Business Analytics

Decision Tree Classifiers

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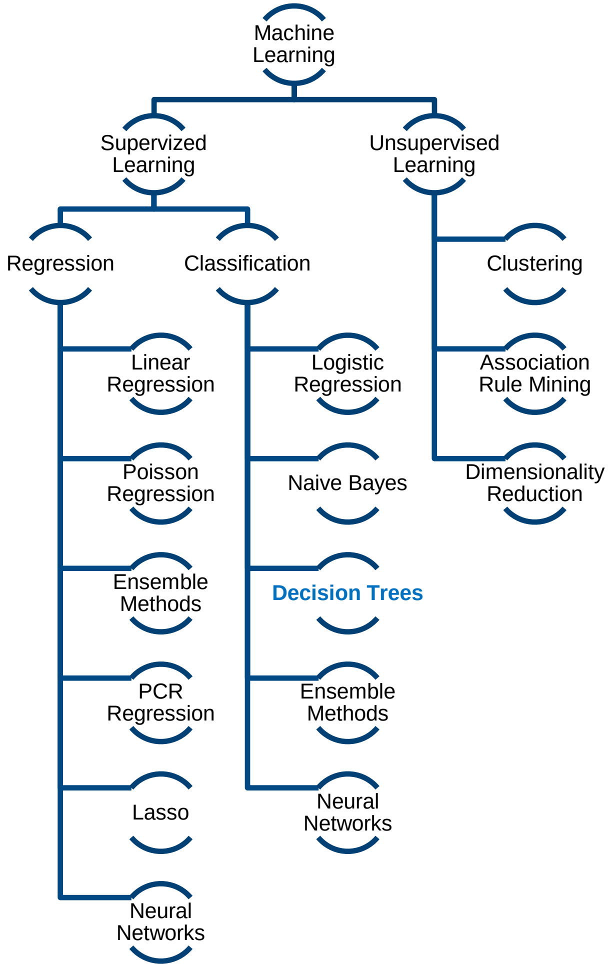
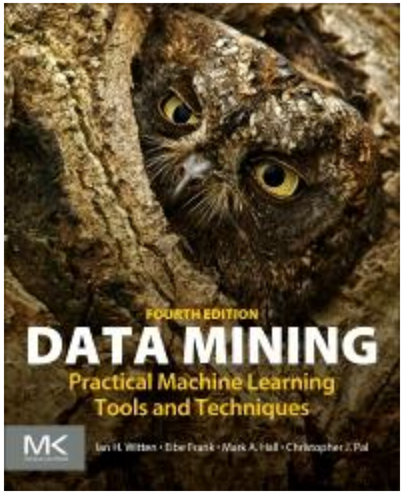
Course Content

- Introduction
- Regression Analysis
- Regression Diagnostics
- Logistic and Poisson Regression
- Naive Bayes and Bayesian Networks
- **Decision Tree Classifiers**
- Data Preparation and Causal Inference
- Model Selection and Learning Theory
- Ensemble Methods and Clustering
- High-Dimensional Problems
- Association Rules and Recommenders
- Neural Networks



Recommended Literature

- **Data Mining: Practical Machine Learning Tools and Techniques**
  - Ian H. Witten,Eibe Frank, Mark A. Hall, Christopher Pal.
  - http://www.cs.waikato.ac.nz/ml/weka/book.html
  - Section: 4.3, 6.1



- **Alternative literature**
  - Machine Learning
    - Tom M. Mitchell, 1997
  - Data Mining: Introductory and Advanced Topics
    - Margaret H. Dunham, 2003

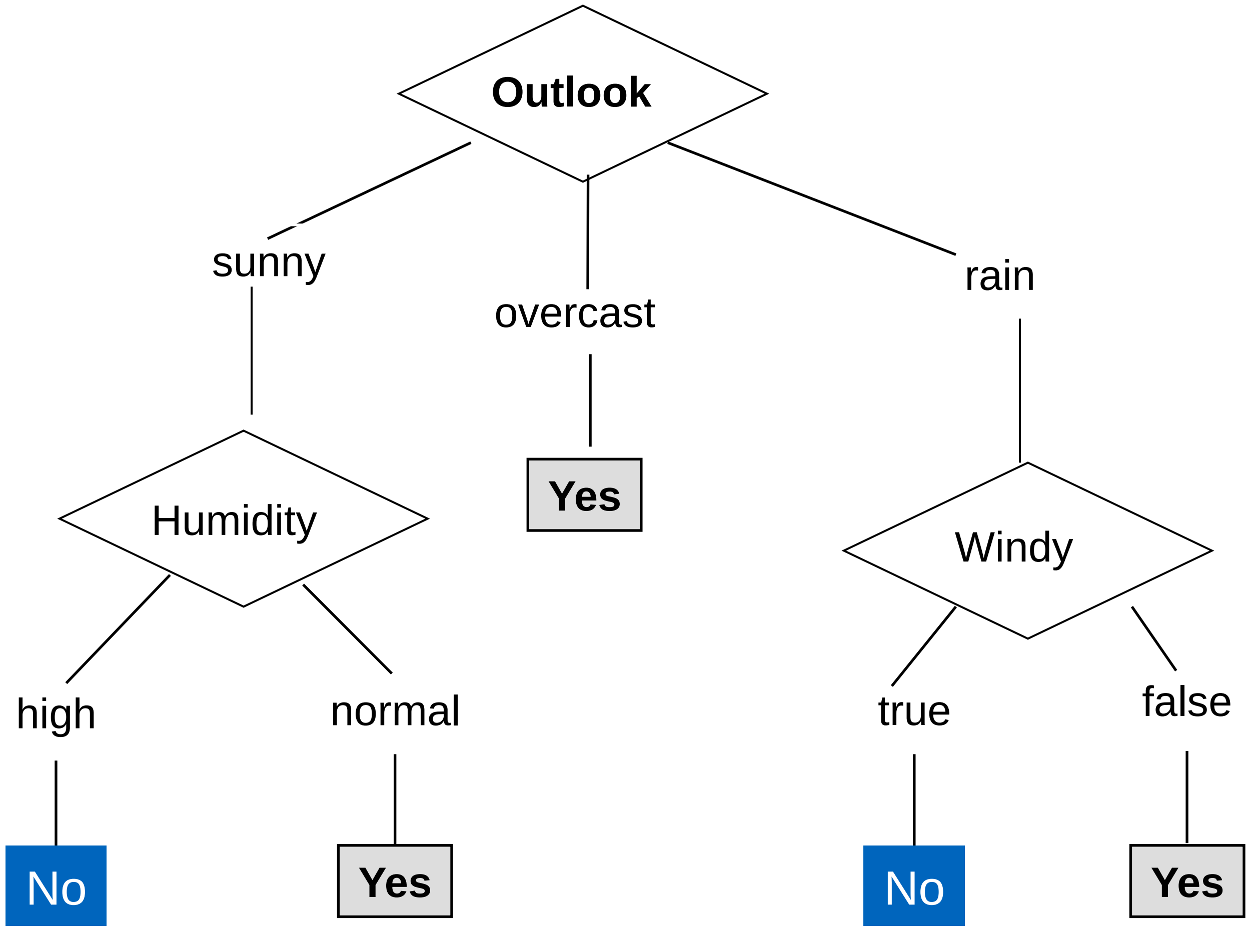
Outline for Today

- **Choosing a splitting attribute in decision trees**
  - Information gain
  - Gain ratio
  - Gini index
- Numeric attributes
- Missing values
- Relational rules

