Elements of Machine Learning & Data Science

Winter semester 2025/26

Lecture 3 – Decision Trees

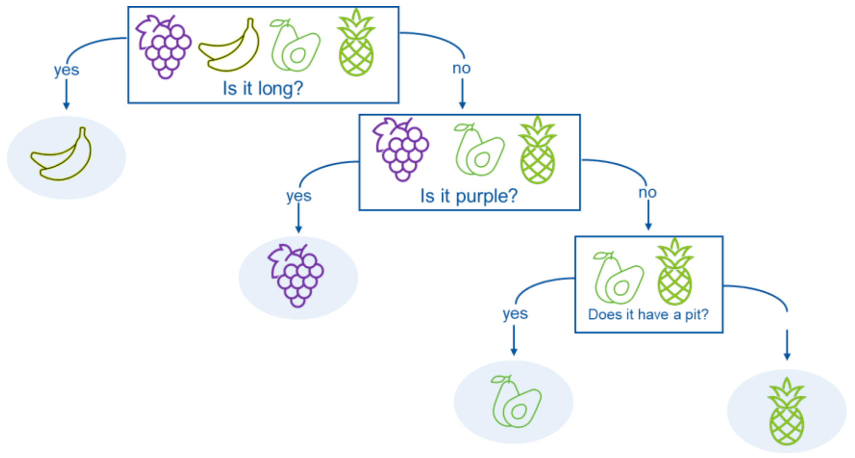
27.10.2025

Prof. Bastian Leibe

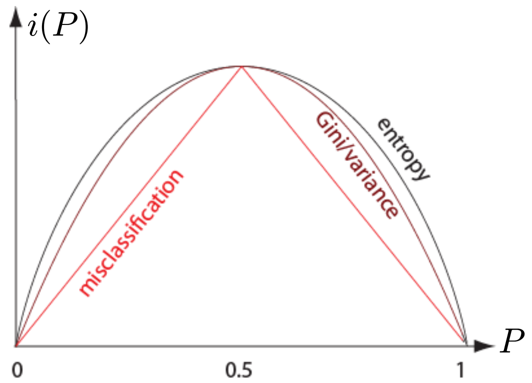
slides by Prof. Wil van der Aalst

Overview of the Lecture Topics

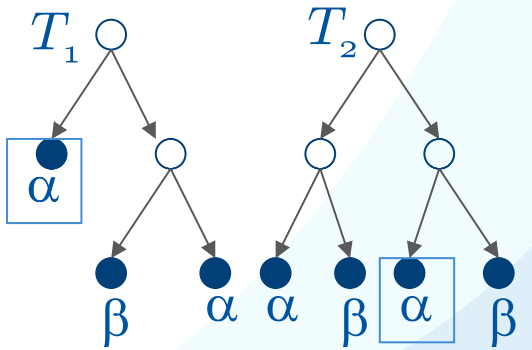
1. Introduction to Data Science
2. **Decision Trees**
3. Clustering
4. Frequent Itemsets
5. Association Rules
6. Time Series



Constructing Decision Trees



Entropy, Information gain, Gini index

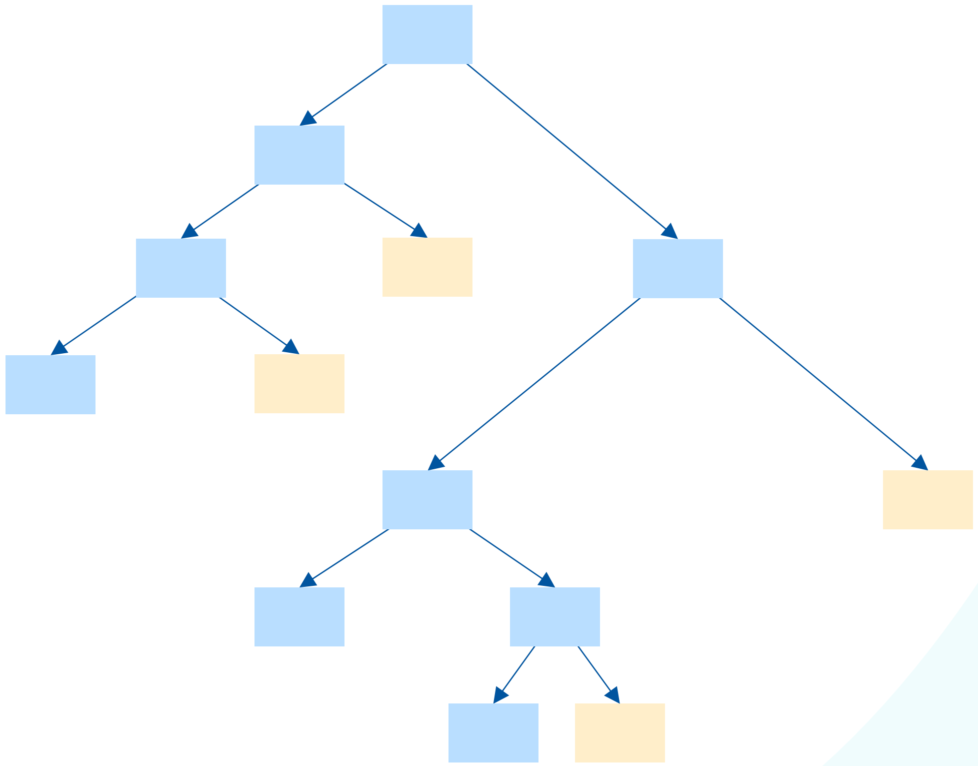


Randomized Forests

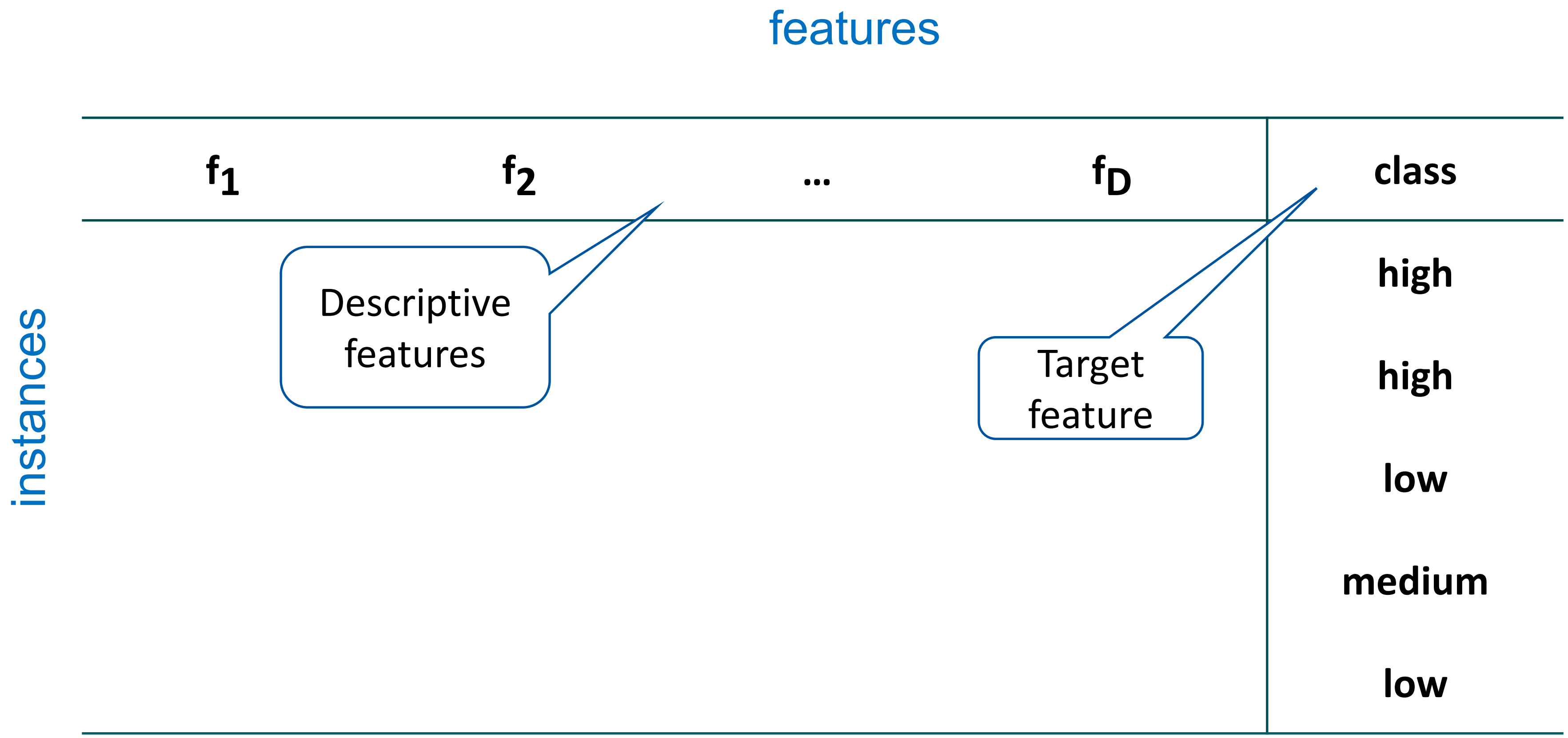
Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

Decision Trees

1. **Introduction to Decision Trees**
2. Entropy and Information Gain
3. ID3 Algorithm
4. Quantifying Information Gain
5. Pruning
6. Continuous Data
7. Ensembles



Intuition and Interpretation



A decision tree aims to explain the target feature in terms of the descriptive features.

