# Decision Trees

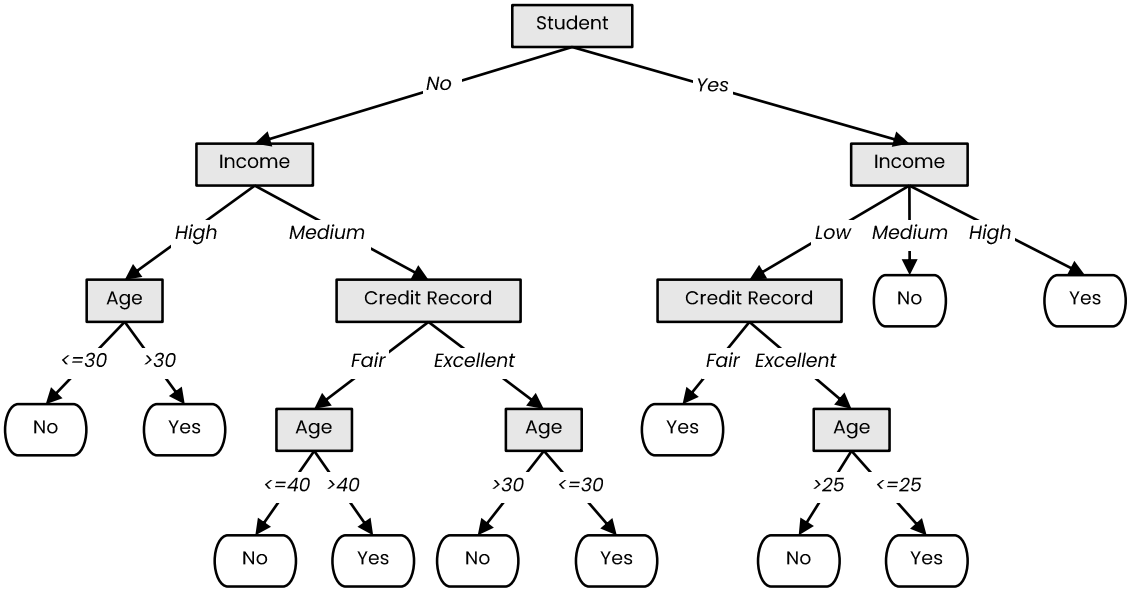
## Making predictions with a **tree-like structure**

**Faculty of Mathematics and Computer Science, University of Bucharest**
and
**Sparktech Software**

*Academic Year 2018/2019, 1st Semester*

# Definition

- A **tree-like model** which illustrates series of events which lead to certain *decisions*.
- Each node of the tree represents a “test” on an attribute and each branch, an outcome of that test.




- Student
- 27 years old
- Low income
- Excellent credit record

**Loan default?**

- Not a student
- 45 years old
- Medium income
- Fair credit record

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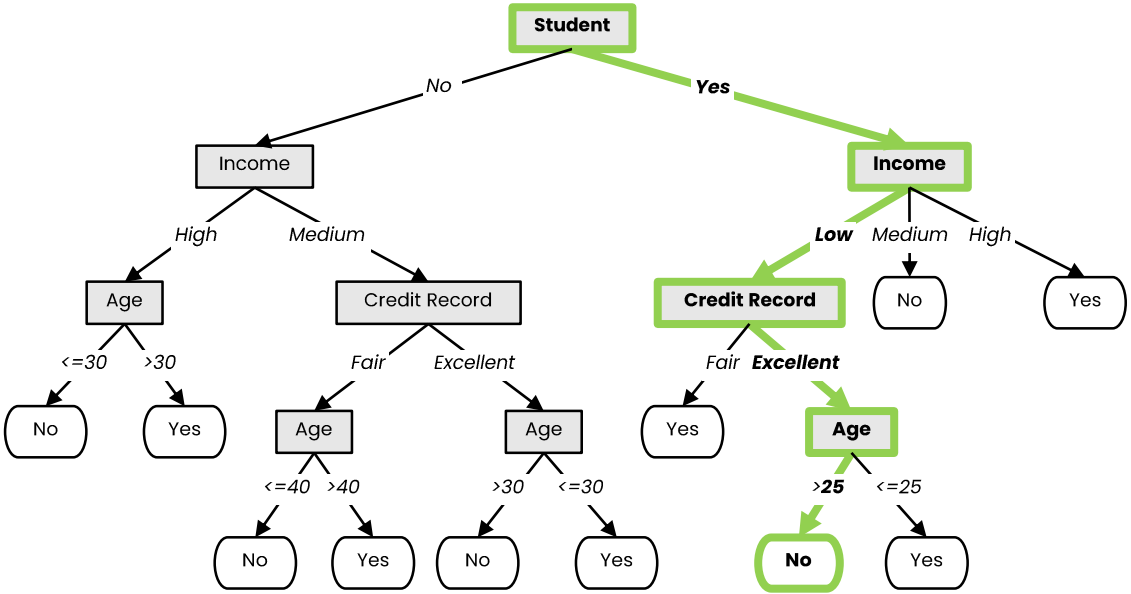


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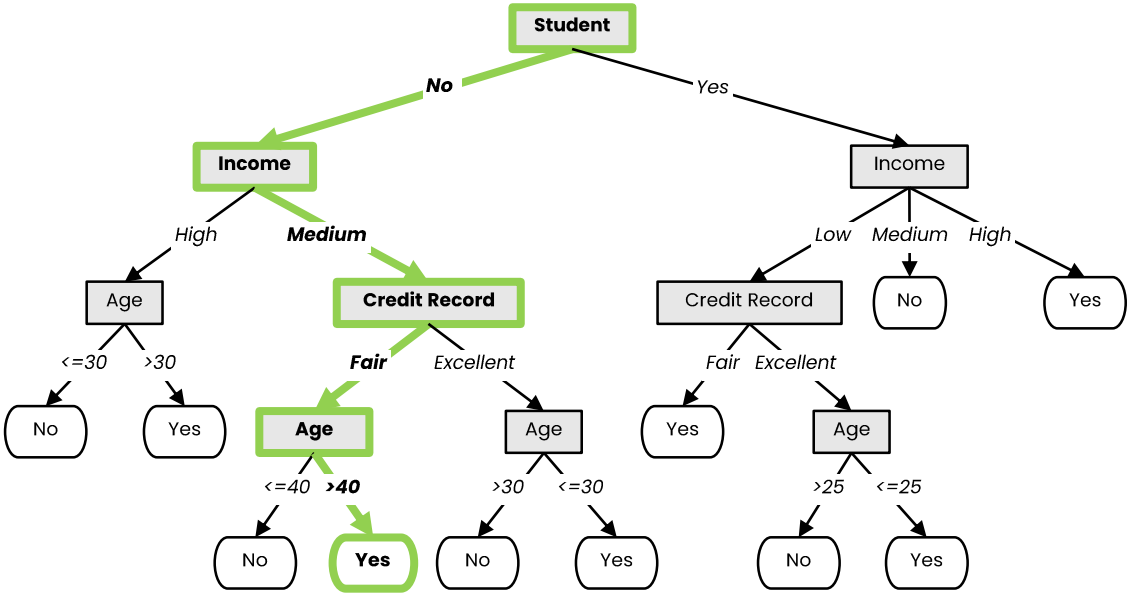


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  - We want a tree which works well on unseen data, while asking as few questions as possible.

| Outlook | Temperature | Humidity | Wind | Play Tennis? |
|---|---|---|---|---|
| Sunny | Hot | High | Weak | **No** |
| Sunny | Hot | High | Strong | **No** |
| Overcast | Hot | High | Weak | **Yes** |
| Rainy | Mild | High | Weak | **Yes** |
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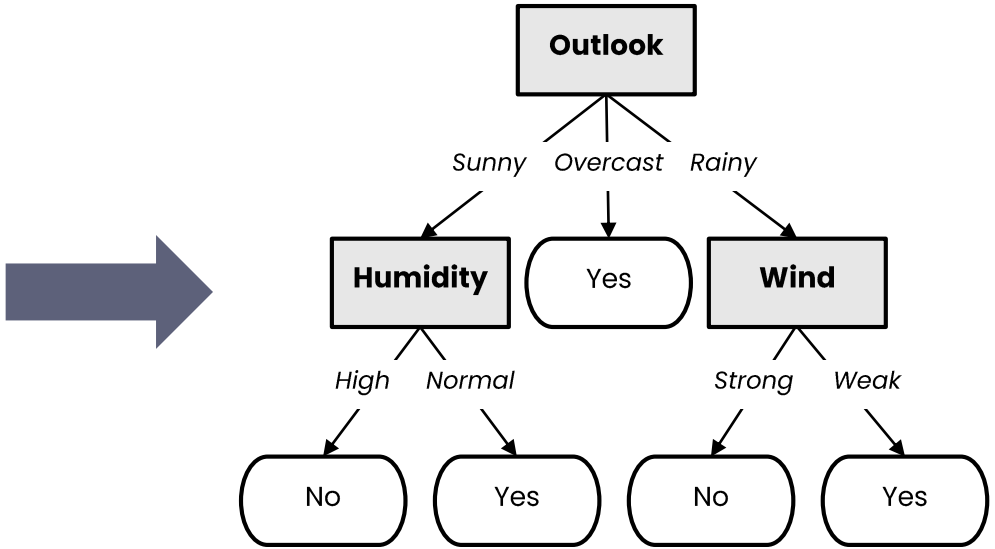

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| Temperature | Humidity | Wind | Play Tennis? |
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| Hot | High | Weak | **No** |
| Hot | High | Strong | **No** |
| Mild | High | Weak | **No** |
| Cool | Normal | Weak | **Yes** |
| Mild | Normal | Strong | **Yes** |

**Outlook** = *Overcast*

| Temperature | Humidity | Wind | Play Tennis? |
|---|---|---|---|
| Hot | High | Weak | **Yes** |
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| Mild | High | Strong | **Yes** |
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**Outlook** = *Rainy*

| Temperature | Humidity | Wind | Play Tennis? |
|---|---|---|---|
| Mild | High | Weak | **Yes** |
| Cool | Normal | Weak | **Yes** |
| Cool | Normal | Strong | **No** |
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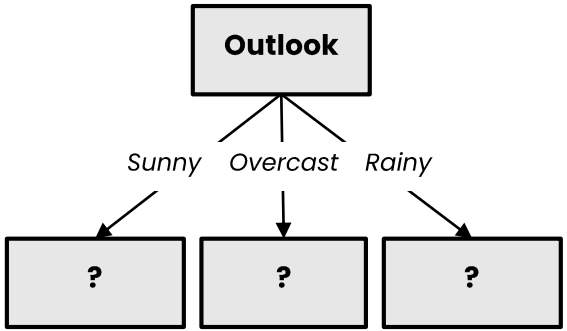
| Mild | High | Strong | **No** |



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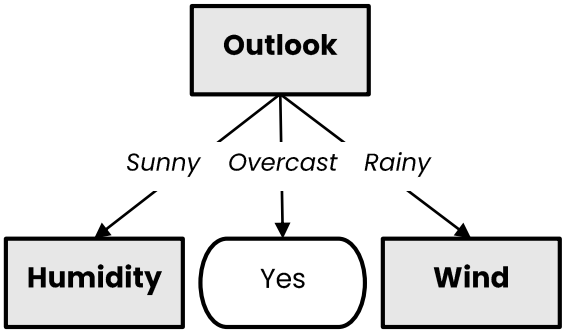

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**Outlook** = *Sunny*

**Humidity** = High

| Temperature | Wind | Play Tennis? |
|---|---|---|
| Hot | Weak | **No** |
| Hot | Strong | **No** |
| Mild | Weak | **No** |

**Humidity** = Normal

| Temperature | Wind | Play Tennis? |
|---|---|---|
| Cool | Weak | **Yes** |
| Mild | Strong | **Yes** |

**Outlook** = *Overcast*

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| Hot | High | Weak | **Yes** |
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**Outlook** = *Rainy*

**Wind** = Strong

| Temperature | Humidity | Play Tennis? |
|---|---|---|
| Cool | Normal | **No** |
| Mild | High | **No** |

**Wind** = Weak

| Temperature | Humidity | Play Tennis? |
|---|---|---|
| Mild | High | **Yes** |
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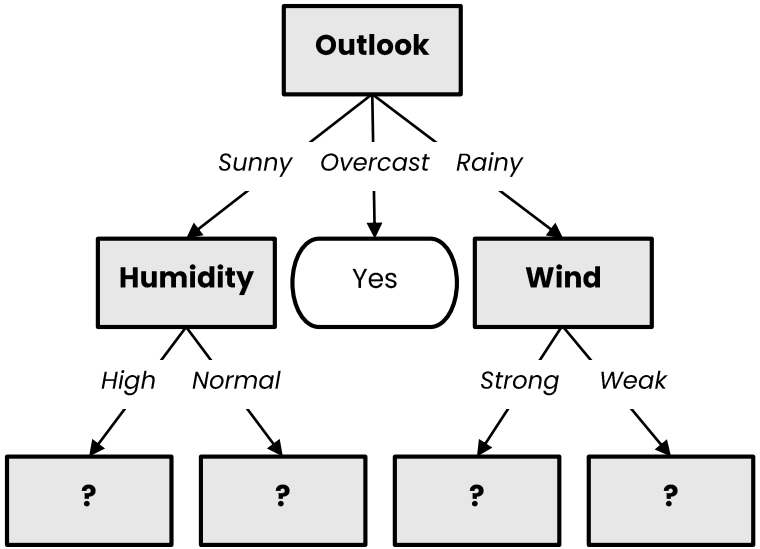

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**Humidity** = Normal

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| Temperature | Humidity | Play Tennis? |
|---|---|---|
| Cool | Normal | **No** |
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**Wind** = Weak

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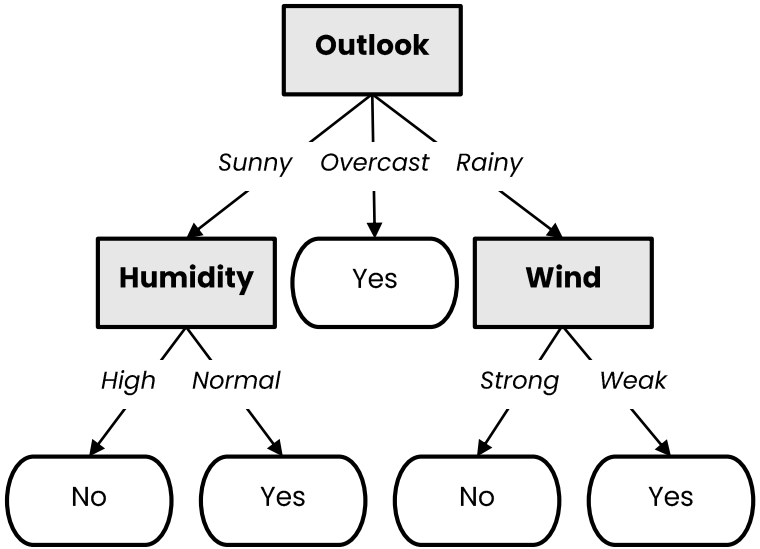

# Decision Tree Learning Algorithm

```
1   def extract_node(X):
2       node = TreeNode(X)
3       if should_be_leaf_node(X):
4           node.label = majority_label(X)
5       else:
6           a = select_best_splitting_attribute(X)
7           for v in values(a):
8               X_v = {x ∈ X | x[a] == v}
9               node.children.append(extract_node(X_v))
10      return node
```

# What makes a “good” attribute?

| Does it fly? | Color | Class |
|---|---|---|
| No | Brown | **Mammal** |
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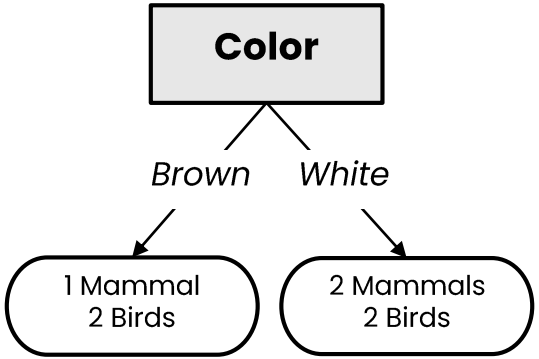


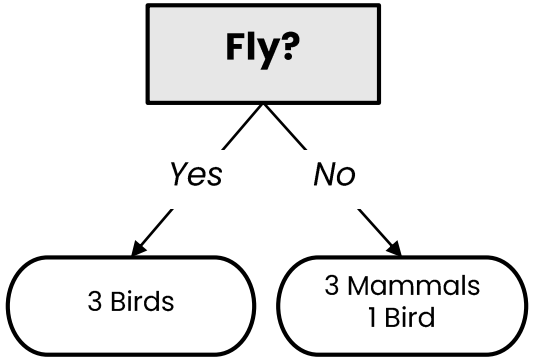


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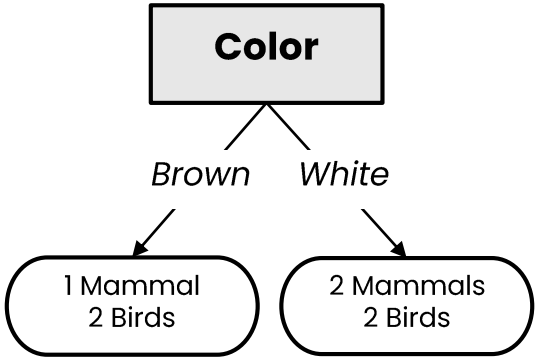


