

Lecture 15: Decision Trees & Random Forest

COMP90049 Knowledge Technologies

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THE UNIVERSITY OF
MELBOURNE

From Decision Stumps to Decision Trees

Decision Tree & Random Forest

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Decision Tree

Definition
Hunt Algorithm
Predicting by DT

Attribute Selection
Information Gain
Gain Ratio

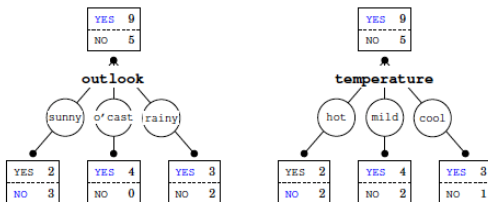
More DT Algorithms

Overfitting

Classifier
Combination
Bagging
Random Tree
Random Forest

Summary
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- We have seen decision stumps in action in the context of 1-R



- Based the same concept we can build a more complex model with the ability to capture complex feature interaction

Decision Tree

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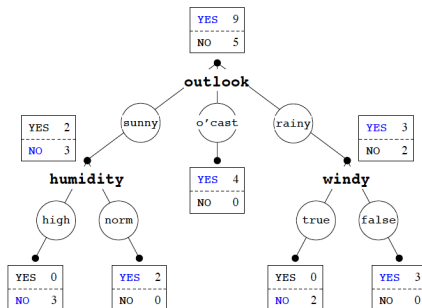
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A flow-chart-like tree structure

- Internal node denotes a test on an *attribute*
- Branch represents an *outcome* of the test (*attribute value*)
- Leaf nodes represent *class labels* or class distribution



Total errors = $\frac{0}{14}$

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Advantages:

- Basic classification model
- Fast
- Scalable
- Interpretable

Disadvantage:

- Not highest accuracy (Random Forest to the rescue)

Training Decision Tree: Hunt's Algorithm

Let D_t be the set of training records that reach a node t

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General Procedure:

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| 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 |
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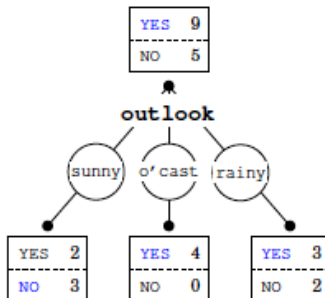
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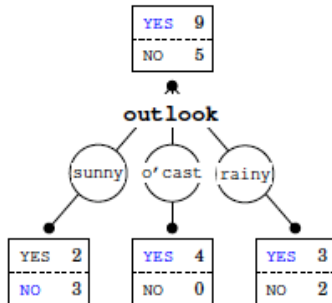
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General Procedure:

- If D_t contains records that belong to more than one class, **use an attribute** to **split** the data into smaller subsets.
- Recursively apply the procedure to each subset.

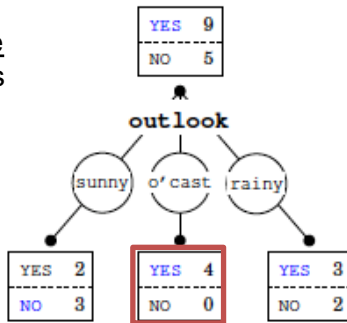
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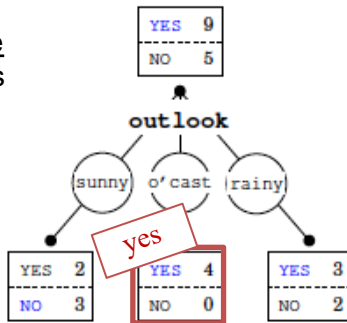
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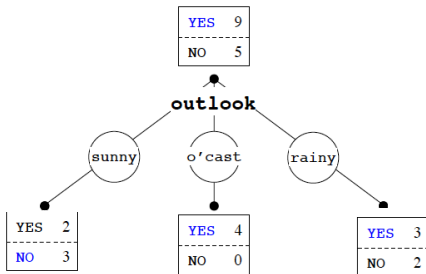
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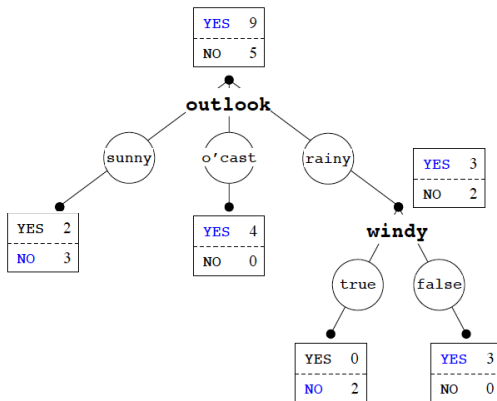
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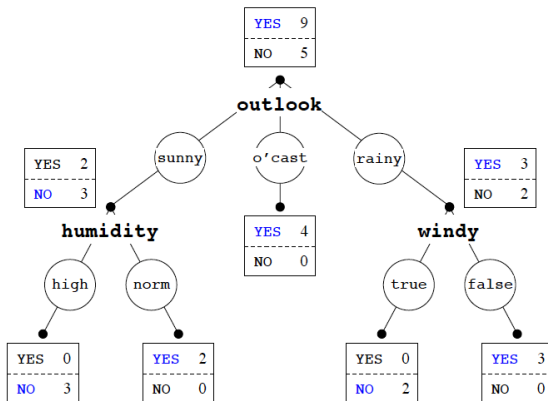
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Attribute Selection Information Gain Gain Ratio

