# Einführung in Web- und Data-Science

Inductive Learning

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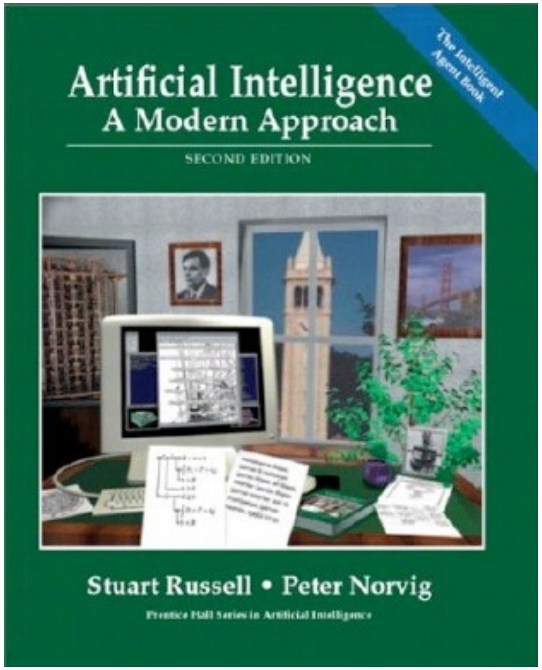
Inductive Learning

# VERSION SPACE

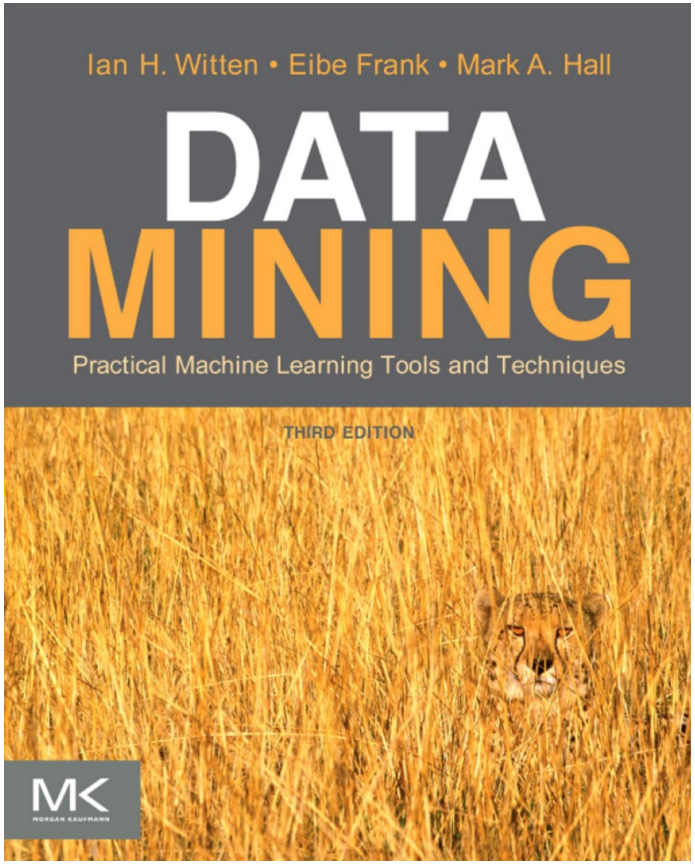
# Inductive Learning

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

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

$(r=1) \vee \ldots \vee (r=10) \Leftrightarrow$ NUM(r)

$(r=J) \vee (r=Q) \vee (r=K) \Leftrightarrow$ FACE(r)

$(s=\spadesuit) \vee (s=\clubsuit) \vee (s=\diamondsuit) \vee (s=\heartsuit) \Leftrightarrow$ ANY-SUIT(s)

$(s=\spadesuit) \vee (s=\clubsuit) \Leftrightarrow$ BLACK(s)

$(s=\diamondsuit) \vee (s=\heartsuit) \Leftrightarrow$ 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 ∈ {a, n, f, 1, …, 10, j, q, k}
- s ∈ {a, b, r, ♣, ♠, ♦, ♥}

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

Inductive Learning

# MOST GENERAL/SPECIFIC HYPOTHESIS

# More General/Specific Relation

- Let $h_1$ and $h_2$ be two hypotheses in H
- $h_1$ is more general than $h_2$ iff the extension of $h_1$ is a proper superset of the extension of $h_2$

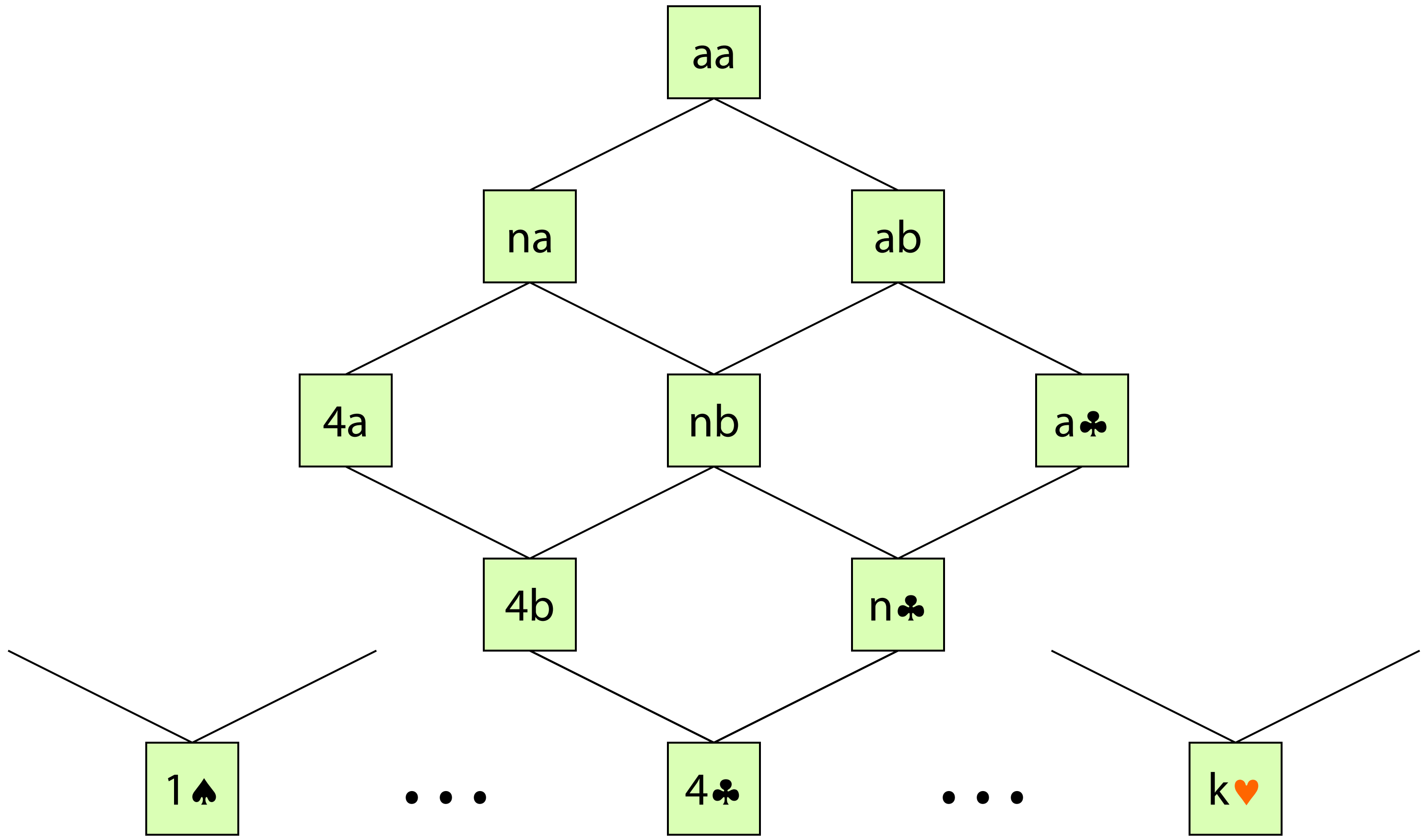
Examples:

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

# More General/Specific Relation

- Let $h_1$ and $h_2$ be two hypotheses in H
- $h_1$ is more general than $h_2$ iff the extension of $h_1$ is a proper superset of the extension of $h_2$
- 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



