (Analysis of Variation, ANOVA), Inter-Cluster-Variation, Intra-Cluster-Variation, F-Statistik, Bonferroni-Korrektur, MANOVA, Discriminant Function Analysis
- Analyse Sozialer Strukturen



# Inductive Learning

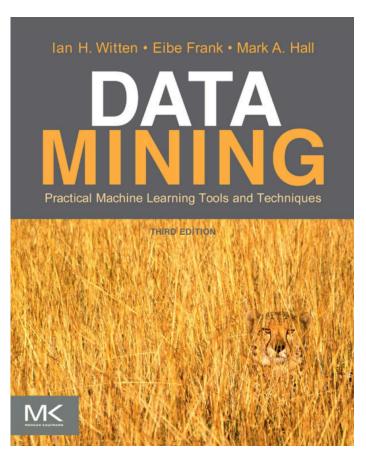




Stuart Russell • Peter Norvig

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?



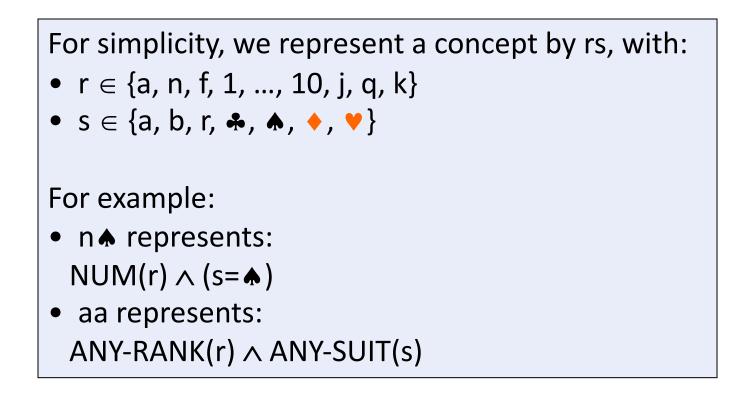
$$(r=1) \vee ... \vee (r=10) \vee (r=J) \vee (r=Q) \vee (r=K) \Leftrightarrow ANY-RANK(r$$
  
 $(r=1) \vee ... \vee (r=10) \Leftrightarrow NUM(r)$   
 $(r=J) \vee (r=Q) \vee (r=K) \Leftrightarrow FACE(r)$   
 $(s=\clubsuit) \vee (s=\clubsuit) \vee (s=\spadesuit) \vee (s=\blacktriangledown) \Rightarrow ANY-SUIT(s)$   
 $(s=\clubsuit) \vee (s=\clubsuit) \Leftrightarrow BLACK(s)$   
 $(s=\bigstar) \vee (s=\blacktriangledown) \Leftrightarrow RED(s)$ 

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)







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

Examples:

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



#### More General/Specific Relation

- Let  $h_1$  and  $h_2$  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

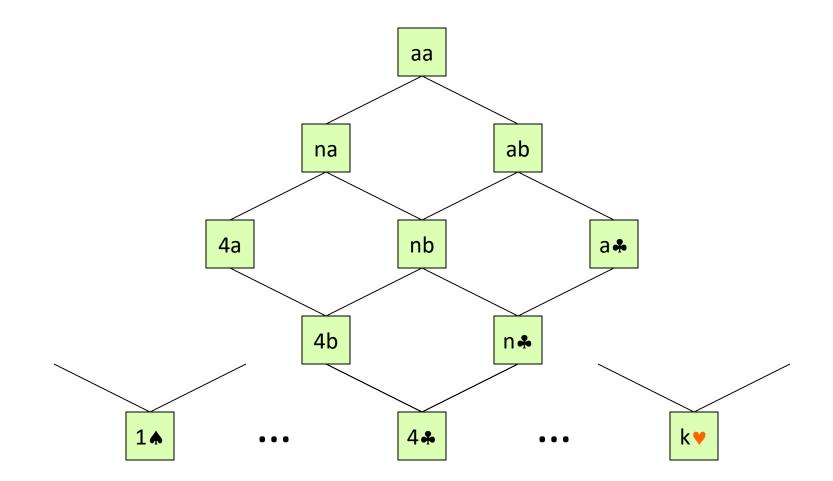


#### More General/Specific Relation

- Let h<sub>1</sub> and h<sub>2</sub> 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





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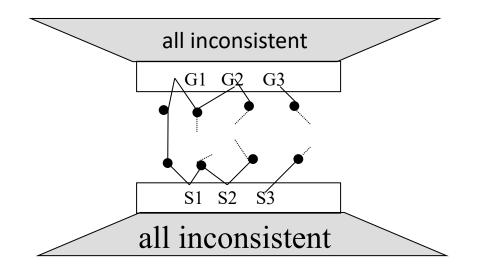
### G-Boundary / S-Boundary of V