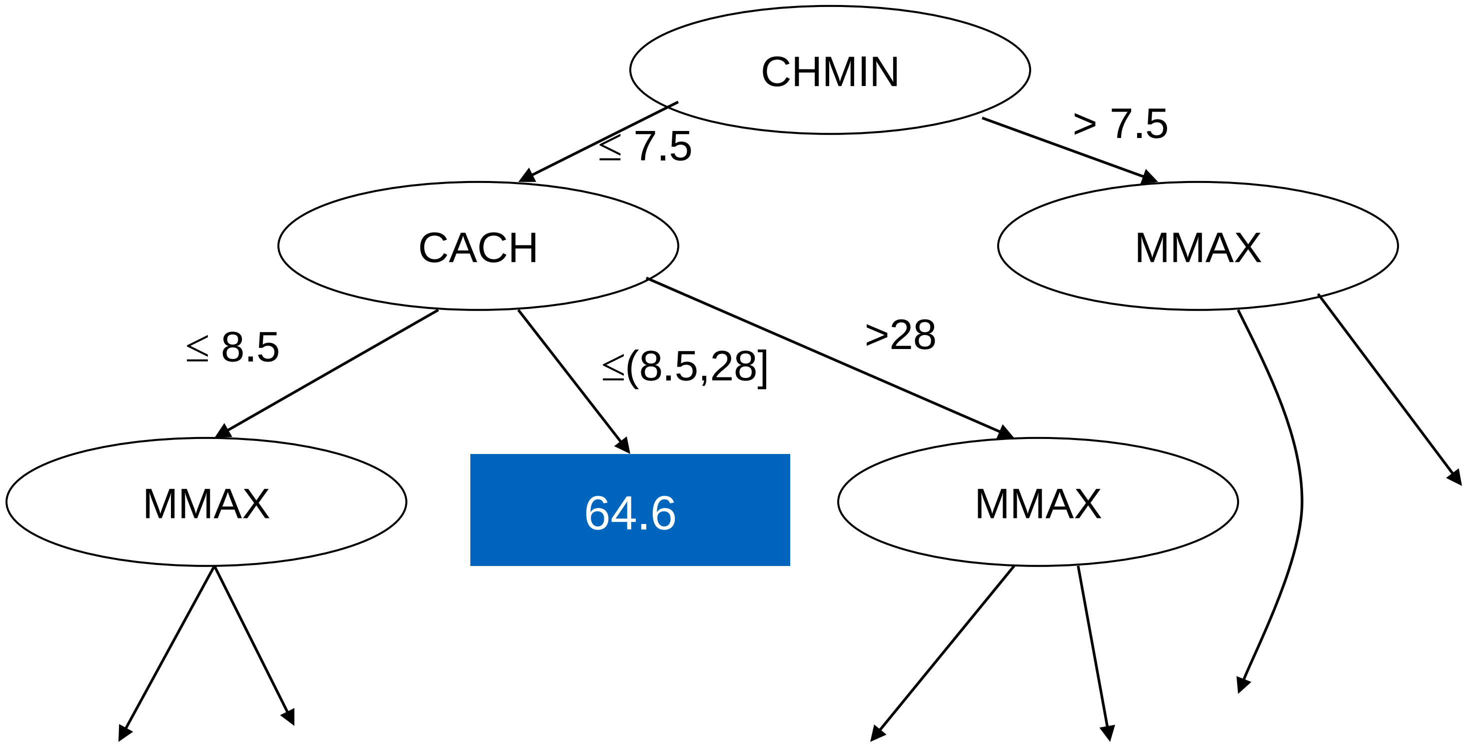
The Weather Data

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**

Example Tree for “Play?”