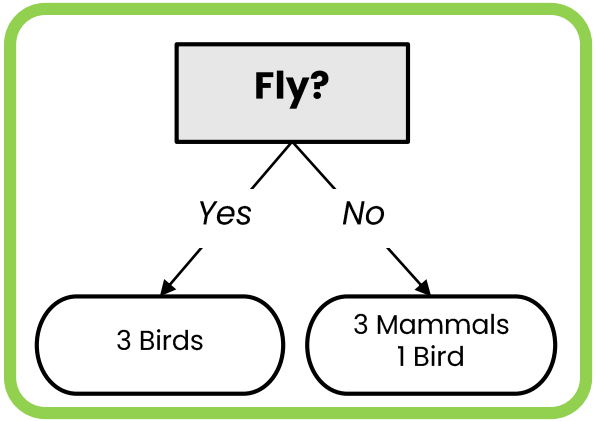


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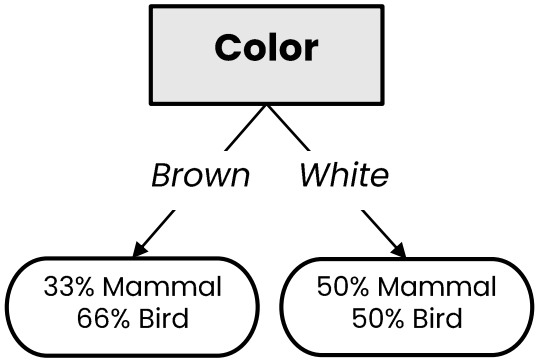


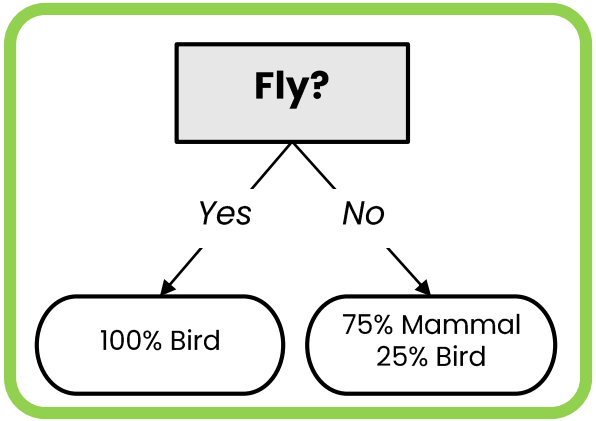


- Which one is a *better* attribute for splitting?
- Why?
  - Because the resulting subsets are more “*pure*”.
  - Knowing the value of this attribute gives us “*more information*” about the label.
    - i.e. The **entropy** of the subsets is lower.

# Information Gain

# Entropy

- **Entropy** measures the *degree of randomness* in a dataset, with lower entropy implying greater *predictability*.

**Low entropy**

**High entropy**

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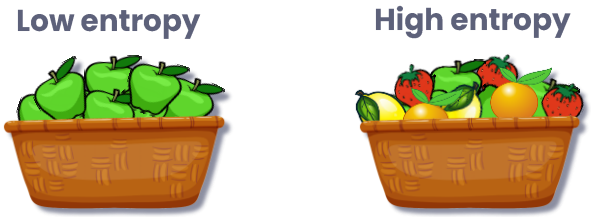
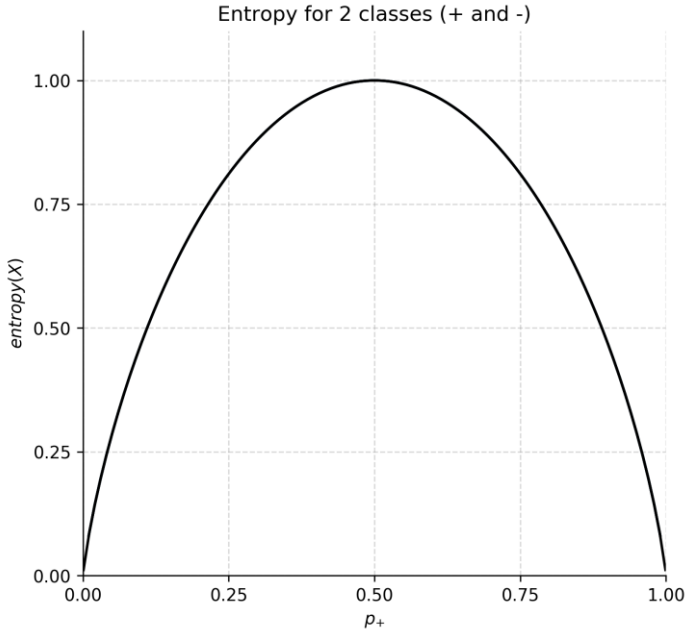



- For a set of samples $X$ with $k$ classes:

$$\textbf{entropy}(X) = -\sum_{i=1}^{k} p_i \log_2(p_i)$$

where $p_i$ is the proportion of elements with class $i$



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$$\mathbf{gain}(X, a) = \mathbf{entropy}(X) - \sum_{v \in \mathbf{values}(a)} \frac{|X_v|}{|X|} \mathbf{entropy}(X_v)$$

where $X_v$ is the subset of $X$ for which $a = v$.

# Best attribute = highest information gain

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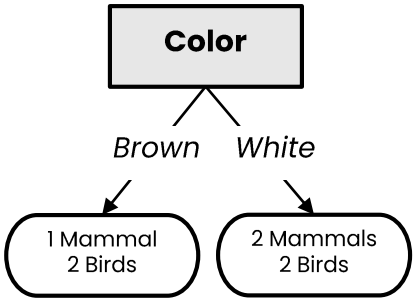


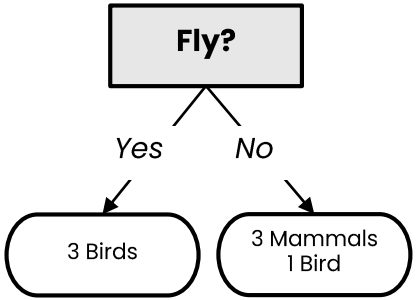


$$\text{entropy}(X) = -p_{\text{mammal}} \log_2 p_{\text{mammal}} - p_{\text{bird}} \log_2 p_{\text{bird}} = -\frac{3}{7}\log_2\frac{3}{7} - \frac{4}{7}\log_2\frac{4}{7} \approx 0.985$$

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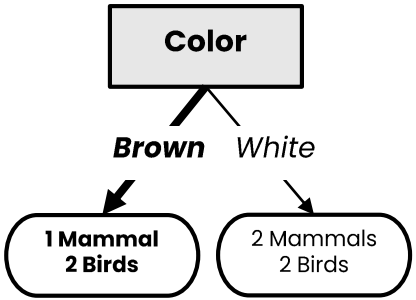


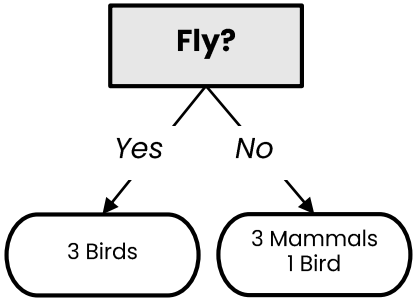


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$$\textbf{entropy}(\mathbf{X}_{\textbf{color=brown}}) = -\frac{\mathbf{1}}{\mathbf{3}}\boldsymbol{log_2}\frac{\mathbf{1}}{\mathbf{3}} - \frac{\mathbf{2}}{\mathbf{3}}\boldsymbol{log_2}\frac{\mathbf{2}}{\mathbf{3}} \approx \mathbf{0.918}$$

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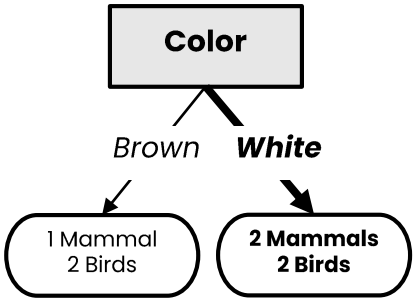


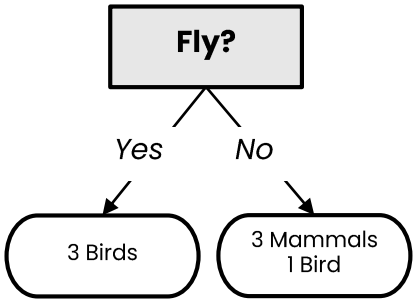


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$$\text{entropy}(\text{X}_{\text{color=brown}}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} \approx 0.918 \qquad \textbf{entropy}(\boldsymbol{X}_{\textbf{color=white}}) = \mathbf{1}$$

# Best attribute = highest information gain

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| No | Brown | **Mammal** |
| No | White | **Mammal** |
| Yes | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
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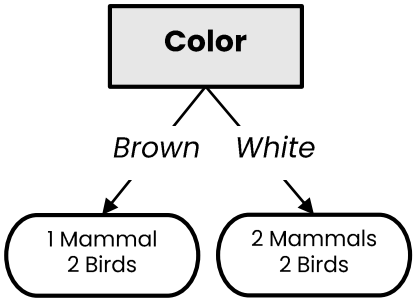
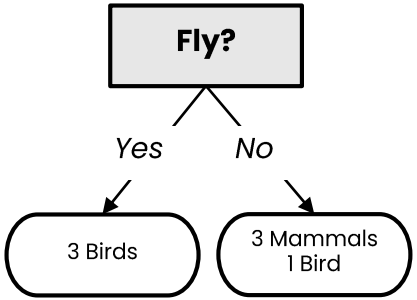


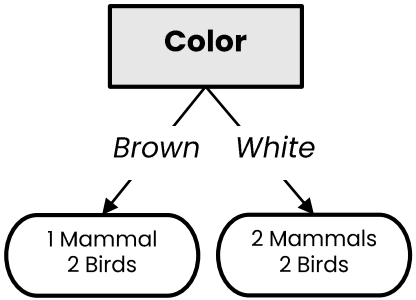

$$\text{entropy}(X) = -p_{\text{mammal}} \log_2 p_{\text{mammal}} - p_{\text{bird}} \log_2 p_{\text{bird}} = -\frac{3}{7}\log_2\frac{3}{7} - \frac{4}{7}\log_2\frac{4}{7} \approx 0.985$$

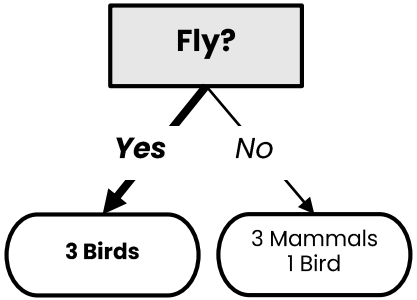
$$\text{entropy}(\text{X}_{\text{color=brown}}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} \approx 0.918 \qquad \text{entropy}(X_{\text{color=white}}) = 1$$

$$\mathbf{gain}(\boldsymbol{X}, \mathbf{color}) = \mathbf{0.985} - \frac{\mathbf{3}}{\mathbf{7}} * \mathbf{0.918} - \frac{\mathbf{4}}{\mathbf{7}} * \mathbf{1} = \mathbf{0.02}$$

# Best attribute = highest information gain

| Does it fly? | Color | Class |
|---|---|---|
| No | Brown | **Mammal** |
| No | White | **Mammal** |
| Yes | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
| Yes | White | **Bird** |




$$\text{entropy}(X) = -p_{\text{mammal}} \log_2 p_{\text{mammal}} - p_{\text{bird}} \log_2 p_{\text{bird}} = -\frac{3}{7}\log_2\frac{3}{7} - \frac{4}{7}\log_2\frac{4}{7} \approx 0.985$$

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$$\mathbf{gain}(X, \mathbf{color}) = \mathbf{0.985} - \frac{\mathbf{3}}{\mathbf{7}} * \mathbf{0.918} - \frac{\mathbf{4}}{\mathbf{7}} * \mathbf{1} = \mathbf{0.02}$$

$$\mathbf{entropy}(X_{\mathbf{fly=yes}}) = \mathbf{0}$$

# Best attribute = highest information gain

| Does it fly? | Color | Class |
|---|---|---|
| No | Brown | **Mammal** |
| No | White | **Mammal** |
| Yes | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
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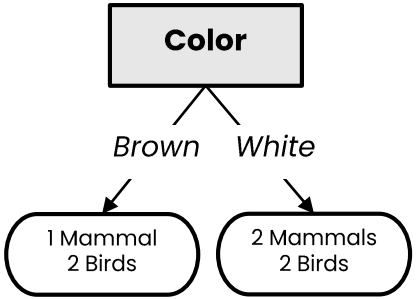


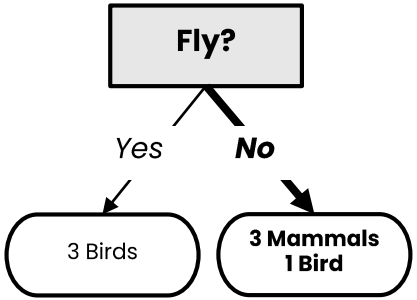


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$$\text{entropy}(X_{\text{fly=yes}}) = 0 \qquad \textbf{entropy}(X_{\textbf{fly=no}}) = -\frac{\mathbf{3}}{\mathbf{4}}\boldsymbol{log_2}\frac{\mathbf{3}}{\mathbf{4}} - \frac{\mathbf{1}}{\mathbf{4}}\boldsymbol{log_2}\frac{\mathbf{1}}{\mathbf{4}} \approx \mathbf{0.811}$$

# Best attribute = highest information gain

| Does it fly? | Color | Class |
|---|---|---|
| No | Brown | **Mammal** |
| No | White | **Mammal** |
| Yes | Brown | **Bird** |
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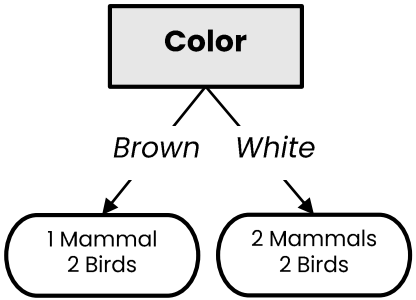


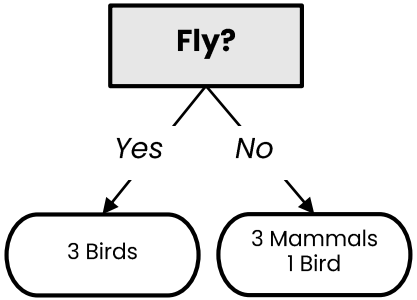


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$$\text{entropy}(X_{\text{color=brown}}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} \approx 0.918 \qquad \text{entropy}(X_{\text{color=white}}) = 1$$

$$\mathbf{gain}(X, \mathbf{color}) = \mathbf{0.985} - \frac{\mathbf{3}}{\mathbf{7}} * \mathbf{0.918} - \frac{\mathbf{4}}{\mathbf{7}} * \mathbf{1} = \mathbf{0.02}$$

$$\text{entropy}(X_{\text{fly=yes}}) = 0 \qquad \text{entropy}(X_{\text{fly=no}}) = -\frac{3}{4}\log_2\frac{3}{4} - \frac{1}{4}\log_2\frac{1}{4} \approx 0.811$$

$$\mathbf{gain}(X, \mathbf{fly}) = \mathbf{0.985} - \frac{\mathbf{3}}{\mathbf{7}} * \mathbf{0} - \frac{\mathbf{4}}{\mathbf{7}} * \mathbf{0.811} = \mathbf{0.521}$$

# Best attribute = highest information gain

| Does it fly? | Color | Class |
|---|---|---|
| No | Brown | **Mammal** |
| No | White | **Mammal** |
| Yes | Brown | **Bird** |
| Yes | White | **Bird** |
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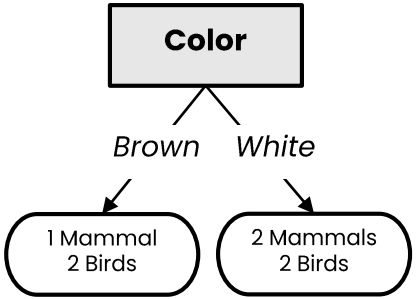
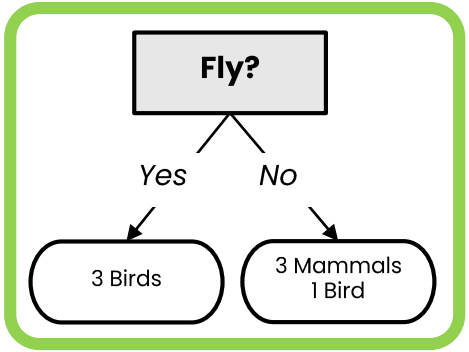



In practice we don't need to compute entropy$(X)$ since it is the same for all attributes.

$$\text{entropy}(X) = -p_{\text{mammal}} \log_2 p_{\text{mammal}} - p_{\text{bird}} \log_2 p_{\text{bird}} = -\frac{3}{7}\log_2\frac{3}{7} - \frac{4}{7}\log_2\frac{4}{7} \approx 0.985$$

$$\text{entropy}(X_{\text{color=brown}}) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} \approx 0.918 \qquad \text{entropy}(X_{\text{color=white}}) = 1$$

$$\textbf{gain}(X, \textbf{color}) = \mathbf{0.985} - \frac{\mathbf{3}}{\mathbf{7}} * \mathbf{0.918} - \frac{\mathbf{4}}{\mathbf{7}} * \mathbf{1} = \mathbf{0.02}$$

$$\text{entropy}(X_{\text{fly=yes}}) = 0 \qquad \text{entropy}(X_{\text{fly=no}}) = -\frac{3}{4}\log_2\frac{3}{4} - \frac{1}{4}\log_2\frac{1}{4} \approx 0.811$$

$$\textbf{gain}(X, \textbf{fly}) = \mathbf{0.985} - \frac{\mathbf{3}}{\mathbf{7}} * \mathbf{0} - \frac{\mathbf{4}}{\mathbf{7}} * \mathbf{0.811} = \boxed{\mathbf{0.521}}$$

# ID3 Algorithm

```
1   def ID3(X):
2       node = TreeNode(X)
3       if all_points_have_same_class(X):
4           node.label = majority_label(X)
5       else:
6           a = select_attribute_with_highest_information_gain(X)
7           if gain(X, a) == 0:
8               node.label = majority_label(X)
9           else:
10              for v in values(a):
11                  X_v = {x ∈ X | x[a] == v}
12                  node.children.append(ID3(X_v))
13      return node
```

ID stands for *"Iterative Dichotomiser"*

# Gini Impurity

# Gini impurity

- Measures how often a randomly chosen element would be incorrectly labeled if it was randomly labeled according to the distribution of labels.