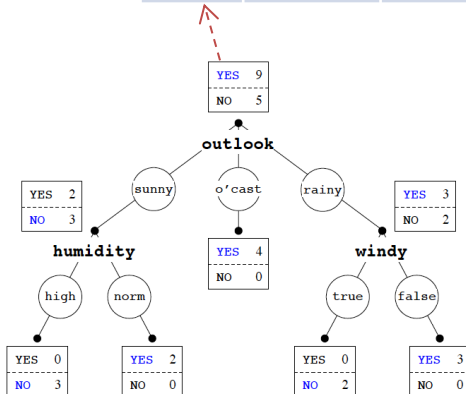
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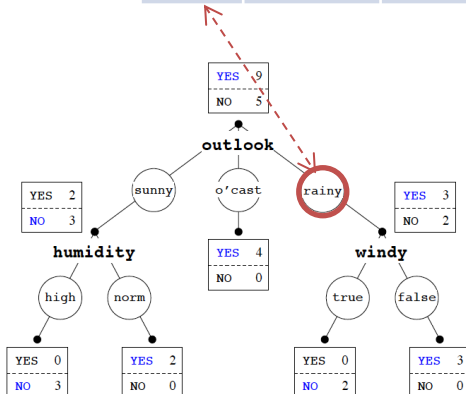
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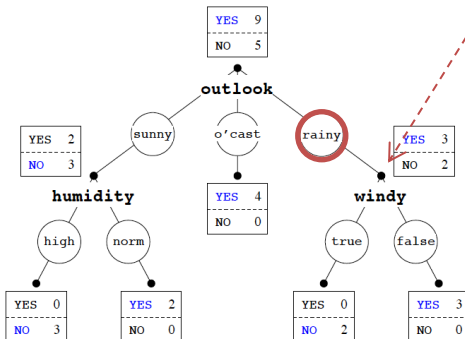
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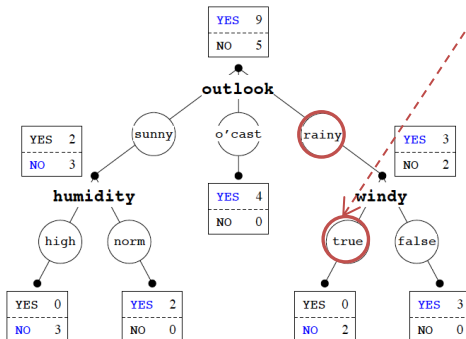
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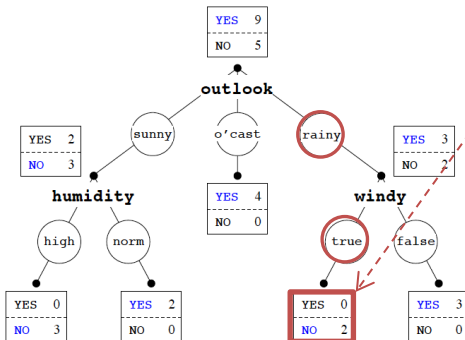
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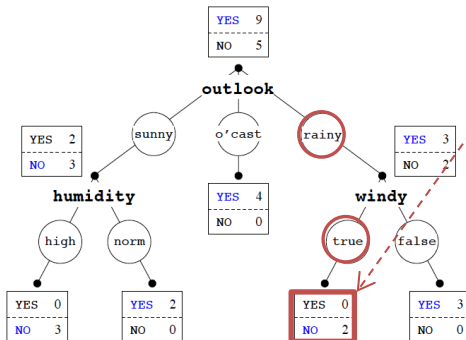
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Criterion for Attribute Selection

- There could be more than one tree that fits the same data!