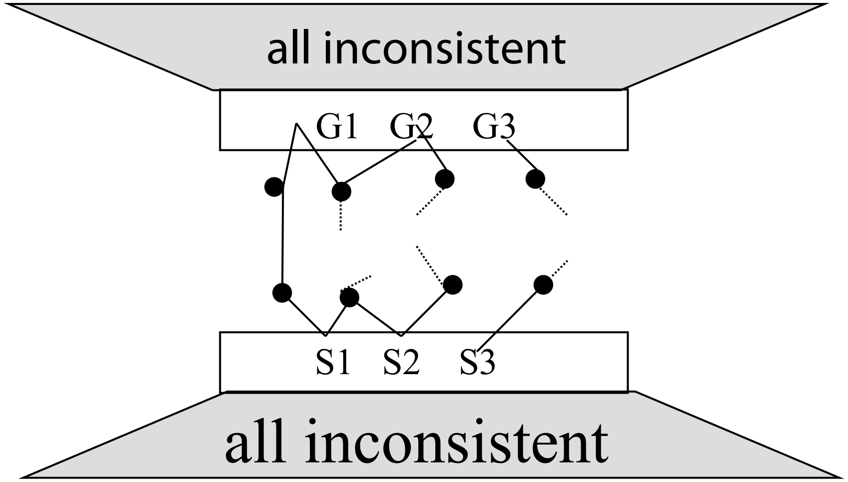
# G-Boundary / S-Boundary of V

- 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

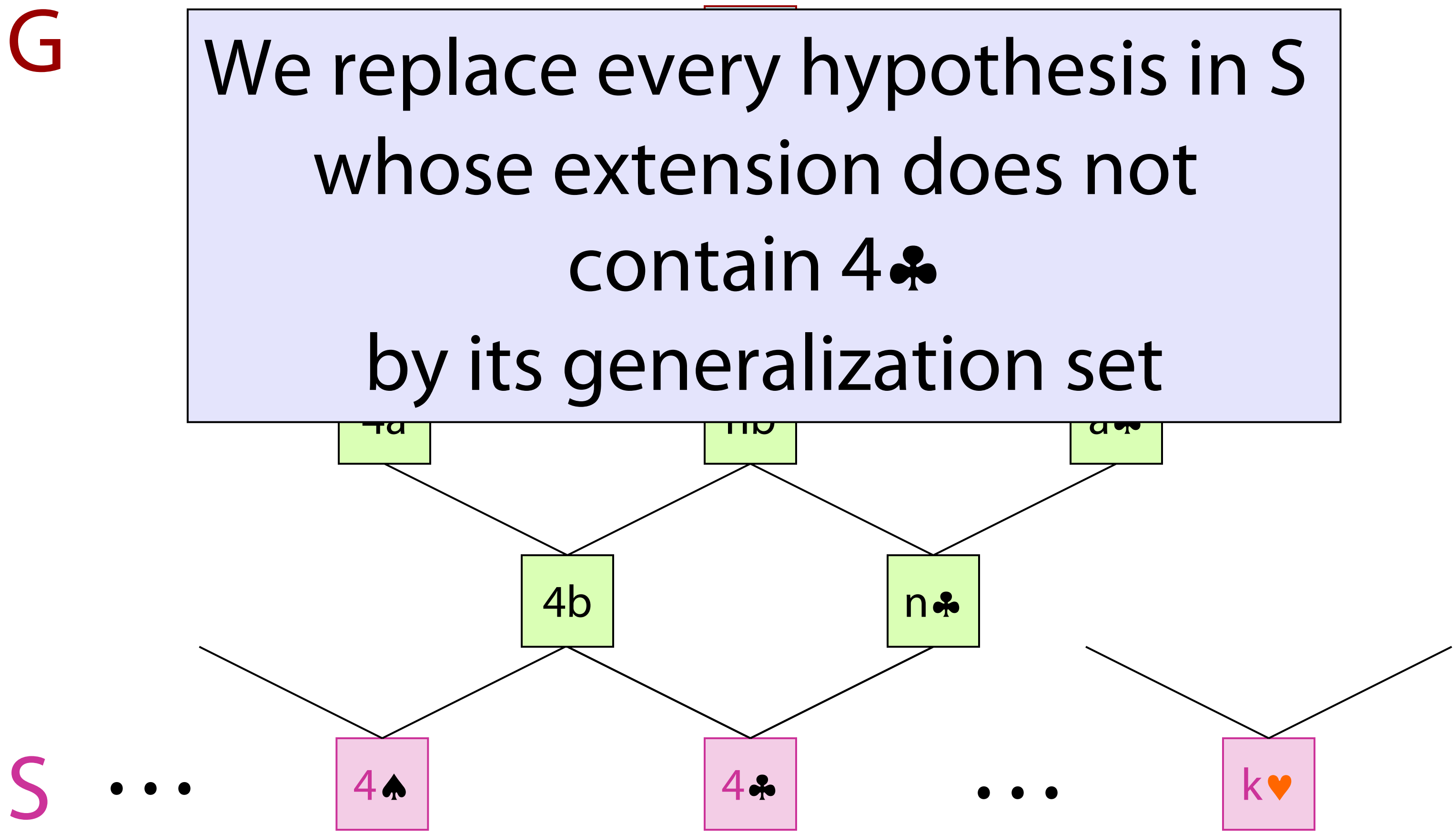
# G-Boundary / S-Boundary of V

- 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



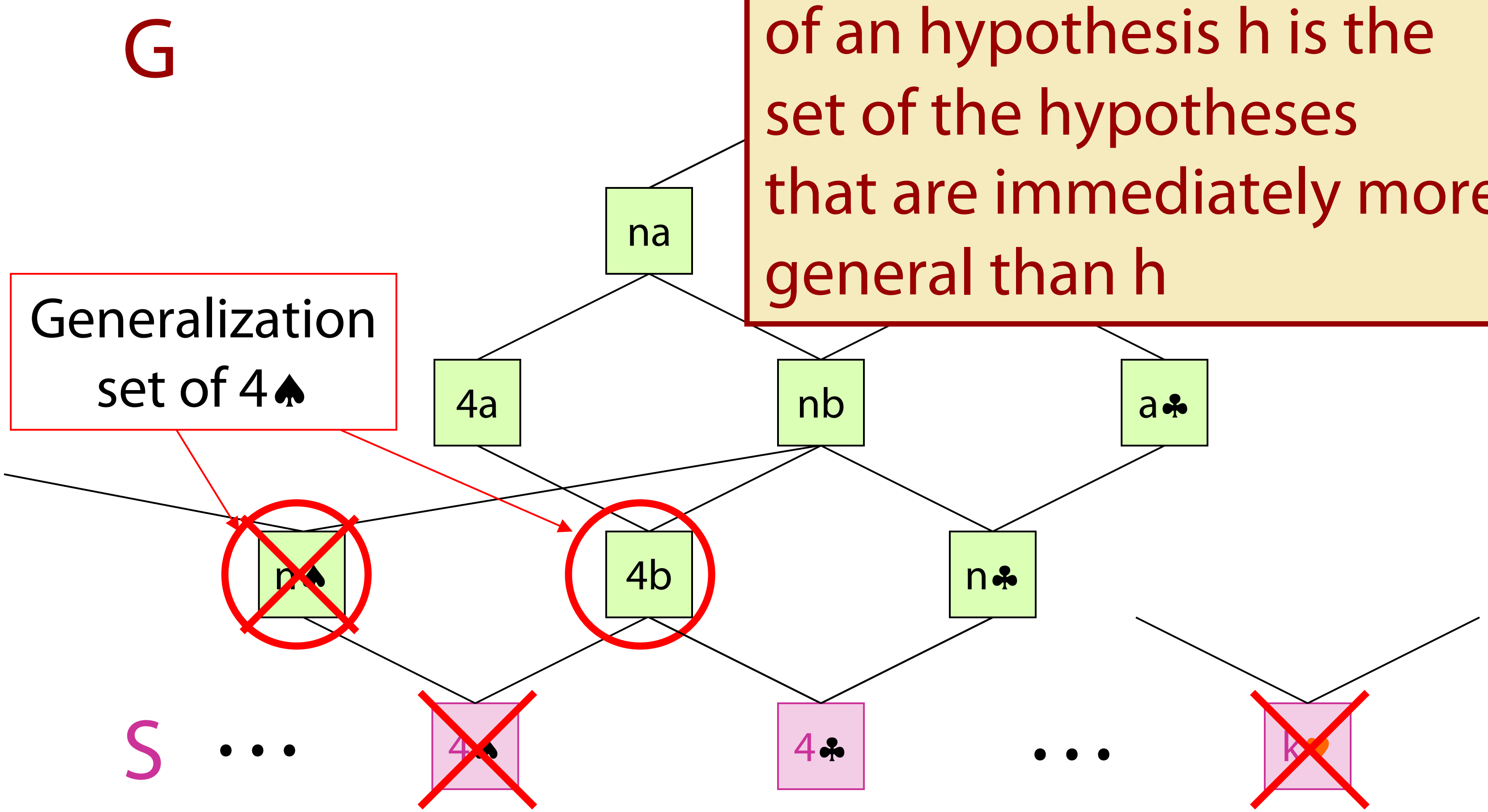
# Example: G-/S-Boundaries of V

We replace every hypothesis in S
whose extension does not
contain 4♣
by its generalization set

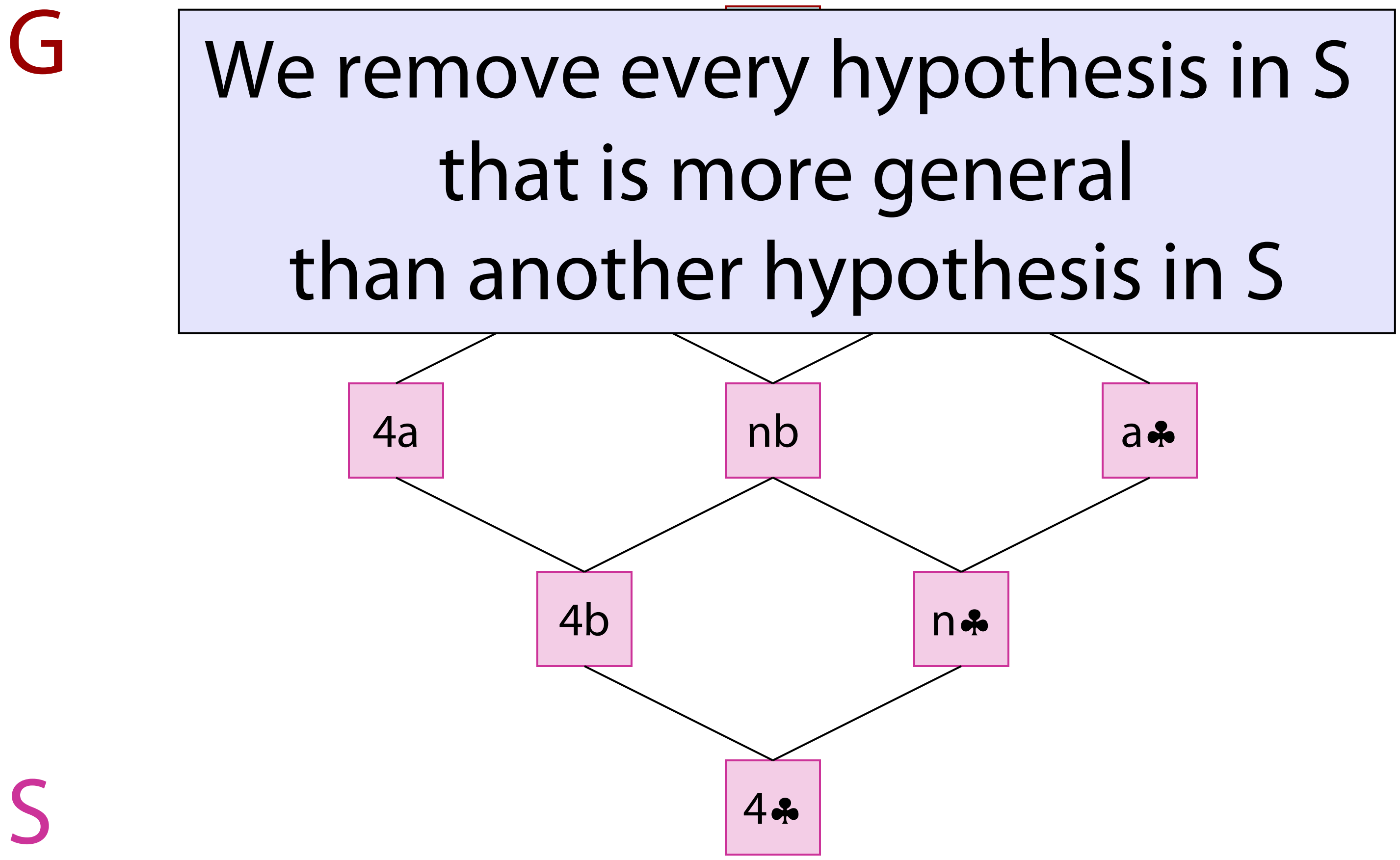


# Example: G-/S-Boundaries of V

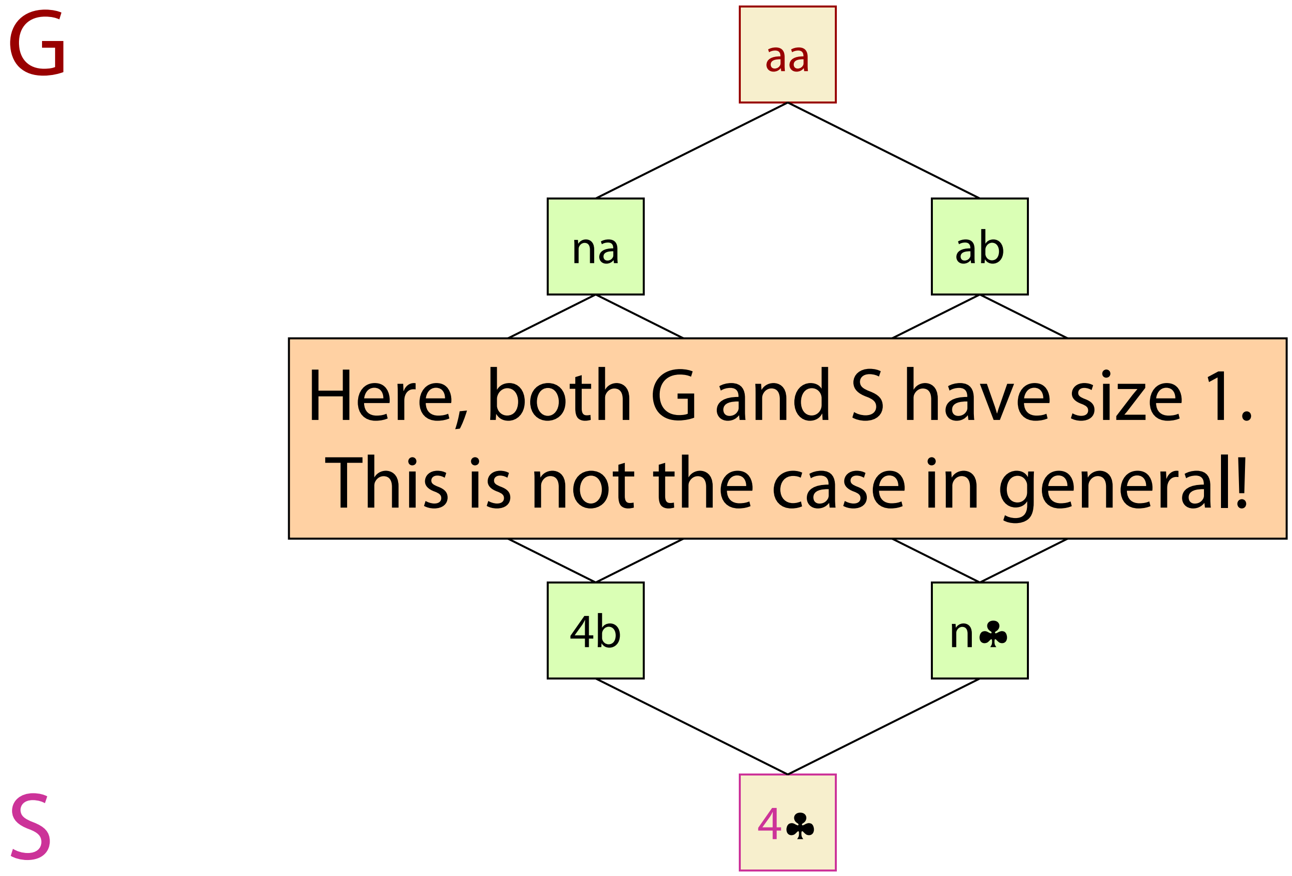
The **generalization set** of an hypothesis h is the set of the hypotheses that are immediately more general than h