Intuition and Interpretation

features

ances

f_1	f_2	…	f_D	
				high
				high
				low
				medium
				low

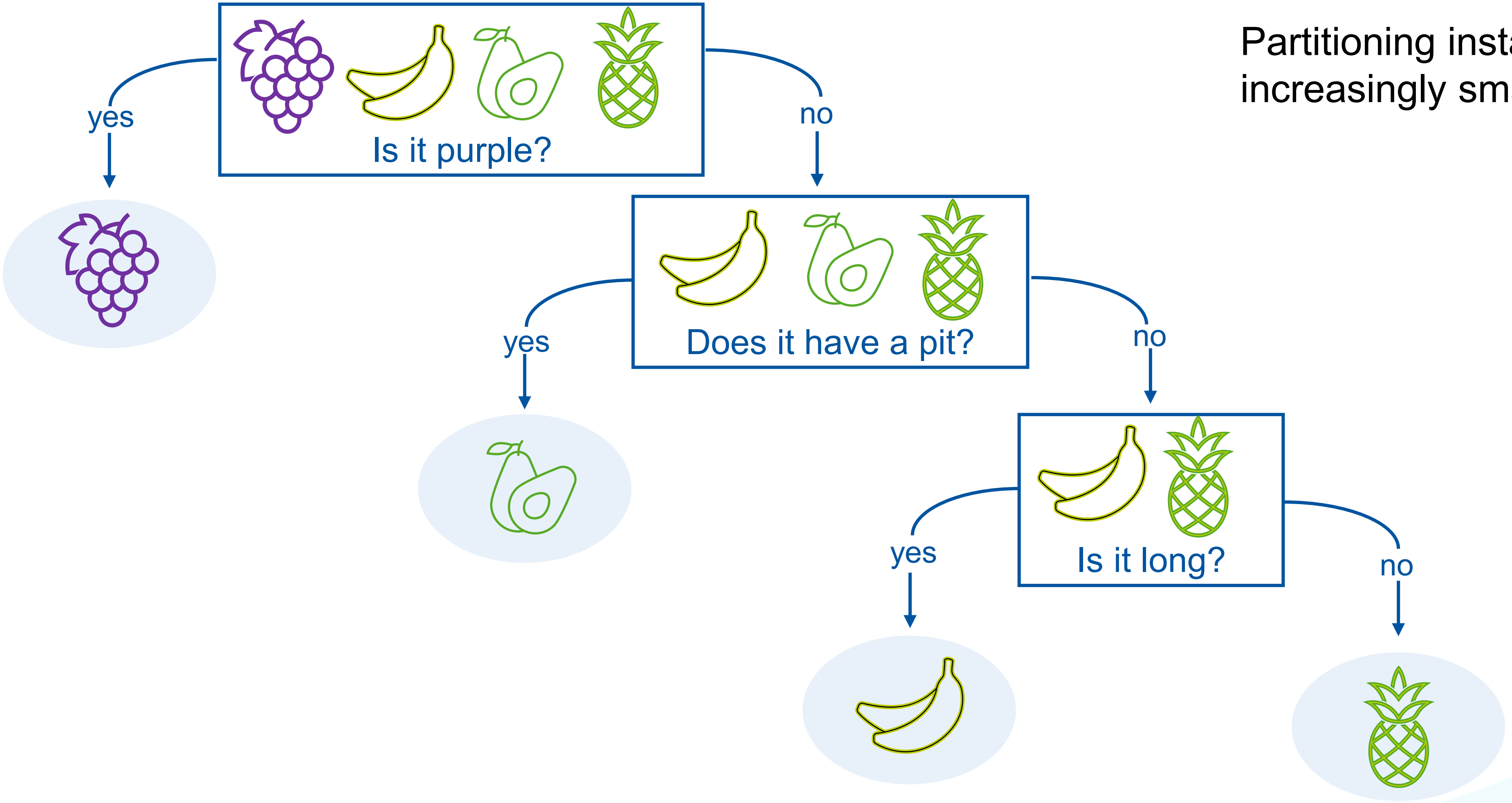
Descriptive featu

Target feature

Remember: We want to learn a function based on labeled training instances!

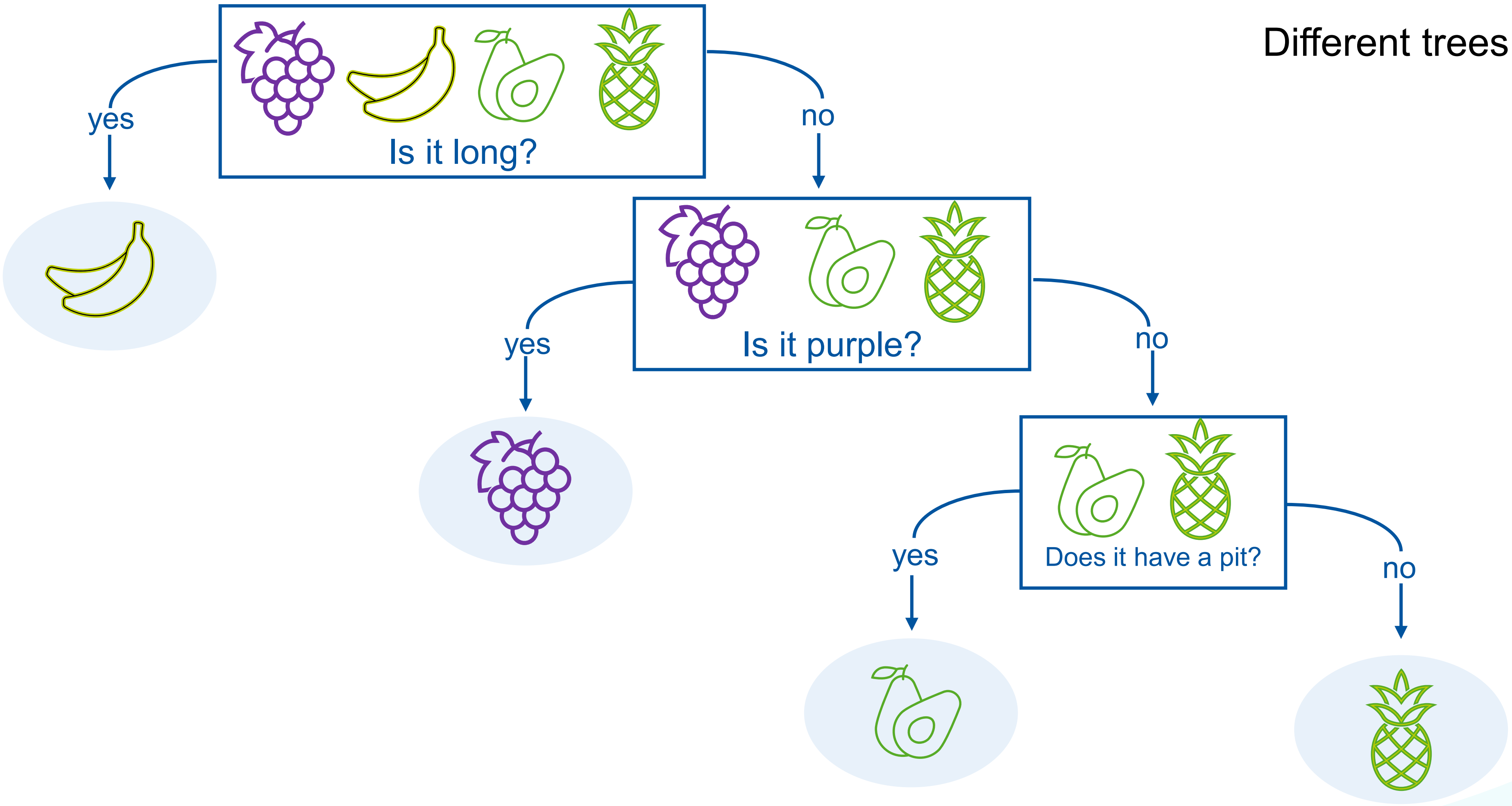
A decision tree aims to explain the target feature in terms of the descriptive features.

Fruity Example



Partitioning instances in increasingly smaller groups

Fruity Example



Different trees are possible

Example 2

Rain	Wind	Temperature (◦C)	Play tennis
Yes	Yes	15	**No**
No	No	34	**Yes**
Yes	No	23	**Yes**
Yes	Yes	20	**Yes**
No	Yes	28	**No**
…	…	…	…