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- There could be more than one tree that fits the same data!
- How do we choose the attribute to partition the instances at a given node?

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- There could be more than one tree that fits the same data!
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- We want to get the **smallest** tree

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- Prefer attributes that create more **homogeneous (pure)** nodes

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- One Measure is **Entropy**

Criterion for Attribute Selection

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- We want to get the **smallest** tree
- Prefer attributes that create more **homogeneous (pure)** nodes
- We need to measure node **purity**
- One Measure is **Entropy** (measure of **predictability**)

Entropy (Recap)

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The entropy of a discrete random event x with possible states $1, \dots, n$ is:

$$H(x) = - \sum_{i=1}^n P(i) \log_2 P(i)$$

(where $0 \log_2(0)$ is 0)

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When **Entropy** is low

- The event is predictable (more homogeneous)

When **Entropy** is high

- The event is unpredictable (less homogeneous)

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When **Entropy** is low

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When **Entropy** is high

- The event is unpredictable (less homogeneous)

In developing a Decision Tree:

- ✓ We prefer **attributes** (for splitting the dataset) that **reduce the entropy** more.

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- The expected reduction in entropy caused by knowing the value of an attribute.
- Compare:
 - the entropy before splitting the tree using the attribute's values
 - the weighted average of the entropy over the children after the split (**Mean Information**)
- If the entropy decreases, then we have a better tree (more predictable)

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- Compare:
 - the entropy before splitting the tree using the attribute's values
 - the weighted average of the entropy over the children after the split (**Mean Information**)
- If the entropy decreases, then we have a better tree (more predictable)
- Information Gain is the difference between the *entropy at the root* (before splitting) and the *Mean Information*

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- We calculate the **Mean Information** for a tree stump with m attribute values as:

$$\text{Mean Info}(x_1, \dots, x_m) = \sum_{i=1}^m P(x_i) H(x_i)$$

where $H(x_i)$ is the entropy of the class distribution for the instances at node x_i

- We calculate the **Mean Information** for a tree stump with m attribute values as:

$$\text{Mean Info}(x_1, \dots, x_m) = \sum_{i=1}^m P(x_i)H(x_i)$$

where $H(x_i)$ is the entropy of the class distribution for the instances at node x_i

- **Information Gain**

$$IG(R_A|R) = H(R) - \sum_{i=1}^m P(x_i)H(x_i)$$

$$IG(R_A|R) = H(R) - \text{Mean Info}(x_1, \dots, x_m)$$

Calculating Information Gain

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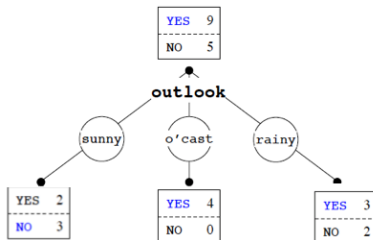
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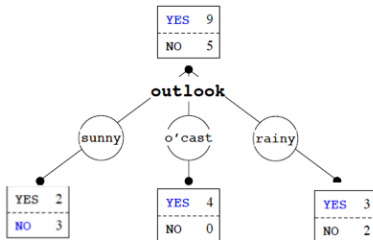
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entropy before splitting the tree (entropy at root)

$$\begin{aligned}
 H(R) &= \\
 &= -((9/14) \log_2(9/14) + (5/14) \log_2(5/14)) = \\
 &= -(-.4098 - 0.5305) = 0.940
 \end{aligned}$$