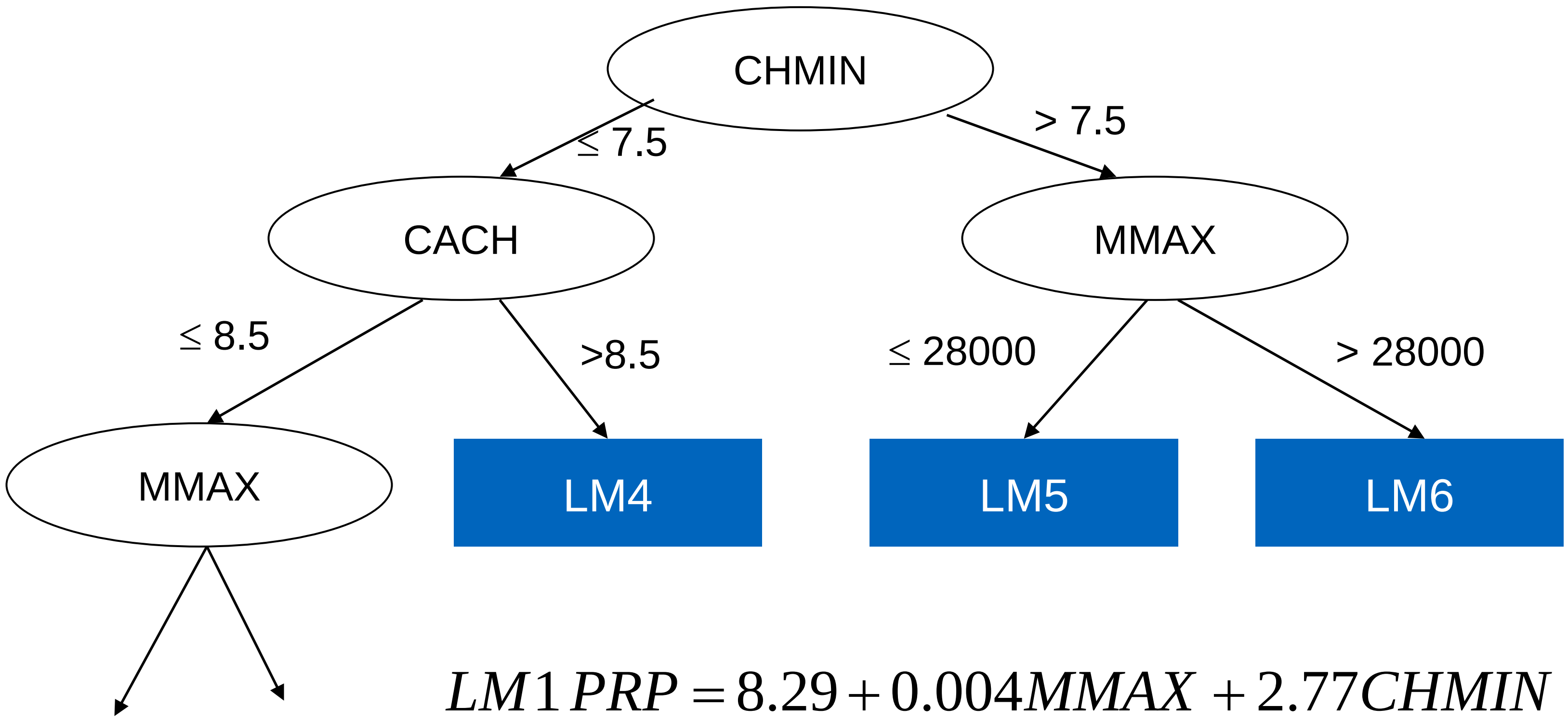


Regression Tree



- High Accuracy
- Large and possibly awkward

Model Trees



$$LM1\ PRP = 8.29 + 0.004MMAX + 2.77CHMIN$$

$$LM2\ PRP = \cdots$$

$$\vdots$$

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

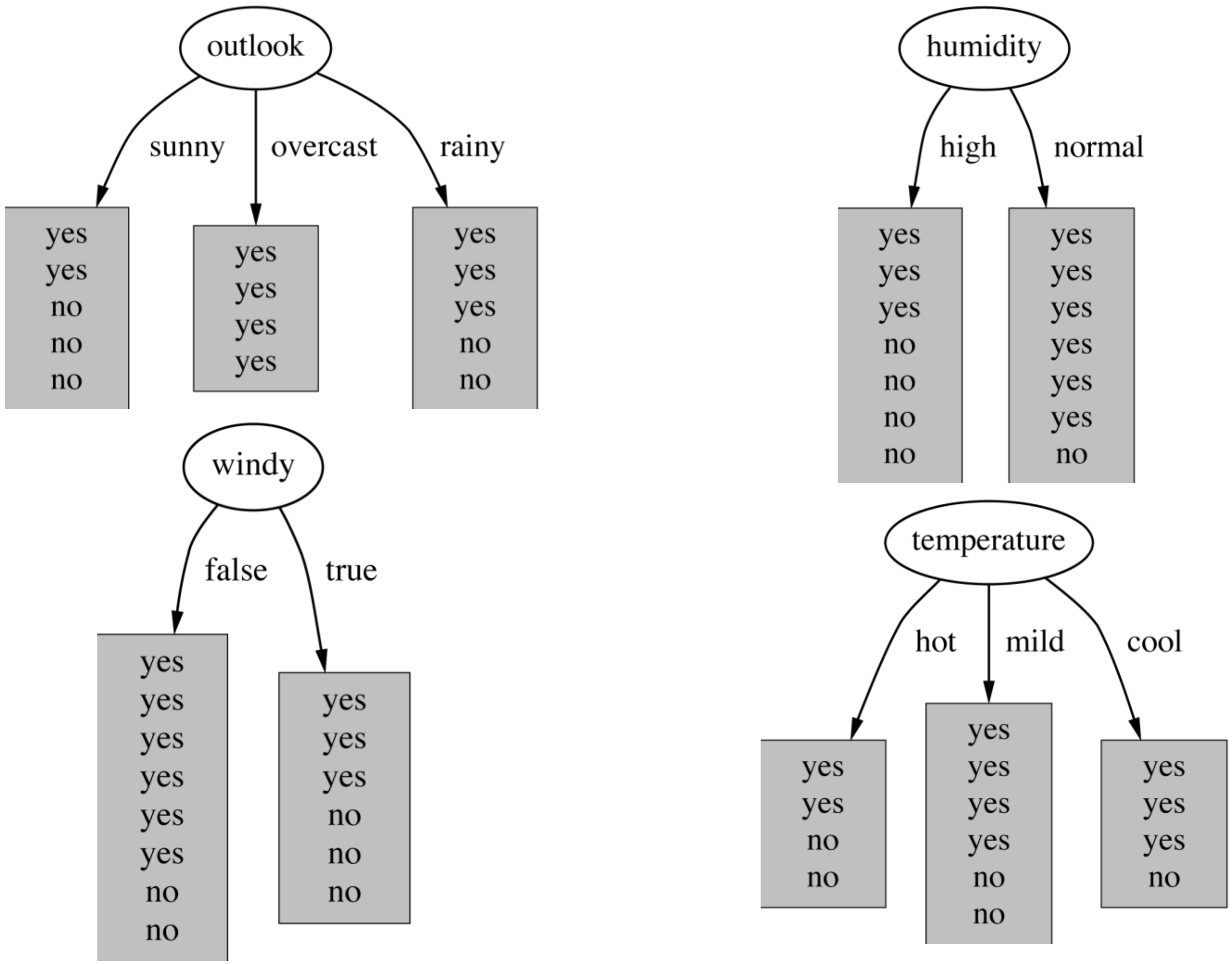
Building Decision Tree

- 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 Splitting Attribute

- At each node, available attributes are evaluated on the basis of separating the classes of the training examples
- A “goodness” function is used for this purpose
- Typical goodness functions:
  - information gain (ID3/C4.5)
  - information gain ratio
  - gini index (CART)

Which Attribute to Select?