- 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

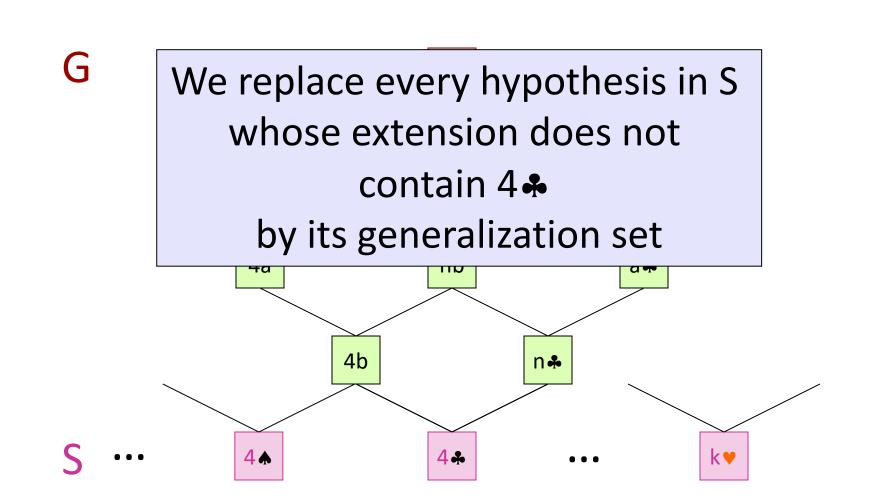


# G-Boundary / S-Boundary of V

- 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

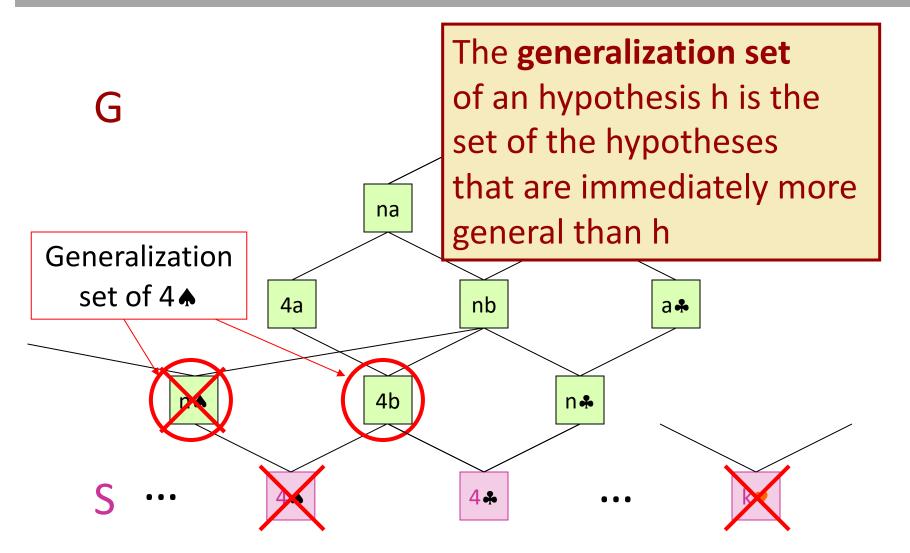




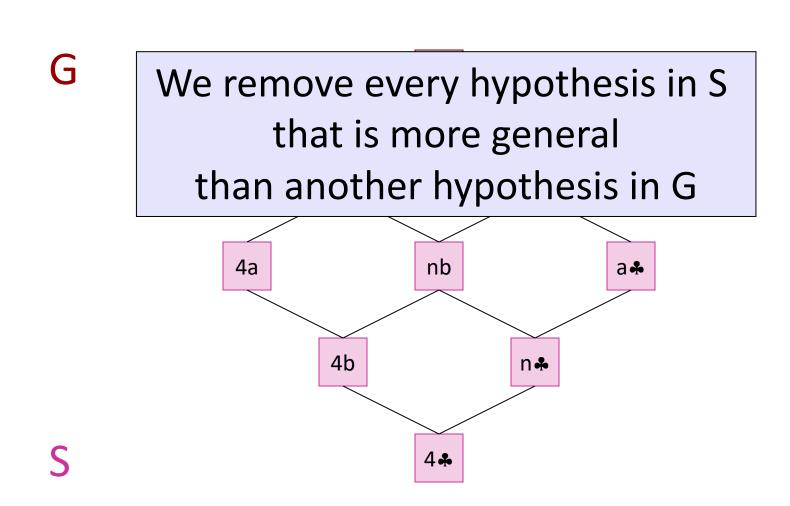




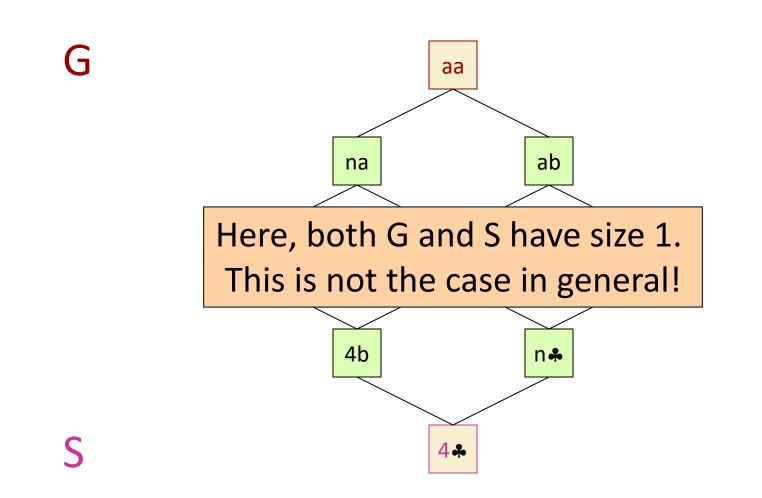
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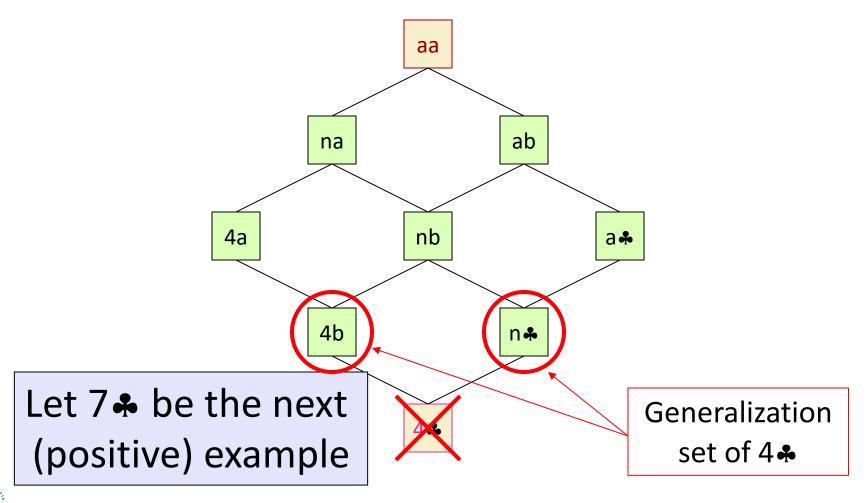