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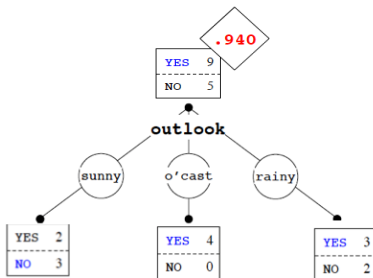
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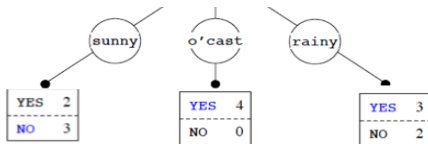
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entropies after splitting the tree (outlook)

$$\begin{aligned} H(\text{rainy}) &= \\ &-(3/5) \log_2(3/5) + (2/5 \log_2(2/5))) = \\ &-(-0.4422 - 0.5288) = 0.971 \end{aligned}$$

$$\begin{aligned} H(\text{overcast}) &= \\ &-((4/4) \log_2(4/4) + (0/4 \log_2(0/4))) = 0 \end{aligned}$$

$$\begin{aligned} H(\text{sunny}) &= \\ &-((2/5) \log_2(2/5) + (3/5 \log_2(3/5))) = 0.971 \end{aligned}$$



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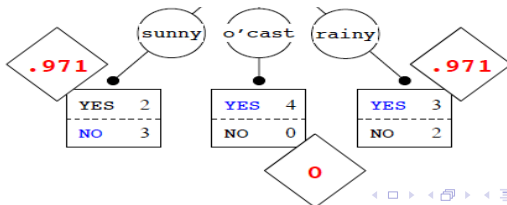
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entropies after splitting the tree (outlook)

$$\begin{aligned} H(\text{rainy}) &= \\ &-(3/5) \log_2(3/5) + (2/5 \log_2(2/5))) = \\ &-(-0.4422 - 0.5288) = 0.971 \end{aligned}$$

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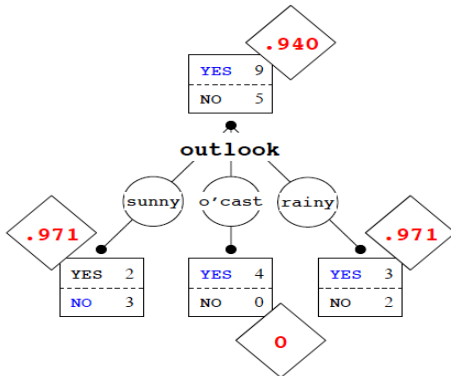
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Mean Information for Outlook

$$\begin{aligned} \text{Mean_info}(\text{outlook}) &= P(\text{rainy})H(\text{rainy}) + P(\text{overcast})H(\text{overcast}) + \\ &P(\text{sunny})H(\text{sunny}) = 5/14 * 0.971 + 0 + 5/14 * 0.971 = 0.693 \end{aligned}$$

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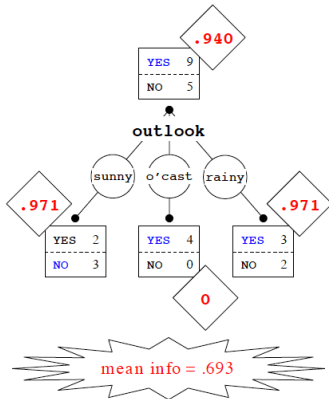
Information Gain

$$IG(R_A | R) = H(R) - \text{Mean Info}(x_1, \dots, x_m)$$

Information Gain

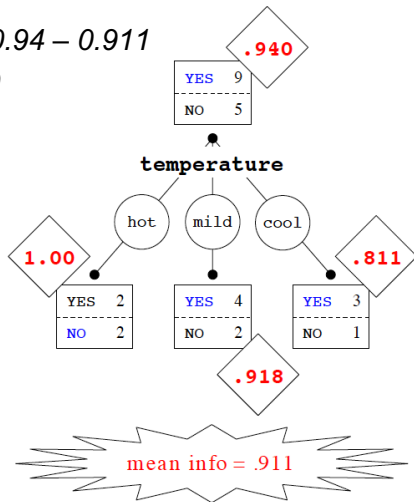
$$IG(R_A | R) = H(R) - \text{Mean Info}(x_1, \dots, x_m)$$

$$IG(\text{outlook} | R) = 0.94 - 0.693 = 0.247$$



Building a tree by using the Information Gain

$$IG(\text{temperature} | R) = 0.94 - 0.911 = 0.029$$



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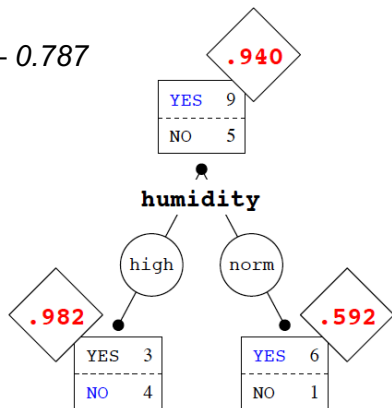
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Building a tree by using the Information Gain