**Error of classifying randomly picked fruit with randomly picked label**

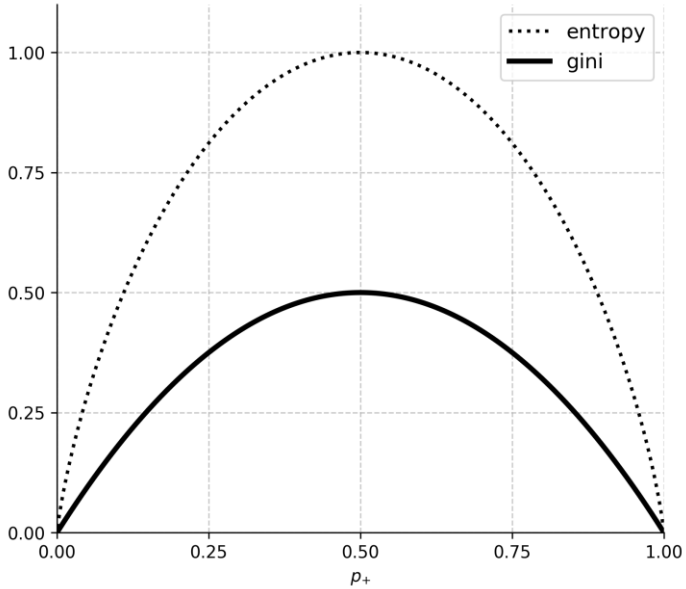
# Gini impurity

- Measures how often a randomly chosen element would be incorrectly labeled if it was randomly labeled according to the distribution of labels.

**Error of classifying randomly picked fruit with randomly picked label**


$$\text{gini}(X) = 1 - \sum_{i=1}^{k} p_i^2$$

- Can be used as an alternative to entropy for selecting attributes.



# Best attribute = highest impurity decrease

| Does it fly? | Color | Class |
|---|---|---|
| No | Brown | **Mammal** |
| No | White | **Mammal** |
| Yes | Brown | **Bird** |
| Yes | White | **Bird** |
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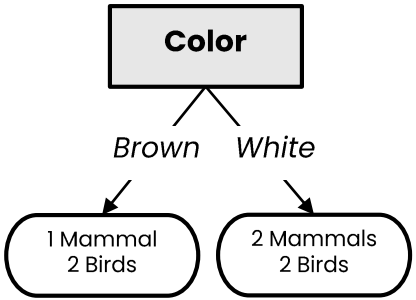
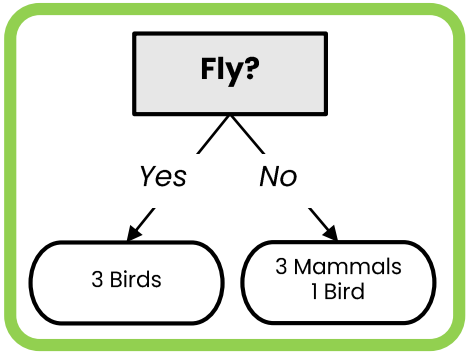



$$\text{gini}(X) = 1 - \left(\frac{3}{7}\right)^2 - \left(\frac{4}{7}\right)^2 \approx 0.489$$

$$\text{gini}(X_{\text{color=brown}}) = 1 - \left(\frac{1}{3}\right)^2 - \left(\frac{2}{3}\right)^2 \approx 0.44 \qquad \text{gini}(X_{\text{color=white}}) = 0.5$$

$$\boldsymbol{\Delta\text{gini}(X, \text{color}) = 0.489 - \frac{3}{7} * 0.44 - \frac{4}{7} * 0.5 \approx 0.01}$$

$$\text{gini}(X_{\text{fly=yes}}) = 0 \qquad \text{gini}(X_{\text{fly=no}}) = 1 - \left(\frac{3}{4}\right)^2 - \left(\frac{1}{4}\right)^2 = 0.375$$

$$\boldsymbol{\Delta\text{gini}(X, \text{fly}) = 0.489 - \frac{3}{7} * 0 - \frac{4}{7} * 0.375 = 0.274}$$

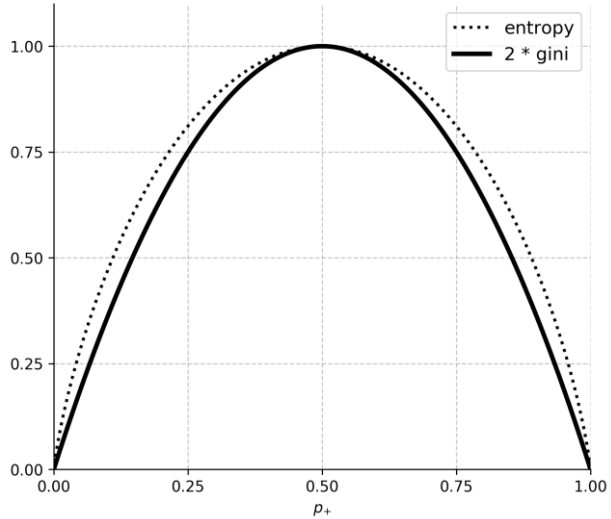
In practice we don't need to compute gini($X$) since it is the same for all attributes.

# Entropy vs. Gini Impurity

- In practice, *entropy* and *gini impurity* are almost the same.
- They only disagree in about 2% of cases:
  - **“Theoretical Comparison between the Gini Index and Information Gain Criteria”**

Laura Elena Raileanu, Kilian Stoffel, 2004

- Entropy might be slower to compute, because of the use of logarithms



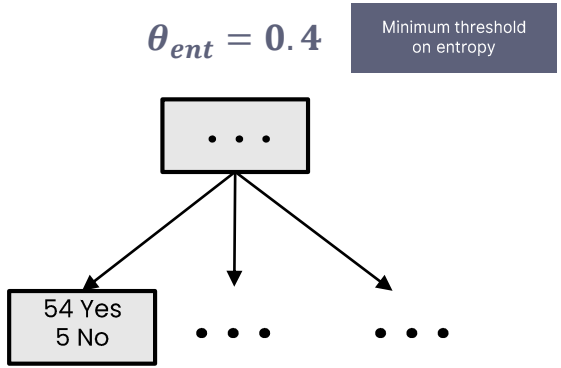

Sklearn uses *gini* by default.

# Pruning

# Pruning

- **Pruning** is a technique which reduces the size of a decision tree by removing parts of the tree which provide little predictive power.
- Pruning is a *regularization* method which reduces the complexity of the final model, and hence reduce overfitting.
  - Decision trees are very prone to *overfitting*.
- *Pre-pruning:*
  - Stop the tree growing algorithm before it fully classifies the data
- *Post-pruning:*
  - Grow the tree completely, then replace some non-leaf nodes with leaf nodes if it improves validation error.

# Pre-pruning




- **Pre-pruning** implies early stopping.
  - If *certain conditions* are met, the current node will *not be split*, even if it is impure and further splitting would be possible.
  - It will become a *leaf node* with the label of the majority class in the current set.
    - It is also possible to use the class distribution as the node's prediction confidence.
- Common stopping criteria include setting a threshold on:
  - Entropy (or impurity) of current set.
  - Number of samples in the current set.
  - Gain of the best-split attribute.
  - Depth of the tree

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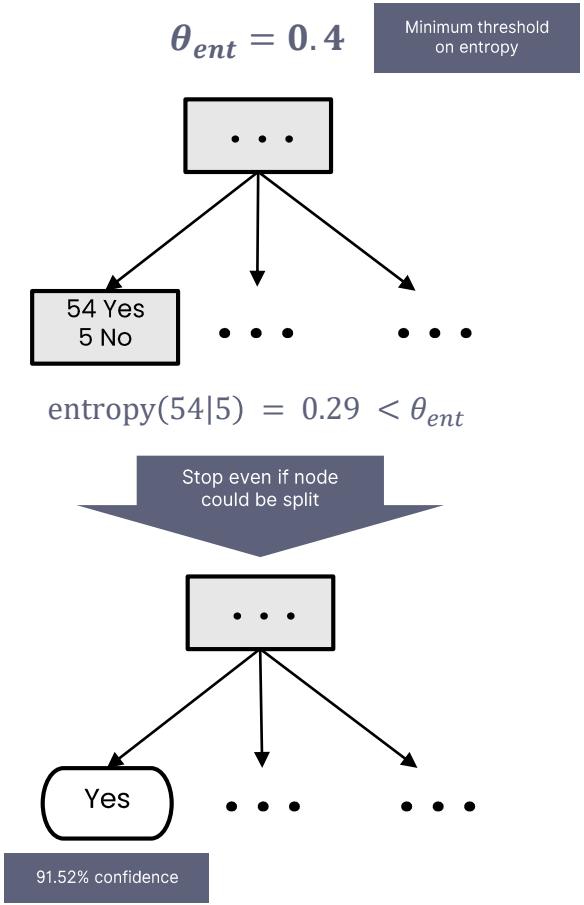
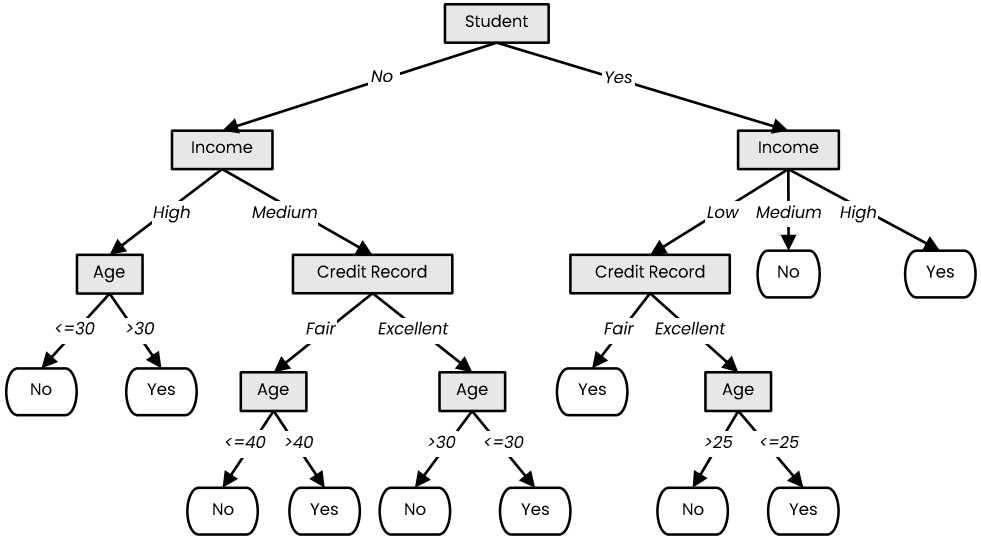
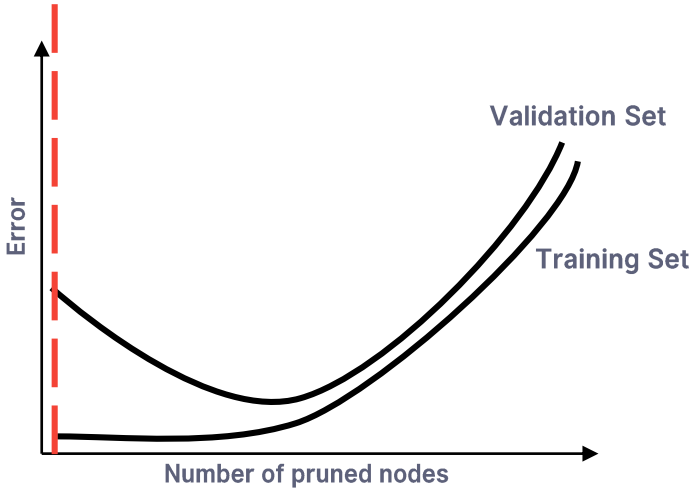


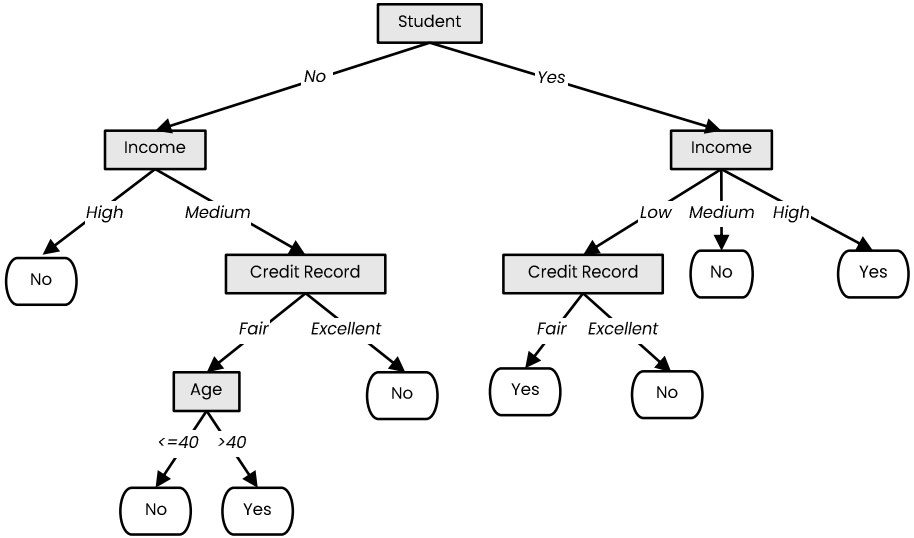
# Post-pruning

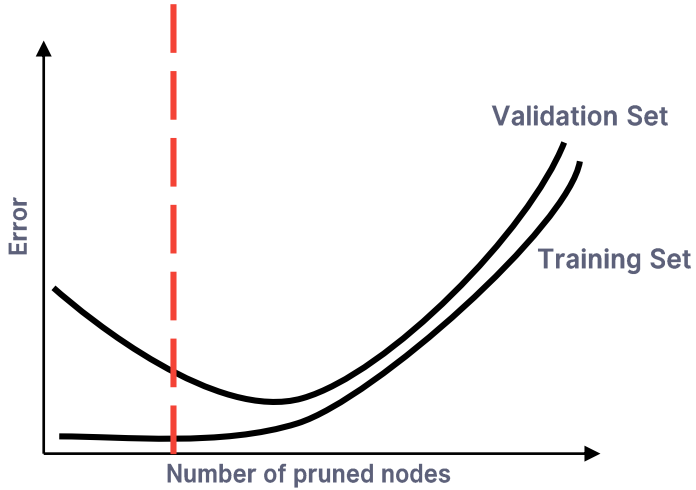



- Prune nodes in a bottom-up manner, if it decreases validation error.