Target feature

Descriptive features

Example 2

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Yes	Yes	15	**No**
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Yes	No	23	**Yes**
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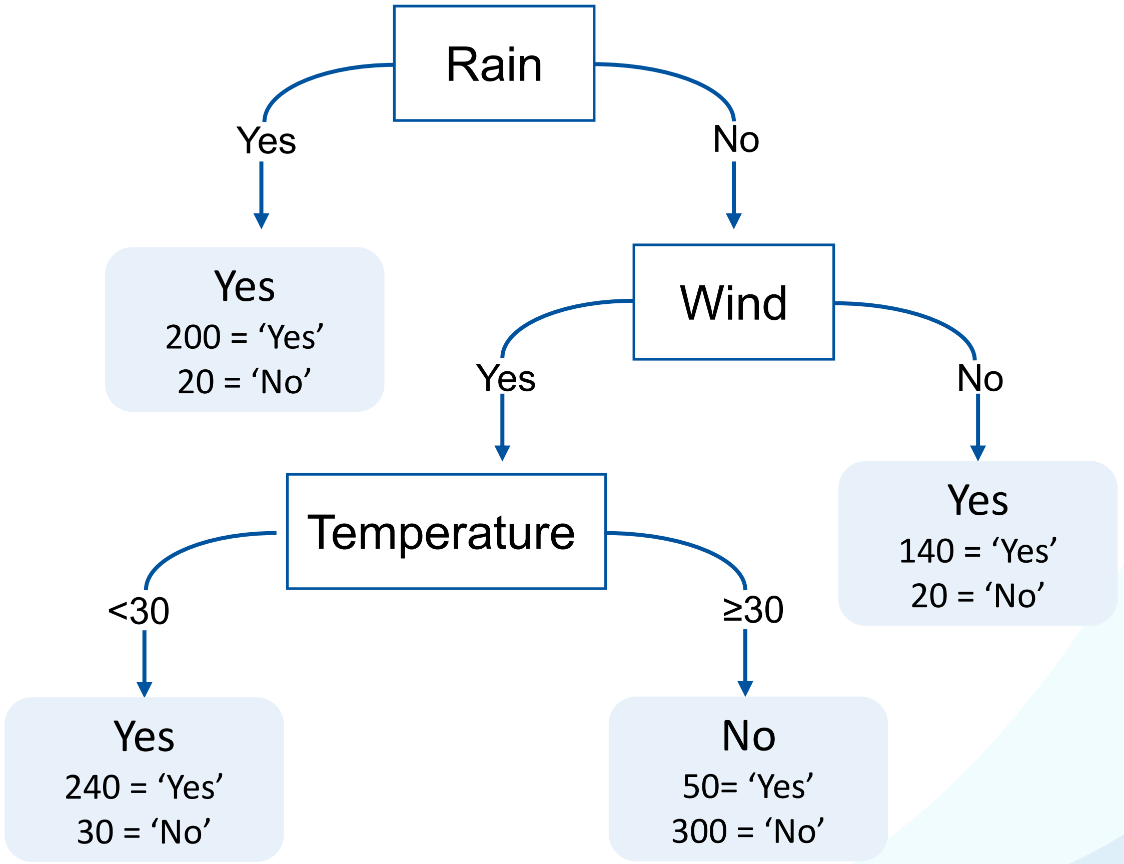
…	…	…	…

1000 Instances



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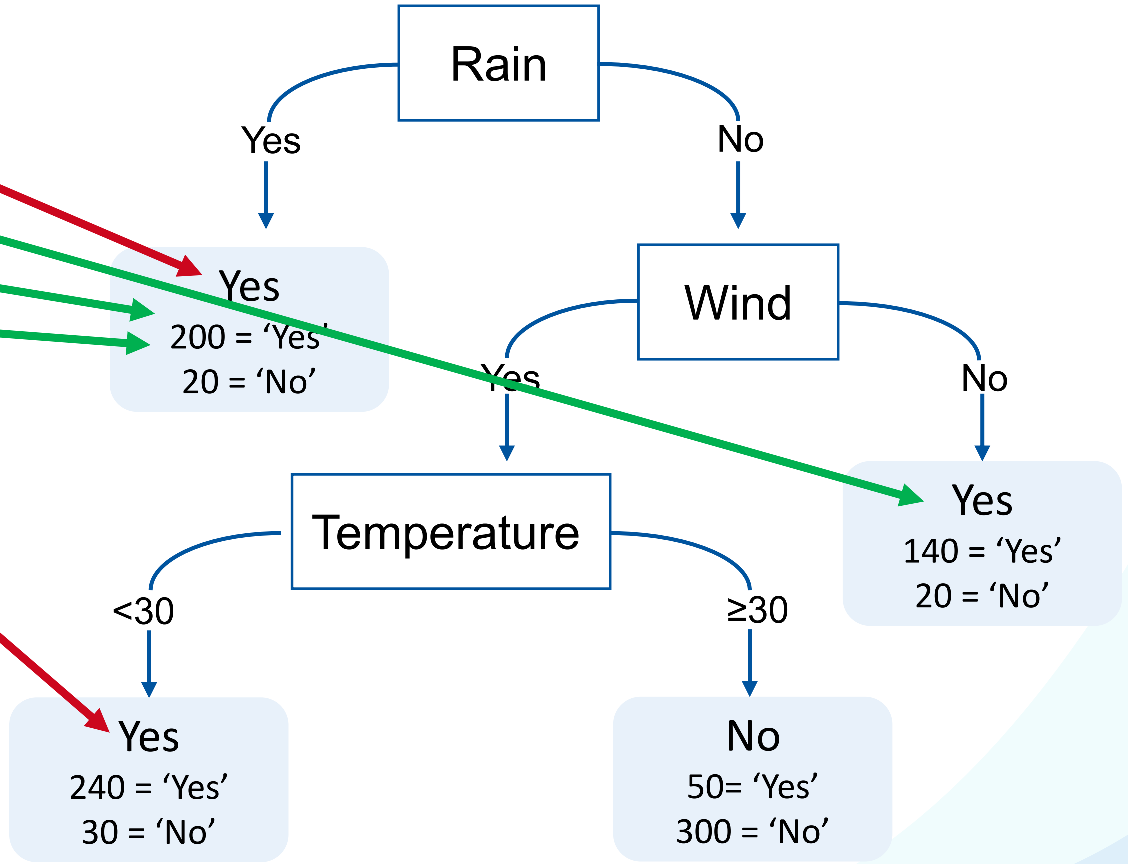

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No	No	34	**Yes**
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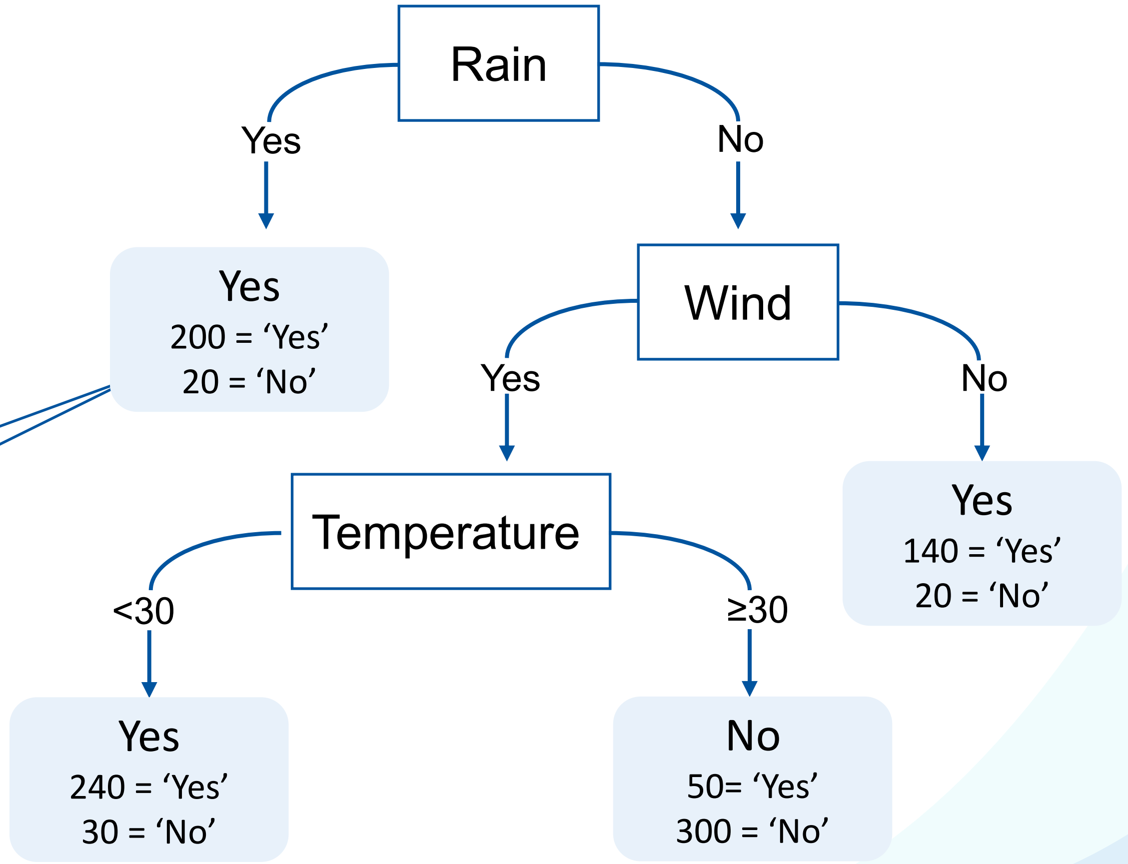
…	…	…	…

220 cases with *Rain = Yes* are classified as 'Yes' (Play tennis), but 20 are classified incorrectly



Decision Tree Construction

Tree Structure

- Three types of nodes: root node, interior nodes and leaf nodes
  - **Root node** refers to all instances
  - **Non-leaf nodes** partition the set of instances based on a descriptive feature
  - **Leaf nodes** have a label (target feature value)
    (usually based on the label of the majority of instances in this node)