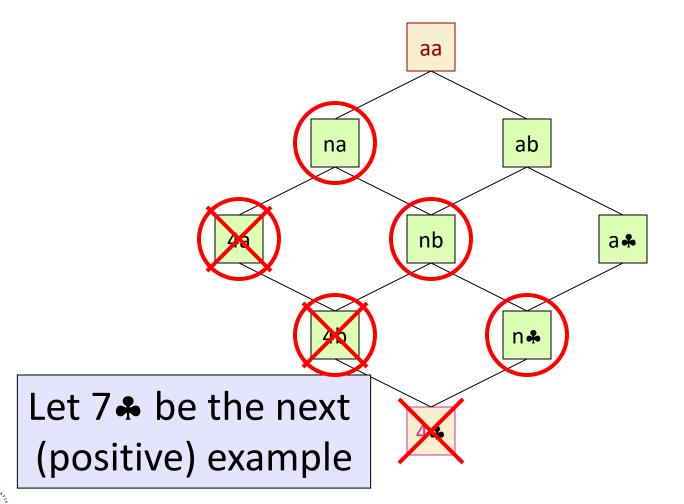


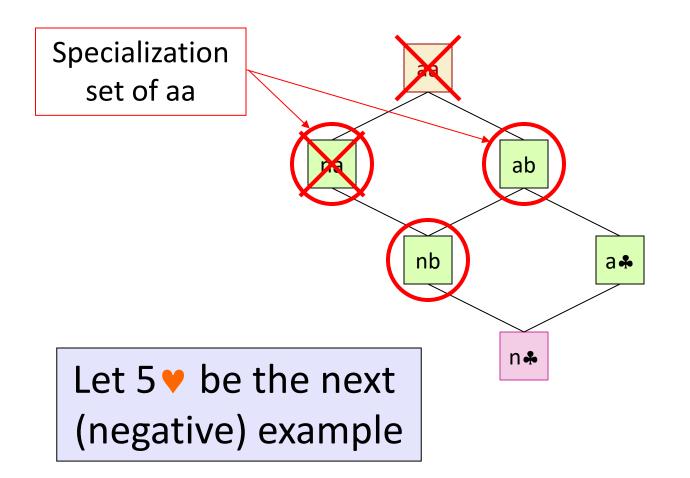






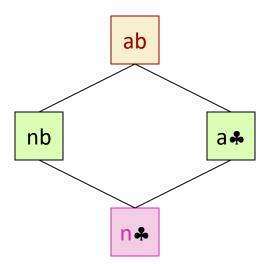
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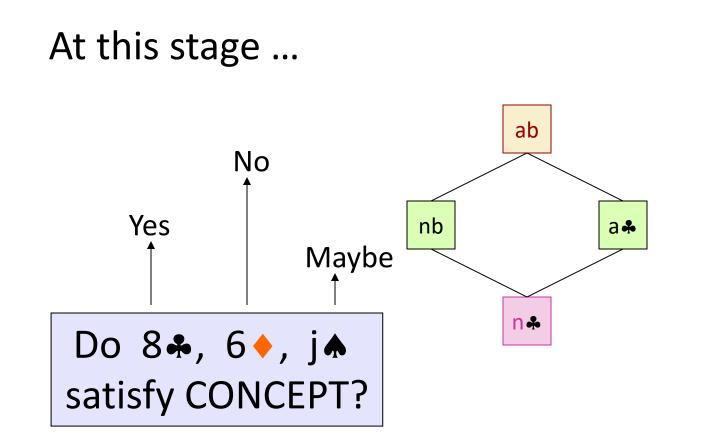




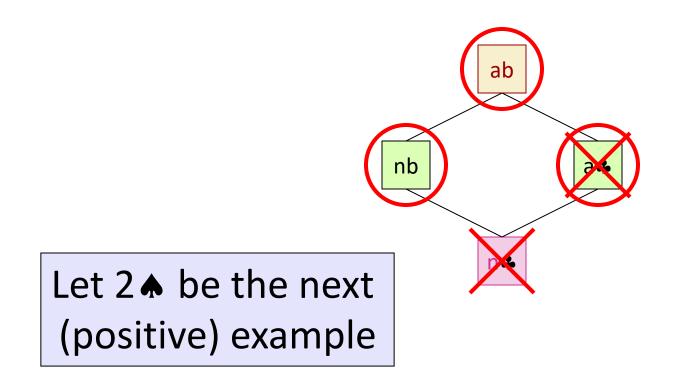
# G and S, and all hypotheses in between form exactly the version space