# Post-pruning

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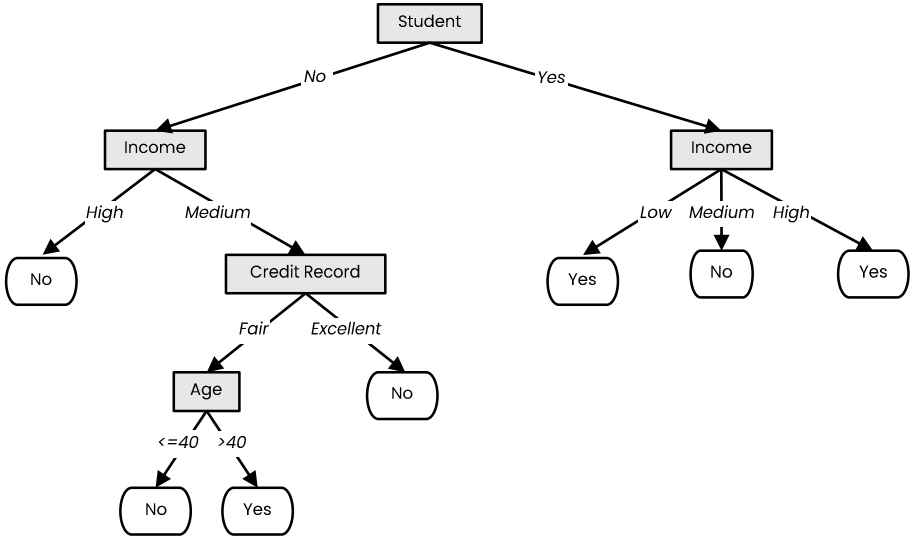
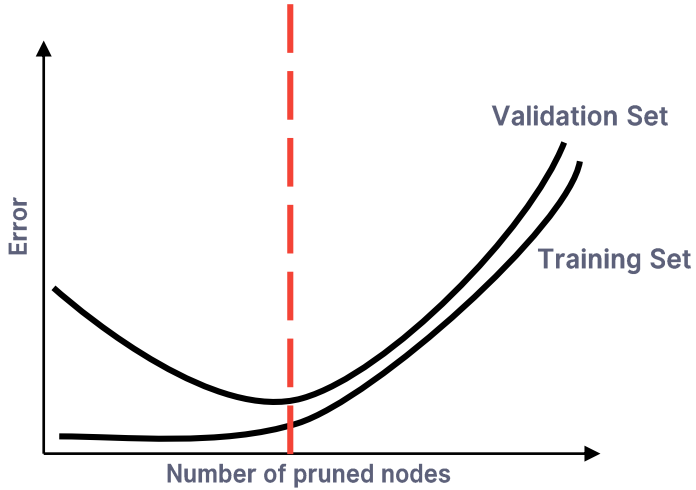
# Post-pruning

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# Handling Numerical Attributes

# Handling numerical data

- How does the ID3 algorithm treat numerical attributes?

| Outlook | Temperature | Humidity | Wind | Play Tennis? |
|---|---|---|---|---|
| Sunny | Hot | 90 | Weak | **No** |
| Sunny | Hot | 87 | Strong | **No** |
| Overcast | Hot | 93 | Weak | **Yes** |
| Rainy | Mild | 89 | Weak | **Yes** |
| Rainy | Cool | 79 | Weak | **Yes** |
| Rainy | Cool | 59 | Strong | **No** |
| Overcast | Cool | 77 | Strong | **Yes** |
| Sunny | Mild | 91 | Weak | **No** |
| Sunny | Cool | 68 | Weak | **Yes** |
| Rainy | Mild | 80 | Weak | **Yes** |
| Sunny | Mild | 72 | Strong | **Yes** |
| Overcast | Mild | 96 | Strong | **Yes** |
| Overcast | Hot | 74 | Weak | **Yes** |
| Rainy | Mild | 97 | Strong | **No** |

Now we have a numerical value for humidity

# Handling numerical data

- How does the ID3 algorithm treat numerical attributes?
  - Any numerical attribute would almost always bring entropy down to zero.
  - This means it will completely overfit the training data.

| Outlook | Temperature | Humidity | Wind | Play Tennis? |
|---|---|---|---|---|
| Sunny | Hot | 90 | Weak | **No** |
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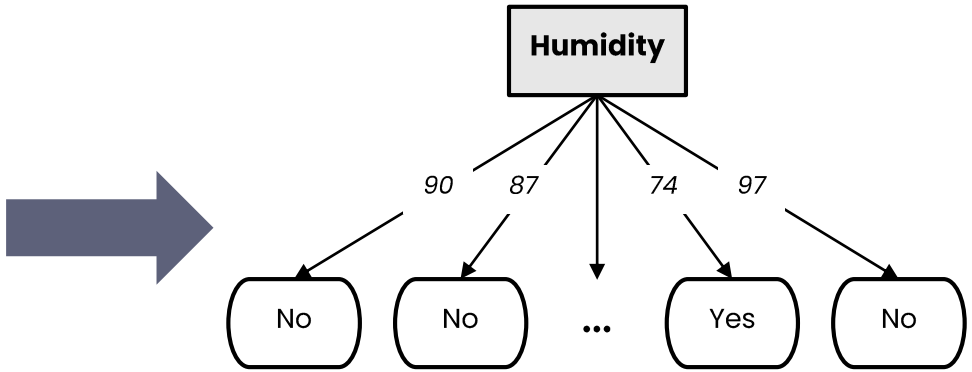

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
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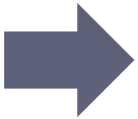
| 72 | Yes |
| 96 | Yes |
| 74 | Yes |
| 97 | No |

Sort



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|---|---|
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| 96 | Yes |
| 74 | Yes |
| 97 | No |

Sort

| Humidity | Play Tennis? |
|---|---|
| 59 | No |
| 68 | Yes |
| 72 | Yes |
| 74 | Yes |
| 77 | Yes |
| 79 | Yes |
| 80 | Yes |
| 87 | No |
| 89 | Yes |
| 90 | No |
| 91 | No |
| 93 | Yes |
| 96 | Yes |
| 97 | No |

Mean of each consecutive pair

| Candidate split values |
|---|
| 63 |
| 70 |
| 73 |
| 75.5 |
| 78 |
| 79.5 |
| 83.5 |
| 88 |
| 89.5 |
| 90.5 |
| 92 |
| 94.5 |
| 96.5 |

Gain of numerical attribute $a$ if it is split on value $t$.

$$\text{gain}(X, a, t) = \text{entropy}(X) - \frac{|X_{a \le t}|}{|X|}\text{entropy}(X_{a \le t}) - \frac{|X_{a > t}|}{|X|}\text{entropy}(X_{a > t})$$

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
| 93 | Yes |
| 89 | Yes |
| 79 | Yes |
| 59 | No |
| 77 | Yes |
| 91 | No |
| 68 | Yes |
| 80 | Yes |
| 72 | Yes |
| 96 | Yes |
| 74 | Yes |
| 97 | No |

Sort

| Humidity | Play Tennis? |
|---|---|
| 59 | No |
| 68 | Yes |
| 72 | Yes |
| 74 | Yes |
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| 79 | Yes |
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| 89 | Yes |
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| Candidate split values |
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| 94.5 |
| 96.5 |

$$\text{gain}(X, a, t) = \text{entropy}(X) - \frac{|X_{a \le t}|}{|X|}\text{entropy}(X_{a \le t}) - \frac{|X_{a > t}|}{|X|}\text{entropy}(X_{a > t})$$

$$\text{gain}(X, \text{hummidity}, 83.5)$$

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
| 93 | Yes |
| 89 | Yes |
| 79 | Yes |
| 59 | No |
| 77 | Yes |
| 91 | No |
| 68 | Yes |
| 80 | Yes |
| 72 | Yes |
| 96 | Yes |
| 74 | Yes |
| 97 | No |

Sort

| Humidity | Play Tennis? |
|---|---|
| 59 | No |
| 68 | Yes |
| 72 | Yes |
| 74 | Yes |
| 77 | Yes |
| 79 | Yes |
| 80 | Yes |
| 87 | No |
| 89 | Yes |
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| 96 | Yes |
| 97 | No |

Mean of each consecutive pair

| Candidate split values |
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| 73 |
| 75.5 |
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| 89.5 |
| 90.5 |
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| 94.5 |
| 96.5 |

$$\text{gain}(X, a, t) = \text{entropy}(X) - \frac{|X_{a \le t}|}{|X|}\text{entropy}(X_{a \le t}) - \frac{|X_{a > t}|}{|X|}\text{entropy}(X_{a > t})$$

$$\text{gain}(X, \text{hummidity}, 83.5) = \mathbf{0.94}$$

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
| 93 | Yes |
| 89 | Yes |
| 79 | Yes |
| 59 | No |
| 77 | Yes |
| 91 | No |
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| 80 | Yes |
| 72 | Yes |
| 96 | Yes |
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| Humidity | Play Tennis? |
|---|---|
| 59 | No |
| 68 | Yes |
| 72 | Yes |
| 74 | Yes |
| 77 | Yes |
| 79 | Yes |
| 80 | Yes |
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| 89.5 |
| 90.5 |
| 92 |
| 94.5 |
| 96.5 |

$$\text{gain}(X, a, t) = \text{entropy}(X) - \frac{|X_{a \le t}|}{|X|}\text{entropy}(X_{a \le t}) - \frac{|X_{a > t}|}{|X|}\text{entropy}(X_{a > t})$$

$$\text{gain}(X, \text{hummidity}, 83.5) = 0.94 - \frac{\mathbf{7}}{\mathbf{14}} * \mathbf{0.591}$$

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
| 93 | Yes |
| 89 | Yes |
| 79 | Yes |
| 59 | No |
| 77 | Yes |
| 91 | No |
| 68 | Yes |
| 80 | Yes |
| 72 | Yes |
| 96 | Yes |
| 74 | Yes |
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Sort

| Humidity | Play Tennis? |
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| 59 | No |
| 68 | Yes |
| 72 | Yes |
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| 77 | Yes |
| 79 | Yes |
| 80 | Yes |
| 87 | No |
| 89 | Yes |
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| 91 | No |
| 93 | Yes |
| 96 | Yes |
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Mean of each consecutive pair

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| 96.5 |

$$\text{gain}(X, a, t) = \text{entropy}(X) - \frac{|X_{a \le t}|}{|X|}\text{entropy}(X_{a \le t}) - \frac{|X_{a > t}|}{|X|}\text{entropy}(X_{a > t})$$

$$\text{gain}(X, \text{hummidity}, 83.5) = 0.94 - \frac{7}{14} * 0.591 - \frac{\mathbf{7}}{\mathbf{14}} * \mathbf{0.985}$$

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
| 93 | Yes |
| 89 | Yes |
| 79 | Yes |
| 59 | No |
| 77 | Yes |
| 91 | No |
| 68 | Yes |
| 80 | Yes |
| 72 | Yes |
| 96 | Yes |
| 74 | Yes |
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Sort

| Humidity | Play Tennis? |
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| 59 | No |
| 68 | Yes |
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| 87 | No |
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| Candidate split values |
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| 63 |
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| 78 |
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| 94.5 |
| 96.5 |

$$\text{gain}(X, a, t) = \text{entropy}(X) - \frac{|X_{a \le t}|}{|X|}\text{entropy}(X_{a \le t}) - \frac{|X_{a > t}|}{|X|}\text{entropy}(X_{a > t})$$

$$\text{gain}(X, \text{hummidity}, 83.5) = 0.94 - \frac{7}{14} * 0.591 - \frac{7}{14} * 0.985 = \mathbf{0.152}$$

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
| 93 | Yes |
| 89 | Yes |
| 79 | Yes |
| 59 | No |
| 77 | Yes |
| 91 | No |
| 68 | Yes |
| 80 | Yes |
| 72 | Yes |
| 96 | Yes |
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Sort

| Humidity | Play Tennis? |
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| 59 | No |
| 68 | Yes |
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| 74 | Yes |
| 77 | Yes |
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| 87 | No |
| 89 | Yes |
| 90 | No |
| 91 | No |
| 93 | Yes |
| 96 | Yes |
| 97 | No |

Mean of each consecutive pair

| Candidate split values |
|---|
| 63 |
| 70 |
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| 75.5 |
| 78 |
| 79.5 |
| 83.5 |
| 88 |
| 89.5 |
| 90.5 |
| 92 |
| 94.5 |
| 96.5 |

Info gain for every candidate

| Information gain |
|---|
| 0.113 |
| 0.01 |
| 0.0004 |
| 0.015 |
| 0.045 |
| 0.09 |
| 0.152 |
| 0.048 |
| 0.102 |
| 0.025 |
| 0.0004 |
| 0.01 |
| 0.113 |

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Humidity | Play Tennis? |
|---|---|
| 90 | No |
| 87 | No |
| 93 | Yes |
| 89 | Yes |
| 79 | Yes |
| 59 | No |
| 77 | Yes |
| 91 | No |
| 68 | Yes |
| 80 | Yes |
| 72 | Yes |
| 96 | Yes |
| 74 | Yes |
| 97 | No |

Sort

| Humidity | Play Tennis? |
|---|---|
| 59 | No |
| 68 | Yes |
| 72 | Yes |
| 74 | Yes |
| 77 | Yes |
| 79 | Yes |
| 80 | Yes |
| 87 | No |
| 89 | Yes |
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| 91 | No |
| 93 | Yes |
| 96 | Yes |
| 97 | No |

Mean of each consecutive pair

| Candidate split values |
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| 63 |
| 70 |
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| 75.5 |
| 78 |
| 79.5 |
| 83.5 |
| 88 |
| 89.5 |
| 90.5 |
| 92 |
| 94.5 |
| 96.5 |

Info gain for every candidate

| Information gain |
|---|
| 0.113 |
| 0.01 |
| 0.0004 |
| 0.015 |
| 0.045 |
| 0.09 |
| **0.152** |
| 0.048 |
| 0.102 |
| 0.025 |
| 0.0004 |
| 0.01 |
| 0.113 |

83.5 is the best split value with a 0.152 gain

# Handling numerical data

- Numerical attributes need to be treated differently.
  - Find the best splitting value.

| Outlook | Temperature | Humidity | Wind | Play Tennis? |
|---|---|---|---|---|
| Sunny | Hot | > 83.5 | Weak | **No** |
| Sunny | Hot | > 83.5 | Strong | **No** |
| Overcast | Hot | > 83.5 | Weak | **Yes** |
| Rainy | Mild | > 83.5 | Weak | **Yes** |
| Rainy | Cool | ≤ 83.5 | Weak | **Yes** |
| Rainy | Cool | ≤ 83.5 | Strong | **No** |
| Overcast | Cool | ≤ 83.5 | Strong | **Yes** |
| Sunny | Mild | > 83.5 | Weak | **No** |
| Sunny | Cool | ≤ 83.5 | Weak | **Yes** |
| Rainy | Mild | ≤ 83.5 | Weak | **Yes** |
| Sunny | Mild | ≤ 83.5 | Strong | **Yes** |
| Overcast | Mild | > 83.5 | Strong | **Yes** |
| Overcast | Hot | ≤ 83.5 | Weak | **Yes** |
| Rainy | Mild | > 83.5 | Strong | **No** |

- 83.5 is the best split value for *Humidity* with a 0.152 information gain.
- *Humidity* is now treated like a categorical attribute with two possible values.
- A new optimal split is computed at every level of the tree.
- Numerical attribute can be used more than once in the tree, with different split values

# Handling Missing Attributes

# Handling Missing Attributes at Training Time

| Does it fly? | Color | Class |
|---|---|---|
| No | **?** | **Mammal** |
| No | White | **Mammal** |
| **?** | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
| Yes | White | **Bird** |

- A dataset might have instances where some attribute values are unknown.
- Simply ignoring them would mean that we throw a lot of information away.
- There are many better ways of handling missing values:

# Handling Missing Attributes at Training Time

| Does it fly? | Color | Class |
|---|---|---|
| No | ***White*** | **Mammal** |
| No | White | **Mammal** |
| ***No*** | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
| Yes | White | **Bird** |

**4 No** 2 Brown
2 Yes **4 White**

- A dataset might have instances where some attribute values are unknown.
- Simply ignoring them would mean that we throw a lot of information away.
- There are many better ways of handling missing values:
  - Set it as the most common value for that attribute.

# Handling Missing Attributes at Training Time

| Does it fly? | Color | Class |
|---|---|---|
| No | ***White*** | **Mammal** |
| No | White | **Mammal** |
| ***Yes*** | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
| Yes | White | **Bird** |

$$\boldsymbol{P(\text{Yes}|\text{Bird}) = \frac{2}{3} = 0.66}$$
$$P(\text{No}|\text{Bird}) = 0.33$$

$$\boldsymbol{P(\text{White}|\text{Mammal}) = 1}$$
$$P(\text{Brown}|\text{Mammal}) = 0$$

- A dataset might have instances where some attribute values are unknown.
- Simply ignoring them would mean that we throw a lot of information away.
- There are many better ways of handling missing values:
  - Set it as the most common value for that attribute.
  - Set it as the most probable value given the label.