Decision Tree Construction

Tree Structure

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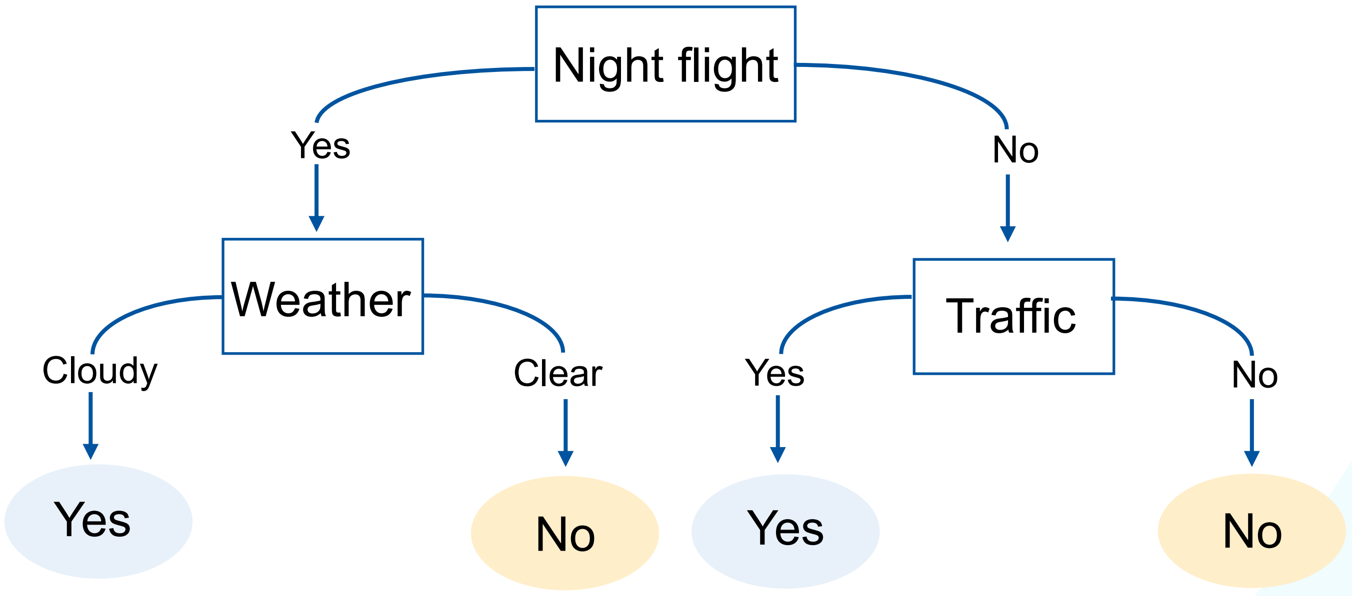
There are two goals (often conflicting)

- The tree is small and simple
- The leaves are homogeneous in terms of the target feature

Comparing Decision Trees (1/2)

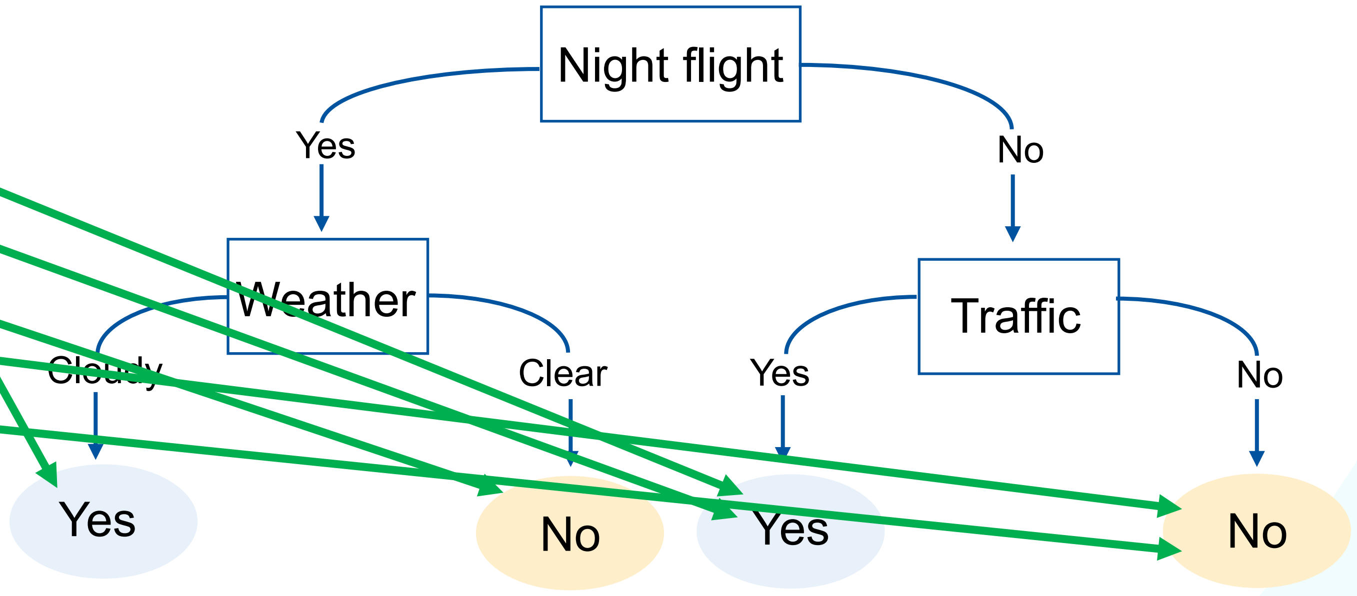
Weather	Traffic	Night flight	Flight delayed
Cloudy	No	Yes	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	No	**No**
Clear	No	No	**No**



Comparing Decision Trees (1/2)

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	Yes	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	No	**No**
Clear	No	No	**No**

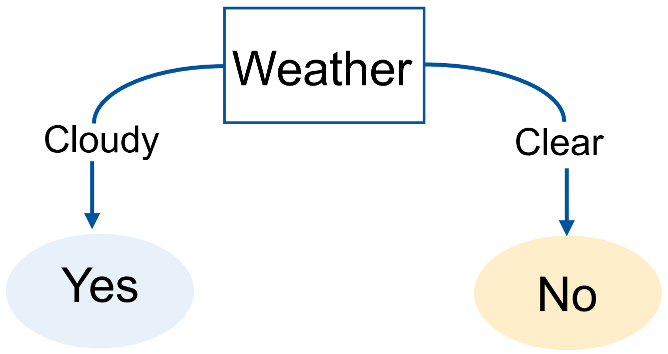
All instances correctly classified



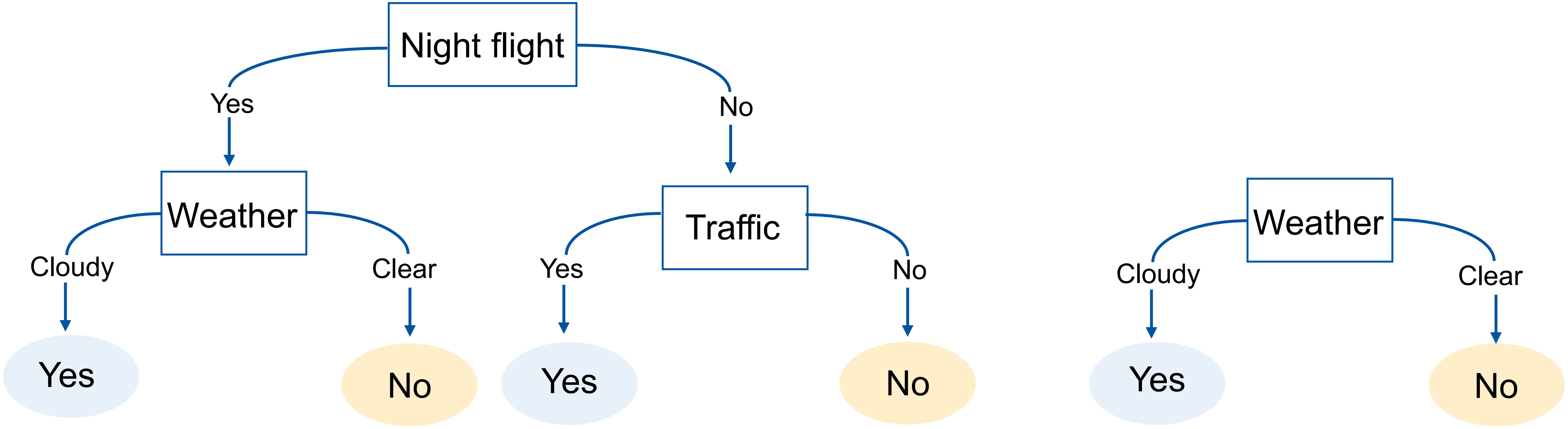
Comparing Decision Trees (2/2)

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	Yes	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	No	**No**
Clear	No	No	**No**

All instances correctly classified



Comparing Decision Trees



Both trees correctly classify all observed instances, but the ‘simpler’ one seems ‘better’.