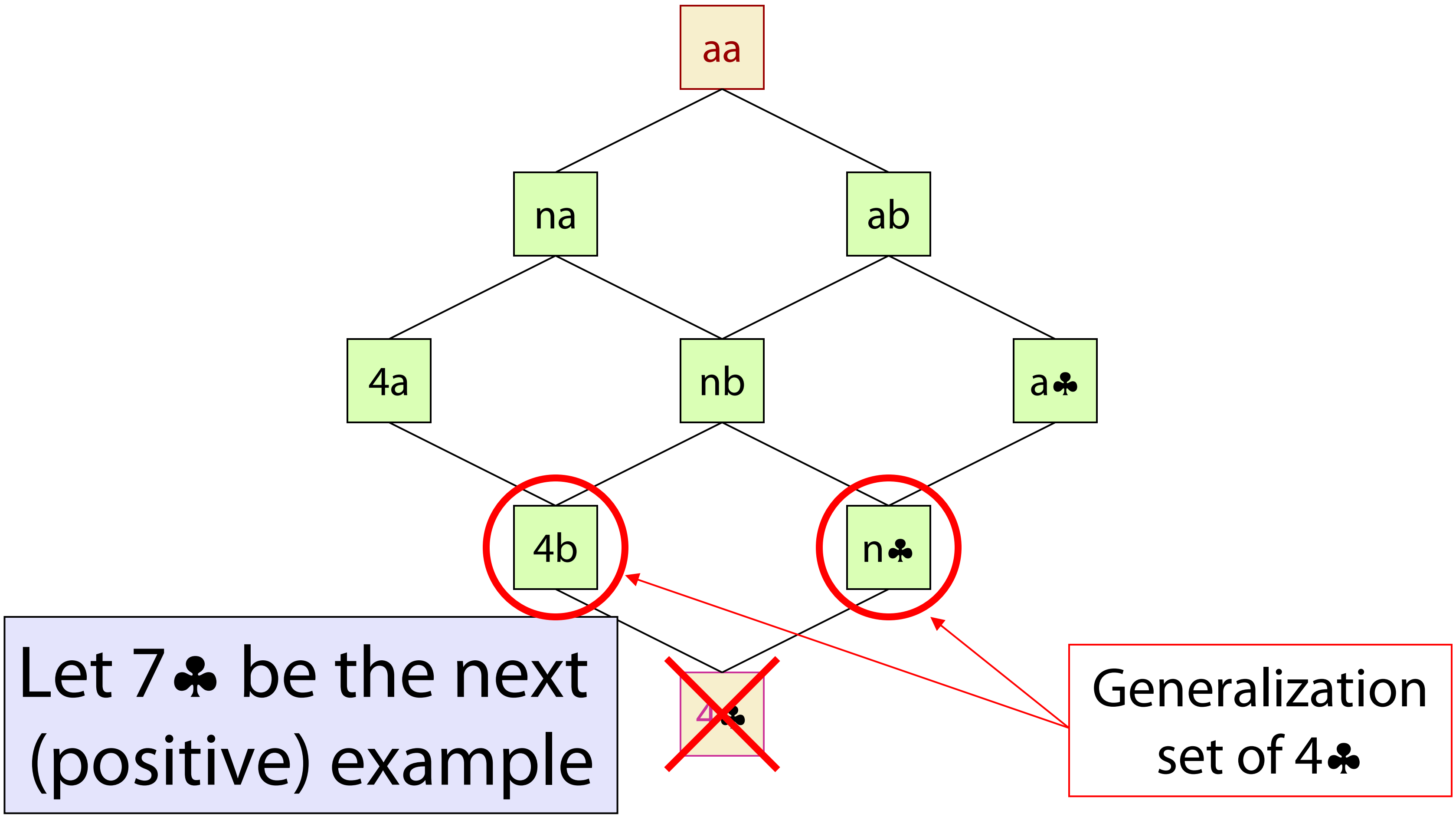
# Example: G-/S-Boundaries of V



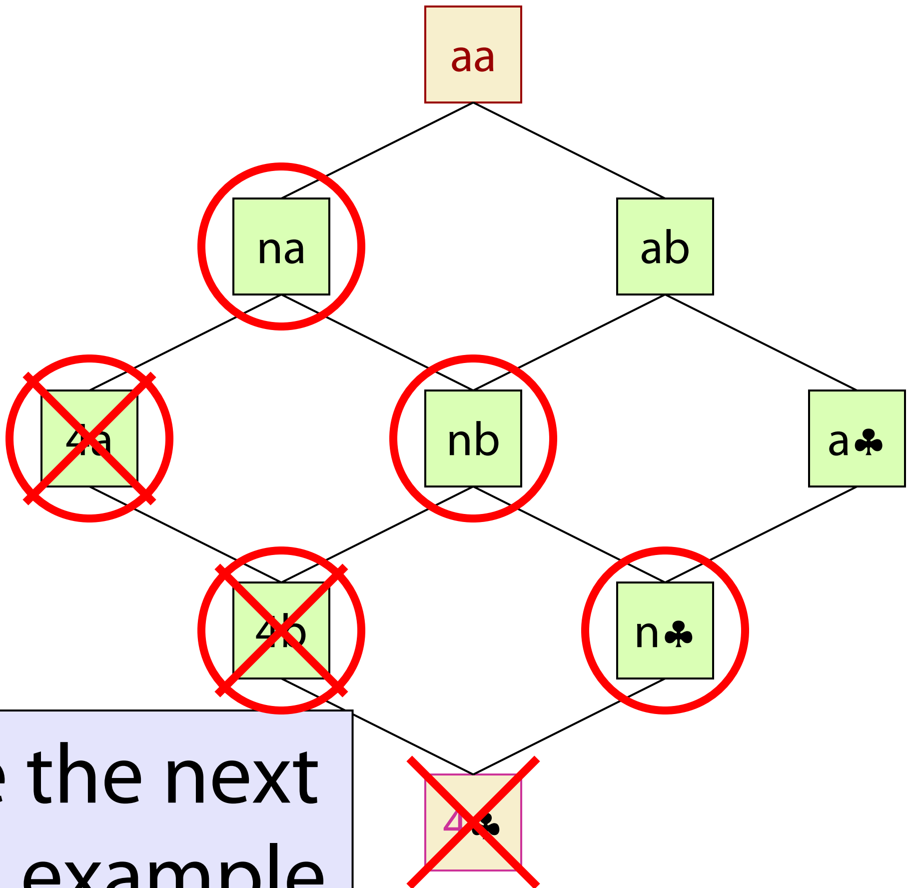
# Example: G-/S-Boundaries of V



# Example: G-/S-Boundaries of V



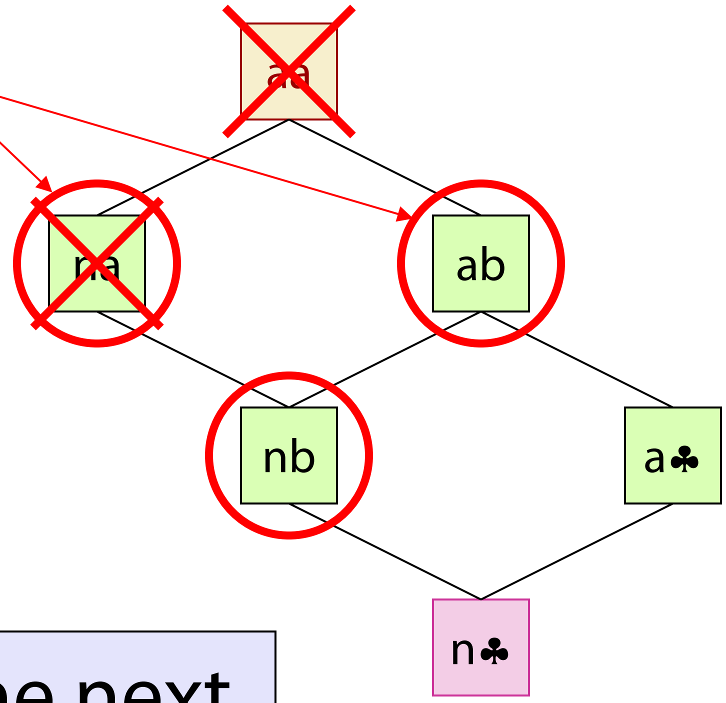
# Example: G-/S-Boundaries of V




Let 7♣ be the next (positive) example

# Example: G-/S-Boundaries of V

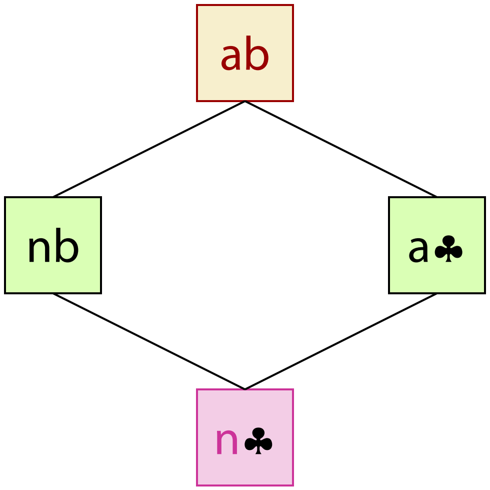
Specialization set of aa




Let 5♥ be the next (negative) example

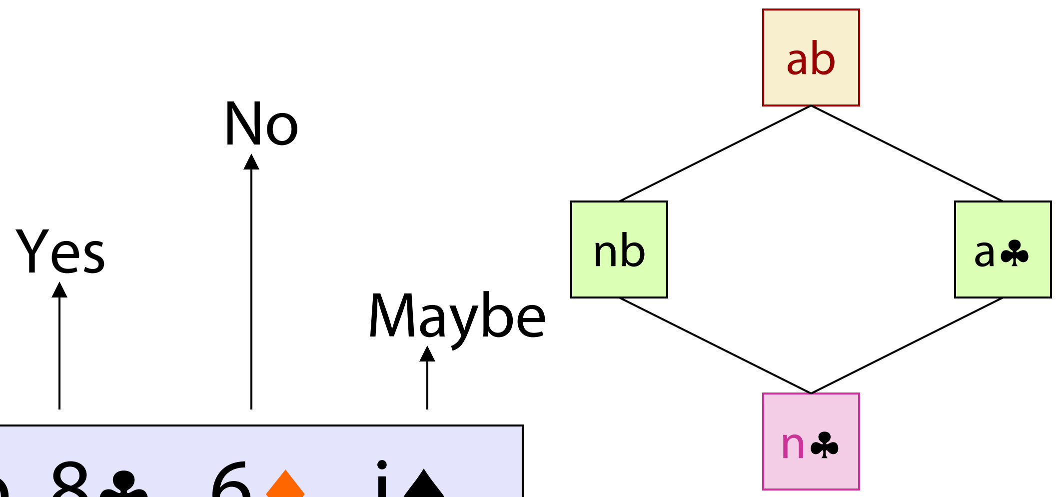
# Example: G-/S-Boundaries of V

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



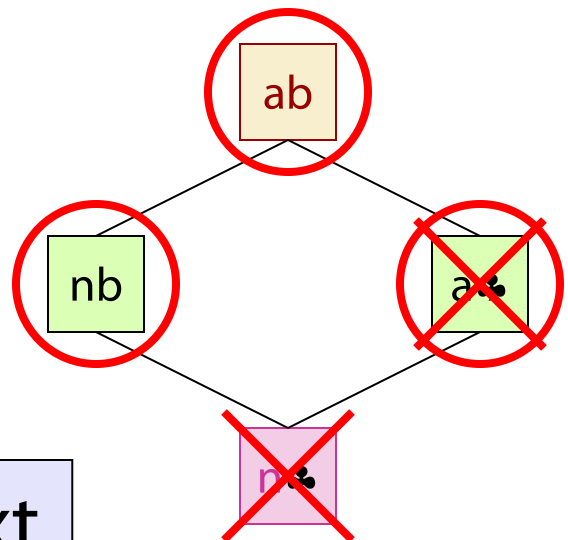
# Example: G-/S-Boundaries of V

At this stage …



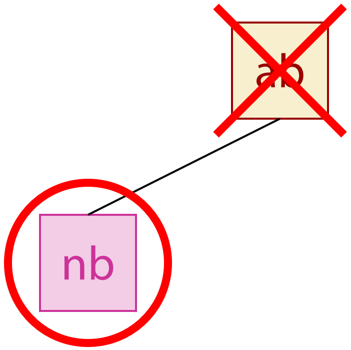

Do 8♣, 6♦, j♠
satisfy CONCEPT?

# Example: G-/S-Boundaries of V




Let 2♠ be the next (positive) example

# Example: G-/S-Boundaries of V




Let j♠ be the next (negative) example

# Example: G-/S-Boundaries of V

+ 4♣ 7♣ 2♠

– 5♥ j♠

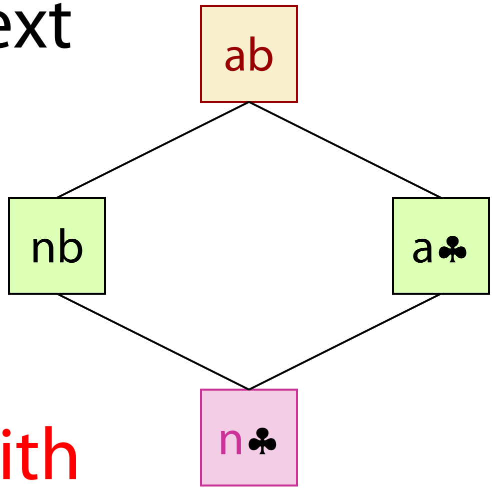
nb

NUM(r) ∧ BLACK(s)

# Example: G-/S-Boundaries of V

Let us return to the version space …

… and let 8♣ be the next (negative) example

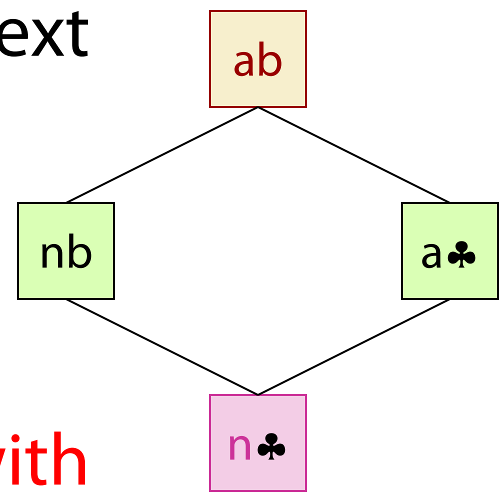



The only most specific hypothesis disagrees with this example, so no hypothesis in H agrees with all examples

# Example: G-/S-Boundaries of V

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

Inductive Learning

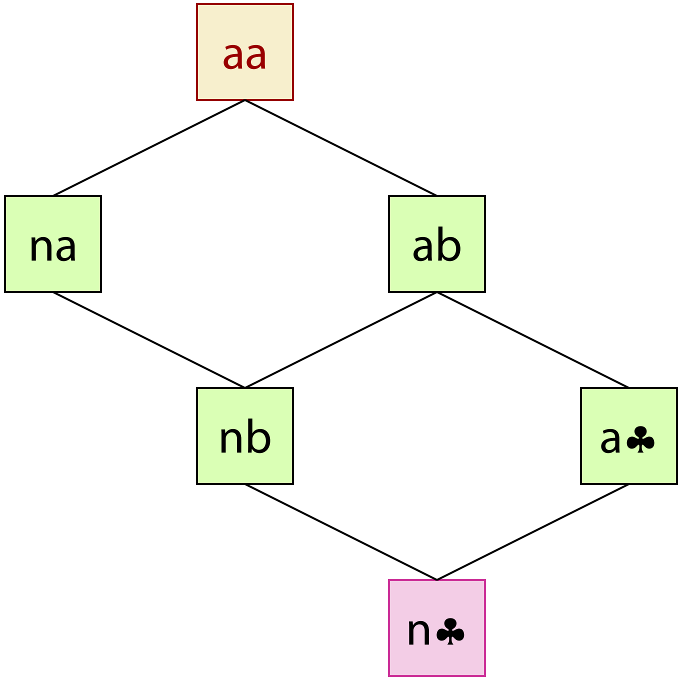
# SELECTION STRATEGY

# 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

- 9♣?
- 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

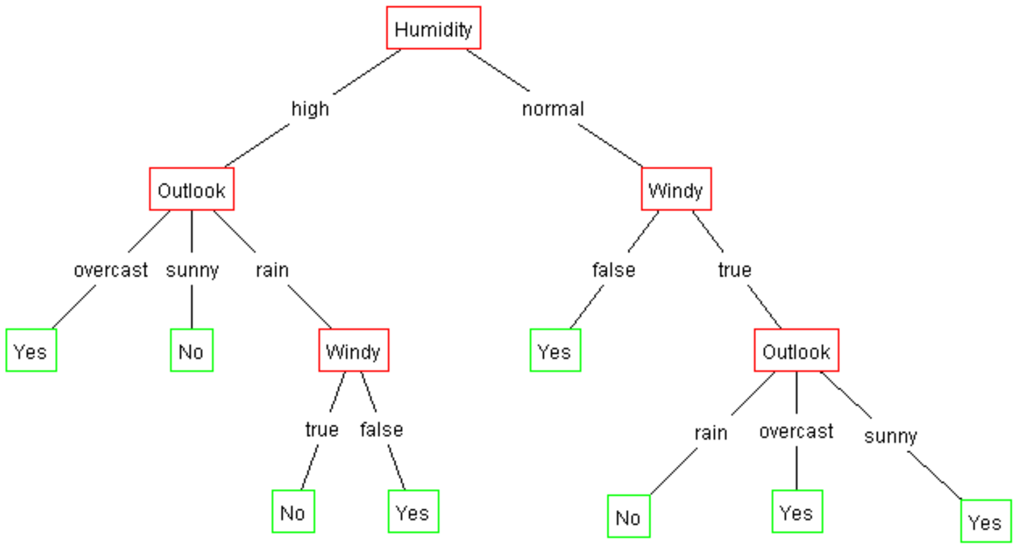
- If some examples are misclassified, the version space may collapse
- Possible solution:
  Maintain several G- and S-boundaries, e.g., consistent with all examples, all examples but one, etc…