# Handling Missing Attributes at Training Time

| Does it fly? | Color | Class |
|---|---|---|
| No | ***White*** | **Mammal** |
| No | ***Brown*** | **Mammal** |
| No | White | **Mammal** |
| ***Yes*** | Brown | **Bird** |
| ***No*** | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
| Yes | White | **Bird** |

- A dataset might have instances where some attribute values are unknown.
- Simply ignoring them would mean that we throw a lot of information away.
- There are many better ways of handling missing values:
  - Set it as the most common value for that attribute.
  - Set it as the most probable value given the label.
  - Add a new instance to the dataset for every possible attribute value.

# Handling Missing Attributes at Training Time

| Does it fly? | Color | Class |
|---|---|---|
| No | ? | Mammal |
| No | White | **Mammal** |
| **?** | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
| Yes | White | **Bird** |

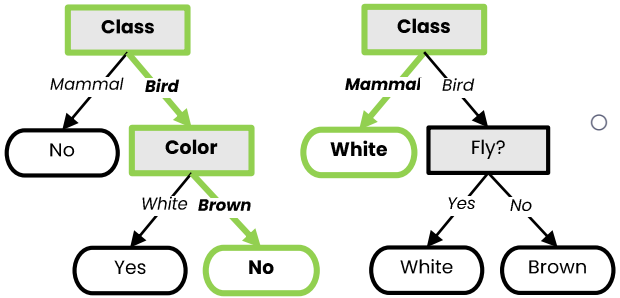
$\text{entropy}(X_{\text{color=brown}}) = 0$
$\text{entropy}(X_{\text{color=white}}) = 1$

$$\textbf{gain}(X, \textbf{color}) = 0.985 - \frac{2}{6} * 0 - \frac{4}{6} * 1 = 0.318$$

- A dataset might have instances where some attribute values are unknown.
- Simply ignoring them would mean that we throw a lot of information away.
- There are many better ways of handling missing values:
  - Set it as the most common value for that attribute.
  - Set it as the most probable value given the label.
  - Add a new instance to the dataset for every possible attribute value.
  - Leave it unknown, but, when evaluating the gain for that attribute, consider only the instances where the attribute is defined.
    - If the attribute is chosen for splitting, send the instances with unknown values to all children.

# Handling Missing Attributes at Training Time

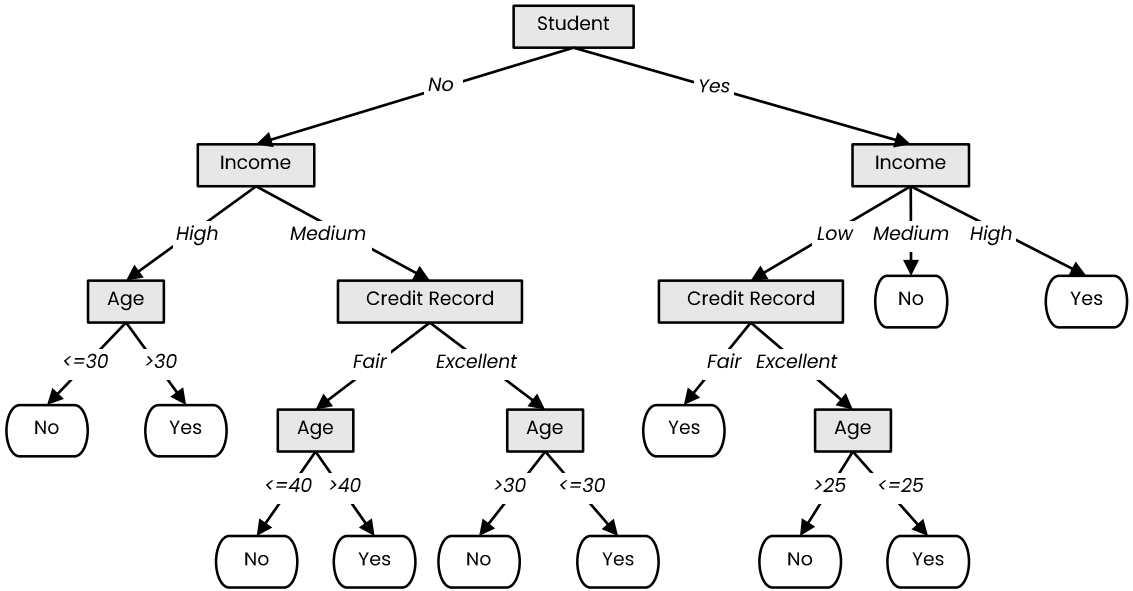
| Does it fly? | Color | Class |
|---|---|---|
| No | ***White*** | **Mammal** |
| No | White | **Mammal** |
| ***No*** | Brown | **Bird** |
| Yes | White | **Bird** |
| No | White | **Mammal** |
| No | Brown | **Bird** |
| Yes | White | **Bird** |




- A dataset might have instances where some attribute values are unknown.
- Simply ignoring them would mean that we throw a lot of information away.
- There are many better ways of handling missing values:
  - Set it as the most common value for that attribute.
  - Set it as the most probable value given the label.
  - Add a new instance to the dataset for every possible attribute value.
  - Leave it unknown, but, when evaluating the gain for that attribute, consider only the instances where the attribute is defined.
    - If the attribute is chosen for splitting, send the instances with unknown values to all children.
  - Grow a decision tree on all other attributes (including label) to predict the missing values.
    - Use instances where the attribute is defined as training data.

# Handling Missing Attributes at Inference Time

- When we encounter a node which checks an attribute with a missing value, we explore all possibilities.

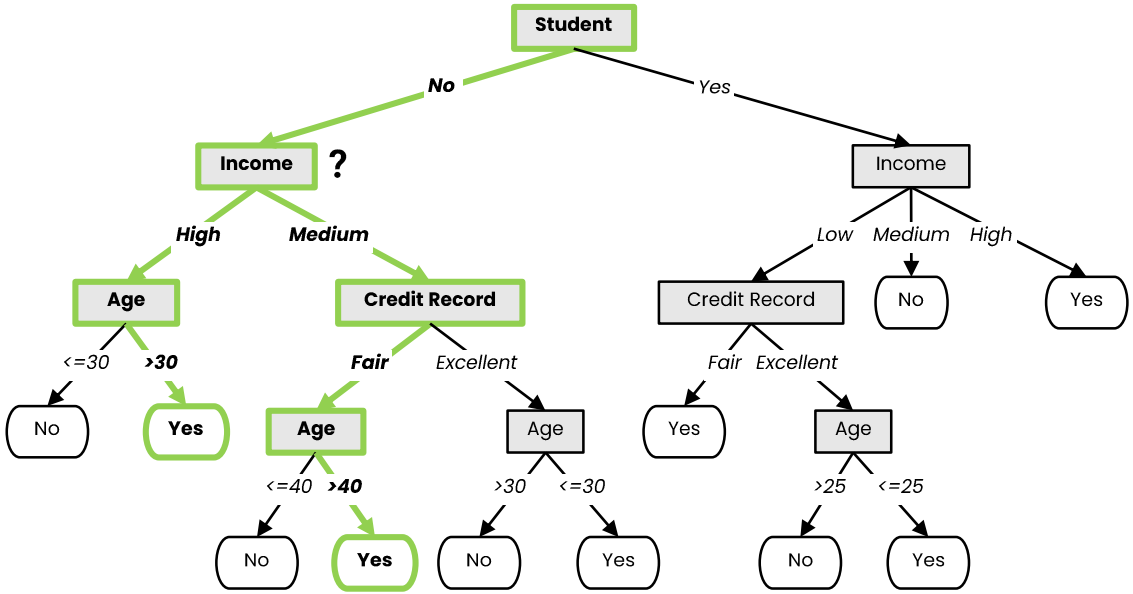



**Loan default?**

- Not a student
- 46 years old
- ***Unknown income***
- Fair credit record

# Handling Missing Attributes at Inference Time

- When we encounter a node which checks an attribute with a missing value, we explore all possibilities.
- We go down all branches and make all leaf nodes take a *(weighted)* vote for the final prediction.




**Loan default?**

- Not a student
- 46 years old
- ***Unknown income***
- Fair credit record

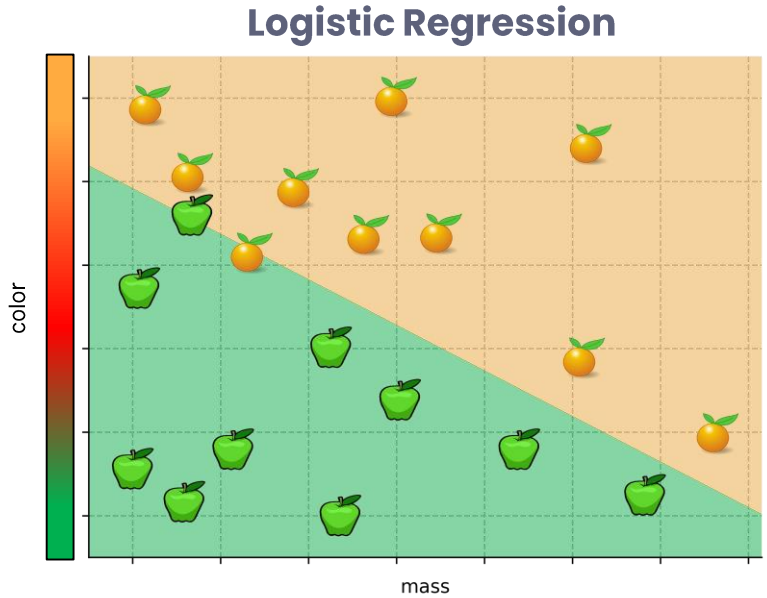
**Yes**

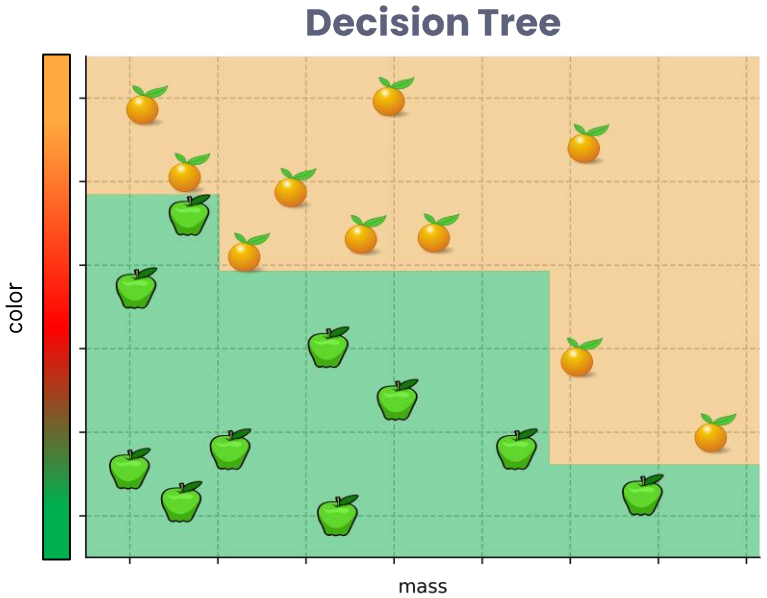
# C4.5 Algorithm

- **C4.5** is a an extension to the ID3 algorithm which brings several improvements:
  - Ability to handle *both discrete and* ***continuous attributes***. Continuous attributes are split by finding a best-splitting threshold.
  - Ability to handle ***missing attributes*** both at training and inference time. Training missing values are not used in information gain computation. Inference missing values are handled by considering all subsequent branches.
  - Ability to handle ***attributes with different costs***.
  - Post-**pruning** in a bottom-up manner for removing branches which decrease validation error.

# Decision Boundaries

- Different algorithms produce different decision boundaries.



# History of Decision Trees

- ***"Automatic Interaction Detection (AID)"*** — Morgan and Sonquist, 1963
  - The first regression tree algorithm.
- ***"Theta Automatic Interaction Detection (THAID)"*** — Messenger and Mandell, 1972
  - The first classification tree algorithm.
- ***"Classification and regression trees (CART)"*** — Breiman L., J. Friedman, R. Olshen, and C. Stone, 1984
- ***"Induction of Decision Trees"*** — J.R. Quinlan, 1986
  - Introduced the ID3 algorithm.
- ***"C4.5: Programs for Machine Learning"*** — J. R. Quinlan, 1993
  - Introduced the C4.5 algorithm.

# Summary

- A **decision tree** is a tool which uses a tree-like graph of decisions and their possible outcomes.
- **Decision tree learning** is a machine learning method which uses a *decision tree* as a predictive model.
- The **ID3** algorithm builds a decision tree by iteratively splitting the data on the values of the attribute with the largest **information gain** (decrease in **entropy**)
  - Using the decrease in **gini impurity** is also an option very common in practice.
- **C4.5** is an extension to *ID3* which handles *attributes with continuous values*, handles *missing attribute values* and adds regularization by *pruning* unnecessary branches.

# Random Forests

## **Ensemble learning** with decision trees

**Faculty of Mathematics and Computer Science, University of Bucharest**
and
**Sparktech Software**

*Academic Year 2018/2019, 1st Semester*

# Random Forests

- **Random Forests** basic idea:
  - Instead of *growing* a single decision tree and use it to make predictions, grow many slightly different trees and combine their predictions.

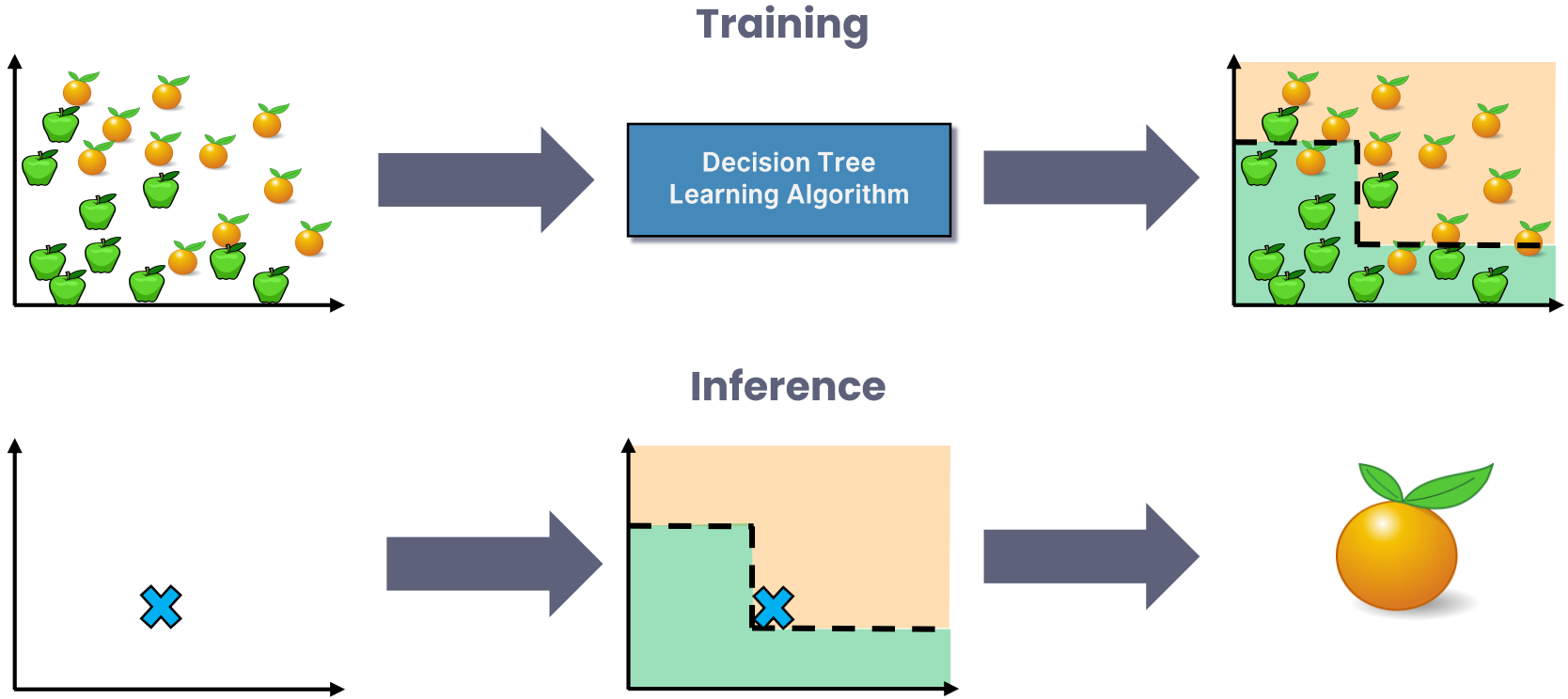
# Random Forests

- **Random Forests** basic idea:
  - Instead of *growing* a single decision tree and use it to make predictions, grow many slightly different trees and combine their predictions.
- We have one dataset, so how do we obtain *slightly different* trees?