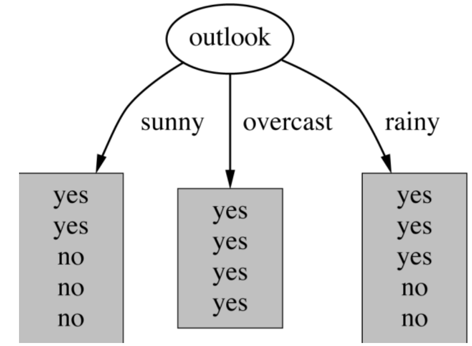
A Criterion for Attribute Selection

- Which is the best attribute?
  - The one which will result in the smallest tree
  - Heuristic: choose the attribute that produces the “purest” nodes
- Popular impurity criterion: information gain
  - Information gain increases with the average purity of the subsets that an attribute produces
- Strategy: choose attribute that results in greatest information gain

Computing Information

- Information is measured in *bits*
  - Given a probability distribution, the info required to predict an event, i.e. if play is yes or no, is the distribution's *entropy*
  - *Entropy* gives the information required in bits (this can involve fractions of bits!)
- Formula for computing the information entropy:

$$\text{entropy}(p_1, p_2, \ldots, p_n) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 \ldots - p_n \log_2 p_n$$



Example: attribute “Outlook”

“Outlook” = “Sunny”:

$$\text{info}([2,3]) = \text{entropy}(2/5,3/5) = -2/5\log_2(2/5) - 3/5\log_2(3/5) = 0.971\,\text{bits}$$

“Outlook” = “Overcast”:

$$\text{info}([4,0]) = \text{entropy}(1,0) = -1\log_2(1) - 0\log_2(0) = 0\,\text{bits}$$

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

“Outlook” = “Rainy”:

$$\text{info}([3,2]) = \text{entropy}(3/5,2/5) = -3/5\log_2(3/5) - 2/5\log_2(2/5) = 0.971\,\text{bits}$$

Expected information for attribute:

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

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

Computing the Information Gain

- Information gain: (information before split) – (information after split)

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

  $= 0.940 - 0.693 = 0.247 \text{ bits}$

- Information gain for attributes from weather data:

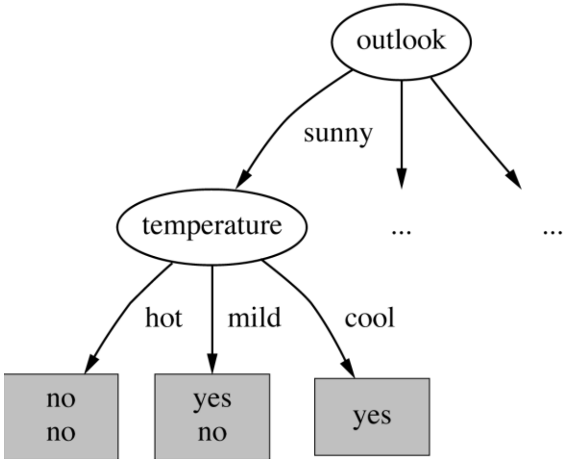
  $\text{gain}(\text{Outlook}) = 0.247 \text{ bits}$

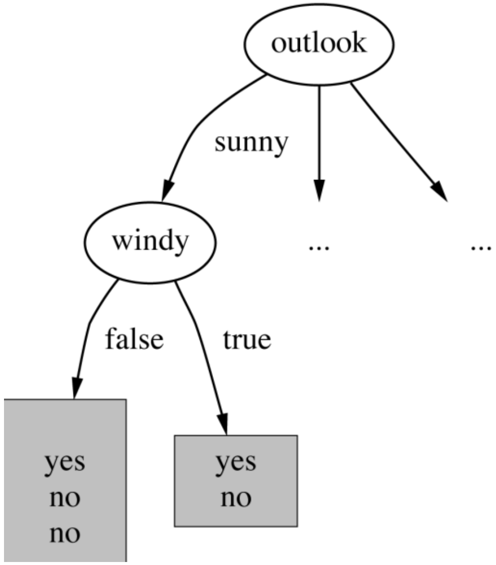
  $\text{gain}(\text{Temperature}) = 0.029 \text{ bits}$

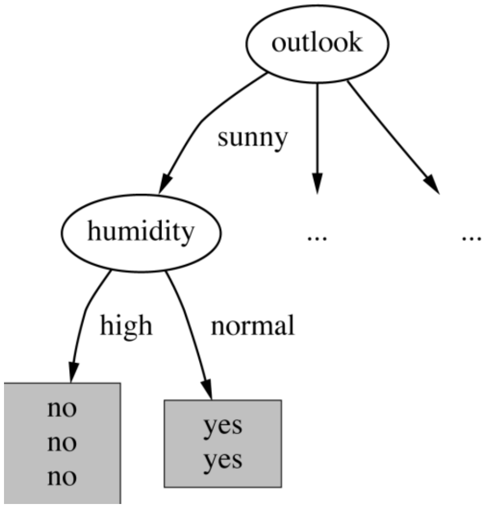
  $\text{gain}(\text{Humidity}) = 0.152 \text{ bits}$

  $\text{gain}(\text{Windy}) = 0.048 \text{ bits}$

Continuing to Split





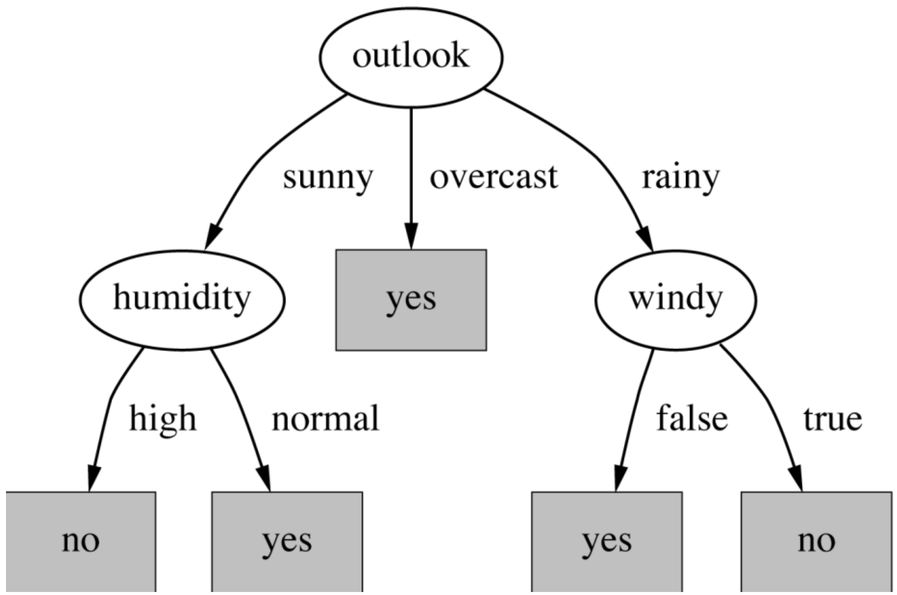


$$\text{gain}(\text{Temperatur}) = 0.571 \text{ bits}$$

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

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

The Final Decision Tree



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

Wish List for a Purity Measure

- Properties we require from a purity measure:
  - When node is pure, measure should be zero (=0)
  - When impurity is maximal (i.e. all classes equally likely), measure should be maximal (e.g., 1 for boolean values)
  - Multistage property: info[2,3,4]=info[2,7]+7/9 info[3,4]

- Entropy is a function that satisfies these properties

Number of classes

$$entropy(S) = \sum_{i=1}^{n} -p_i \, log_2 \, p_i$$

(scales from 0 to max $\log_2 n$)

Training data (instances)

Probability of *S being* classified to *i*

Entropy

- Entropy in general, describes the randomness of a system
  - $\mathrm{entropy} = 0$ describes a perfectly ordered system
- The term was used in thermodynamics and and statistical mechanics
- „ A Mathematical Theory of Communication“ by Claude Shannon 1948 defines entropy and information theory
  - „uncertainty about the contents of a message“

Claude Shannon

Born: 30 April 1916, Died: 23 February 2001

Shannon is famous for having founded information theory with one landmark paper published in 1948 (*A Mathematical Theory of Communication*).