Inductive Learning

# DECISION TREES

# 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 |



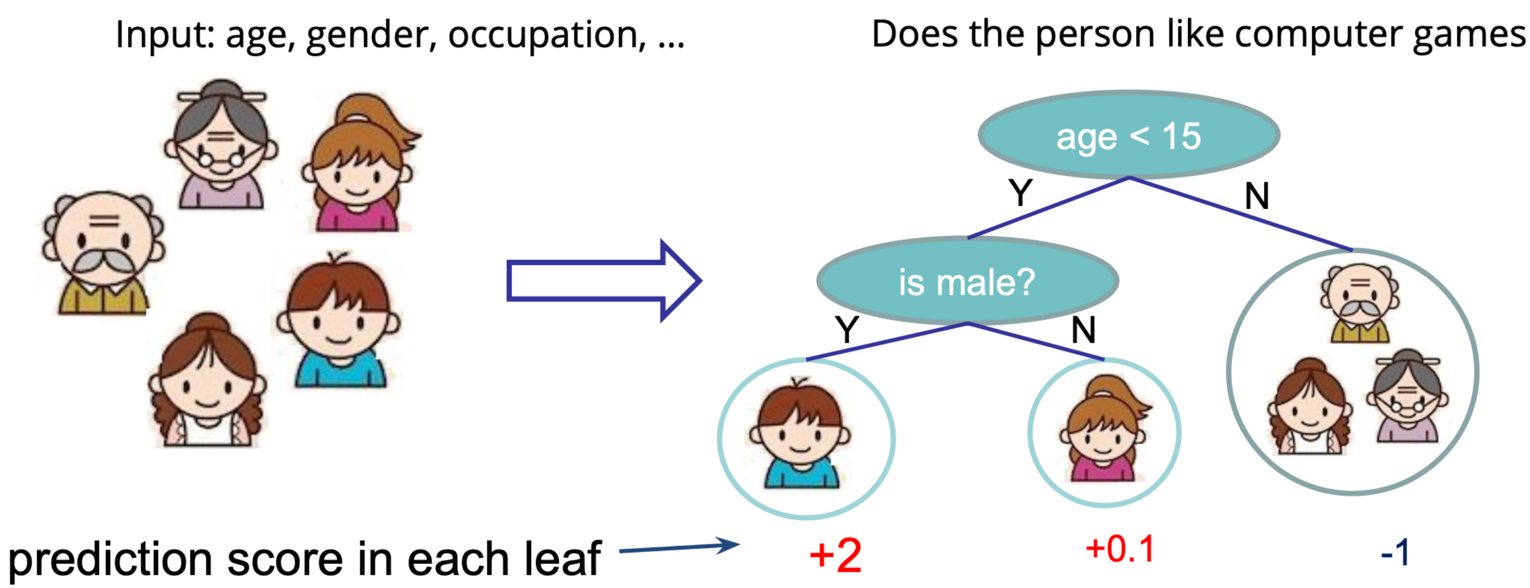
# Decision trees

- 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

- 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.

# Regression Trees

- Regression tree (also known as CART)
- This is what it would looks like for a commercial system

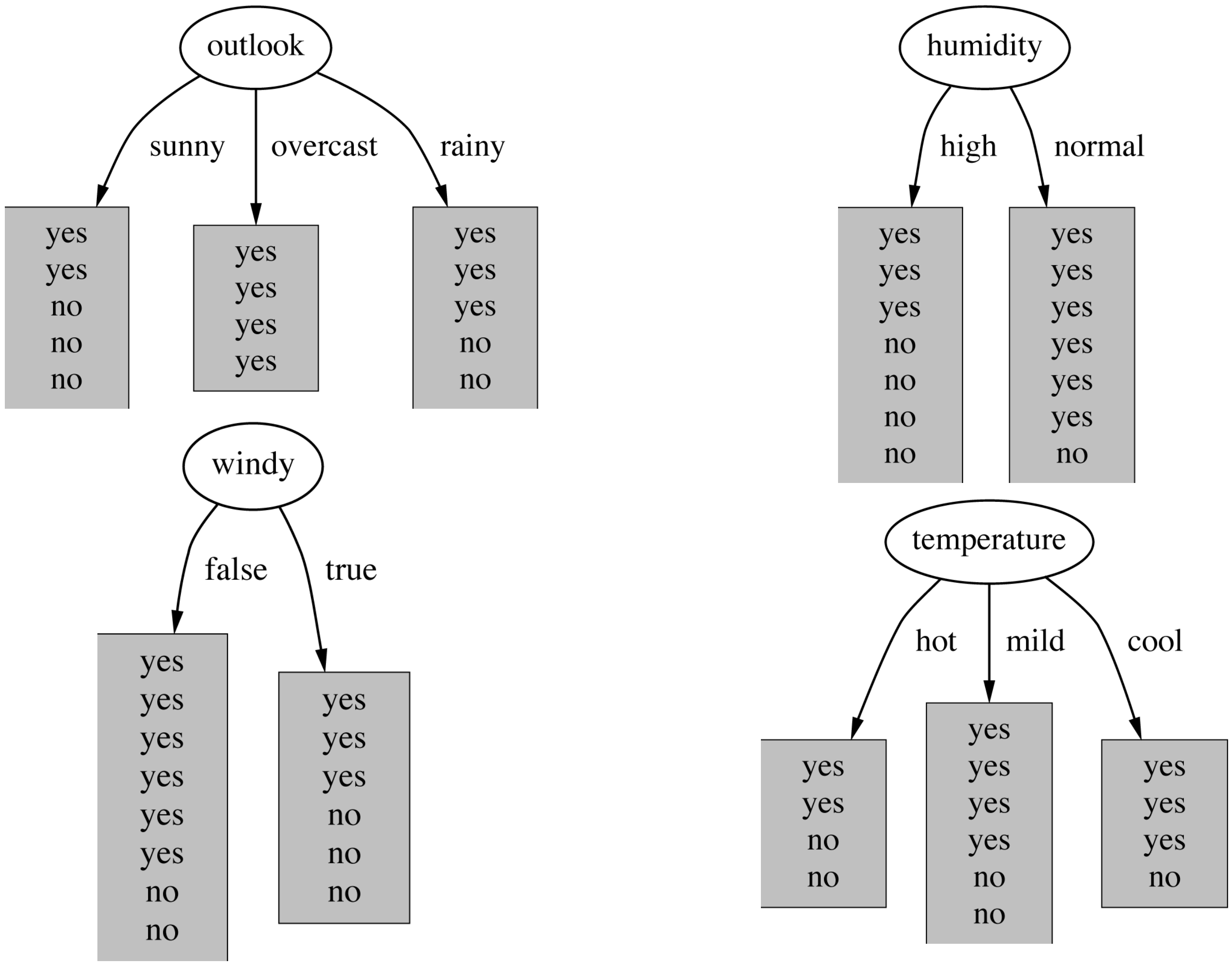


# Building Decision Trees

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

R. Quinlan, Learning efficient classification procedures, Machine Learning: an artificial intelligence approach, Michalski, Carbonell & Mitchell (eds.), Morgan Kaufmann, p. 463-482., **1983**

# 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.

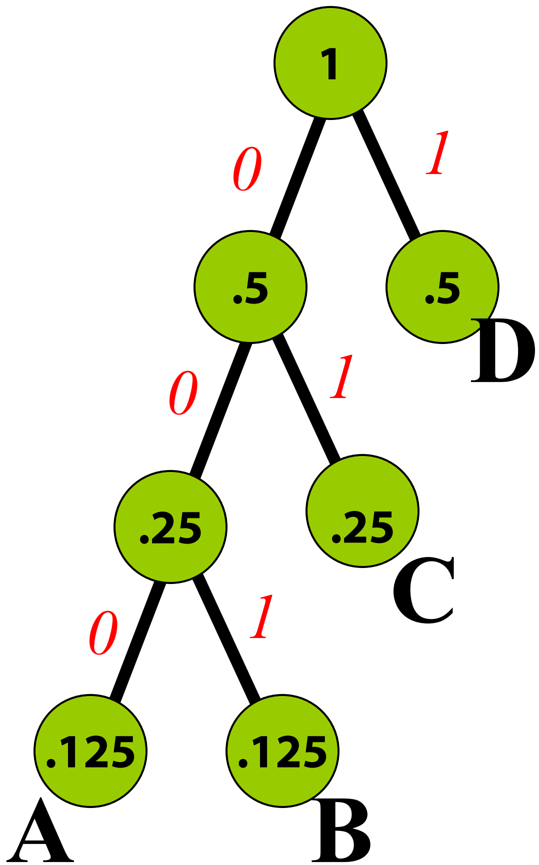
Inductive Learning

# INFORMATION THEORY

# 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 | Exp. len |
| --- | --- | --- | --- | --- |
| A | 000 | 3 | 0,125 | 0,375 |
| B | 001 | 3 | 0,125 | 0,375 |
| C | 01 | 2 | 0,250 | 0,500 |
| D | 1 | 1 | 0,500 | 0,500 |
| average message length | | | | 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:

  $I(P) = -(p_1*\log(p_1) + p_2*\log(p_2) + .. + p_n*\log(p_n))$
- 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":

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

- "Outlook" = "Overcast":

$$\text{info}([4,0]) = \text{entropy}(1,0) = -1\log(1) - 0\log(0) = 0\,\text{bits}$$

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

- "Outlook" = "Rainy":

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

- Expected information for attribute:

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

$$= 0.693\,\text{bits}$$

# Computing the information gain

- Information gain:

(information before split) – (information after split)

$$\text{gain}(\text{"Outlook"}) = \text{info}([9,5]) - \text{info}([2,3],[4,0],[3,2]) = 0.940 - 0.693$$

$$= 0.247 \text{ bits}$$

# Computing the information gain

- Information gain:

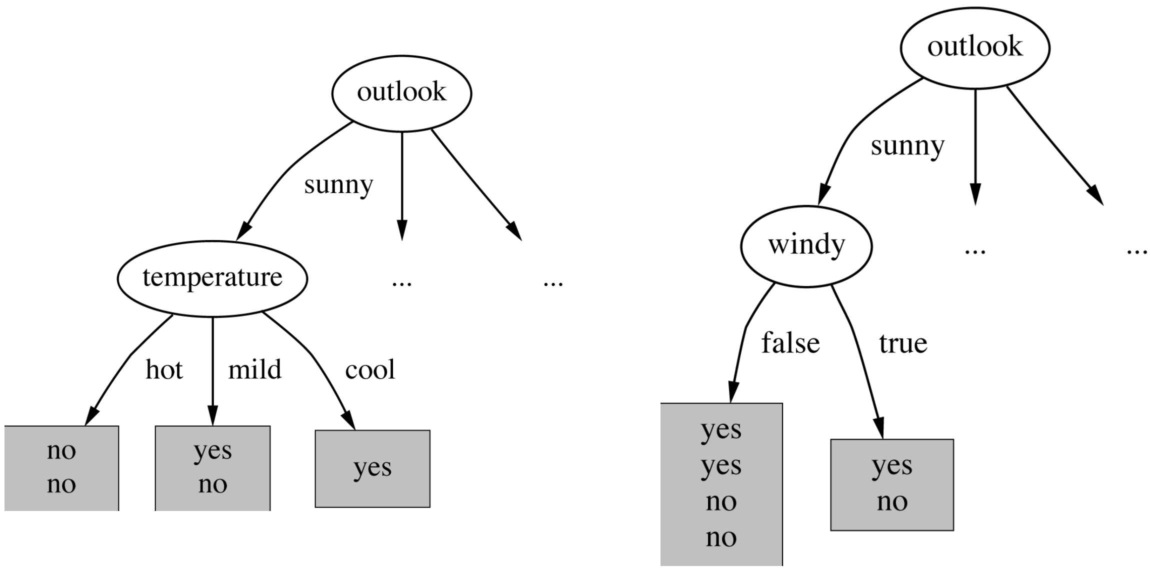
(information before split) – (information after split)

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

- Information gain for attributes from weather data:

$$\text{gain}(\text{"Outlook"}) = 0.247 \text{ bits}$$
$$\text{gain}(\text{"Temperature"}) = 0.029 \text{ bits}$$
$$\text{gain}(\text{"Humidity"}) = 0.152 \text{ bits}$$
$$\text{gain}(\text{"Windy"}) = 0.048 \text{ bits}$$

# Continuing to split

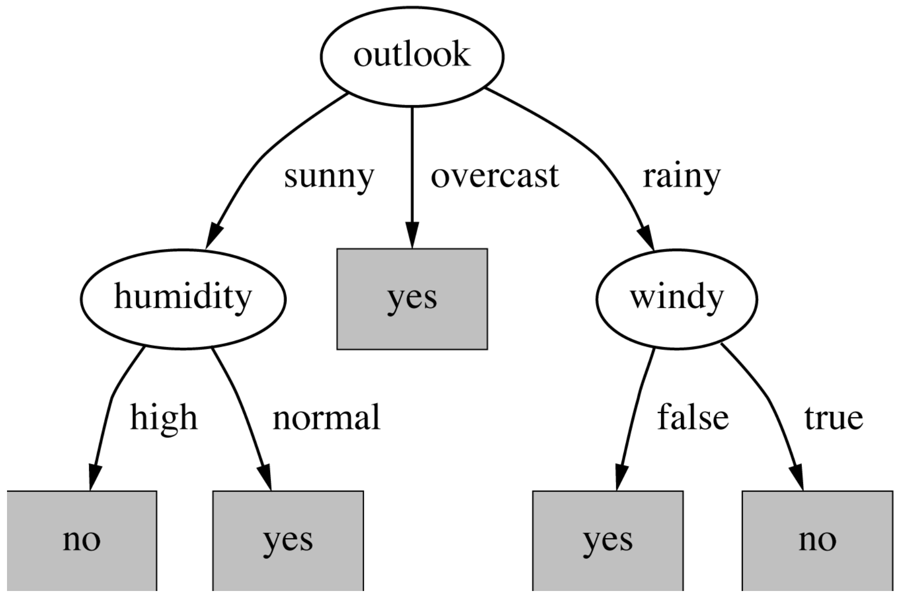



$$\text{gain}(\text{"Humidity"}) = 0.971\,\text{bits}$$

$$\text{gain}(\text{"Temperature"}) = 0.571\,\text{bits}$$

$$\text{gain}(\text{"Windy"}) = 0.020\,\text{bits}$$

# The final decision tree



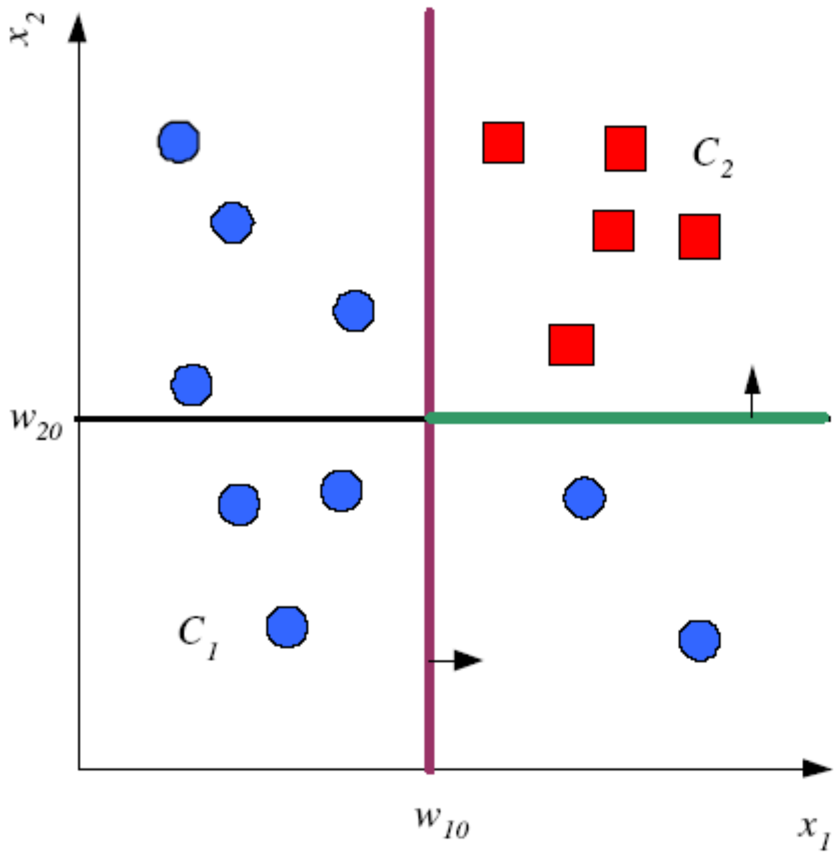

- Note: not all leaves need to be pure; sometimes identical instances have different classes