# Random Forests

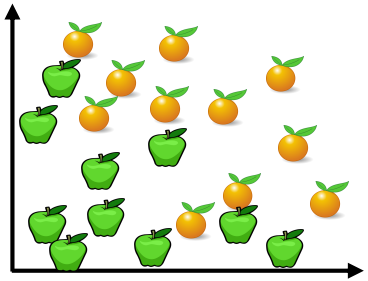
- **Random Forests** basic idea:
  - Instead of *growing* a single decision tree and use it to make predictions, grow many slightly different trees and combine their predictions.
- We have one dataset, so how do we obtain *slightly different* trees?
  - **Bagging** (**B**ootstrap **Agg**regat**ing**)
    - Take random subsamples of data points from the large dataset to create *N* smaller datasets
    - Fit a different model on each of small datasets.
  - **Random Subspace Method** (a.k.a. Feature Bagging)
    - Fit *N* different models, but allow each one to see a random subsample of features from the original dataset.

# Reminder – Single Decision Tree Flow

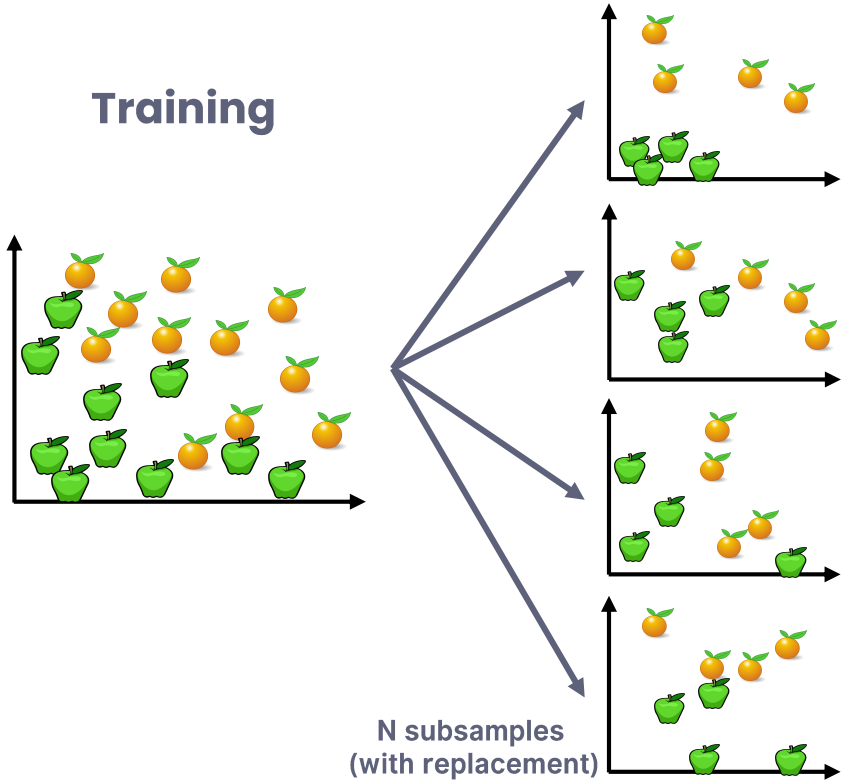


# Bagging

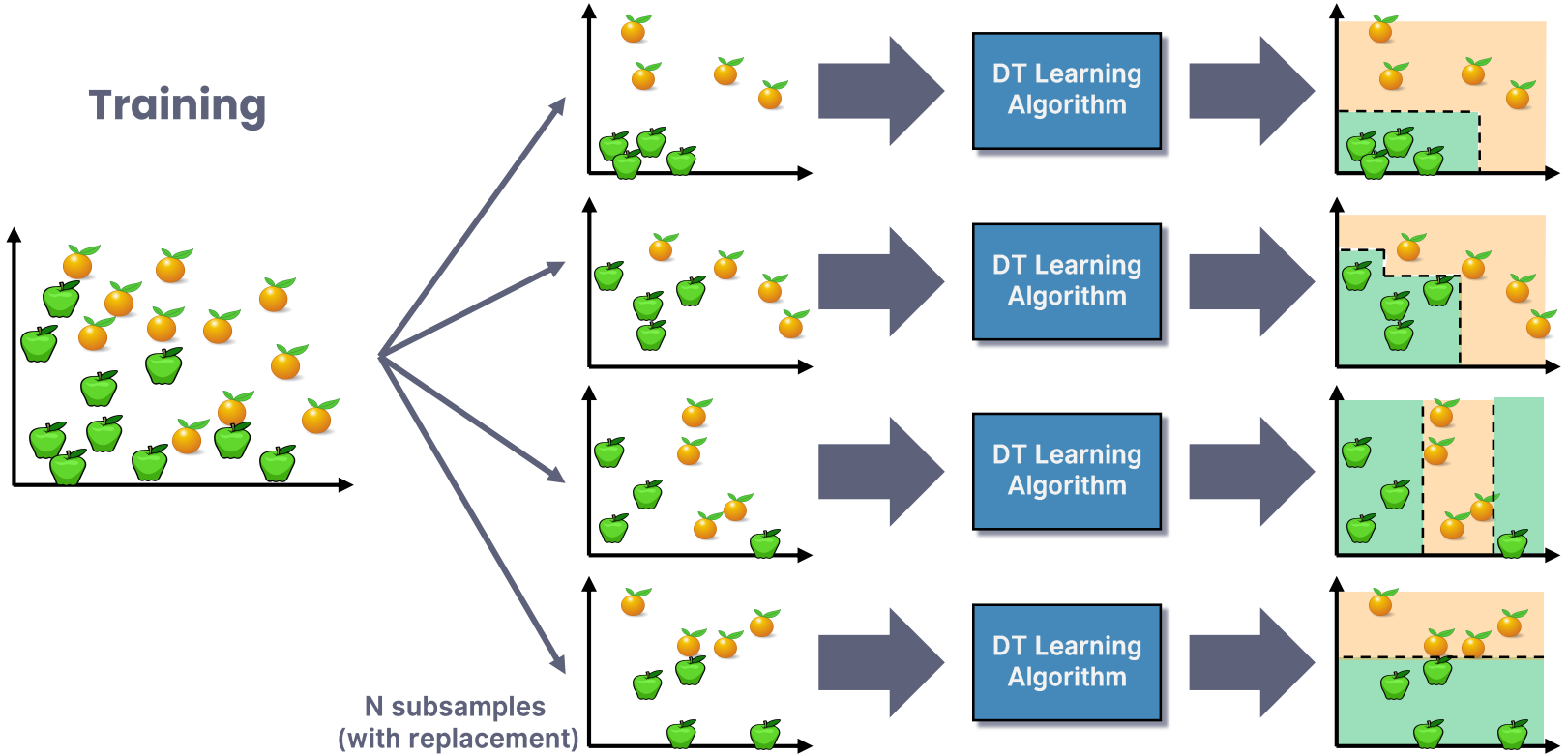
## Training



# Bagging

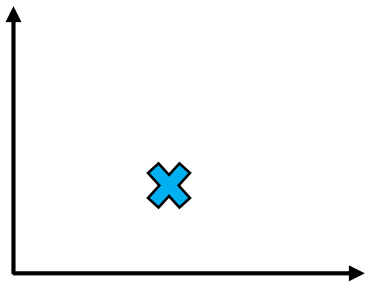


# Bagging


Training
DT Learning Algorithm
DT Learning Algorithm
DT Learning Algorithm
DT Learning Algorithm
N subsamples
(with replacement)

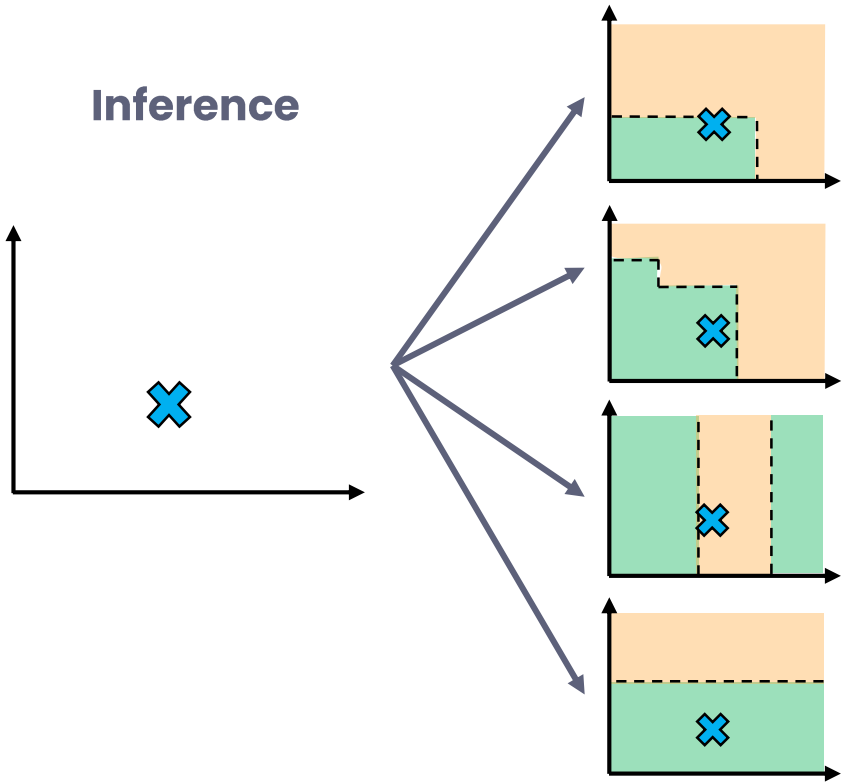
# Bagging

## Inference

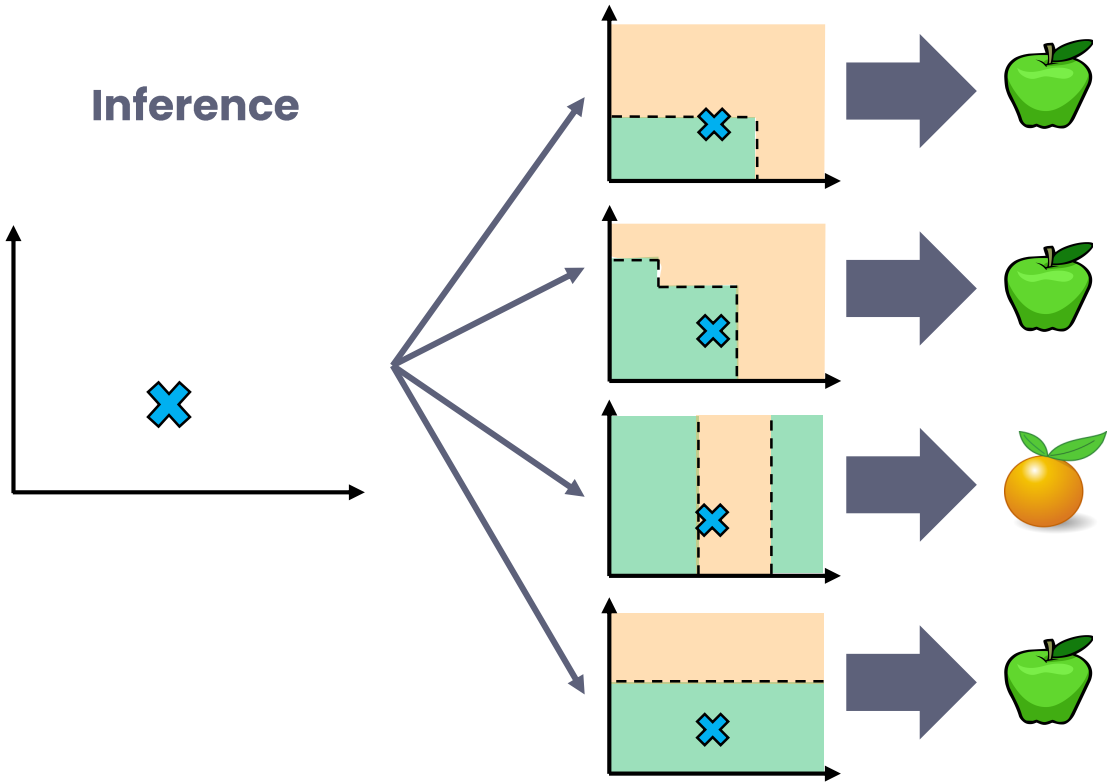


# Bagging

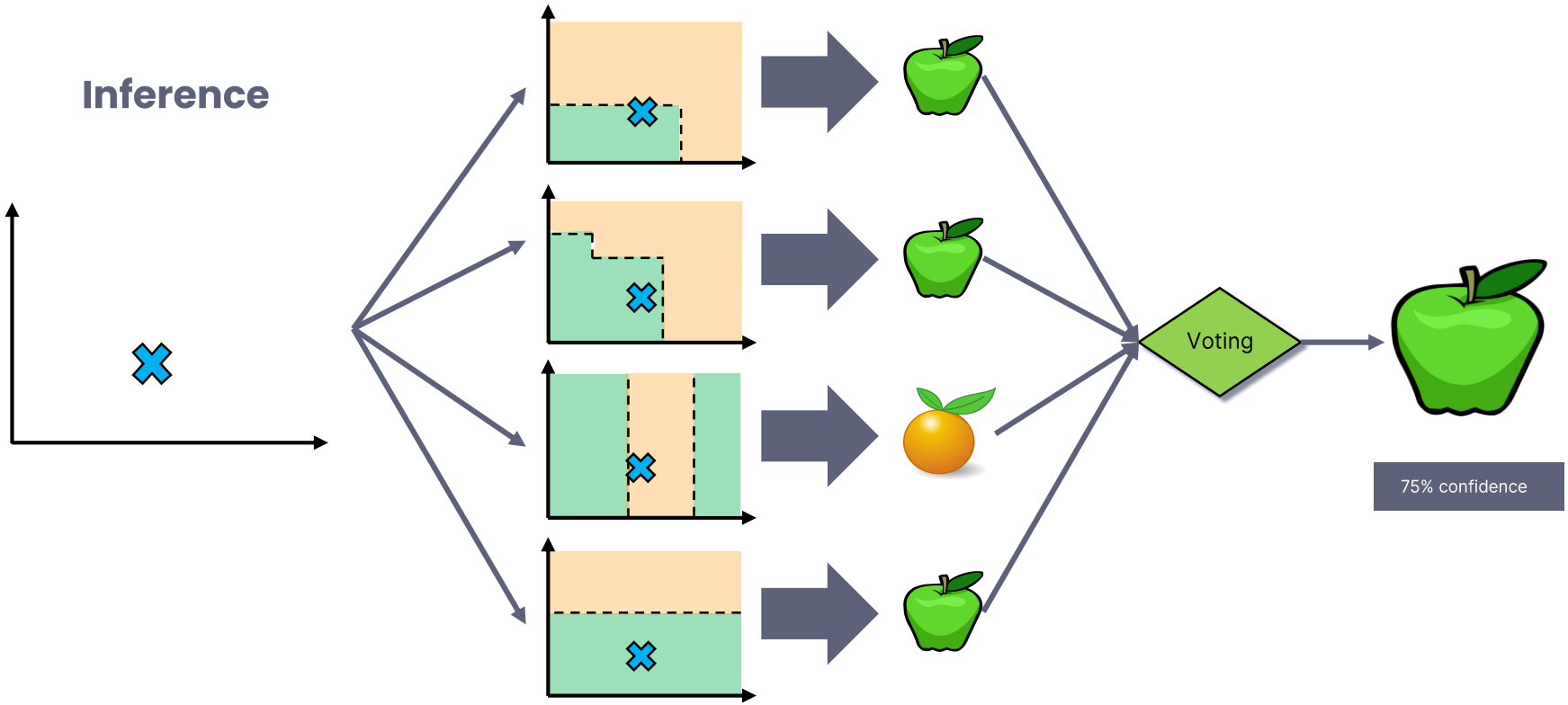
## Inference



# Bagging



# Bagging



# Random Subspace Method

## Training

| Mass (g) | Color | Texture | pH | Label |
|---|---|---|---|---|
| 84 | Green | Smooth | 3.5 | **Apple** |
| 121 | Orange | Rough | 3.9 | **Orange** |
| 85 | Red | Smooth | 3.3 | **Apple** |
| 101 | Orange | Smooth | 3.7 | **Orange** |
| 111 | Green | Rough | 3.5 | **Apple** |
| ... | | | | |
| 117 | Red | Rough | 3.4 | **Orange** |