Information theory was developed to find fundamental limits on compressing and reliably communicating data. Communications over a channel was the primary motivation. Channels (such as a phone line) often fail to produce exact reconstruction of a signal; noise, periods of silence, and other forms of signal corruption often degrade quality. How much information can one hope to communicate over a noisy (or otherwise imperfect) channel?

An important application of information theory is coding theory:

- Data compression (by removing redundancy in data)
- Error-correcting codes add just the right kind of redundancy (i.e. error correction) needed to transmit the data efficiently and faithfully across a noisy channel.

Expected Information Gain

$$\text{gain}(S, a) = \text{entropy}(S) - \sum_{v \in Values(a)} \frac{|S_v|}{|S|} \text{entropy}(S_v)$$

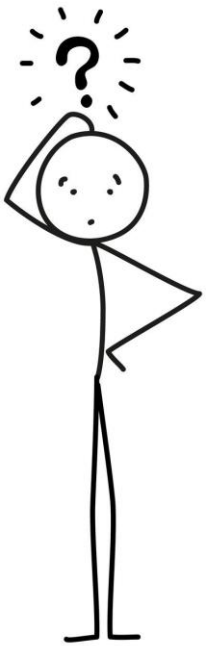
$$S_v = \{s \in S : a(s) = v\}$$

All possible values for attribute a

$\text{gain}(S, a)$ is the information gained adding a sub-tree
(Reduction in number of bits needed to classify an instance)

Problems?

Which splitting attribute would be selected in the following example?

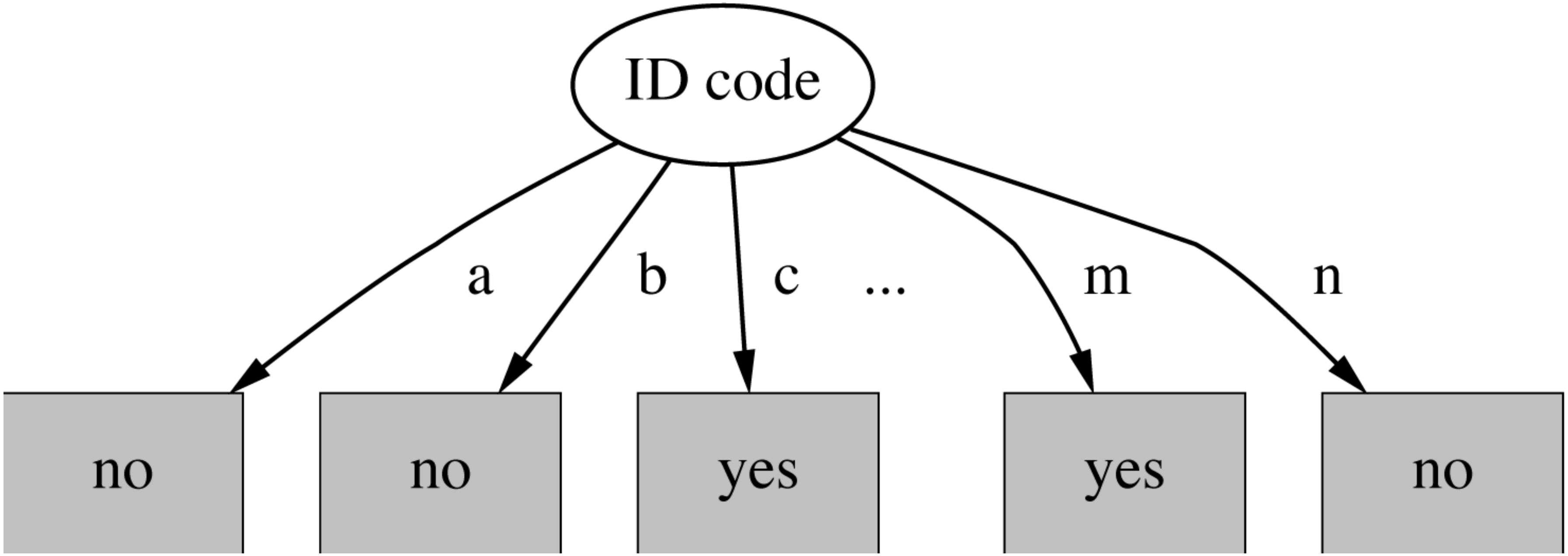


ID	Outlook	Temperature	Humidity	Windy	Play?
A	sunny	hot	high	false	**No**
B	sunny	hot	high	true	**No**
C	overcast	hot	high	false	**Yes**
D	rain	mild	high	false	**Yes**
E	rain	cool	normal	false	**Yes**
F	rain	cool	normal	true	**No**
G	overcast	cool	normal	true	**Yes**
H	sunny	mild	high	false	**No**
I	sunny	cool	normal	false	**Yes**
J	rain	mild	normal	false	**Yes**
K	sunny	mild	normal	true	**Yes**
L	overcast	mild	high	true	**Yes**
M	overcast	hot	normal	false	**Yes**
N	rain	mild	high	true	**No**

Weather Data with ID Code

ID	Outlook	Temperature	Humidity	Windy	Play?
A	sunny	hot	high	false	**No**
B	sunny	hot	high	true	**No**
C	overcast	hot	high	false	**Yes**
D	rain	mild	high	false	**Yes**
E	rain	cool	normal	false	**Yes**
F	rain	cool	normal	true	**No**
G	overcast	cool	normal	true	**Yes**
H	sunny	mild	high	false	**No**
I	sunny	cool	normal	false	**Yes**
J	rain	mild	normal	false	**Yes**
K	sunny	mild	normal	true	**Yes**
L	overcast	mild	high	true	**Yes**
M	overcast	hot	normal	false	**Yes**
N	rain	mild	high	true	**No**

Split for ID Code Attribute



Entropy of split = 0 (since each leaf node is “pure”), having only one case.