$$IG (humidity | R) = 0.94 - 0.787 \\ = 0.152$$



mean info = .787

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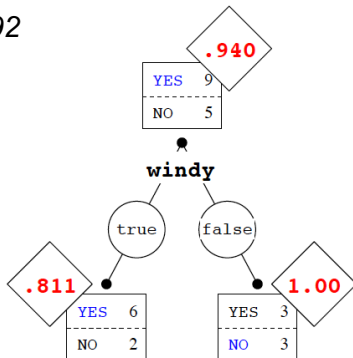
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$$IG(windy | R) = 0.94 - 0.892 = 0.048$$



mean info = .892

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$$IG (outlook \mid R) = 0.247$$

$$IG (temperature \mid R) = 0.029$$

$$IG (humidity \mid R) = 0.152$$

$$IG (windy \mid R) = 0.048$$

Building a tree by using the Information Gain

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$IG (outlook \mid R) = 0.247$ *higher Information Gain*

$IG (temperature \mid R) = 0.029$

$IG (humidity \mid R) = 0.152$

$IG (windy \mid R) = 0.048$

Shortcomings of Information Gain

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| ID | Outlook | Temperature | Humidity | Windy | Play |
|----|----------|-------------|----------|-------|------|
| 1 | sunny | hot | high | FALSE | no |
| 2 | sunny | hot | high | TRUE | no |
| 3 | overcast | hot | high | FALSE | yes |
| 4 | rainy | mild | high | FALSE | yes |
| 5 | rainy | cool | normal | FALSE | yes |
| 6 | rainy | cool | normal | TRUE | no |
| 7 | overcast | cool | normal | TRUE | yes |
| 8 | sunny | mild | high | FALSE | no |
| 9 | sunny | cool | normal | FALSE | yes |
| 10 | rainy | mild | normal | FALSE | yes |

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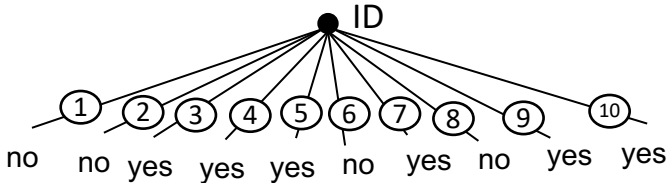
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Shortcomings of Information Gain

- Information gain tends to prefer highly-branching attributes:
 - A subset of instances is more likely to be homogeneous (all of a single class) if there are only a few instances
 - Attribute with many values will have fewer instances at each child node

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- Information gain tends to prefer highly-branching attributes:
 - A subset of instances is more likely to be homogeneous (all of a single class) if there are only a few instances
 - Attribute with many values will have fewer instances at each child node
- This may result in **overfitting/fragmentation**

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- Information gain tends to prefer highly-branching attributes:
 - A subset of instances is more likely to be homogeneous (all of a single class) if there are only a few instances
 - Attribute with many values will have fewer instances at each child node
- This may result in **overfitting/fragmentation**
- Solution → **Gain Ratio**

- **Gain ratio (GR)** reduces the bias for information gain towards highly-branching attributes by normalizing relative to the split information
- **Split info (SI)** is the entropy of a given split (evenness of the distribution of instances to attribute values)

$$\begin{aligned} GR(R_A|R) &= \frac{IG(R_A|R)}{SI(R_A|R)} = \frac{IG(R_A|R)}{H(R_A)} \\ &= \frac{H(R) - \sum_{i=1}^m P(x_i)H(x_i)}{-\sum_{i=1}^m P(x_i) \log_2 P(x_i)} \end{aligned}$$

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- **Note:** Split Info is entropy of distribution of instances to attribute values (disregarding classes, unlike Mean Info)