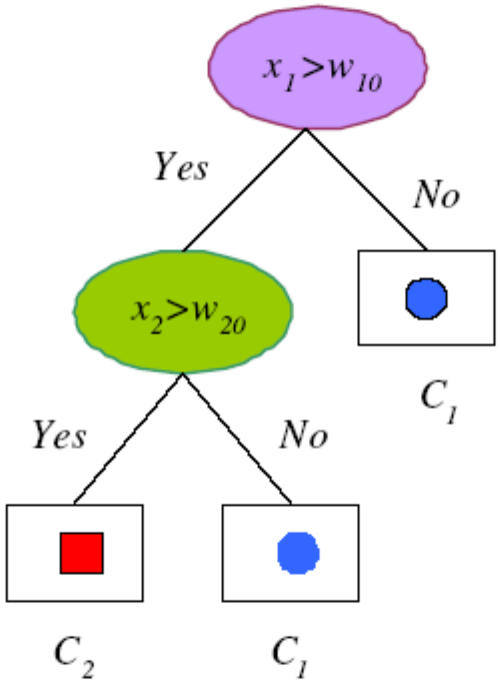
  ⇒ Splitting stops when data can't be split any further

Inductive Learning

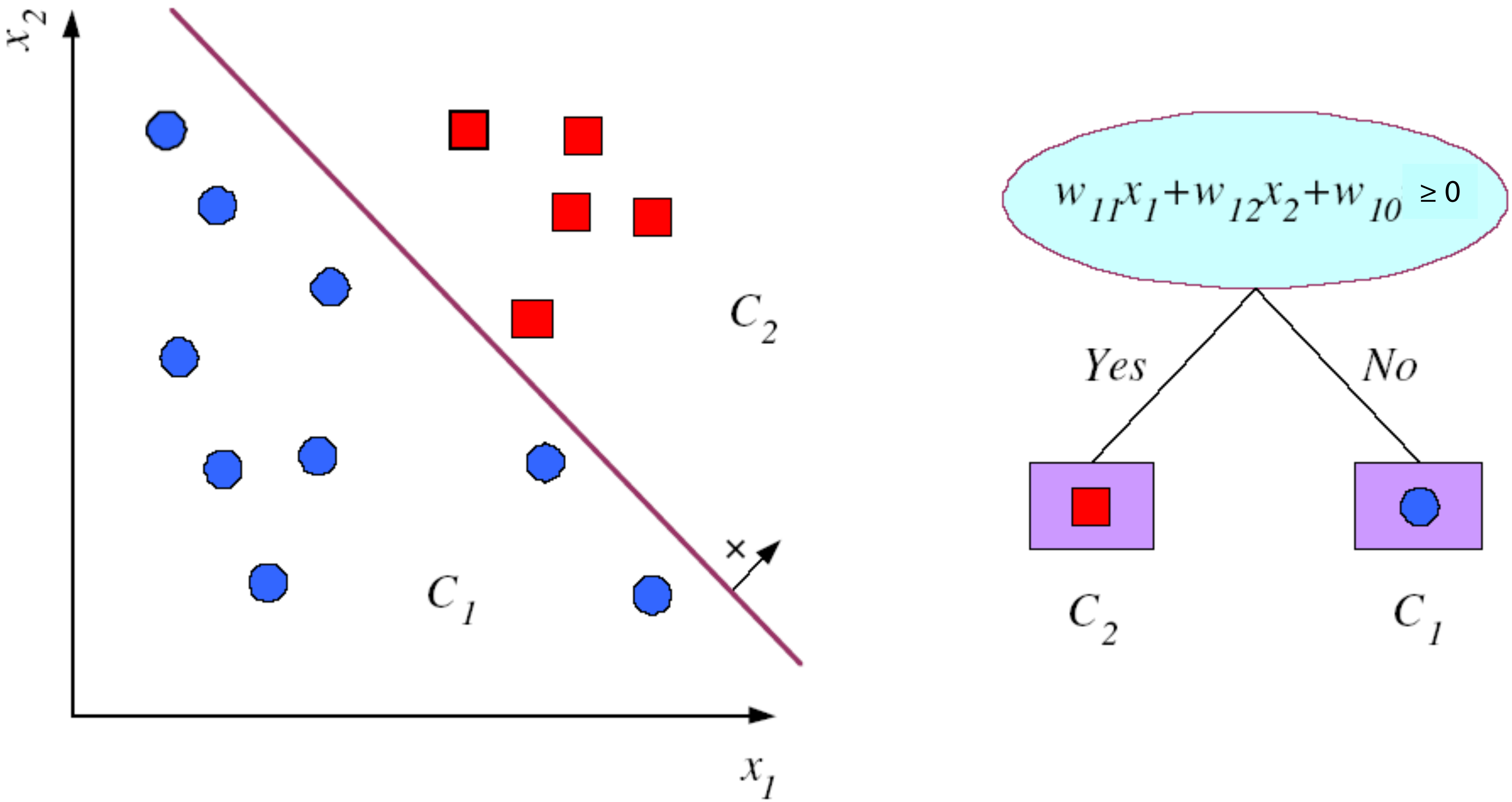
# EVALUATING DECISION TREES

# 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 → No | 2/5 | 4/14 |
| | Overcast → Yes | 0/4 | |
| | Rainy → Yes | 2/5 | |
| Temp | Hot → No* | 2/4 | 5/14 |
| | Mild → Yes | 2/6 | |
| | Cool → Yes | 1/4 | |
| Humidity | High → No | 3/7 | 4/14 |
| | Normal → Yes | 1/7 | |
| Windy | False → Yes | 2/8 | 5/14 |
| | True → No* | 3/6 | |