Information gain is maximal for ID code

Highly-Branching Attributes

- Problematic: attributes with a large number of values (extreme case: ID code)
- Subsets are more likely to be pure if there is a large number of values
  - Information gain is biased towards choosing attributes with a large number of values
  - This may result in overfitting (selection of an attribute that is non-optimal for prediction)

Gain Ratio

- Gain ratio: a modification of the information gain that reduces its bias on high-branch attributes
- Gain ratio takes number and size of branches into account when choosing an attribute
- It corrects the information gain by taking the intrinsic information of a split into account (i.e. how much info do we need to tell which branch an instance belongs to)

Computing the Gain Ratio

Example: intrinsic information for ID code

$$\mathrm{intrinsic\_info}(1,1,\ldots,1) = 14 * \left(-\frac{1}{14} * \log_2\left(\frac{1}{14}\right)\right) = 3.807\ \mathrm{bits}$$

Importance of attribute decreases as intrinsic information grows.

Example of gain ratio: $\mathrm{gainRatio}(S, a) = \frac{\mathrm{gain(S,a)}}{\mathrm{intrinsic\_info(S,a)}}$

Example: $\mathrm{gainRatio}(\mathrm{ID\_Code}) = \frac{0.940\mathrm{bits}}{3.807\mathrm{bits}} = 0.246$

Gain Ratios for Weather Data

Outlook		**Temperature**	
Info:	0.693	Info:	0.911
Gain: 0.940-0.693	0.247	Gain: 0.940-0.911	0.029
Split info: info([5,4,5])	1.577	Split info: info([4,6,4])	1.557
Gain ratio: 0.247/1.577	0.156	Gain ratio: 0.029/1.557	0.019

Humidity		**Windy**	
Info:	0.788	Info:	0.892
Gain: 0.940-0.788	0.152	Gain: 0.940-0.892	0.048
Split info: info([7,7])	1.000	Split info: info([8,6])	0.985
Gain ratio: 0.152/1	0.152	Gain ratio: 0.048/0.985	0.049

More on the Gain Ratio

- „Outlook” still comes out top
- However:
  - “ID code” has still greater gain ratio (0.246)
  - Standard fix: ad hoc test to prevent splitting on that type of attribute
- Problem with gain ratio: it may overcompensate
  - May choose an attribute just because its intrinsic information is very low
  - Standard fix:
    - First, only consider attributes with greater than average information gain
    - Then, compare them on gain ratio

The Splitting Criterion in CART

- Classification and Regression Tree (CART)
- Developed 1974-1984 by 4 statistics professors
  - Leo Breiman (Berkeley), Jerry Friedman (Stanford), Charles Stone (Berkeley), Richard Olshen (Stanford)
- Gini Index is used as a splitting criterion
- Both C4.5 and CART are robust tools
- No method is always superior – experiment!

Gini Index for 2 Attribute Values

- For example, two classes, *Pos* and *Neg*, and dataset *S* with p *Pos*-elements and n *Neg*-elements. The frequency of positives and negative classes is:

$$-P = p \,/\, (p+n)$$
$$-N = n \,/\, (p+n)$$

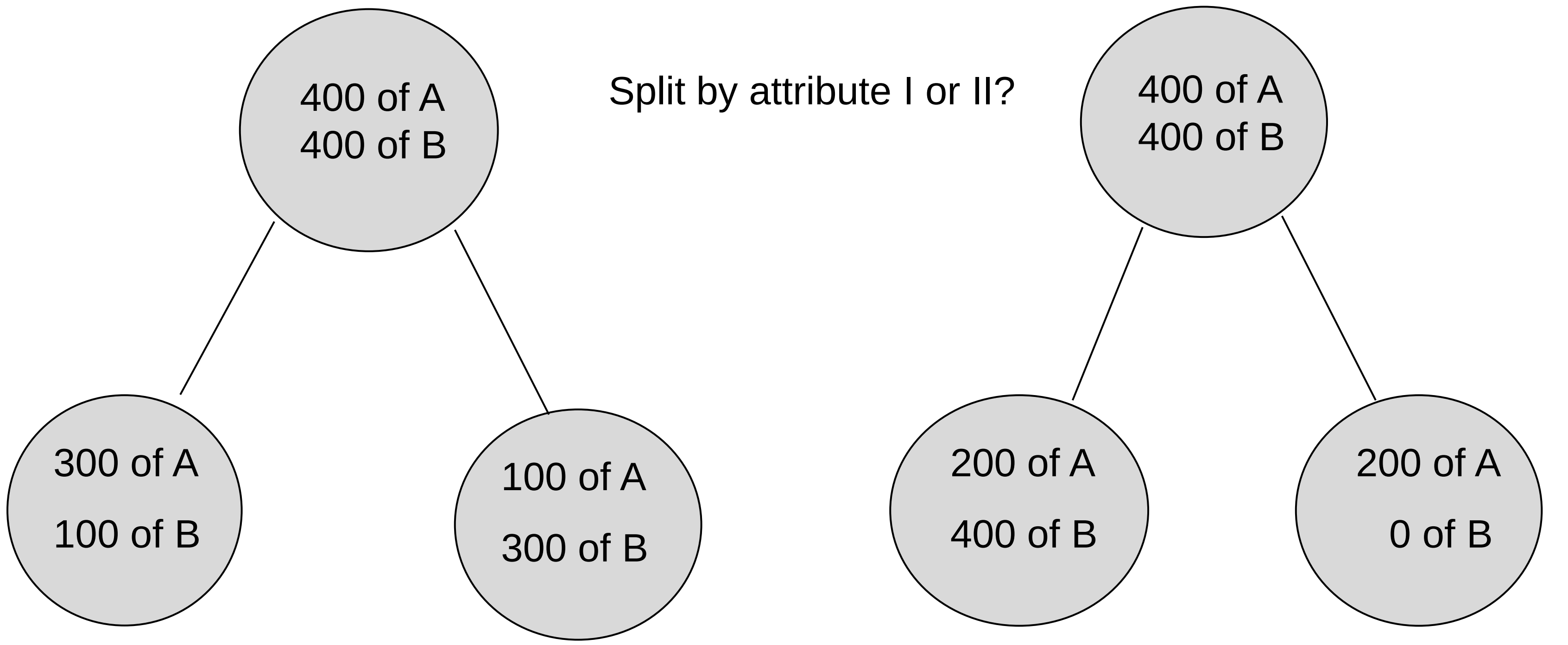
$$Gini(S) = 1 - P^2 - N^2 \qquad \in [0,0.5]$$

- If dataset S is split into S_1, S_2 then

$$Gini_{split}(S_1, S_2) = (p_1 + n_1)/(p+n) \cdot Gini(S_1) + (p_2 + n_2)/(p+n) \cdot Gini(S_2)$$

Example

Split by attribute I or II?