Key concepts:

- avoid overfitting
- apply Occam's razor
- prefer shallow trees

Characteristics Decision Trees

- A very simple model!
- In some cases, preferable to more complex and modern models (such as neural networks):
  - Fewer data points/attributes (managing overfitting is easier)
  - Well-suited for tabular data, where some attributes may be missing from table entries.
  - In domains where explainability and transparency are required
  - The choices of a tree are very easy to explain and show!
- There are extensions of decision trees that aim to combine simplicity and transparency with the ability to handle more complex data

Decision Trees

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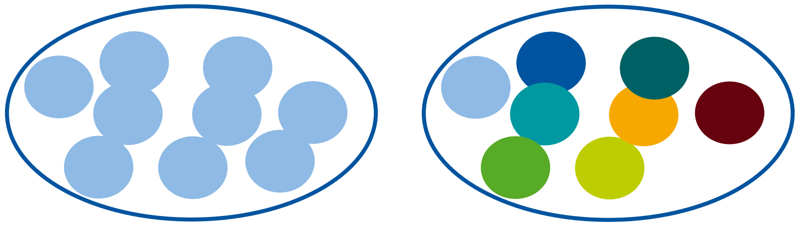
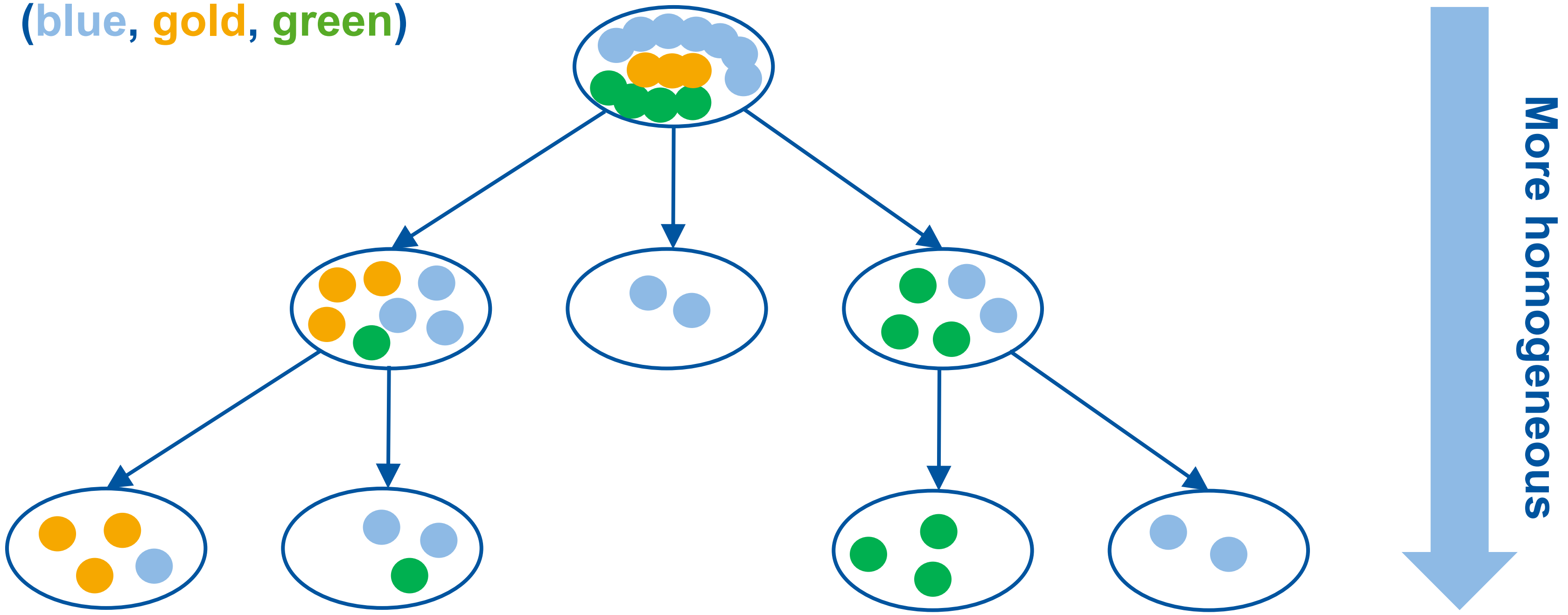


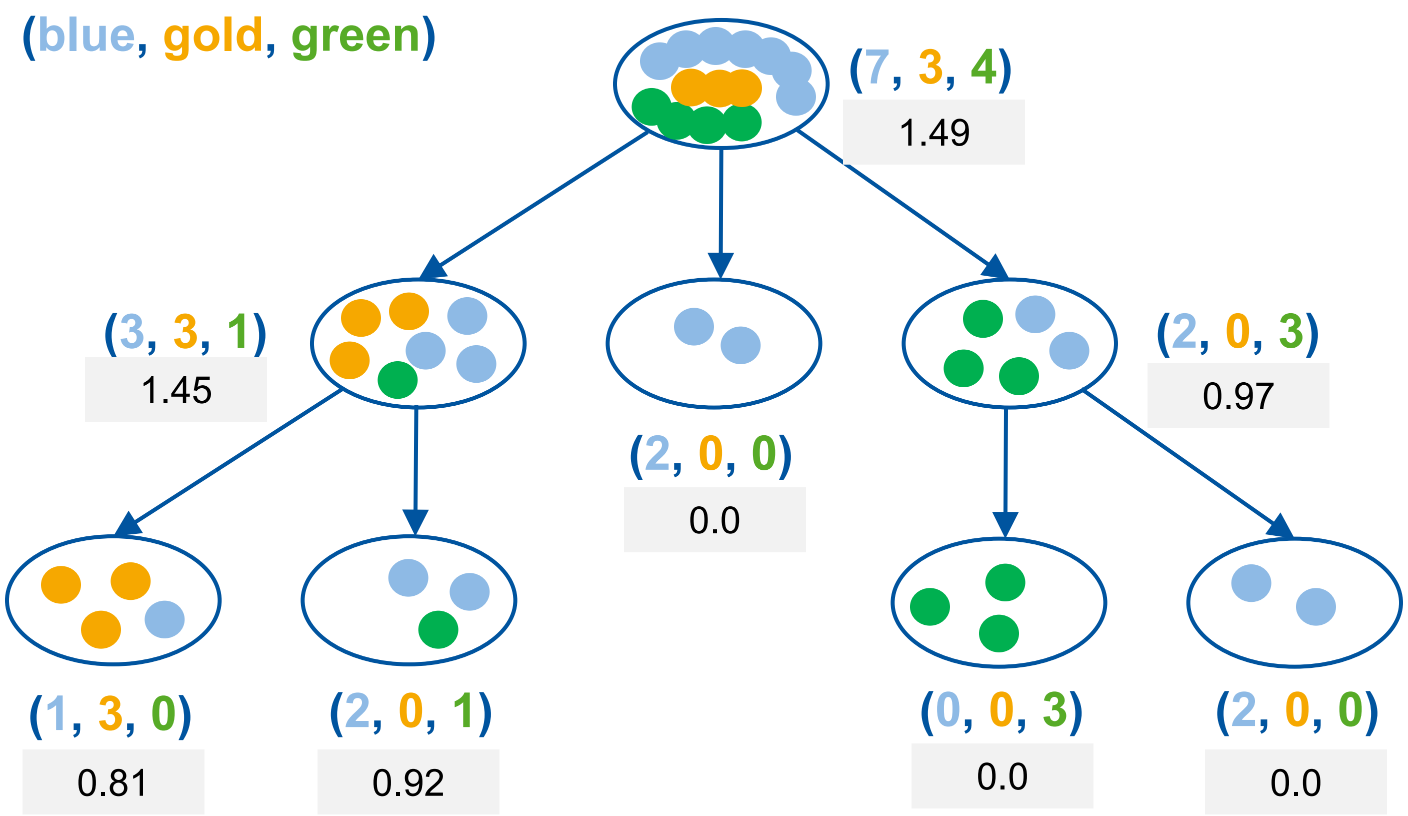
Information Gain

(blue, gold, green)



Information gain = improvement in knowledge
(predictability of target label in nodes)

Entropy - Intuition



Idea

- Measure of impurity
- Uncertainty when guessing
- Incompressibility

Worst case entropy for 3 values: ≈ 1.58

Entropy - Formula

$$H(t) = -\sum_{k=1}^{K} (P(t=k) \cdot log_s(P(t=k)))$$

(7, 3, 4)

$$H(color) = -(\frac{7}{14} \cdot log_2(\frac{7}{14}) + \frac{3}{14} \cdot log_2(\frac{3}{14}) + \frac{4}{14} \cdot log_2(\frac{4}{14})) \approx 1.49$$

t: examined target feature ($color$ in the example)

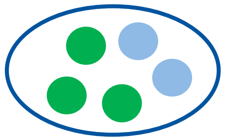
K: number of possible values of the target feature ($K = |\{blue, gold, green\}| = 3$ in the example)

$P(t=k) \in [0,1]$: probability that a random value in t equals the kth value in the set of possible values

s: logarithm base (we use $s = 2$ by convention)

Entropy - Example

$$H(t) = -\sum_{k=1}^{K}(P(t=k) \cdot log_s(P(t=k)))$$

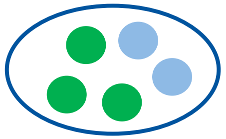


(2, 0, 3)

$$H(color) = -(\tfrac{2}{5} \cdot log_2(\tfrac{2}{5}) + \tfrac{0}{5} \cdot log_2(\tfrac{0}{5}) + \tfrac{3}{5} \cdot log_2(\tfrac{3}{5})) \approx 0.97$$

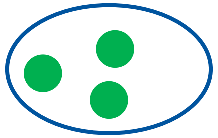
Entropy - Example

$$H(t) = -\sum_{k=1}^{K}(P(t=k)\cdot log_s(P(t=k)))$$



(2, 0, 3)

$$H(color) = -(\tfrac{2}{5}\cdot log_2(\tfrac{2}{5}) + \underbrace{\tfrac{0}{5}\cdot log_2(\tfrac{0}{5})}_{\text{Interpreted as 0}} + \tfrac{3}{5}\cdot log_2(\tfrac{3}{5})) \approx 0.97$$

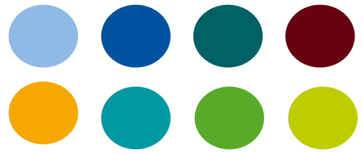


(0, 0, 3)

$$H(color) = -(\tfrac{0}{3}\cdot log_2(\tfrac{0}{3}) + \tfrac{0}{3}\cdot log_2(\tfrac{0}{3}) + \tfrac{3}{3}\cdot log_2(\tfrac{3}{3})) = 0$$

Questions

Suppose that we have K possible values (colors) and N instances (balls).