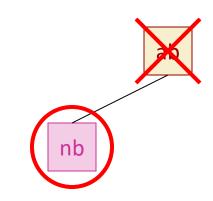












# Let j he the next (negative) example



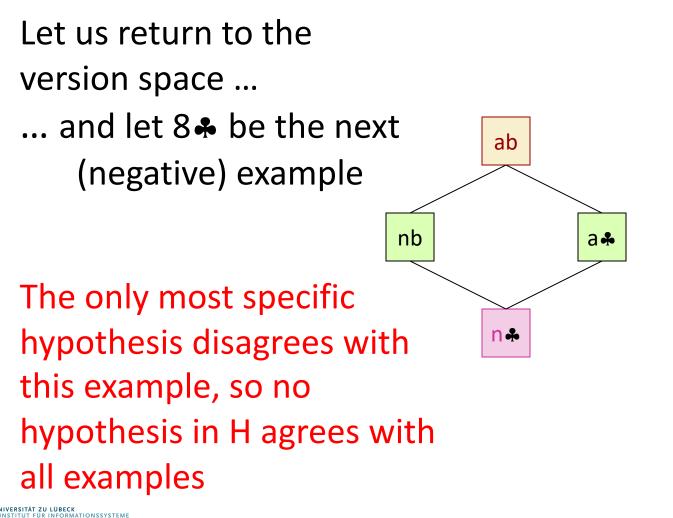
#### + 4♣ 7♣ 2♠ - 5♥ j♠

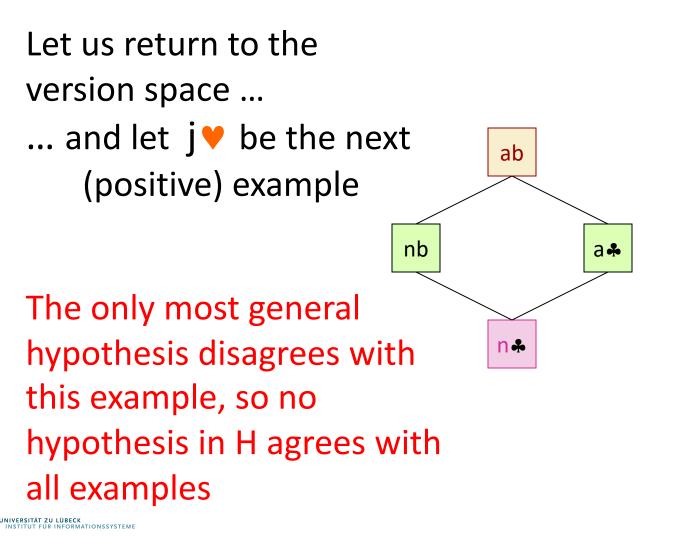
nb

#### NUM(r) ∧ BLACK(s)



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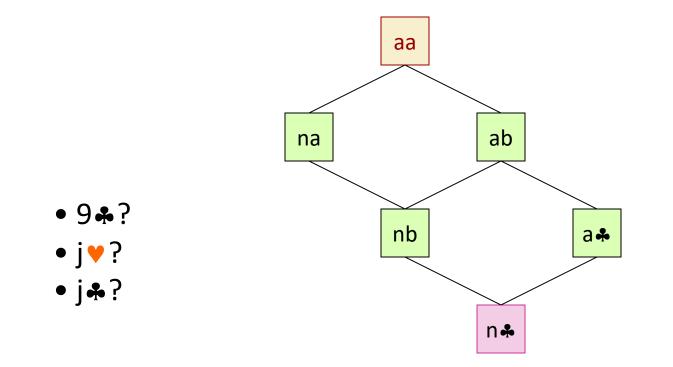


# **Example-Selection Strategy**

- 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





# **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

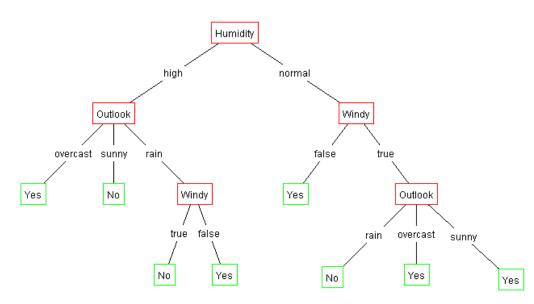
- If some examples are misclassified, the version space may collapse
- Possible solution:

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





- 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.



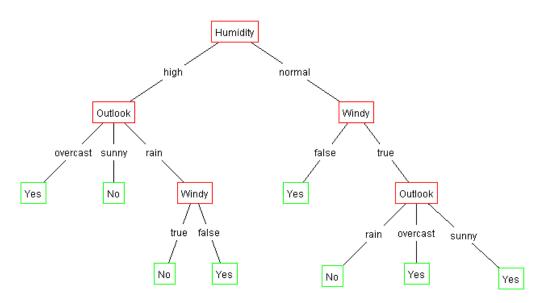
# Choosing the Best Attribute

- 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.