# Random Subspace Method

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| ... | | | | |
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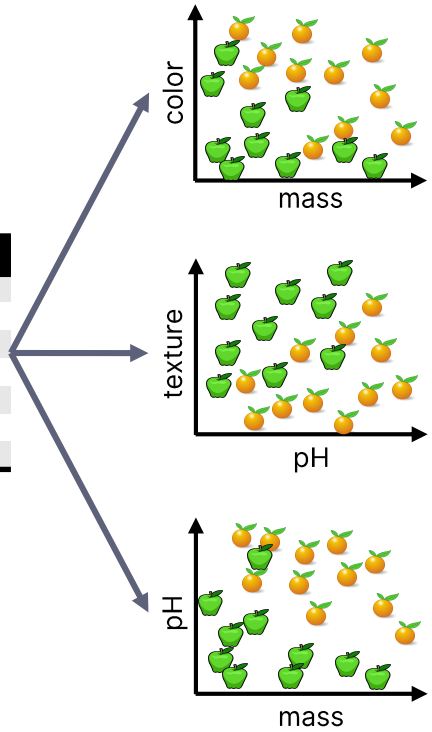

# Random Subspace Method

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| 84 | Green | Smooth | 3.5 | **Apple** |
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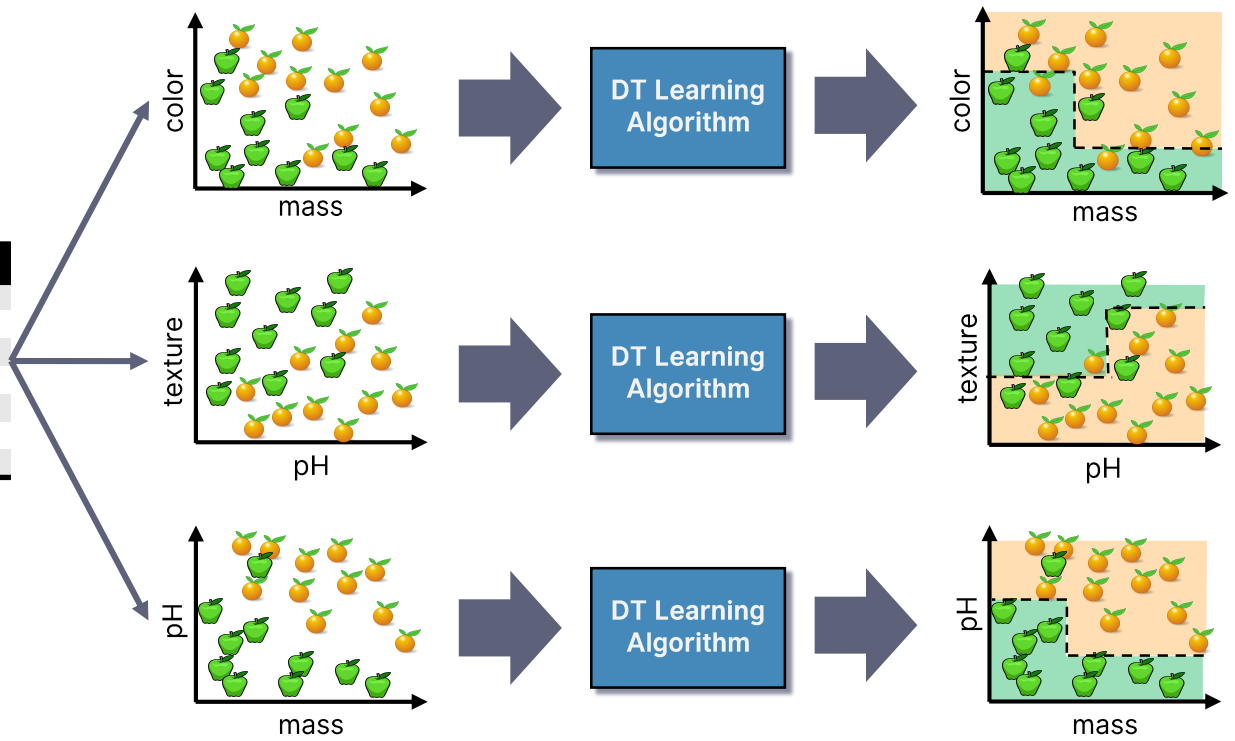
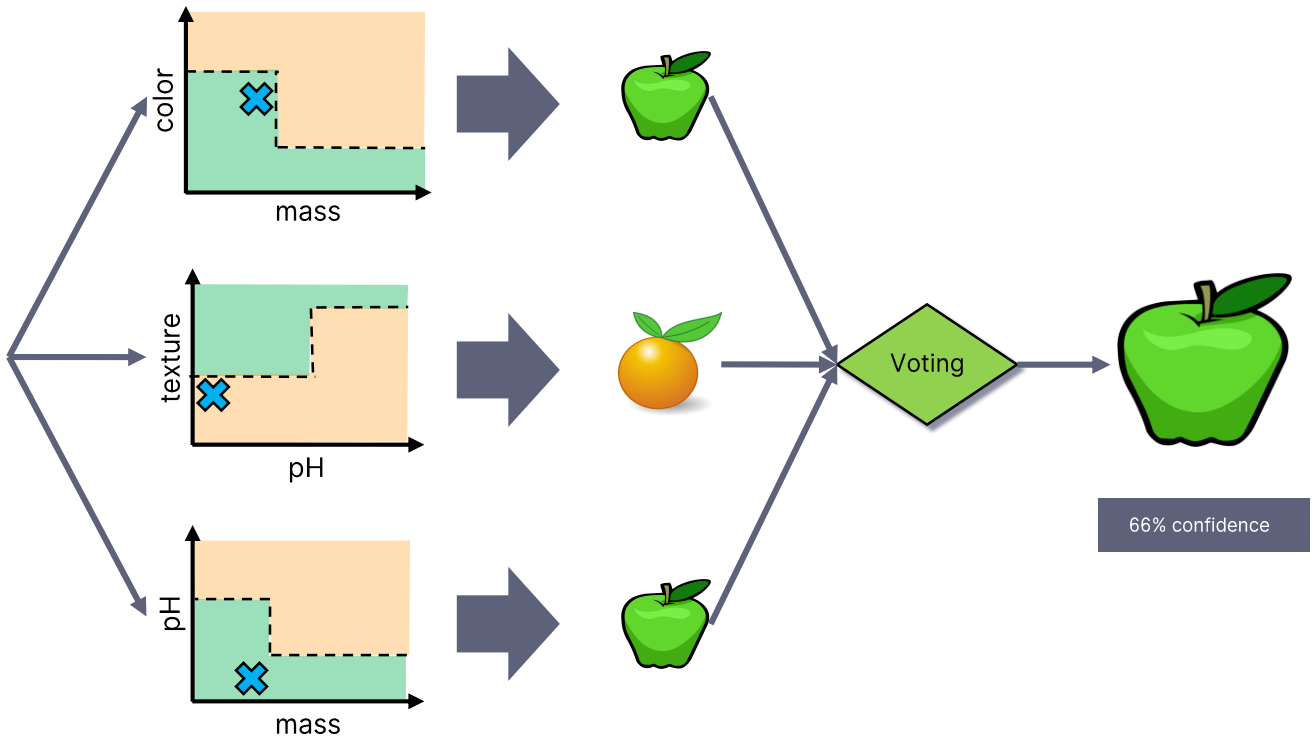


# Random Subspace Method

## Inference

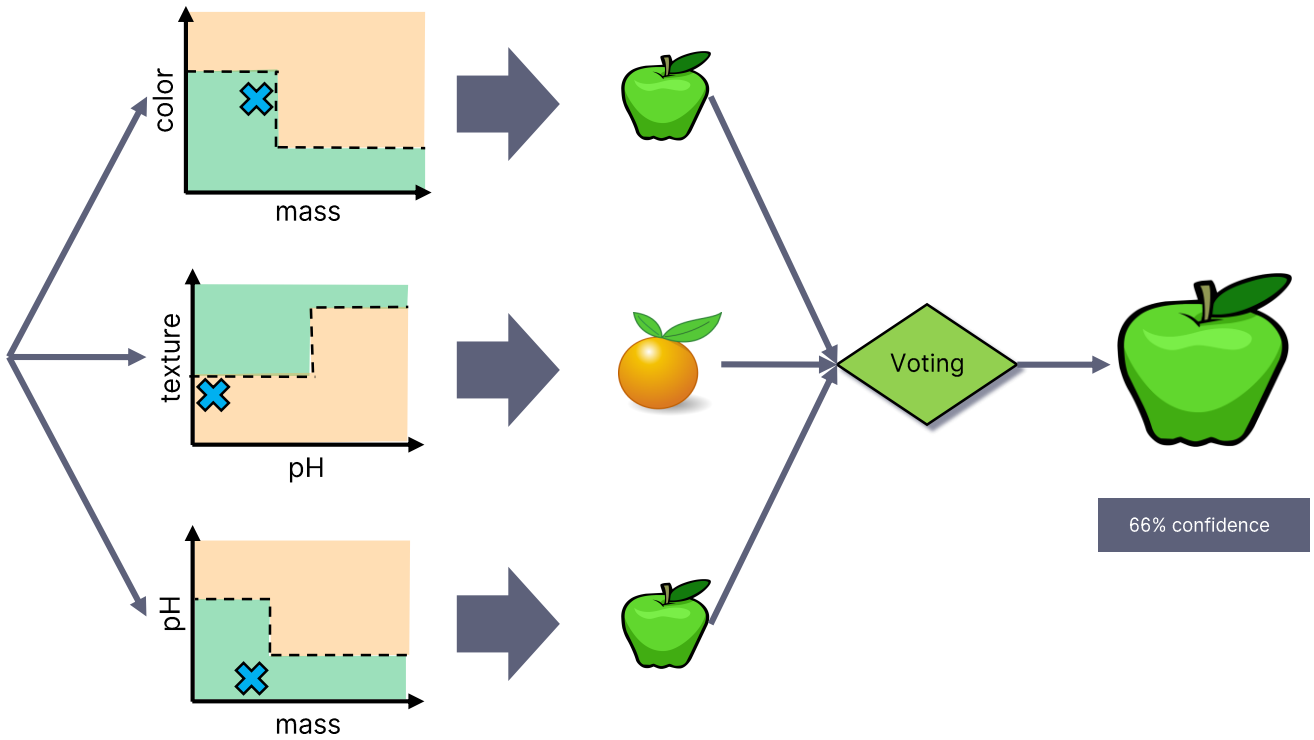
| | | | |
|---|---|---|---|
| 87 | Red | Smooth | 3.1 |



# Random Subspace Method

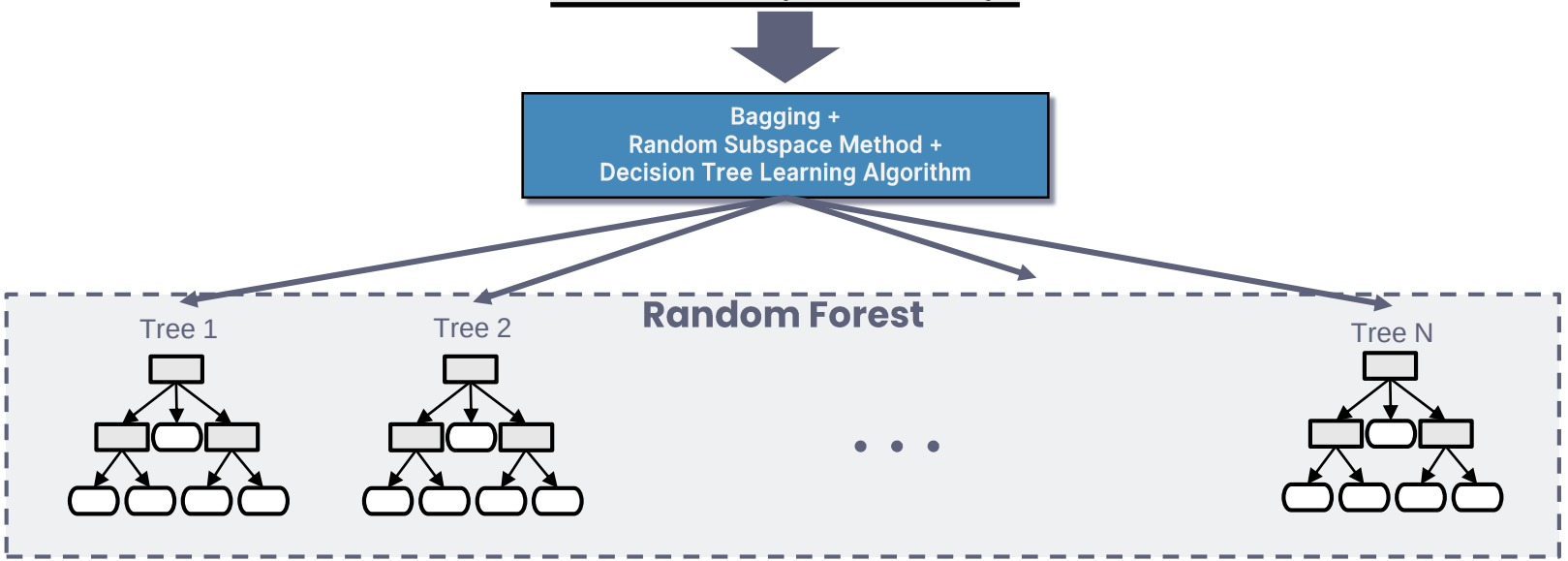
## Inference

| | | | |
|---|---|---|---|
| 87 | Red | Smooth | 3.1 |



# Random Forests

| Mass (g) | Color | Texture | pH | Label |
|---|---|---|---|---|
| 84 | Green | Smooth | 3.5 | **Apple** |
| 121 | Orange | Rough | 3.9 | **Orange** |
| 85 | Red | Smooth | 3.3 | **Apple** |
| 101 | Orange | Smooth | 3.7 | **Orange** |
| 111 | Green | Rough | 3.5 | **Apple** |
| ... | | | | |
| 117 | Red | Rough | 3.4 | **Orange** |



# History of Random Forests

- ***"Random Decision Forests"*** and ***"The Random Subspace Method for Constructing Decision Forests"***

  Tin Kam Ho, 1995 and 1998

  - Introduced the *Random Subspace Method*

- ***"Random Forests"***

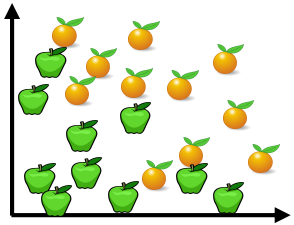
  Leo Breiman, 2001

  - Combined the Random subspace method with *Bagging*
  - Introduced the term *random forest*™, which is a trademark of Leo Breiman and Adele Cutler

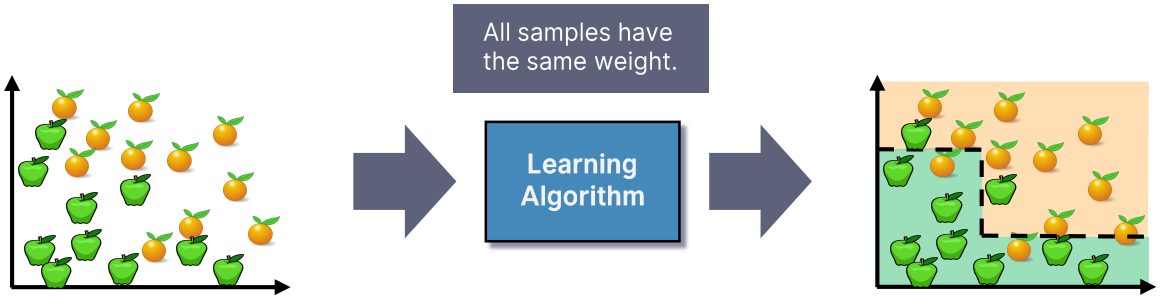
# Ensemble Learning

- **Ensemble Learning** is a generic term for methods which combine *multiple learning algorithms* to obtain better performance than could be obtained from any constituent algorithm alone.
- *Random Forests* are one of the most common instances of ensemble learning.
- Common ensemble techniques:
  - **Bagging** – multiple models on random subsamples of data
  - **Random Subspace Method** – multiple models on random subsamples of features
  - **Boosting** – iteratively train models, while making the current model focus more on the mistakes of previous ones by increasing the weight of misclassified samples.