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$$\text{Mean Info}(x_1, \dots, x_m) = \sum_{i=1}^m P(x_i) H(x_i)$$

$$\text{Split Info}(x_1, \dots, x_m | R) = - \sum_{i=1}^m P(x_i) \log_2 P(x_i)$$

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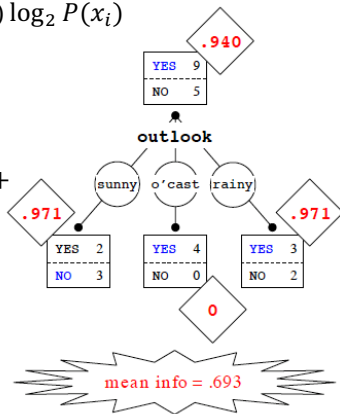
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$$\text{Mean Info}(x_1, \dots, x_m) = \sum_{i=1}^m P(x_i) H(x_i)$$

$$\text{Split Info}(x_1, \dots, x_m | R) = - \sum_{i=1}^m P(x_i) \log_2 P(x_i)$$

$$\begin{aligned} \text{Split Info}(\text{outlook} | R) = \\ - \left(\left(\frac{5}{14} \right) \log_2 \left(\frac{5}{14} \right) + \left(\frac{4}{14} \right) \log_2 \left(\frac{4}{14} \right) + \right. \\ \left. \left(\frac{5}{14} \right) \log_2 \left(\frac{5}{14} \right) \right) = 1.577 \end{aligned}$$



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$$IG(\text{outlook}|R) = 0.247$$

$$IG(\text{humidity}|R) = 0.152$$

$$IG(\text{temperature}|R) = 0.029$$

$$IG(\text{windy}|R) = 0.048$$

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$$SI(\text{outlook}|R) = 1.577$$

$$IG(\text{humidity}|R) = 0.152$$

$$SI(\text{humidity}|R) = 1.000$$

$$IG(\text{temperature}|R) = 0.029$$

$$SI(\text{temperature}|R) = 1.557$$

$$IG(\text{windy}|R) = 0.048$$

$$SI(\text{windy}|R) = 0.985$$

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$$IG(\text{outlook}|R) = 0.247$$

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$$GR(\text{humidity}|R) = 0.152$$

$$IG(\text{temperature}|R) = 0.029$$

$$SI(\text{temperature}|R) = 1.557$$

$$GR(\text{temperature}|R) = 0.019$$

$$IG(\text{windy}|R) = 0.048$$

$$SI(\text{windy}|R) = 0.985$$

$$GR(\text{windy}|R) = 0.049$$

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$$IG(\text{outlook}|R) = 0.247 \quad \leftarrow$$

$$SI(\text{outlook}|R) = 1.577$$

$$GR(\text{outlook}|R) = 0.156$$

$$IG(\text{humidity}|R) = 0.152 \quad \leftarrow$$

$$SI(\text{humidity}|R) = 1.000$$

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Ross Quinlan

- **ID3** uses the Hunt's algorithm with information gain criterion and gain ratio
 - Available in WEKA (no discretization, no missing values)
- **C4.5** improves **ID3**
 - Needs entire data to fit in memory
 - Handles missing attributes and continuous attributes
 - Performs tree post-pruning
 - Available in WEKA as **J48**

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Breiman et al.

- **CART** builds multivariate decision (binary) trees
 - Supports numerical target variables (regression)
 - Available in WEKA as **SimpleCART**

Determine When to Stop Splitting

- When a node is homogenous

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Summary Resources

- When a node is homogenous
- When the subsample size is smaller than a threshold

Determine When to Stop Splitting

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Summary Resources

- When a node is homogenous
- When the subsample size is smaller than a threshold

Remember: our goal is not to sub-divide the data perfectly

- Over-subdivision leads to a complicated decision boundary (over-fitting)

Determine When to Stop Splitting

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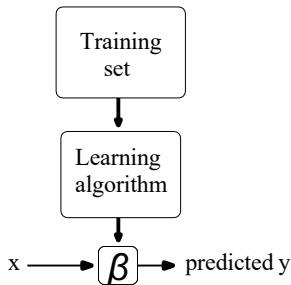
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Metrics to control the complexity of the tree

- Total number of nodes
- Tree depth
- Minimum number of data points for a split
- IG/GR is smaller than a threshold

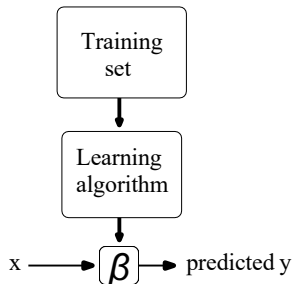
- We have discussed individual classification algorithms and considered each of them in isolation
- We have discussed ways of comparing the performance of individual classifiers over a given dataset/task, which allows us to choose the “dataset optimal” classifier



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- **Classifier combination
(ensemble learning)**

constructs a set of base classifiers from a given set of training data and aggregates the outputs into a single meta-classifier