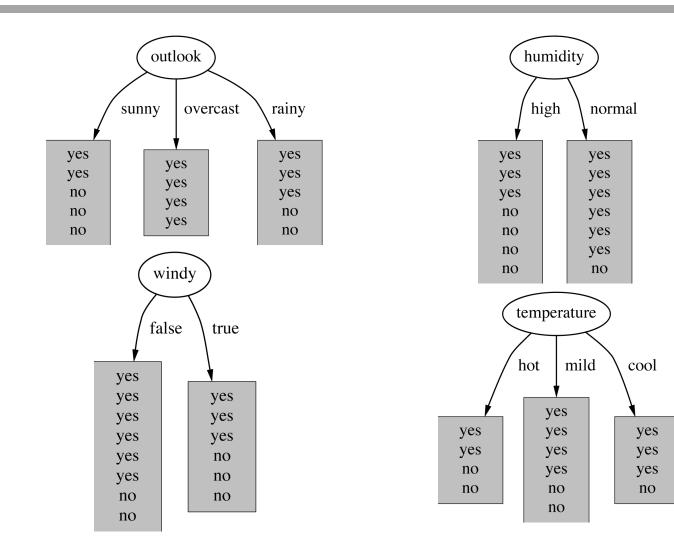
#### **Decision Trees**

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





#### Which attribute to select?





Anmeldung zur Klausur wird nach der Vorlesung freigeschaltet

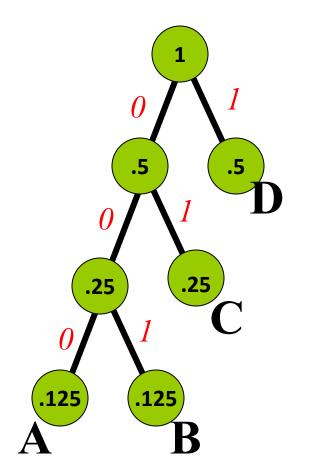
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# Huffman code example





Μ	code 1	ength	prob	Exp. len
А	000	3	0,125	0,375
В	001	3	0,125	0,375
С	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 (number of bits) 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

 $P = (p_1, p_2, .., p_n)$ 

• the information conveyed by distribution (aka entropy of P) is:

 $I(P) = -(p_1^* \log(p_1) + p_2^* \log(p_2) + ... + p_n^* \log(p_n))$ = - \sum\_i p\_i^\* \log(p\_i)



# **Information Theory Background**

- Information conveyed by distribution (aka entropy of P) is:
   I(P) = -(p<sub>1</sub>\*log(p<sub>1</sub>) + p<sub>2</sub>\*log(p<sub>2</sub>) + .. + p<sub>n</sub>\*log(p<sub>n</sub>))
- 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":

 $info([2,3]) = entropy(2/5,3/5) = -2/5\log(2/5) - 3/5\log(3/5) = 0.971$  bits

- "Outlook" = "Overcast": info([4,0]) = entropy(1,0) = -1log(1) - 0log(0) = 0 bitsNote: log( not define we evalue
- "Outlook" = "Rainy":

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

 $info([3,2]) = entropy(3/5,2/5) = -3/5\log(3/5) - 2/5\log(2/5) = 0.971$  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)

gain("Outlook") = info([9,5]) - info([2,3],[4,0],[3,2]) = 0.940 - 0.693= 0.247 bits



### Computing the information gain

• Information gain:

(information before split) – (information after split)

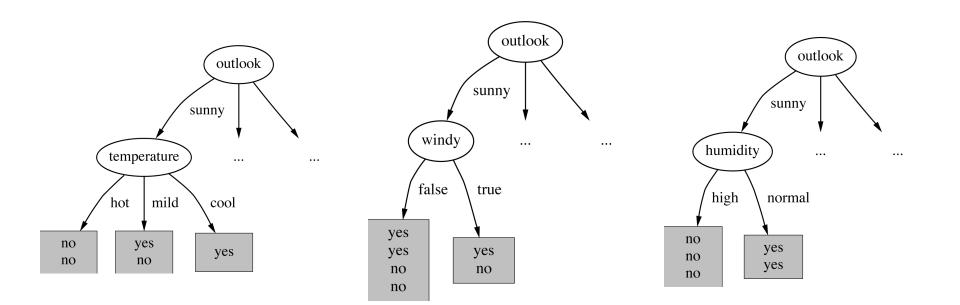
gain("Outlook") = info([9,5]) - info([2,3],[4,0],[3,2]) = 0.940 - 0.693= 0.247 bits