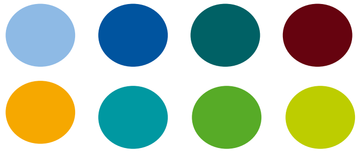


$$H(t) = -\sum_{k=1}^{K}(P(t=k) \cdot log_s(P(t=k)))$$

What distribution of the N instances over the K possible values yields the lowest entropy?

Questions

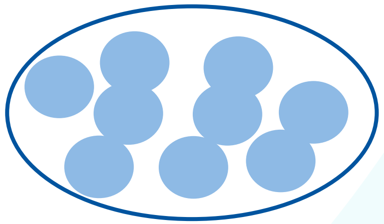
Suppose that we have *K* <u>possible</u> values (colors) and *N* instances (balls).



$$H(t) = -\sum_{k=1}^{K}(P(t=k)\cdot log_s(P(t=k)))$$

What distribution of the *N* instances over the *K* <u>possible</u> values yields the lowest entropy?

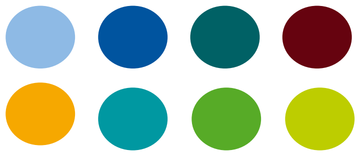
$$H(color) = -(1\cdot log_2(1)) = 0$$



→ all instances have the same value

Questions

Suppose that we have K <u>possible</u> values (colors) and N instances (balls).



$$H(t) = -\sum_{k=1}^{K} \left(P(t=k) \cdot log_s(P(t=k))\right)$$

What distribution of the N instances over the K <u>possible</u> values yields the highest entropy?

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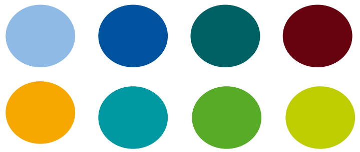
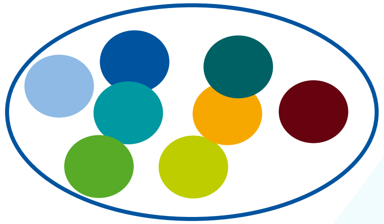


$$H(t) = -\sum_{k=1}^{K}(P(t=k) \cdot log_s(P(t=k)))$$

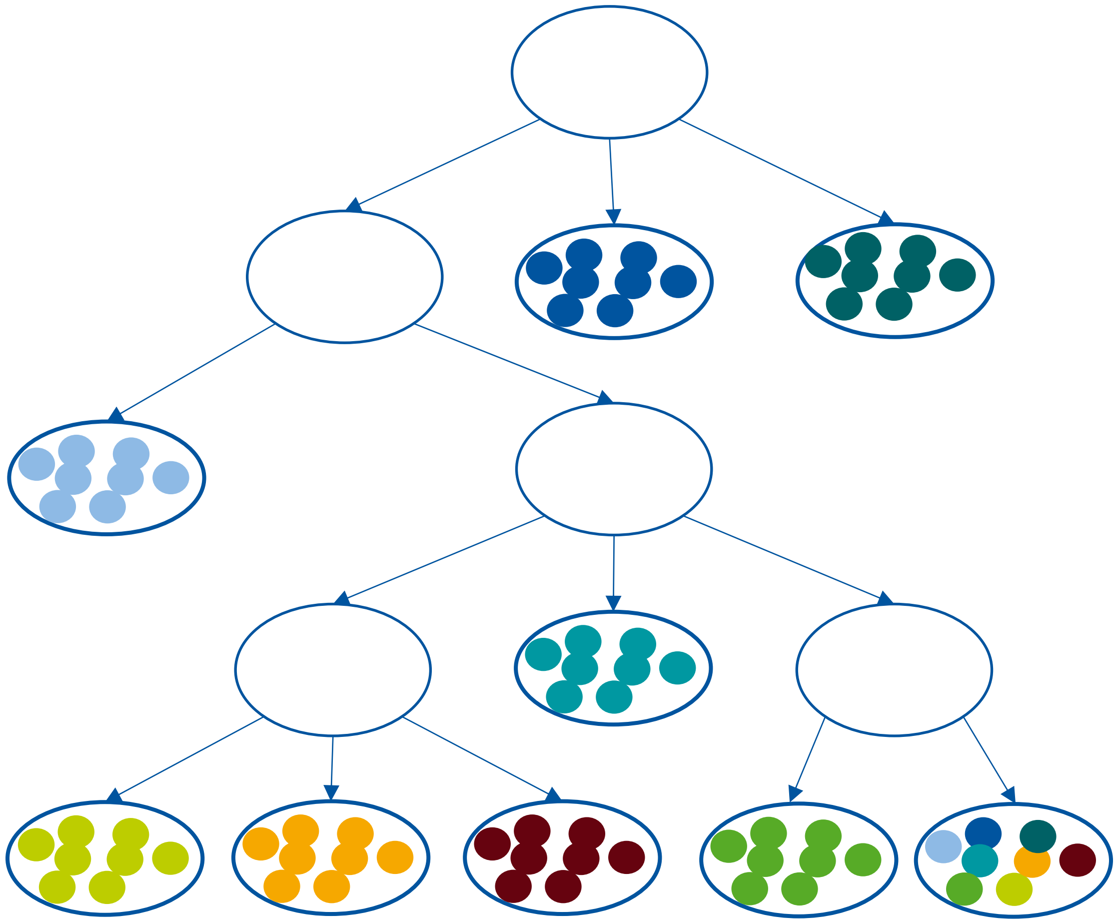
What distribution of the N instances over the K possible values yields the highest entropy?

$$\begin{aligned} H(color) &= -\sum_{k=1}^{K}(\frac{1}{K} \cdot log_2(\frac{1}{K})) \\ &= -(K \cdot \frac{1}{K} \cdot log_2(\frac{1}{K})) \\ &= -log_2(\frac{1}{K}) \\ &= log_2(K) \end{aligned}$$



→ Even distribution over all possible values

Overall Entropy

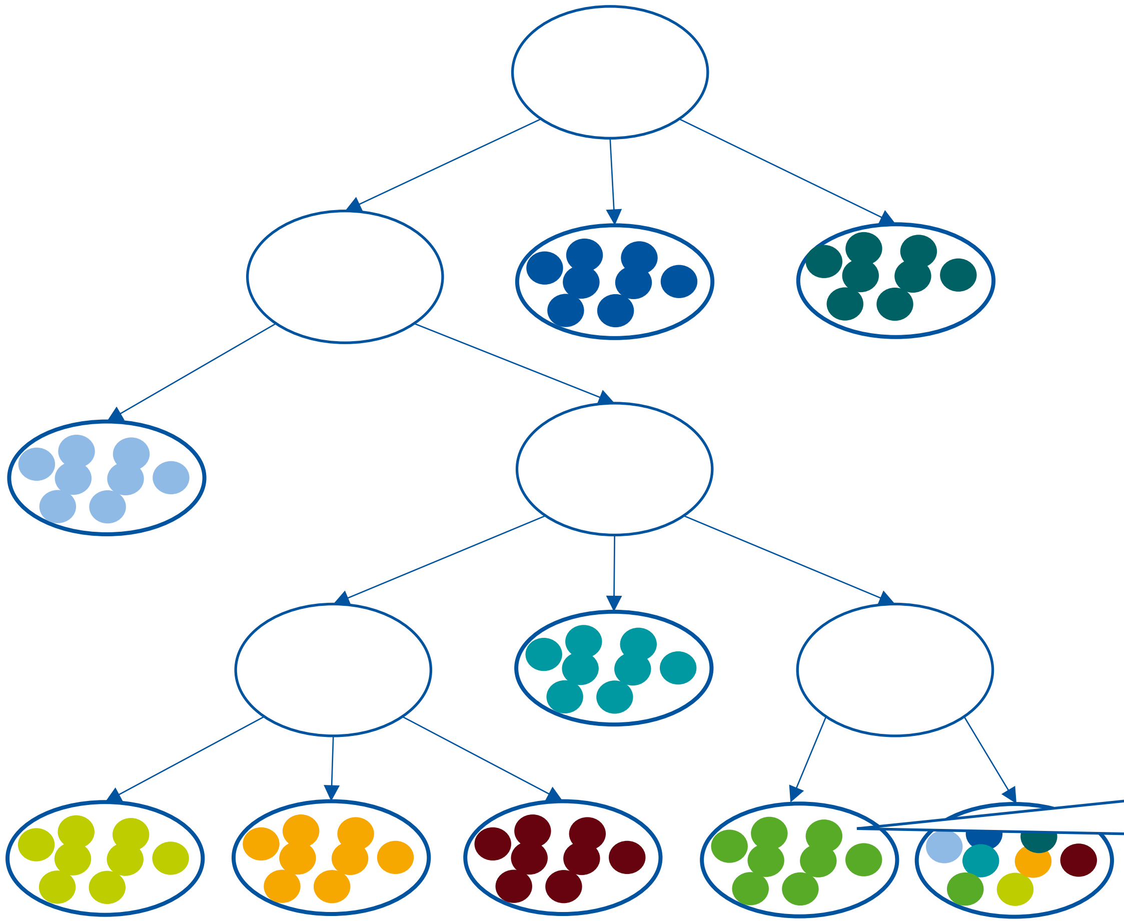


Overall entropy H_W is the weighted average of the individual entropies:

$$H_W(t) = \sum_{node \in nodes} \left(\frac{|node|}{N} \cdot H^{node}(t) \right)$$