Classifier Combination

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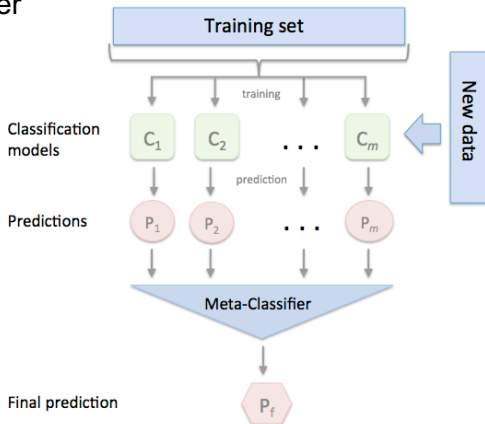
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▪ **Classifier combination (ensemble learning)**

constructs a set of base classifiers from a given set of training data and aggregates the outputs into a single meta-classifier



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- **Motivation 1:** the combination of lots of weak classifiers can be at least as good as one strong classifier
- **Motivation 2:** the combination of a selection of strong classifiers is (usually) at least as good as the best of the base classifiers

Classifier Combination

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- **Instance manipulation:** generate multiple training datasets through sampling, and train a base classifier over each
- **Feature manipulation:** generate multiple training datasets through different feature subsets, and train a base classifier over each
- **Class label manipulation:** generate multiple training datasets by manipulating the class labels in a reversible manner
- **Algorithm manipulation:** semi-randomly “tweak” internal parameters within a given algorithm to generate multiple base classifiers over a given dataset

Bagging

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- **Basic intuition:** the more data, the better the performance, so how can we get ever more data out of a fixed training dataset?
- **Method:** Randomly sample the original dataset N times, with replacement

Original training dataset:

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|----|

Bootstrap samples:

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|----|
| 7 | 2 | 6 | 7 | 5 | 4 | 8 | 8 | 1 | 10 |
|---|---|---|---|---|---|---|---|---|----|

| | | | | | | | | | |
|---|---|---|----|---|---|---|----|---|---|
| 1 | 3 | 8 | 10 | 3 | 5 | 8 | 10 | 1 | 9 |
|---|---|---|----|---|---|---|----|---|---|

| | | | | | | | | | |
|---|---|---|---|---|---|---|----|---|----|
| 2 | 9 | 4 | 2 | 7 | 9 | 3 | 10 | 1 | 10 |
|---|---|---|---|---|---|---|----|---|----|

A “Random Tree” is a Decision Tree where:

- At each node, only some of the possible attributes are considered
- For example, a fixed proportion of all of the attributes, except the ones used earlier in the tree
- Attempts to control for unhelpful attributes in the feature set
- Much faster to build than a “deterministic” Decision Tree, but increases model variance

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A “Random Forest” is:

- An ensemble of Random Trees (many trees = forest)
- Each tree is built on a random subset of records of the data: **Tree bagging**
- Each tree is built on a random subset of features of the data: **Random subspace**
- Decision via **majority voting**

Random Forest

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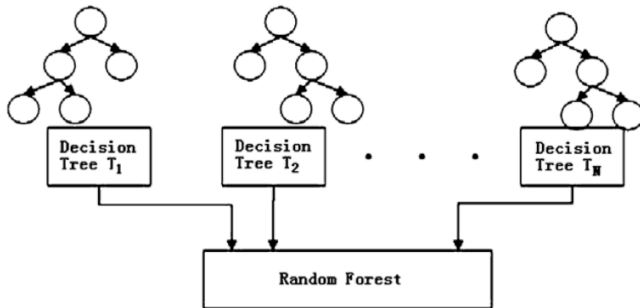
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Community of Experts

Practical Properties of Random Forests

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- Generally a very strong performer
- Embarrassingly parallelisable
- Surprisingly efficient
- Robust to overfitting
- Interpretability sacrificed

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This lecture was prepared using some material adapted from:

- <https://www-users.cs.umn.edu/~kumar/dmbook/ch4.pdf>
- http://www-users.cs.umn.edu/~kumar/dmbook/dmslides/chap4_basic_classification.ppt
- Mitchell, Tom (1997). Machine Learning. Chapter 3: Decision Tree Learning.
- Tan et al (2006) Introduction to Data Mining. Section 4.3, pp 150-171.
- Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Introduction to Data Mining. Addison Wesley, 2006