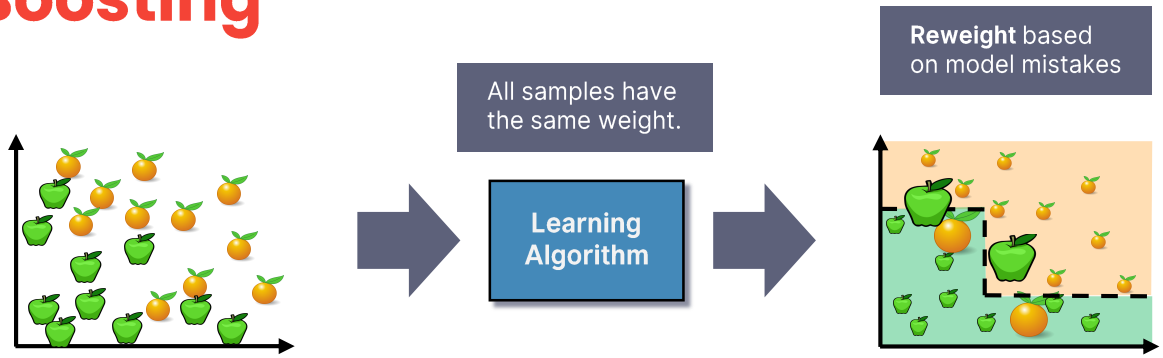
# Boosting



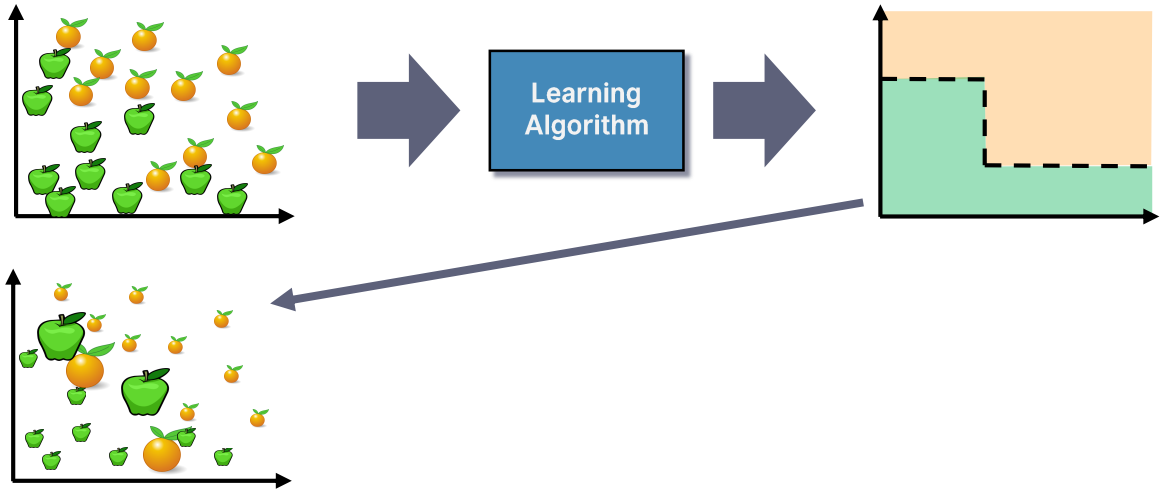
# Boosting



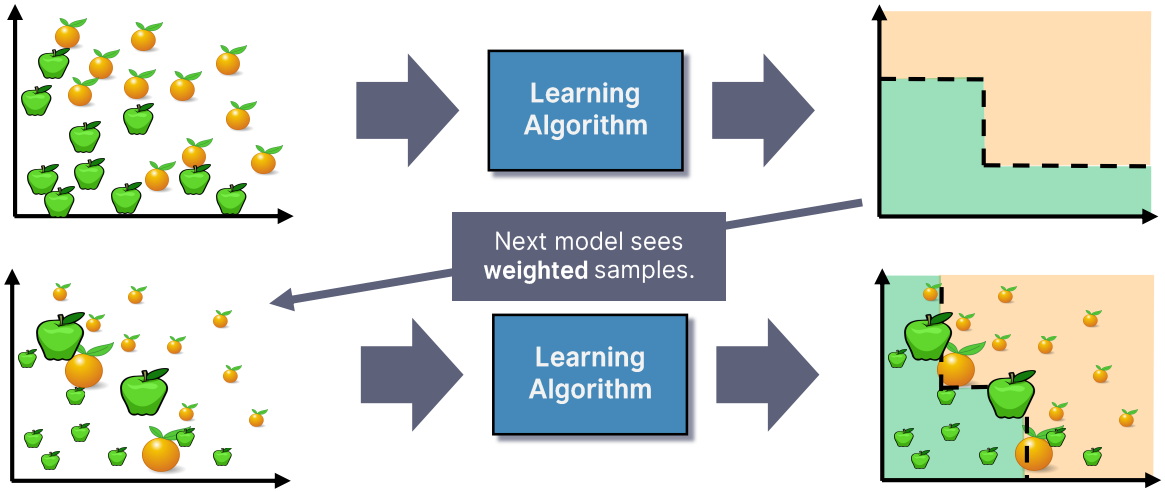
# Boosting


All samples have the same weight.
Learning Algorithm
**Reweight** based on model mistakes

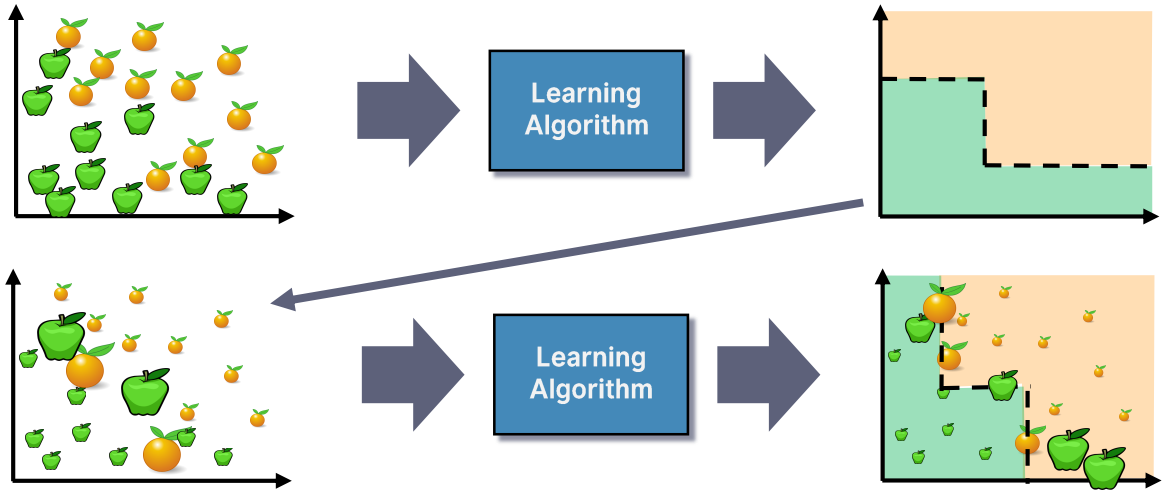
# Boosting



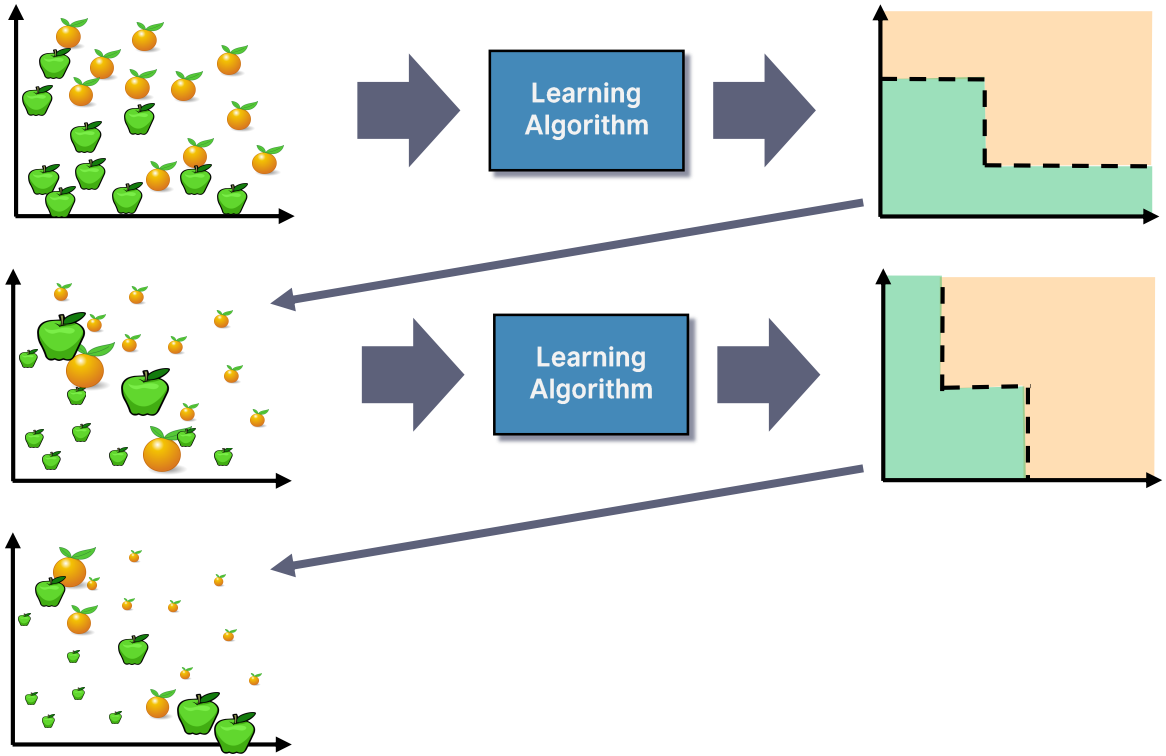
# Boosting


Learning Algorithm
Next model sees **weighted** samples.
Learning Algorithm

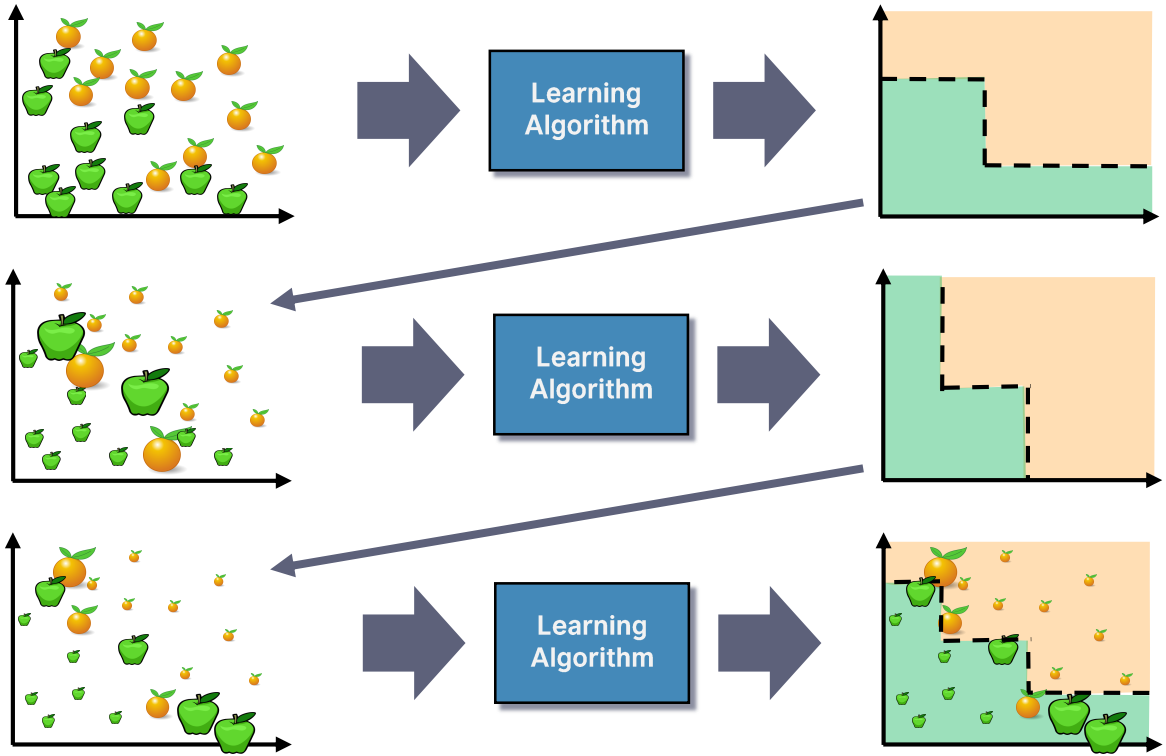
# Boosting



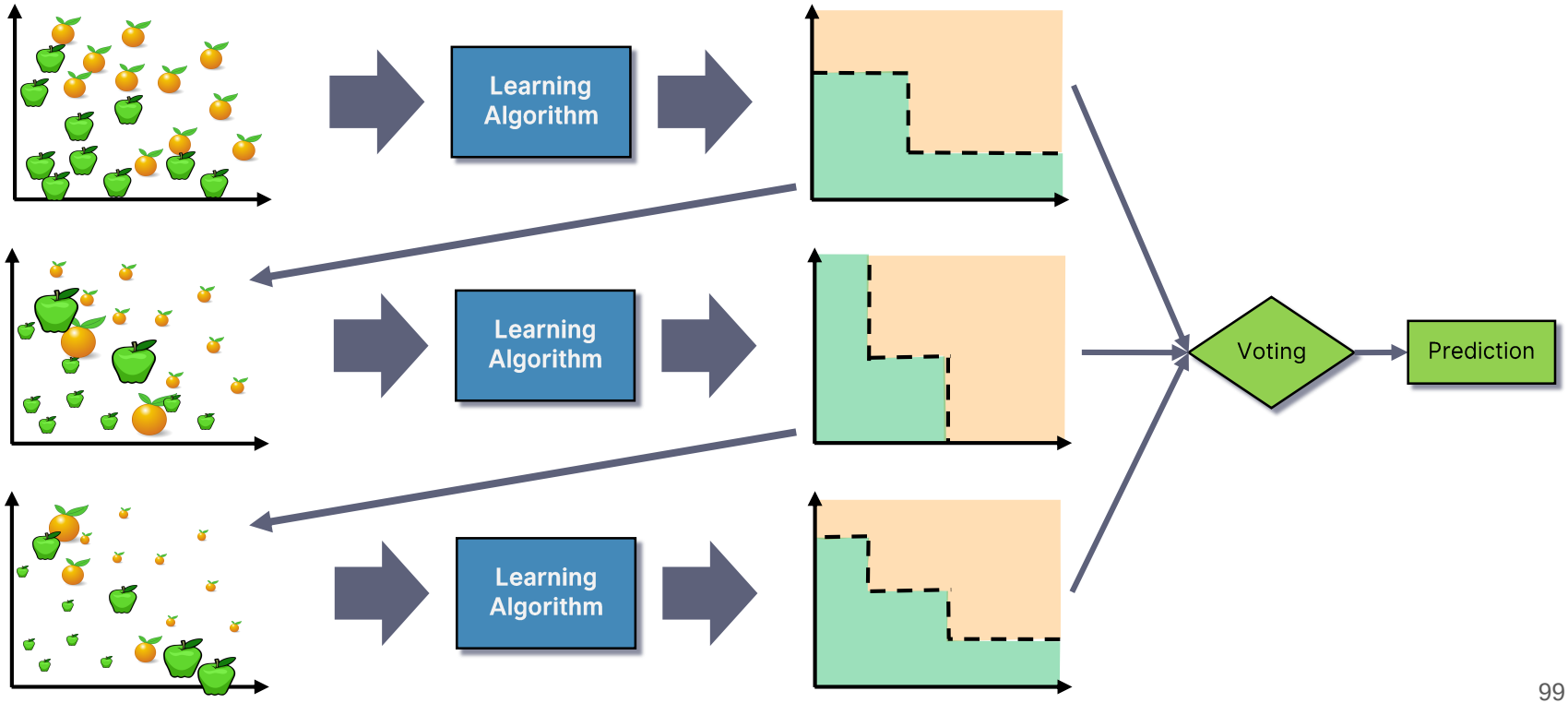
# Boosting



# Boosting


Learning Algorithm
Learning Algorithm
Learning Algorithm

# Boosting


Learning Algorithm
Learning Algorithm
Learning Algorithm
Voting
Prediction

# Summary

- **Ensemble learning** methods combine multiple learning algorithms to obtain better performance that could be obtained from any of the constituent algorithms alone.

- Common ensemble techniques include **bagging** (obtaining multiple models from *random subsamples of data*), the **random subspace method** (multiple models on *random subsamples of features*) and **boosting** (iteratively train models, while making the current model *focus more on the mistakes of previous* ones by increasing the weight of misclassified samples)

- **Random Forests** are an ensemble learning method which uses a *decision tree learning* algorithm to obtain multiple trees by *bagging* and the *random subspace method*. They are used to rectify decision trees' habit of overfitting.

# Decision Trees and Random Forests in Python

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier

clf = DecisionTreeClassifier(criterion = “entropy”, min_samples_leaf = 3)
     # lots of parameters: criterion = ”gini” / “entropy”; max_depth; min_impurity_split; …
clf.fit(X, y) # Note: It can only handle numerical attributes!
              # Categorical attributes need to be encoded, see LabelEncoder and OneHotEncoder
clf.predict([x]) # predict class for x

clf.feature_importances_ # importance of each feature
clf.tree_ # the underlying tree object

clf = RandomForestClassifier(n_estimators = 20) # random forest with 20 trees
```

# Keywords

Decision Tree

ID3 | Entropy | Information Gain | Gini Impurity

C4.5 | Pruning

Random Forests | Ensemble Learning

Bagging | Random Subspace Method | Boosting