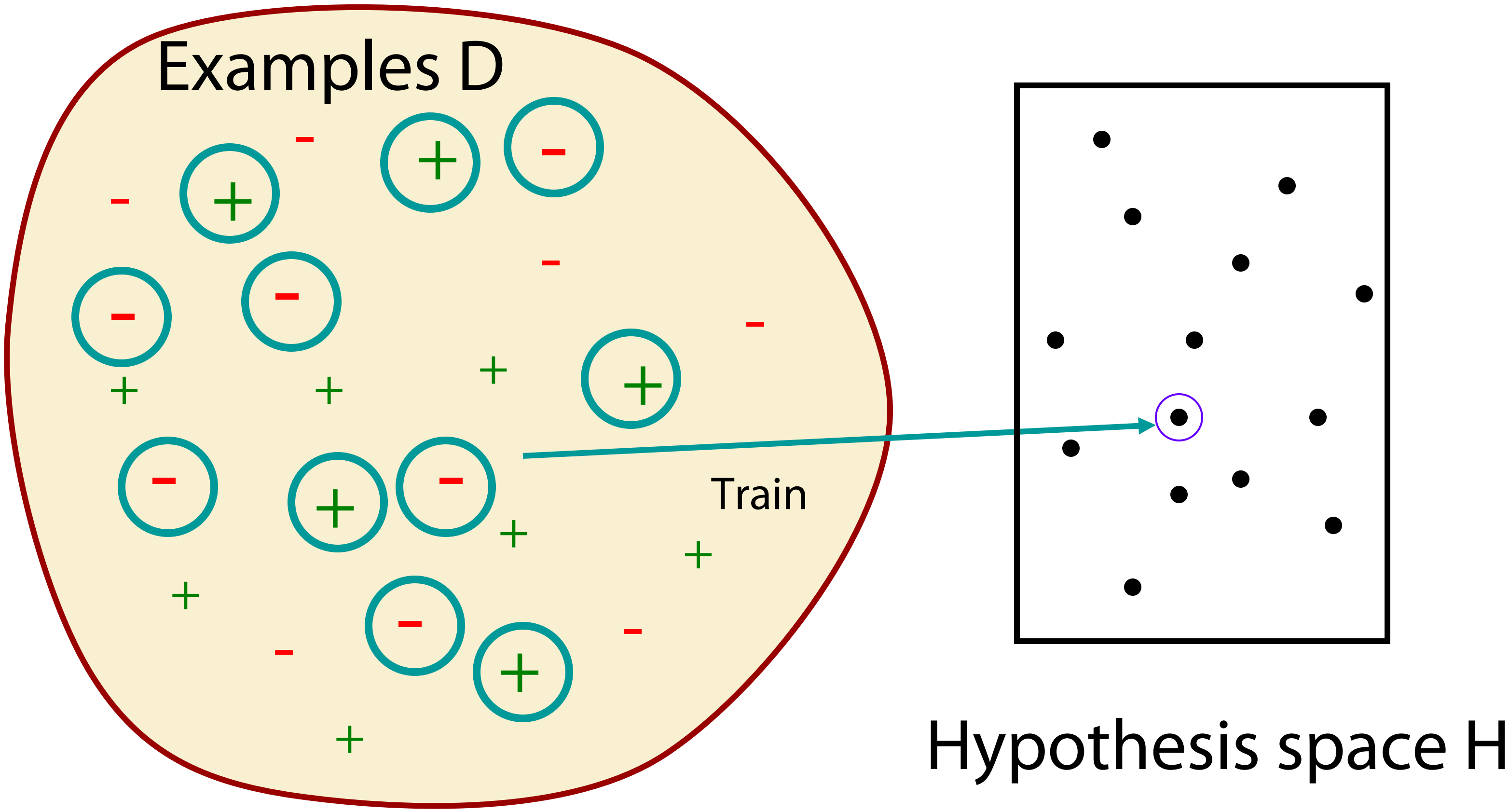
* indicates a tie

# 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*

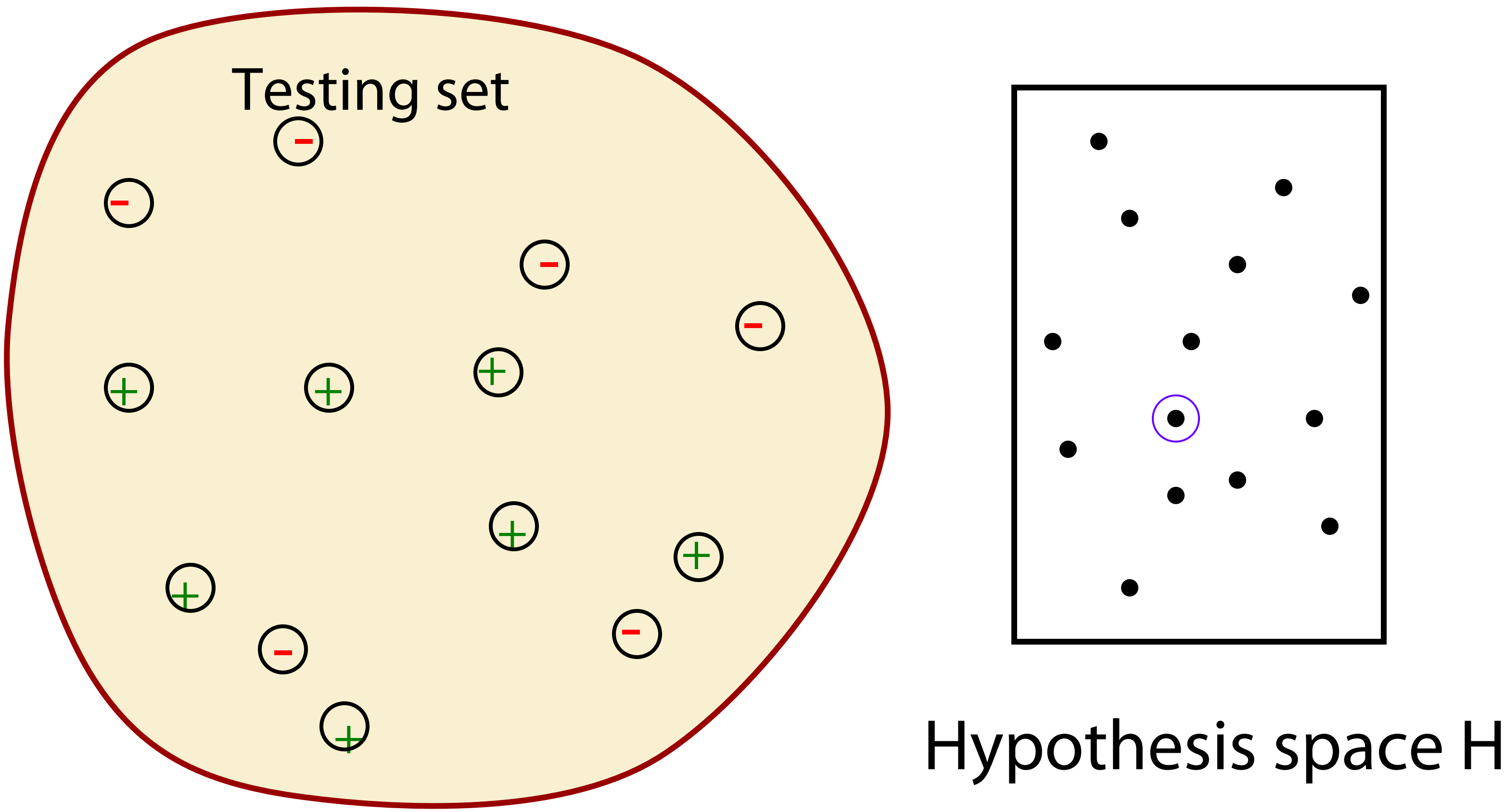
# Cross-Validation

- Split original set of examples, train



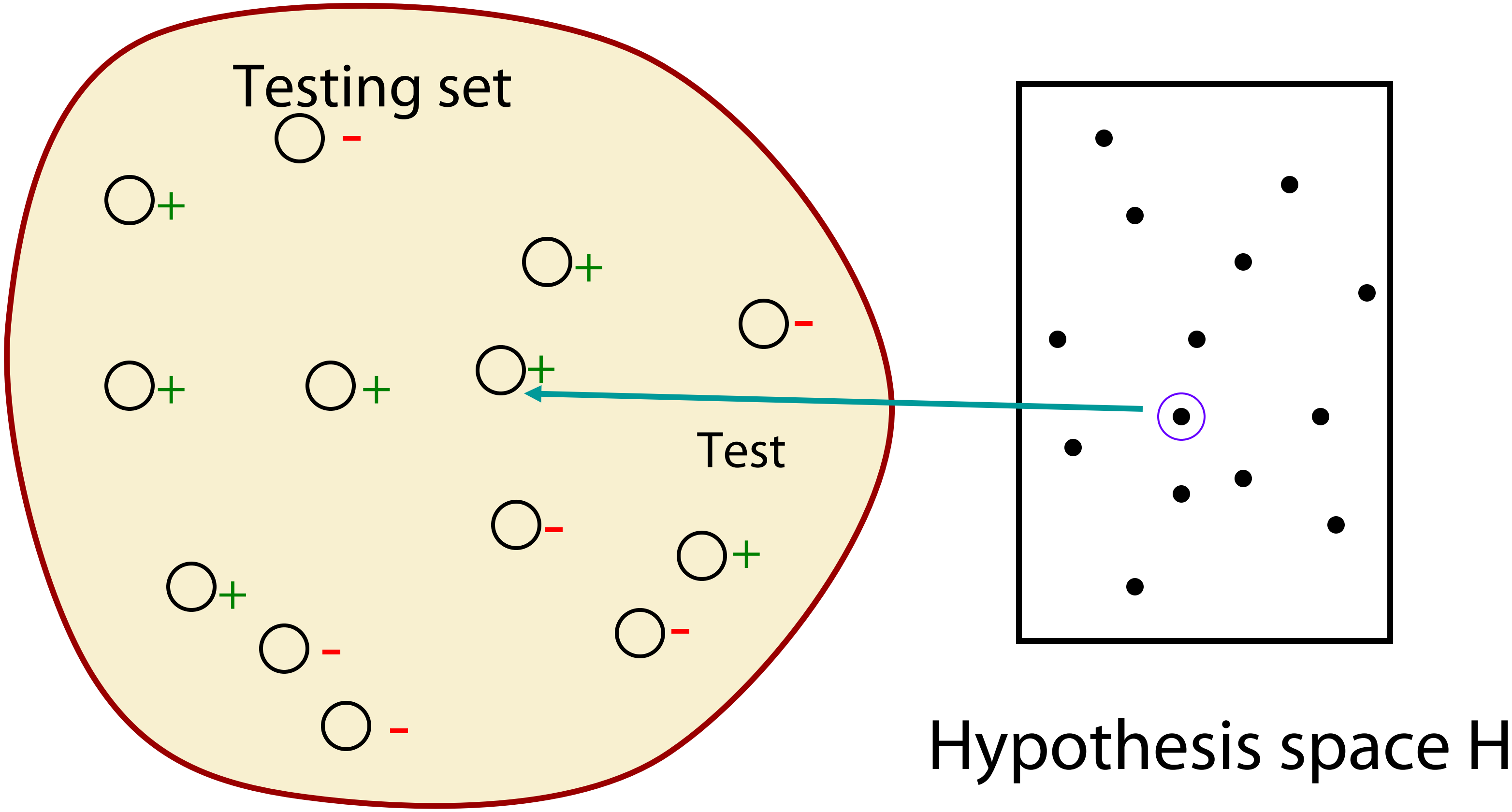
# Cross-Validation

- Evaluate hypothesis on testing set



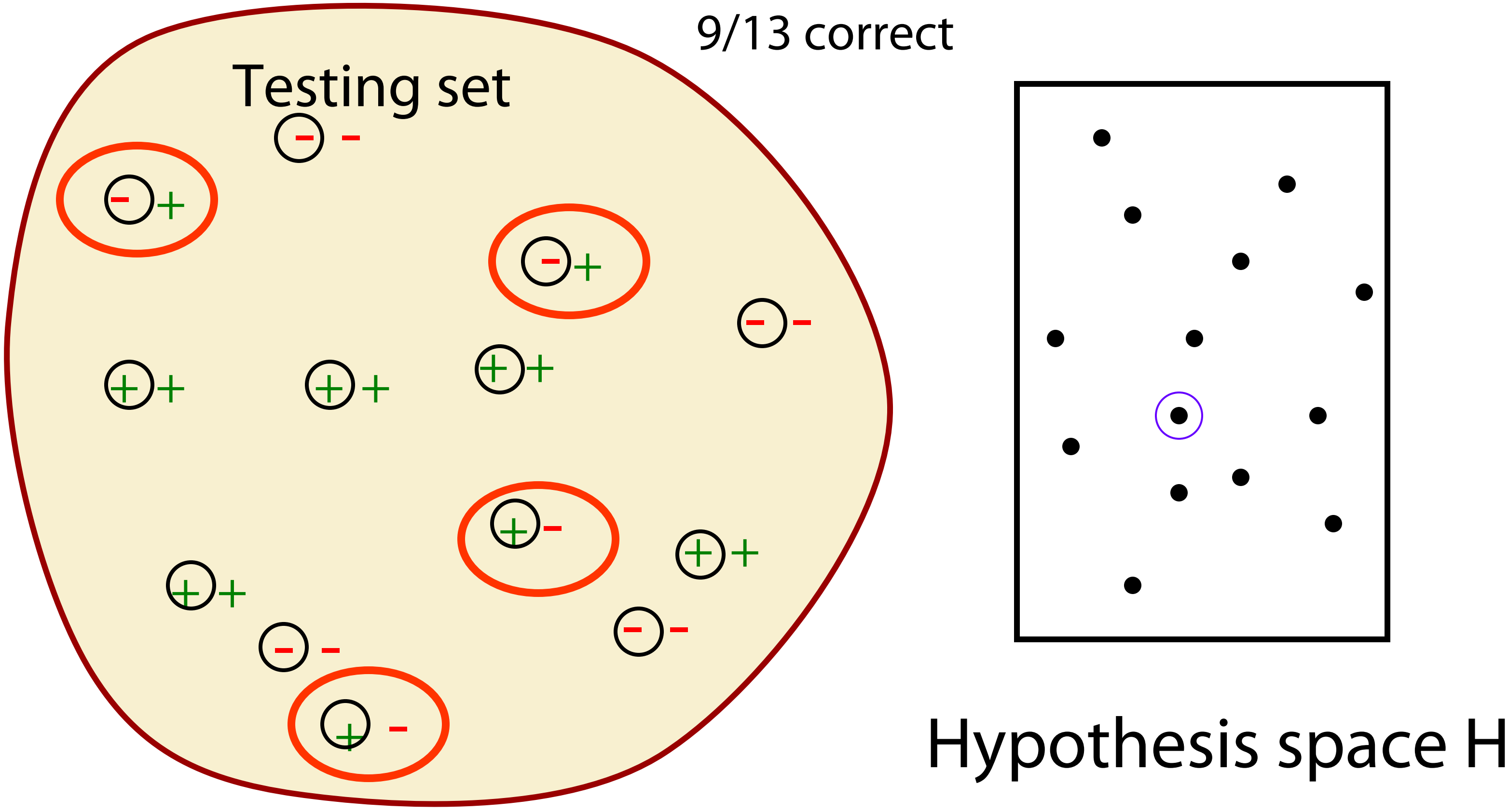
# Cross-Validation

- Evaluate hypothesis on testing set



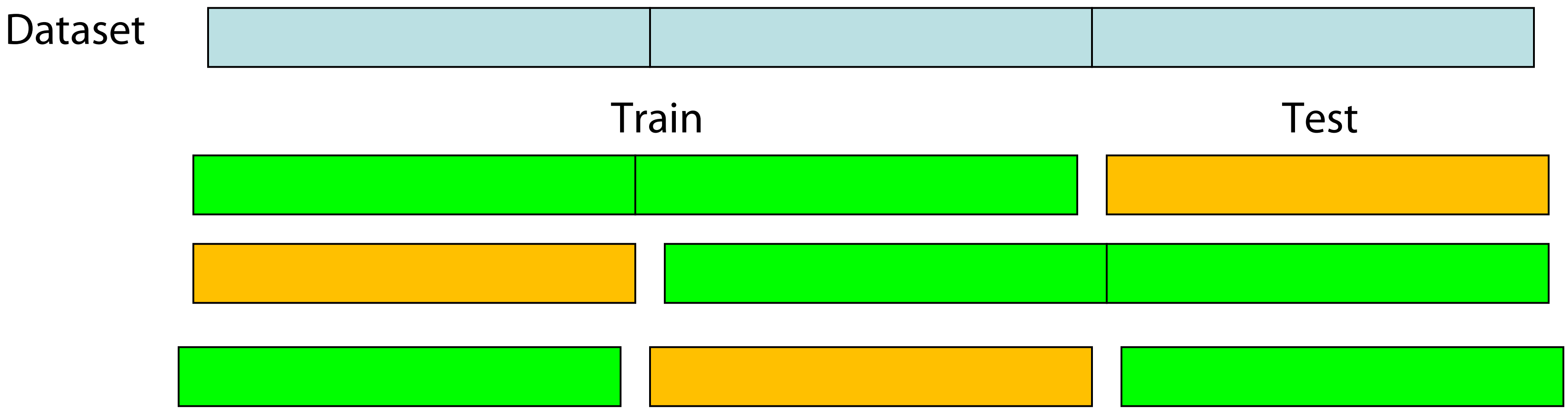
# Cross-Validation

- Compare true concept against prediction



# Common Splitting Strategies

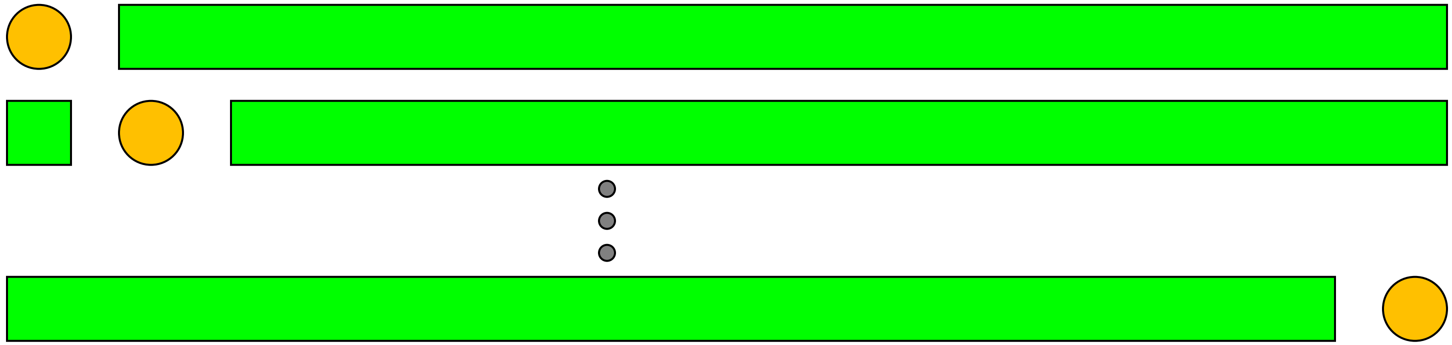
- k-fold cross-validation: k random partitions



# 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!

Robert C. Holte, Very Simple Classification Rules Perform Well on Most Commonly Used Datasets, Journal Machine Learning Volume 11, Issue 1 , pp 63-90, **1993**

# 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):

```
64       65       68    69    70       71    72    72       75    75       80       81       83       85
Yes  |   No   |   Yes   Yes   Yes   |  No    No  |   Yes   Yes   Yes   |  No  |   Yes      Yes  |   No
```

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   |  No    No    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 | ≤ 77.5 → Yes | 3/10 | 5/14 |
| | > 77.5 → No* | 2/4 | |
| Humidity | ≤ 82.5 → Yes | 1/7 | 3/14 |
| | > 82.5 and ≤ 95.5 → 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:

| 64 | 65 | 68 | 69 | 70 | 71 | 72 | 72 | 75 | 75 | 80 | 81 | 83 | 85 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Yes | No | Yes | Yes | Yes | No | No | Yes | Yes | Yes | No | Yes | Yes | No |

  - E.g. temperature $<$ 71.5: yes/4, no/2
    temperature $\geq$ 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:

$$\begin{aligned}\text{Gain}(X) &= \text{probability that A is known} * (\text{info}(T) - \text{info}_X(T)) + \\ &\quad\ \text{probability that A is unknown} * 0 \\ &= F * (\text{info}(T) - \text{info}_X(T))\end{aligned}$$