• 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



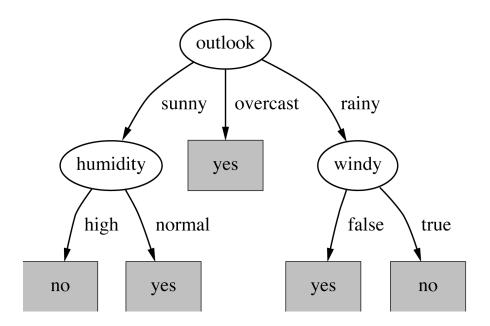
gain("Humidity") = 0.971 bits

gain("Temperature") = 0.571 bits

gain("Windy") = 0.020 bits



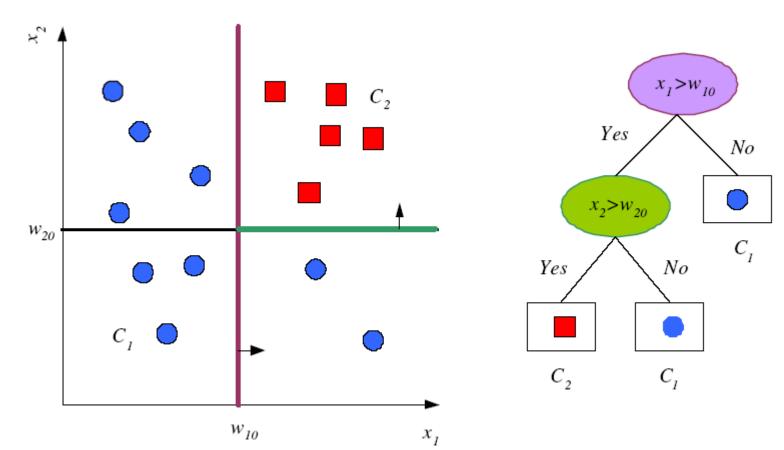
### The final decision tree



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

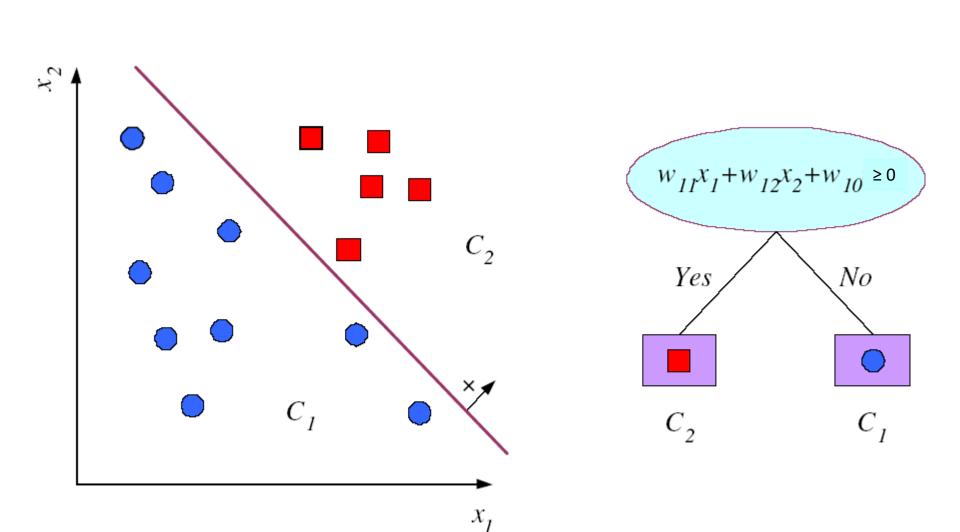


#### **Univariate Splits**





#### **Multivariate Splits**



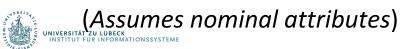


# 1R – Simplicity First!

#### 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



#### Outlook Windv Humidity Plav Temp False Sunny Hot High No Sunnv Hot Hiah True No Overcast High False Yes Hot False Rainv Mild Hiah Yes Normal Rainy Cool False Yes Normal Rainy Cool True No Overcast Cool Normal True Yes Sunny False No Mild High Normal False Sunnv Cool Yes Rainy Mild Normal False Yes Sunny Mild Normal Yes True Overcast Mild Hiah True Yes Normal False Yes **Overcast** Hot Rainv Mild High True No

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Classification

### **Evaluating the Weather Attributes**

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			
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#### Classification