Example: $N = 72, K = 8$

Overall Entropy



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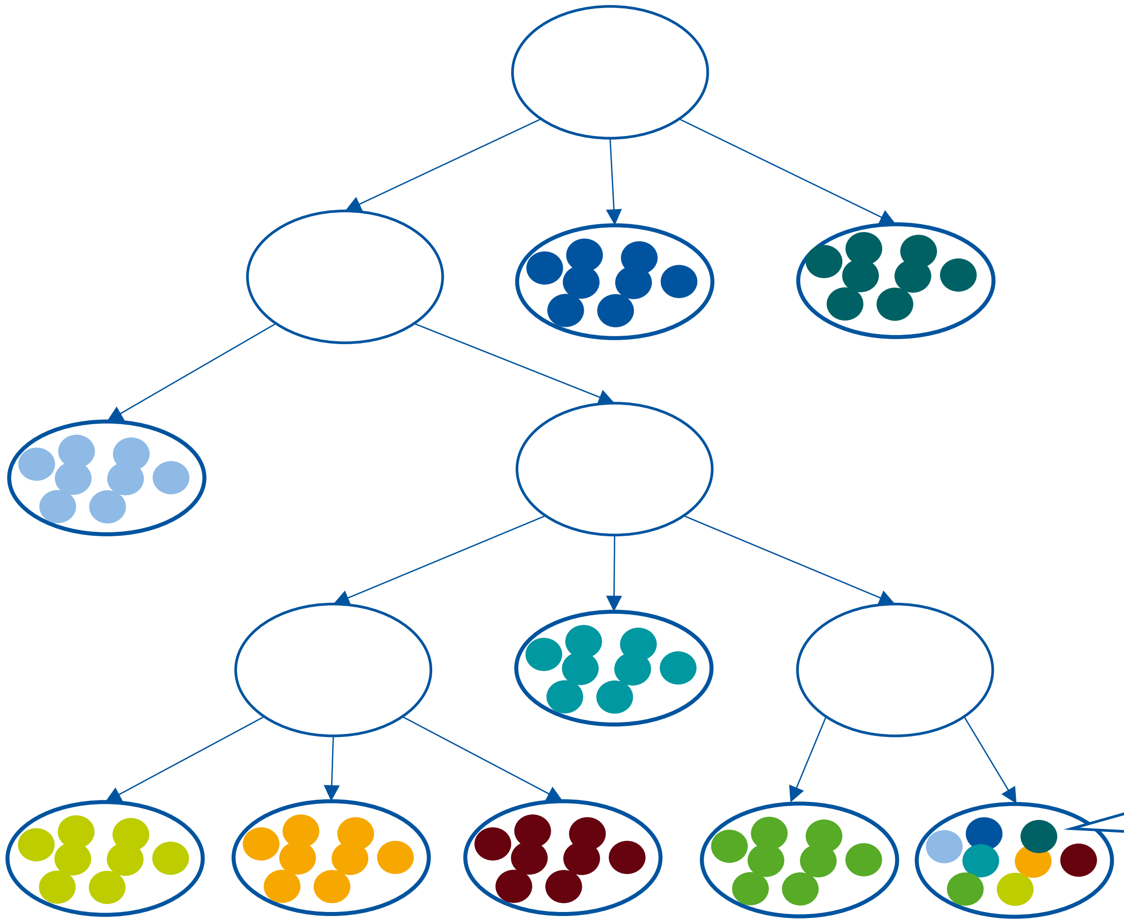
8 homogeneously colored balls:
$H^{node}(color) = -(\frac{8}{8} \cdot \log_2(\frac{8}{8})) = 0$

Overall Entropy



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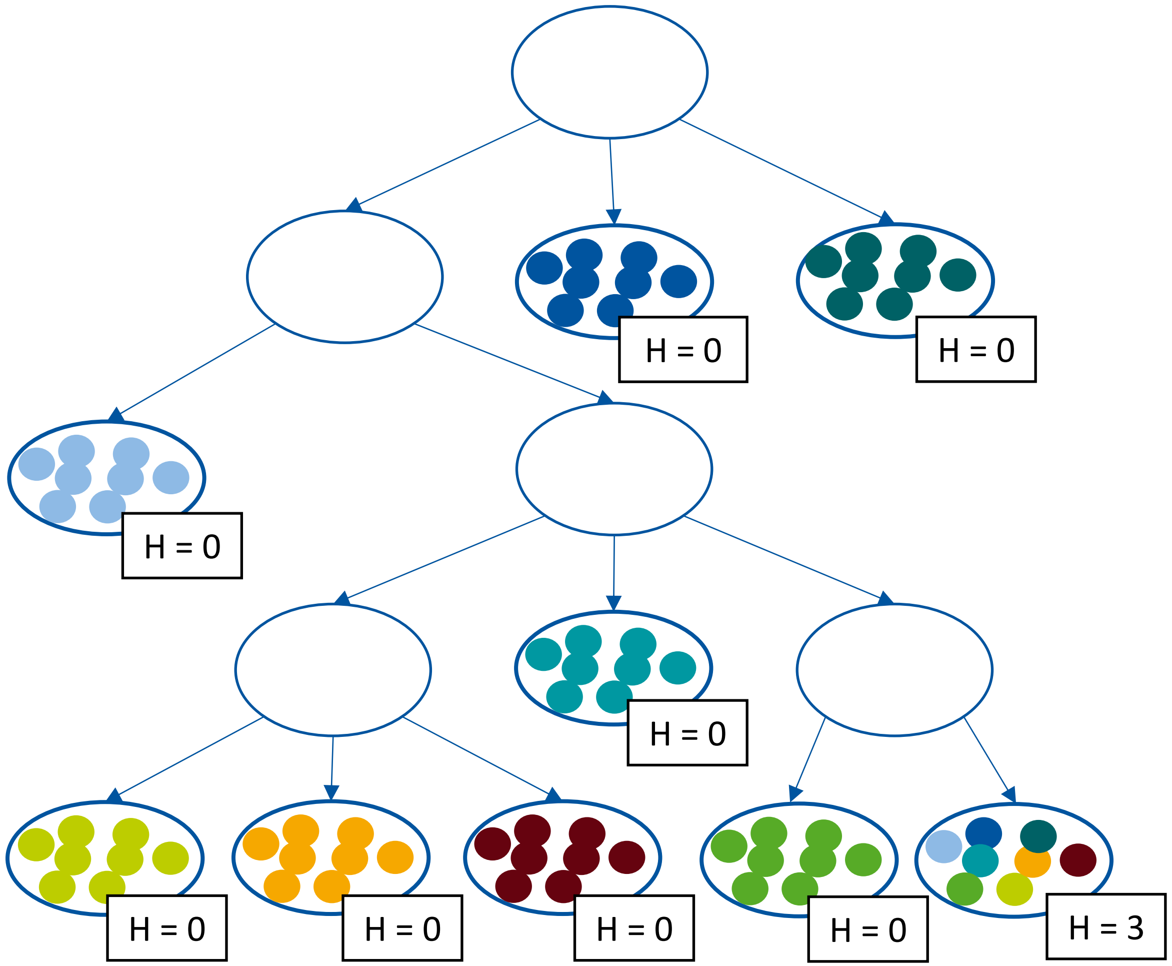
Even distribution of 8 colors over 8 balls:
$H^{node}(color) = -\sum_{k=1}^{8} \frac{1}{8} \cdot log_2(\frac{1}{8}) = \log_2(8) = 3$

Overall Entropy



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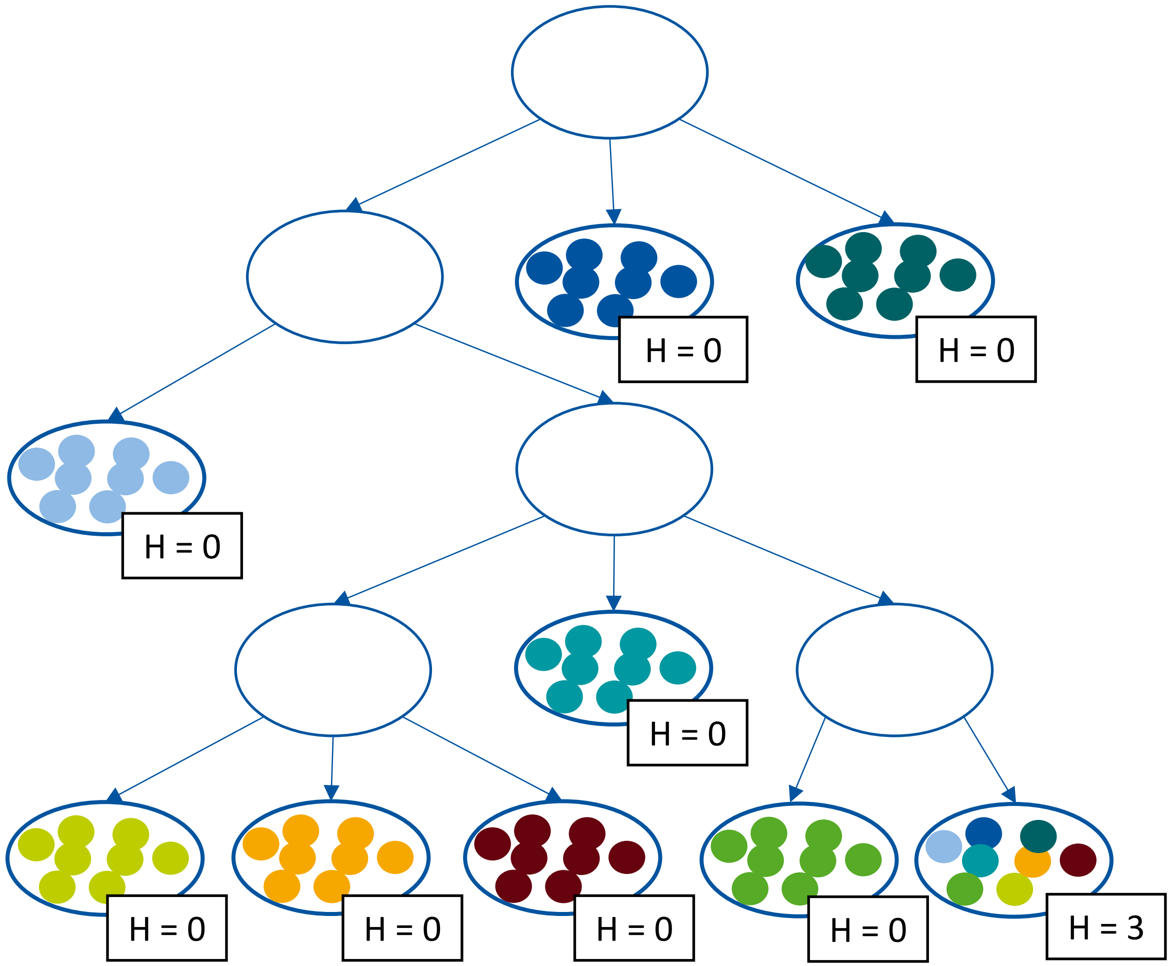