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

Inductive Learning

# PRUNING

# Pruning

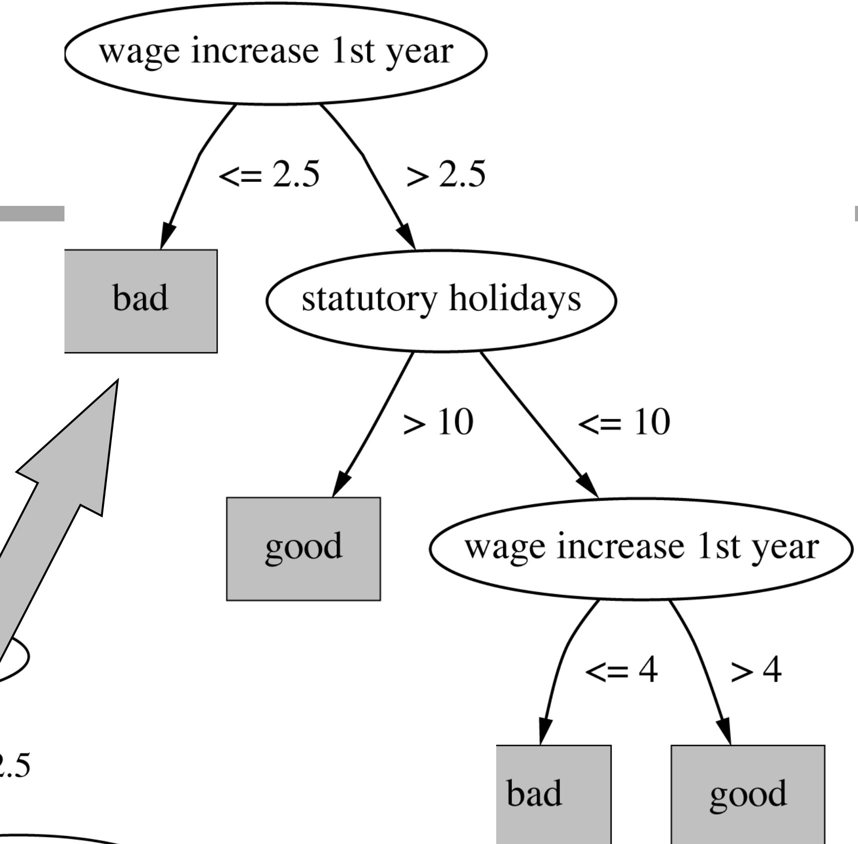
- Goal: Prevent overfitting to noise in the data
- Two strategies for "pruning" the decision tree:
  - Postpruning - take a fully-grown decision tree and discard unreliable parts
  - Prepruning - stop growing a branch when information becomes unreliable
- Postpruning preferred in practice—prepruning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

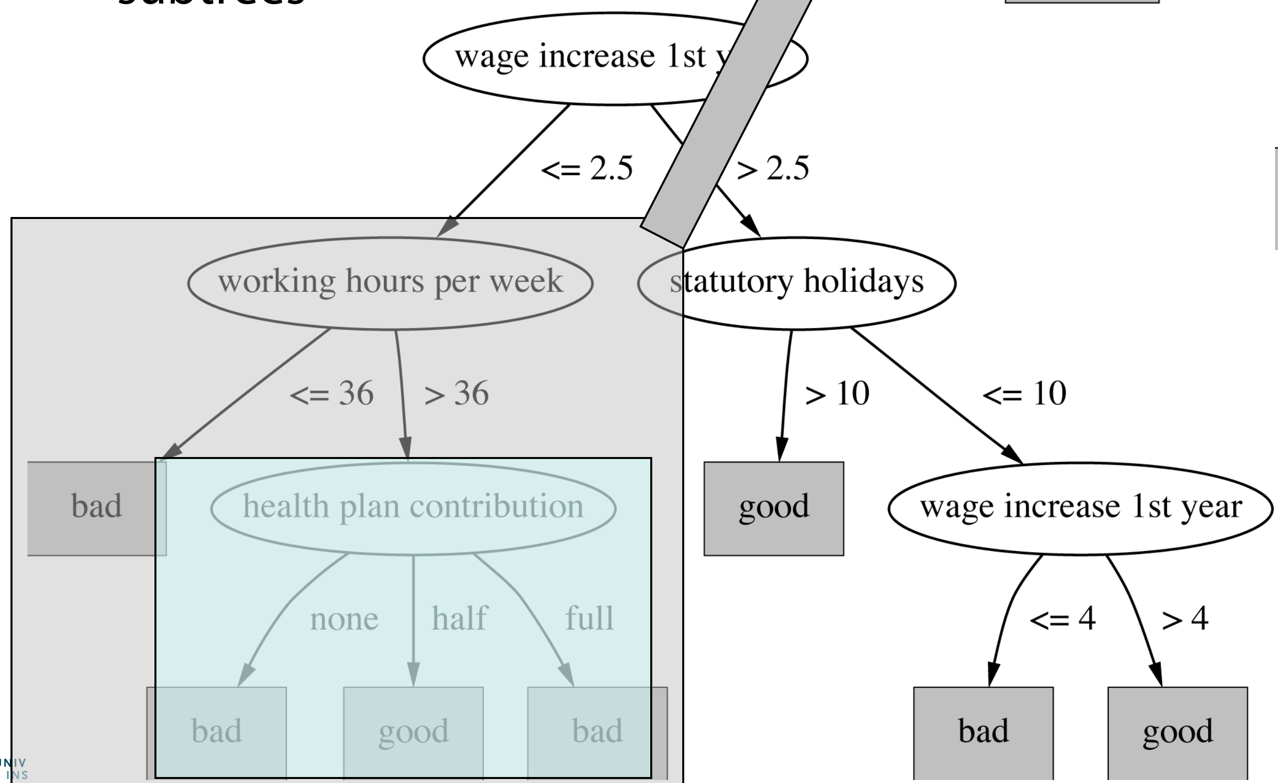
# Post-pruning

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

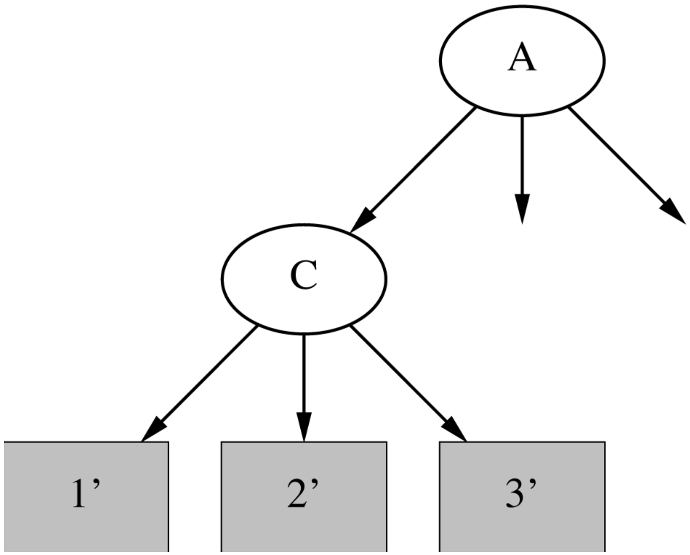
# Subtree replacement

- *Bottom-up*
- Consider replacing a tree only after considering all its subtrees

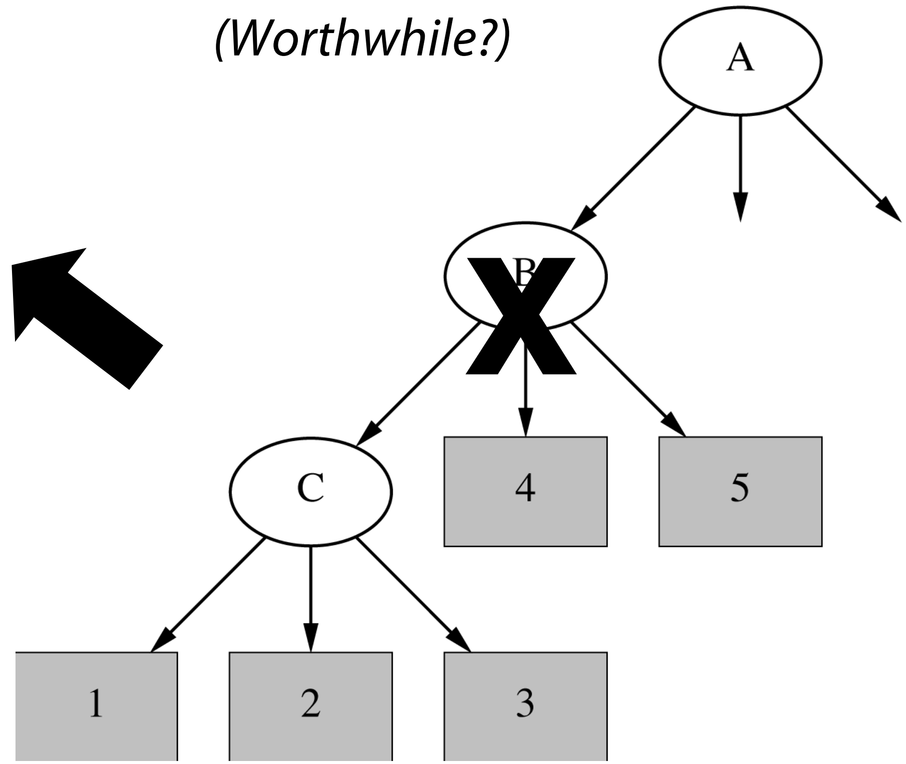


# *Subtree raising




- Delete node
- Redistribute instances
- Slower than subtree replacement
  *(Worthwhile?)*



# 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 $Node_1$, $Node_2$, etc.
  - Probabilities can be estimated by relative frequencies of attribute values in sets of examples that fall into child nodes

$$BackedUpError(Node) = \sum_i P_i \times Error(Node_i)$$

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

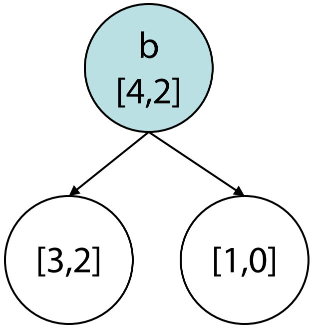
# Example Calculation

- 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

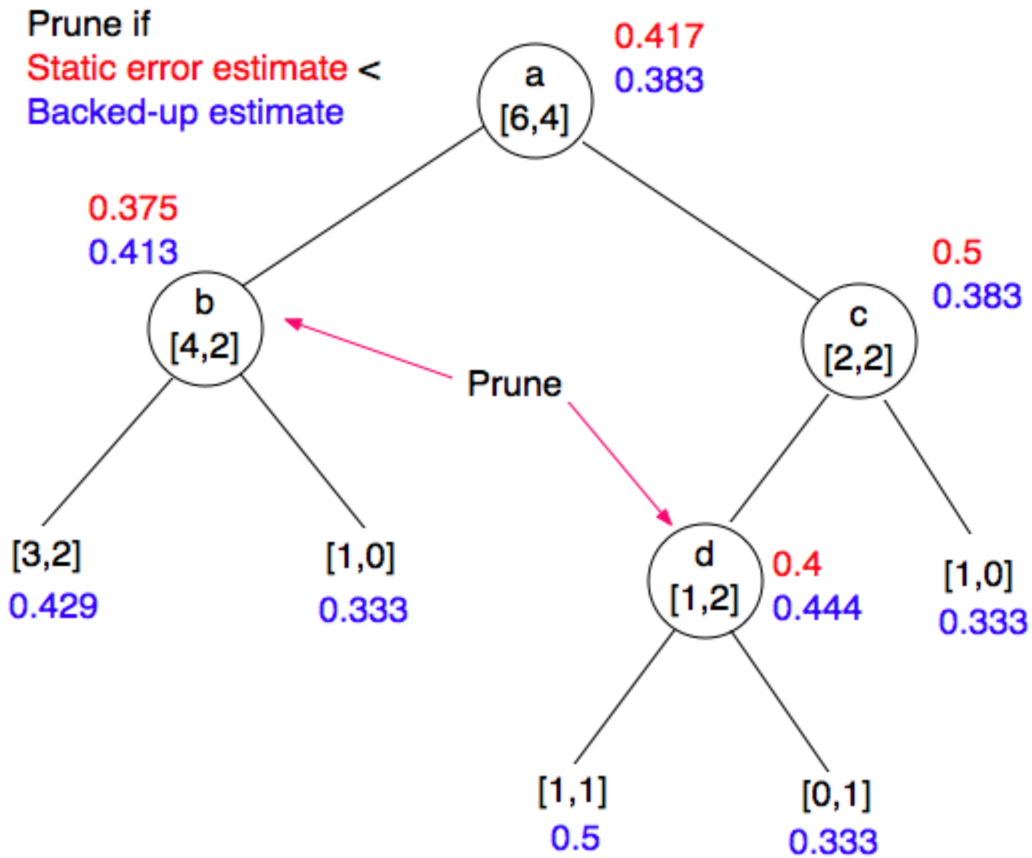
$$E([1,0]) = \frac{1 - 1 + 2 - 1}{1 + 2} = 0{,}333$$

- 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

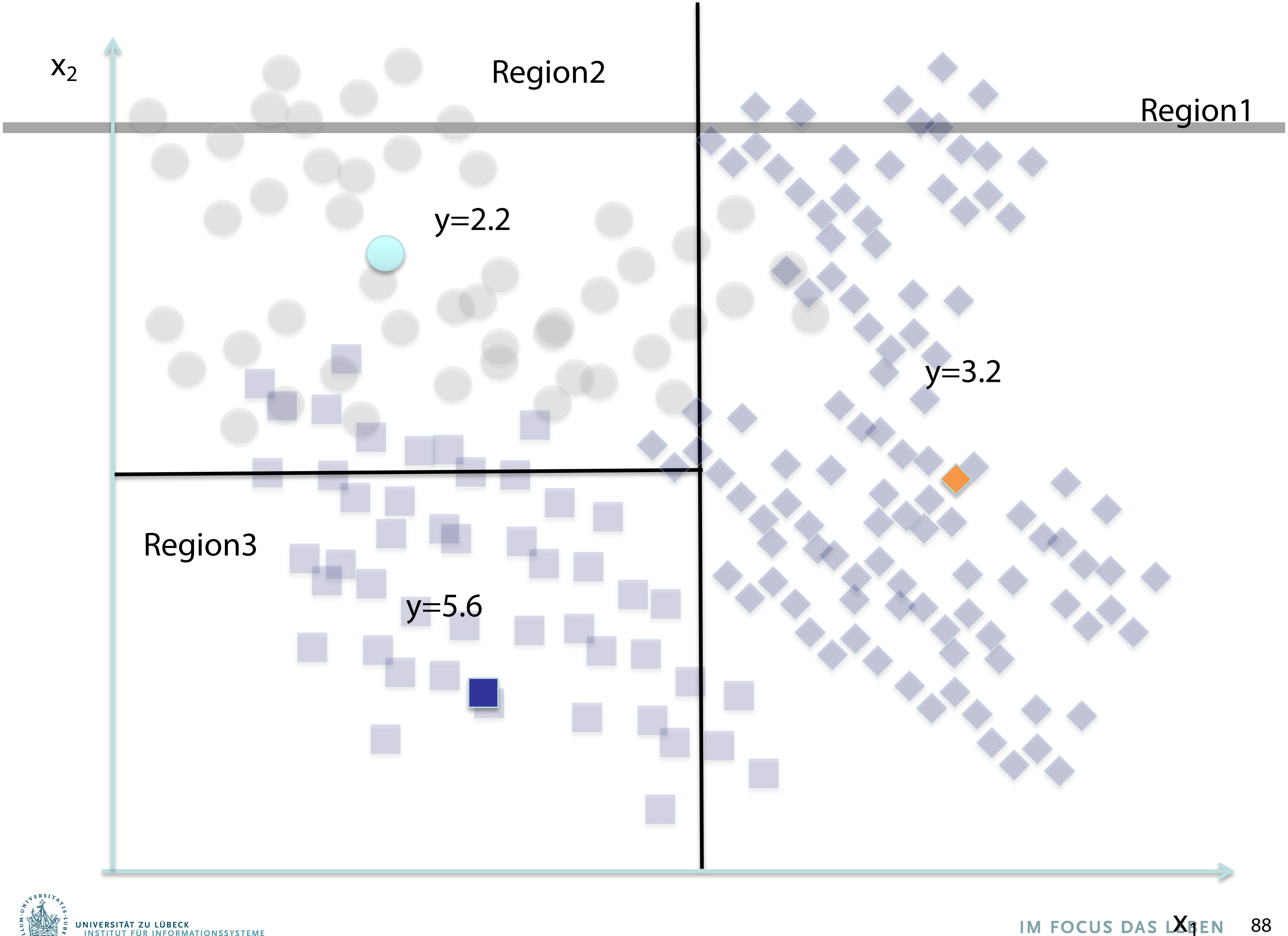

Prune if
Static error estimate <
Backed-up estimate
a
[6,4]
0.417
0.383
b
[4,2]
0.375
0.413
c
[2,2]
0.5
0.383
Prune
[3,2]
0.429
[1,0]
0.333
d
[1,2]
0.4
0.444
[1,0]
0.333
[1,1]
0.5
[0,1]
0.333