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

#### \* indicates a tie

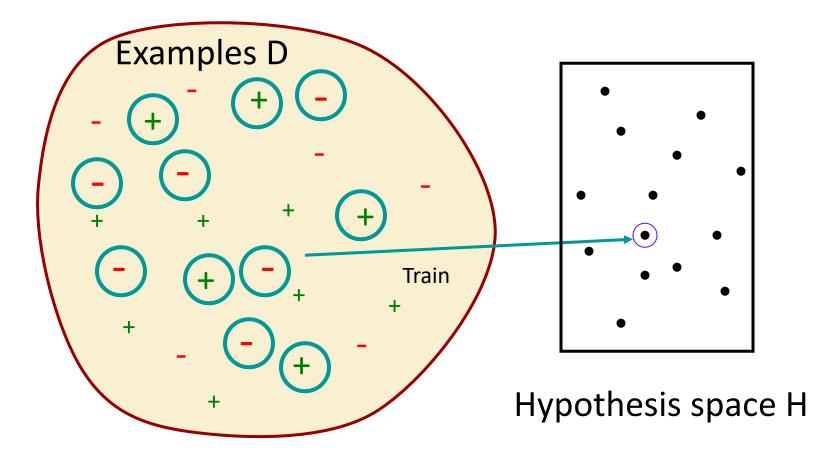


#### Assessing Performance of a Learning Algorithm

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

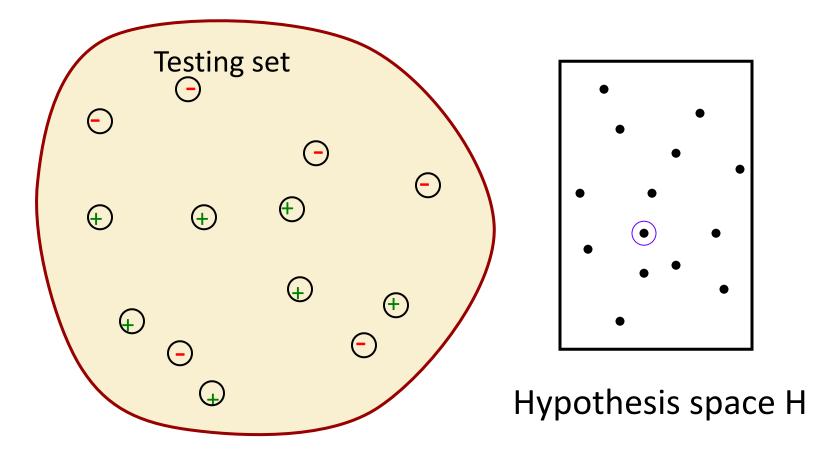


• Split original set of examples, train



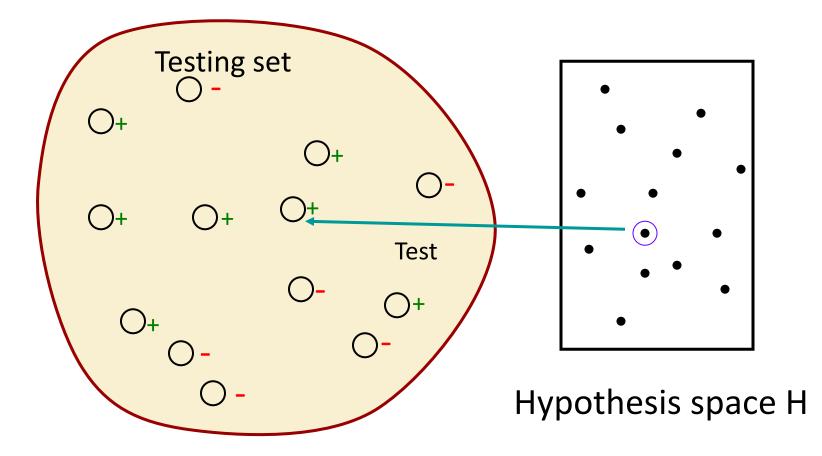


• Evaluate hypothesis on testing set



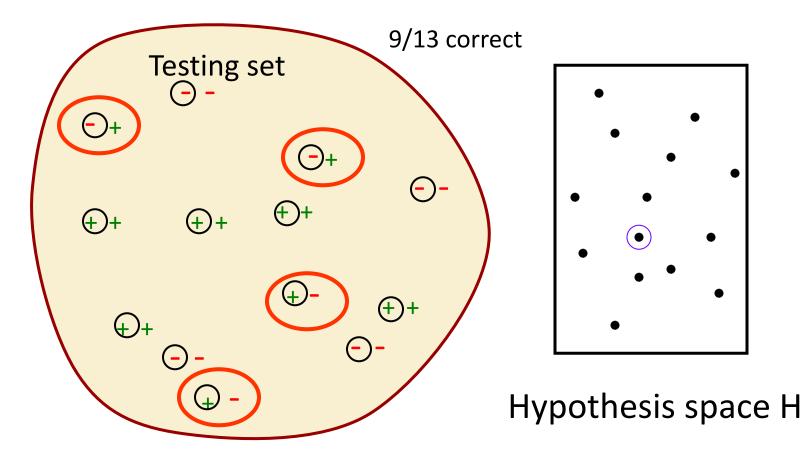


• Evaluate hypothesis on testing set





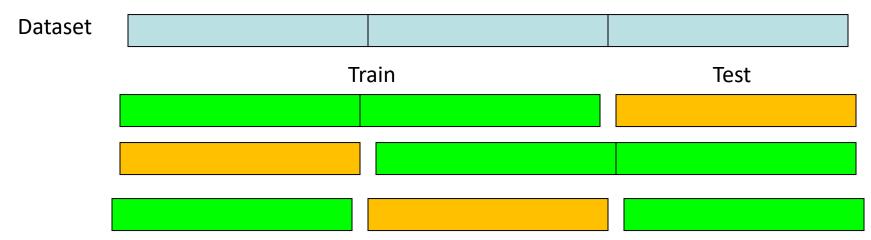
• Compare true concept against prediction





#### **Common Splitting Strategies**

• k-fold cross-validation: k random partitions

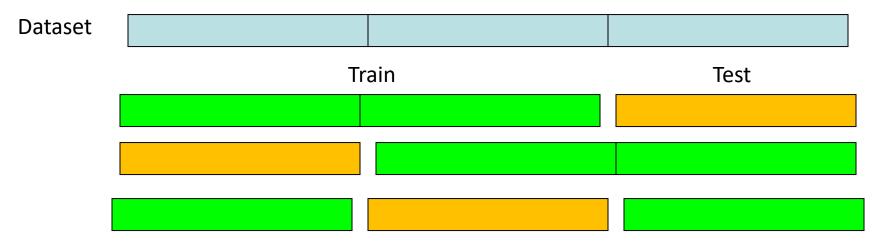




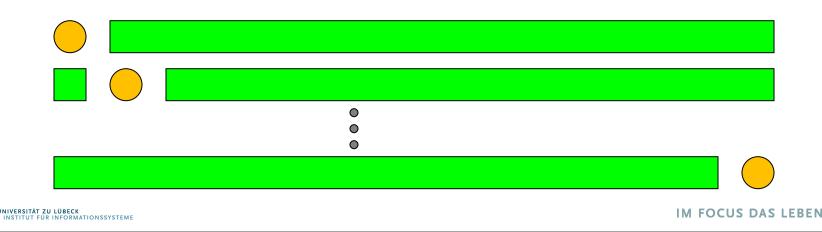
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#### **Common Splitting Strategies**