Example

$$\mathrm{Gini}(p) = 1 - \sum_j p_j^2$$

Numbers of Cases		Proportion of Cases				Gini Index
A	B	A	B			
		p_A	p_B	p^2_A	p^2_B	$1- p^2_A- p^2_B$
400	400	0.5	0.5	0.25	0.25	0.5

Select the split that decreases the Gini Index most. This is done over all possible places for a split and all possible variables to split.

Gini Index Example

Number of Cases		Proportion of Cases				Gini Index	Info required	
A	B	A	B					
		p_A	p_B	p^2_A	p^2_B	$1- p^2_A - p^2_B$		
300	100	0.75	0.25	0.5625	0.0625	0.375	0.1875	0.5*Gini(i)
100	300	0.25	0.75	0.0625	0.5625	0.375	0.1875	
						Total	0.375	
200	400	0.33	0.67	0.1111	0.4444	0.4444	0.3333	0.75*Gini(i)
200	0	1	0	1	0	0	0	
						Total	<u>0.3333</u>	

Generate_DT(samples, attribute_list)

- Create a new node N;
- If samples are all of class C then label N with C and exit;
- If attribute_list is empty then label N with majority_class(samples) and exit;
- Select best_split from attribute_list;
- For each value v of attribute best_split:
  - Let S_v = set of samples with best_split=v ;
  - Let N_v = **Generate_DT**(S_v, attribute_list \ best_split) ;
  - Create a branch from N to N_v labeled with the test best_split=v;

Time Complexity of Basic Algorithm

- Let m be the number of attributes
- Let n be the number of instanes
- Assumption: Depth of tree is $\mathcal{O}(\log n)$
  - Usual assumption if the tree is not degenerate
- For each level of the tree all n instances are considered (best = $\mathrm{v_i}$)
  - $\mathcal{O}(n \log n)$ work for a single attribute over the entire tree
- Total cost is $\mathcal{O}(mn \log n)$ since all attributes are eventually considered.
  - Without pruning (see next class)

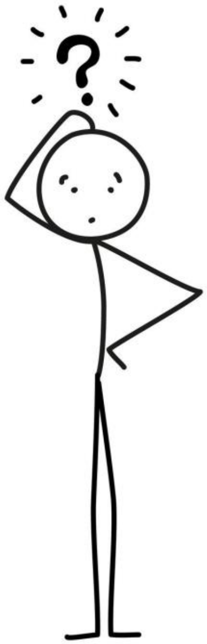
Scalability of DT Algorithms

- Need to design for large amounts of data

- Two things to worry about:
  - Large number of attributes
    - Leads to a large tree
    - Takes a long time

  - Large amounts of data
    - Can the data be kept in memory?
    - Some new algorithms do not require all the data to be memory resident

How would you deal with missing values in the training data?



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- Choosing a splitting attribute in decision trees
  - Information gain
  - Gain ratio
  - Gini index
- **Numeric attributes**
- Missing values
- Relational rules

C4.5 History

- The above procedure is the basis for Ross Quinlain’s ID3 algorithm (so far works only for nominal attributes)
  - ID3, CHAID – 1960s

- The algorithm was improved and is now most widely used as C4.5 or C5.0 respectively, available in most DM software packages
  - Commercial successor: C5.0

- Witten et al. write “a landmark decision tree program that is probably the machine learning workhorse most widely used in practice to date”

C4.5 An Industrial-Strength Algorithm

- For an algorithm to be useful in a wide range of real-world applications it must:
  - Permit numeric attributes
  - Allow missing values
  - Be robust in the presence of noise

- Basic algorithm needs to be extended to fulfill these requirements

Numeric Attributes

- Unlike nominal attributes, every attribute has many possible split points
  - Standard method: binary splits
  - E.g. temp < 45

- 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 highest info gain for attribute

- Numerical attributes can be used several times in a decision tree, nominal attributes only once

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

Binary Splits on Numeric Attributes

- Splitting (multi-way) on a nominal attribute exhausts all information in that attribute
  - Nominal attribute is tested (at most) once on any path in the tree

- Not so for binary splits on numeric attributes!
  - Numeric attributes may be tested several times along a path in the tree

- Disadvantage: tree is hard to read

- Remedy:
  - pre-discretize numeric attributes, or
  - allow for multi-way splits instead of binary ones using the Information Gain criterion

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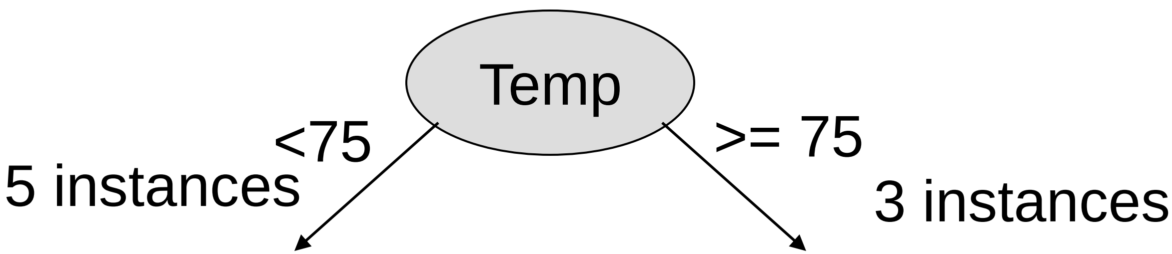
- Choosing a splitting attribute in decision trees
  - Information gain
  - Gain ratio
  - Gini index
- Numeric attributes
- **Missing values**
- Relational rules

Handling Missing Values / Training

- Ignore instances with missing values
  - Pretty harsh, and missing value might not be important
- Ignore attributes with missing values
  - Again, may not be feasible
- Treat missing value as another nominal value
  - Fine if missing a value has a significant meaning
- Estimate missing values
  - Data imputation: regression, nearest neighbor, mean, mode, etc.