# Regression Trees

**Build a regression tree**:

Divide the predictor space into $J$ distinct not overlapping regions $R_1, R_2, R_3, \ldots, R_J$

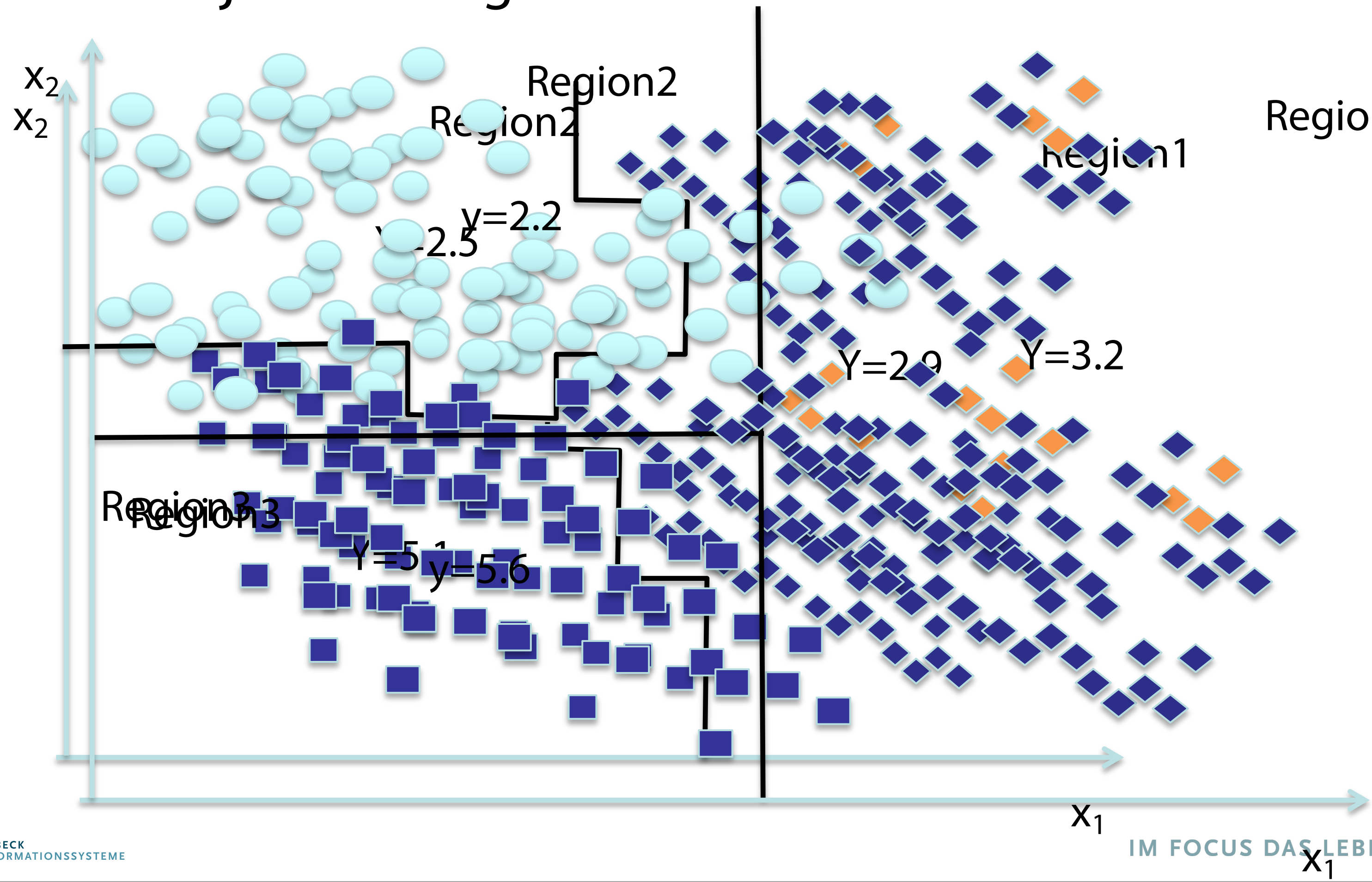
We make the same prediction for all observations in the same region; use the mean of responses for all training observations that are in the region


$x_2$
Region2
Region1
y=2.2
y=3.2
Region3
y=5.6
$x_1$

# Finding the sub-regions

The regions could have any shape.

But we choose just rectangles



## Find boxes $R_1, \ldots, R_J$ that minimize the RSS

$$RSS = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

where $\hat{y}_{R_j}$ is the mean response value of all training observations in the $R_j$ region

This computationally very expensive!

**Solution:** Top down approach, greedy approach

**recursive binary splitting**

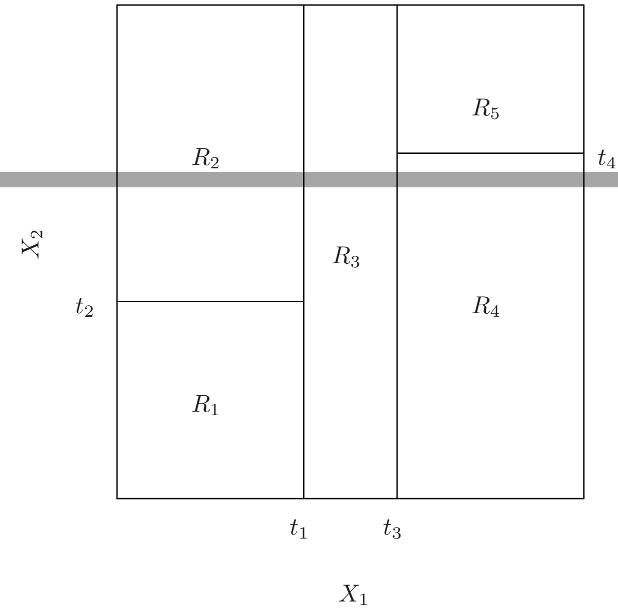
# Recursive Binary Splitting

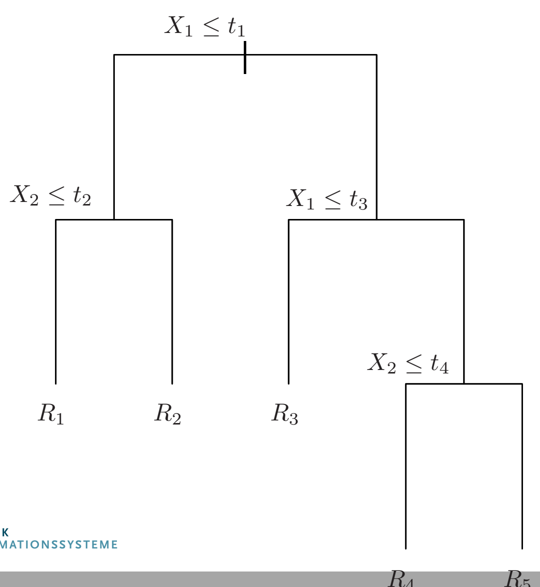
1. Consider all predictor $X_p$ and all the all possible values of the cutpoints *s* for each of the predictors. Choose the predictor and cutpoint s.t. it minimizes the RSS

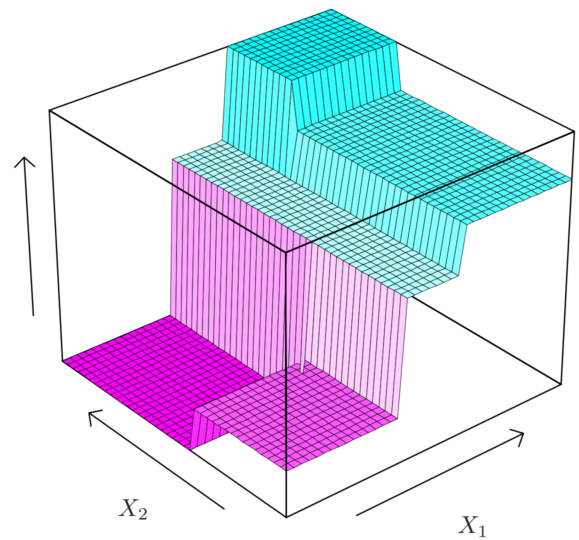
$$\sum_{i:x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

   This can be done quickly, assuming number of predictors is not very large

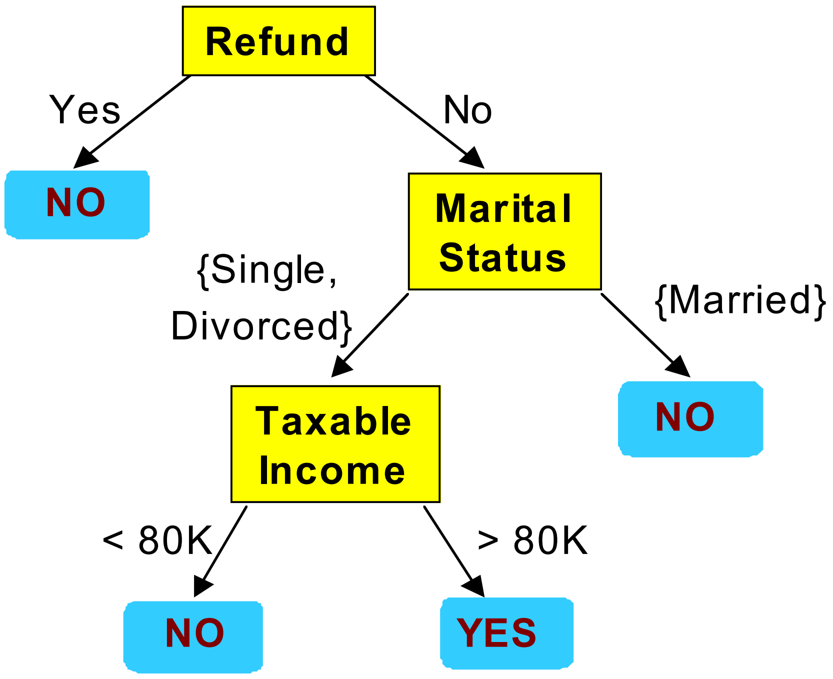
2. Repeat #1 but only consider the sub-regions
3. Stop: node contains only one class or node contains less than *n* data points or max depth is reached


$R_5$
$R_2$
$t_4$
$X_2$
$R_3$
$t_2$
$R_4$
$R_1$
$t_1$
$t_3$
$X_1$


$X_1 \leq t_1$
$X_2 \leq t_2$
$X_1 \leq t_3$
$X_2 \leq t_4$
$R_1$
$R_2$
$R_3$
$R_4$
$R_5$


$X_2$
$X_1$

# From Decision Trees to Rules

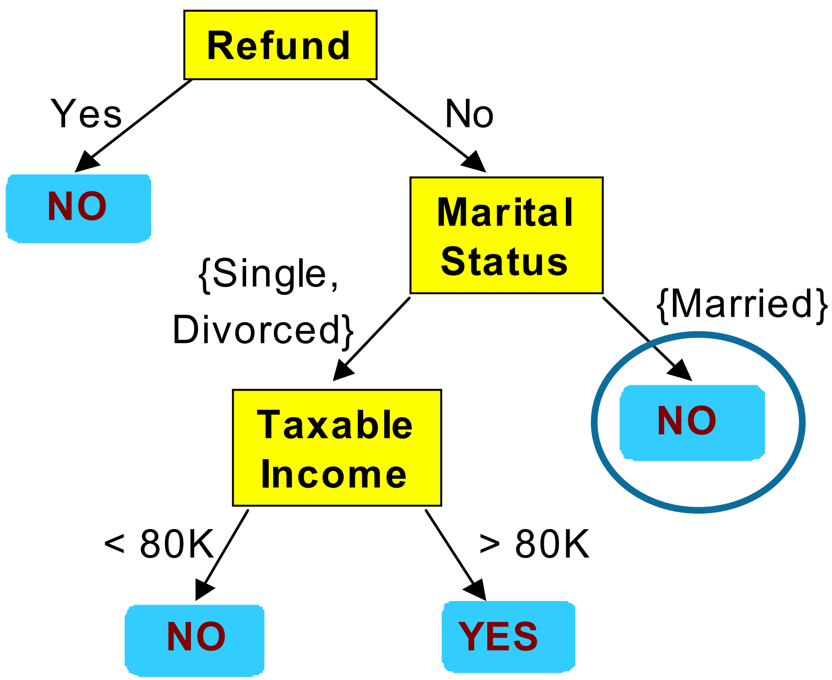



- Refund = Yes $\rightarrow$ No
- Refund = No $\wedge$
  Marital Status = {Single, Divorced}
  $\wedge$ Taxable Income < 80k $\rightarrow$ No
- Refund = No $\wedge$
  Marital Status = {Single, Divorced}
  $\wedge$ Taxable Income > 80k $\rightarrow$ Yes
- Refund = No $\wedge$
  Marital Status = Married $\rightarrow$ 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: $(\text{Refund}=\text{No}) \wedge (\text{Status}=\text{Married}) \rightarrow \text{No}$

# 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