• 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

	Outlool	K	Те	mpera	ture		Humi	dity	Wi	indy	F	Play	
	Sunny				85.3			85	Fa	lse	ſ	Vo	
	Sunny				80.2			90	Tru	Je	ſ	No	
(	Overca	st			83.8			86	Fa	lse		les	
1	Rainy				75.2			80	Fa	lse		les	
	65	68	60	70	71	70	72	-	75	75	80	01	83

• Discretize numeric attributes

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- 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

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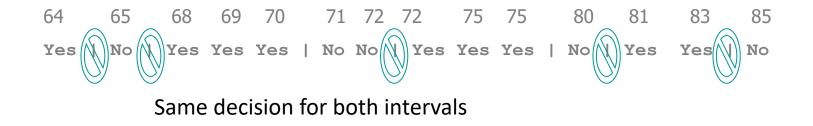
### The problem of Overfitting

- 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

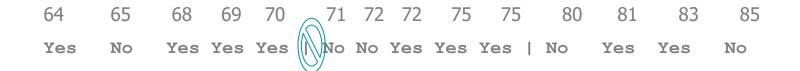


#### **Discretization Example**

• Example (with min = 3):



• Final result for temperature attribute





## With Overfitting Avoidance

#### • Resulting rule set:

Attribute	Rules	Errors	Total errors
Outlook	Sunny $\rightarrow$ No	2/5	4/14
	$Overcast \rightarrow Yes$	0/4	
	Rainy $\rightarrow$ 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 $\rightarrow$ Yes	0/1	
Windy	$False \to Yes$	2/8	5/14
	$True \to No^*$	3/6	



#### Numeric Attributes – Advanced

- Standard method: binary splits
  - E.g. temp < 45</p>
- 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: 68 69 70 72 72 75 75 80 71 65 64 81 83 85 No Yes Yes Yes No Yes Yes Yes No Yes No Yes Yes No
  - 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?



- 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
- → 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 Node<sub>1</sub>, Node<sub>2</sub>, 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*))



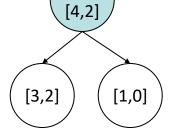
#### **Example Calculation**

- Static Expected Error of b  $E([4,2]) = \frac{N - n + k - 1}{N + k} =$
- Left child of b

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

Right child of b

$$E([1,0]) = \frac{1 - 1 + 2 - 1}{1 + 2} = 0,333$$



b

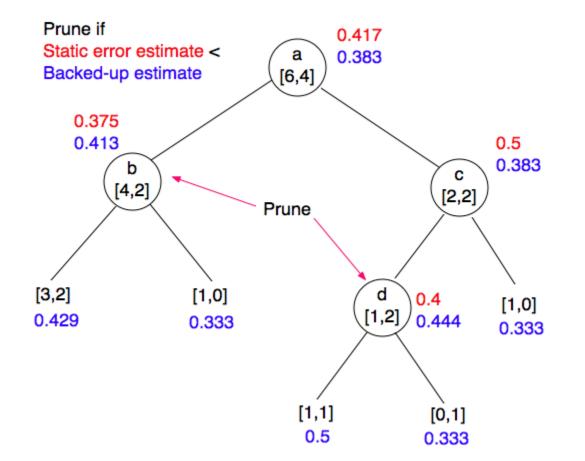
• Backed Up Error of b

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

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

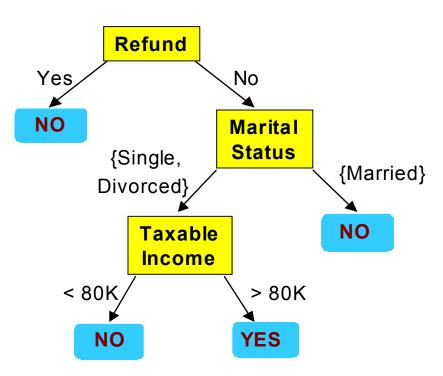


#### Example





#### From Decision Trees To Rules



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

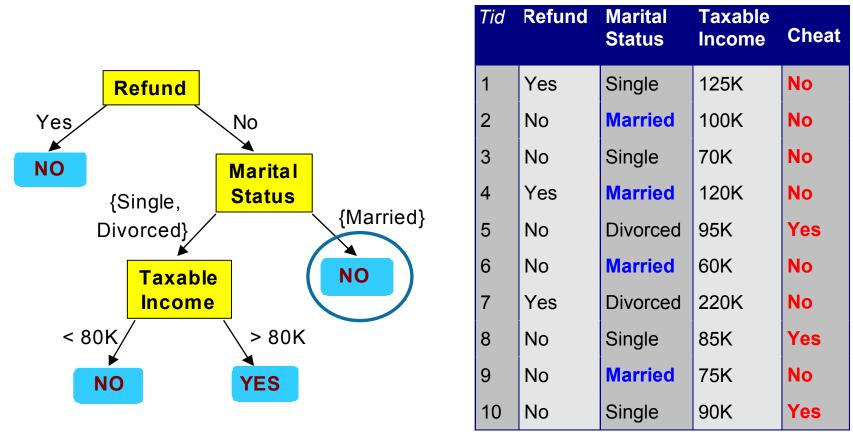


#### From Decision Trees to Rules

- 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**



Initial Rule: (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