Handling Missing Values / Classification

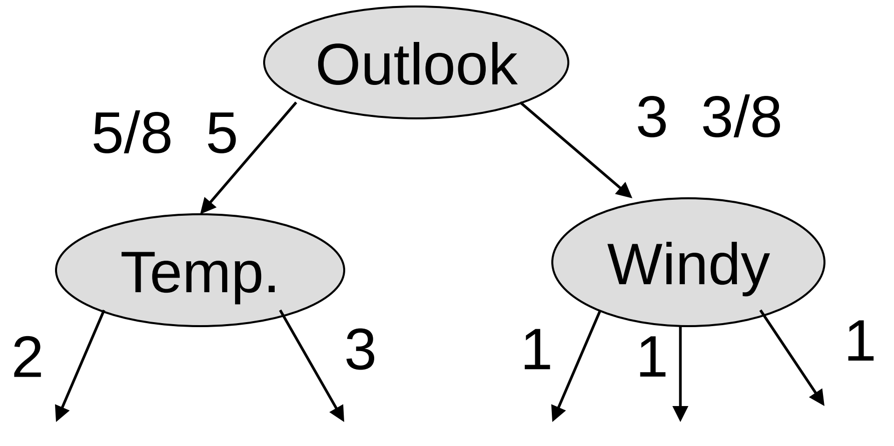
- Follow the leader
  - An instance with a missing value for a tested attribute (temp) is sent down the branch with the most instances



Instance included on the left branch

Handling Missing Values / Classification

- "Partition" the instance
  - branches show # of instances
  - Send down parts of the instance (e.g. 3/8 on Windy and 5/8 on Sunny) proportional to the number of training instances
  - Resulting leaf nodes get weighted in the result



Overfitting

- Two sources of abnormalities
  - Noise (randomness)
  - Outliers (measurement errors)

- Chasing every abnormality causes overfitting
  - Decision tree gets too large and complex
  - Good accuracy on training set, poor accuracy on test set
  - Does not generalize to new data any more

- Solution: prune the tree

Decision Trees - Summary

- Decision trees are a classification technique
- The output of decision trees can be used for descriptive as well as predictive purposes
- They can represent any function in the form of propositional logic
- Heuristics such as information gain are used to select relevant attributes
- Pruning is used to avoid overfitting

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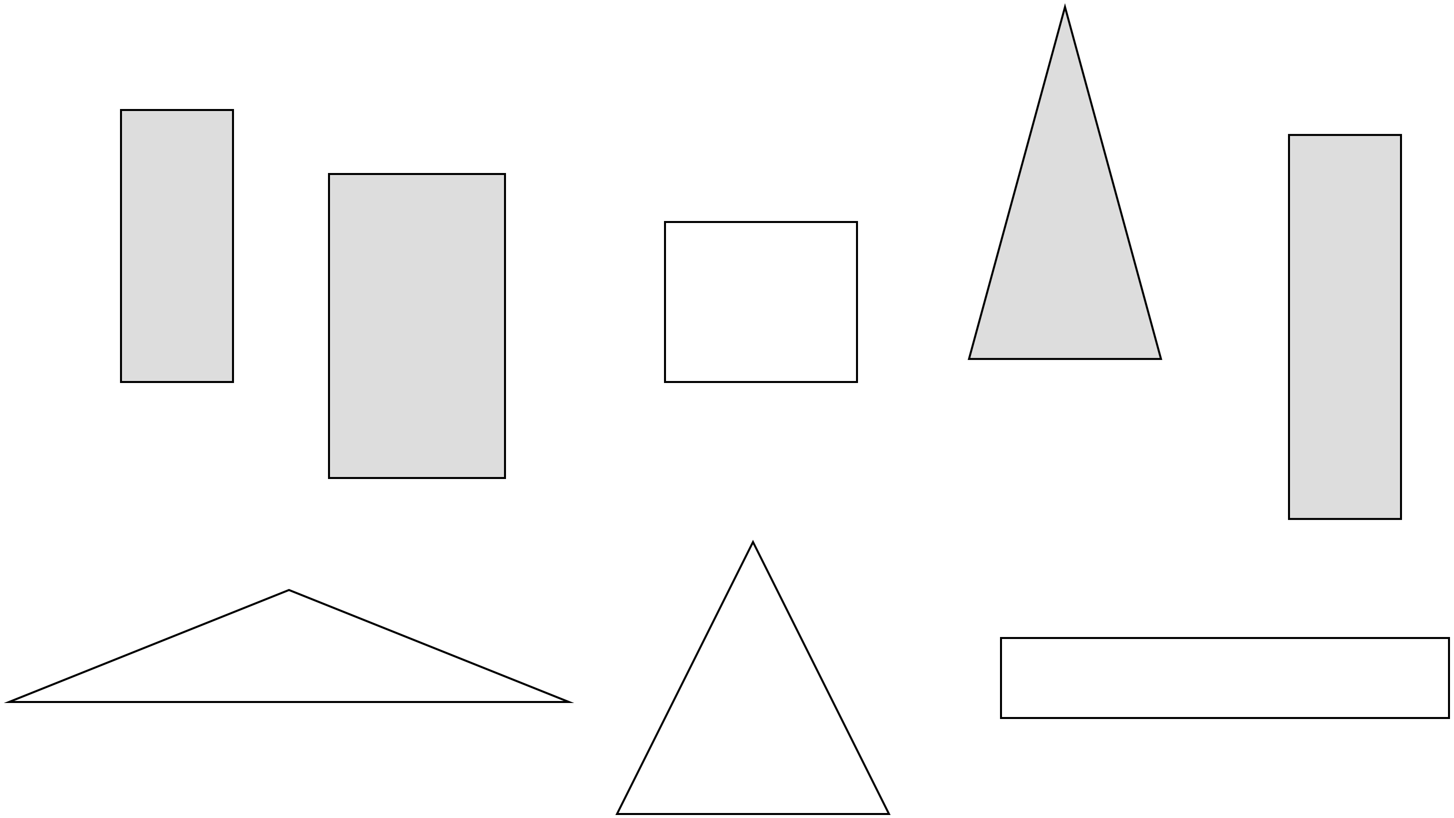
- Missing values
- **Relational rules**

The Shapes Problem



Shaded=standing
Unshaded=lying

Instances

Width	Height	Sides	Class
2	4	4	**Standing**
3	6	4	**Standing**
4	3	4	**Lying**
7	8	3	**Standing**
7	6	3	**Lying**
2	9	4	**Standing**
9	1	4	**Lying**
10	2	3	**Lying**

```
If width ≥ 3.5 and height < 7.0  then lying
If height ≥ 3.5 then standing
```

Classification Rules

```
If width ≥ 3.5 and height < 7.0  then lying
If height ≥ 3.5 then standing
```

- Work well to classify these instances ... but not necessarily for new ones.

- Problems?

Relational Rules

```
If width > height then lying
If height > width then standing
```

- Rules comparing attributes to constants are called propositional rules (propositional data mining)

- Relational rules are more expressive in some cases
  - define relations between attributes (relational data mining)
  - most DM techniques do not consider relational rules

- As a workaround for some cases, one can introduce additional attributes, describing if width > height
  - allows using conventional “propositional” learners

Propositional Logic

- Essentially, decision trees can represent any function in propositional logic
  - A, B, C: propositional variables
  - and, or, not, => (implies), <=> (equivalent): connectives

- A proposition is a statement that is either true or false
  - The sky is blue: color of sky = blue

- Decision trees are an example of a propositional learner.