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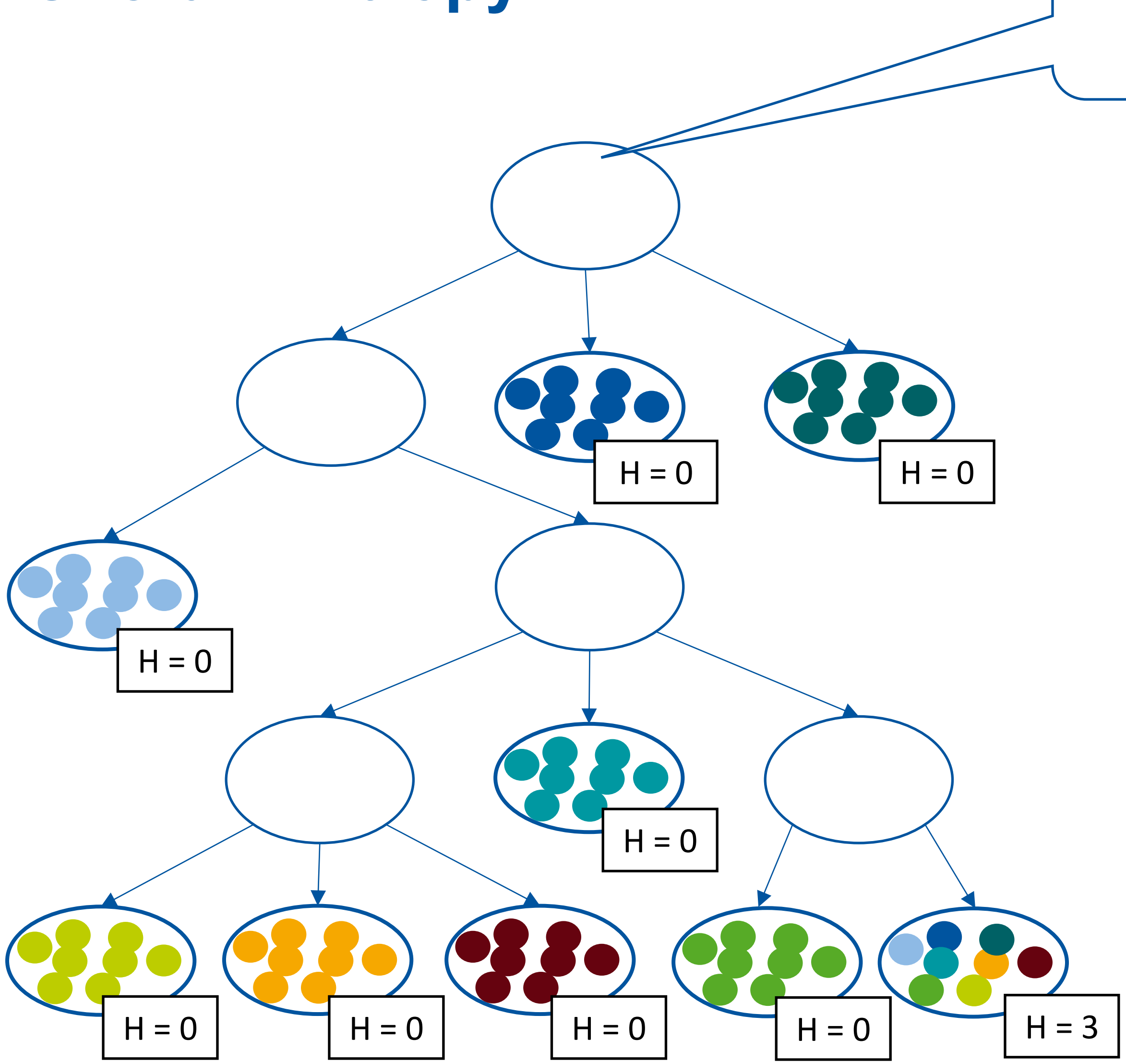
Example: $N = 72, K = 8$

$$H_W(color) = \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 0 + \frac{8}{72} \cdot 3 = \frac{24}{72} \approx 0.33$$

Overall Entropy

Even distribution of 8 colors over 72 balls:



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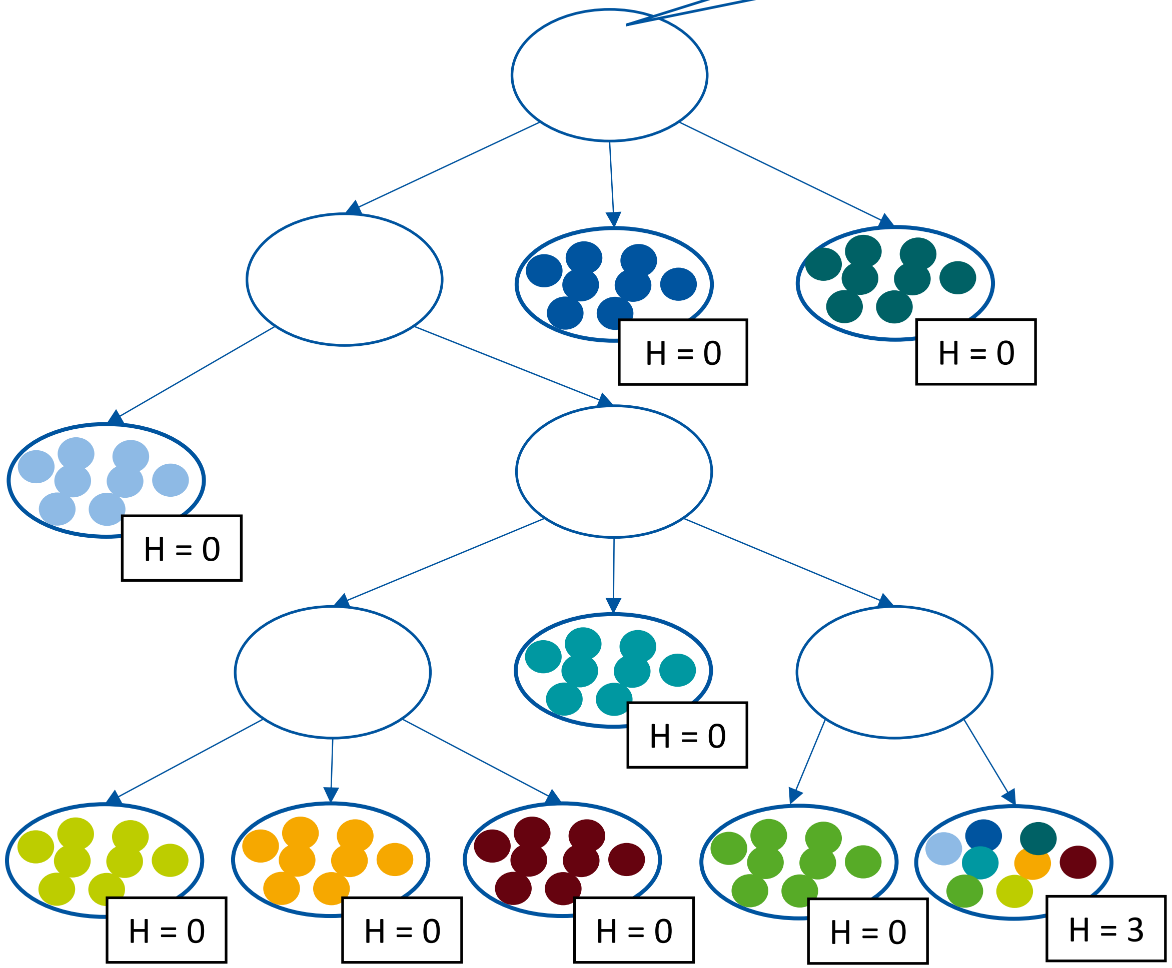
Overall Entropy

Even distribution of 8 colors over 72 balls:

$$H_W(color) = \frac{72}{72} \cdot \left(-\sum_{k=1}^{8} \left(\frac{9}{72} \cdot log_2(\frac{9}{72})\right)\right) = \log_2(8) = 3$$



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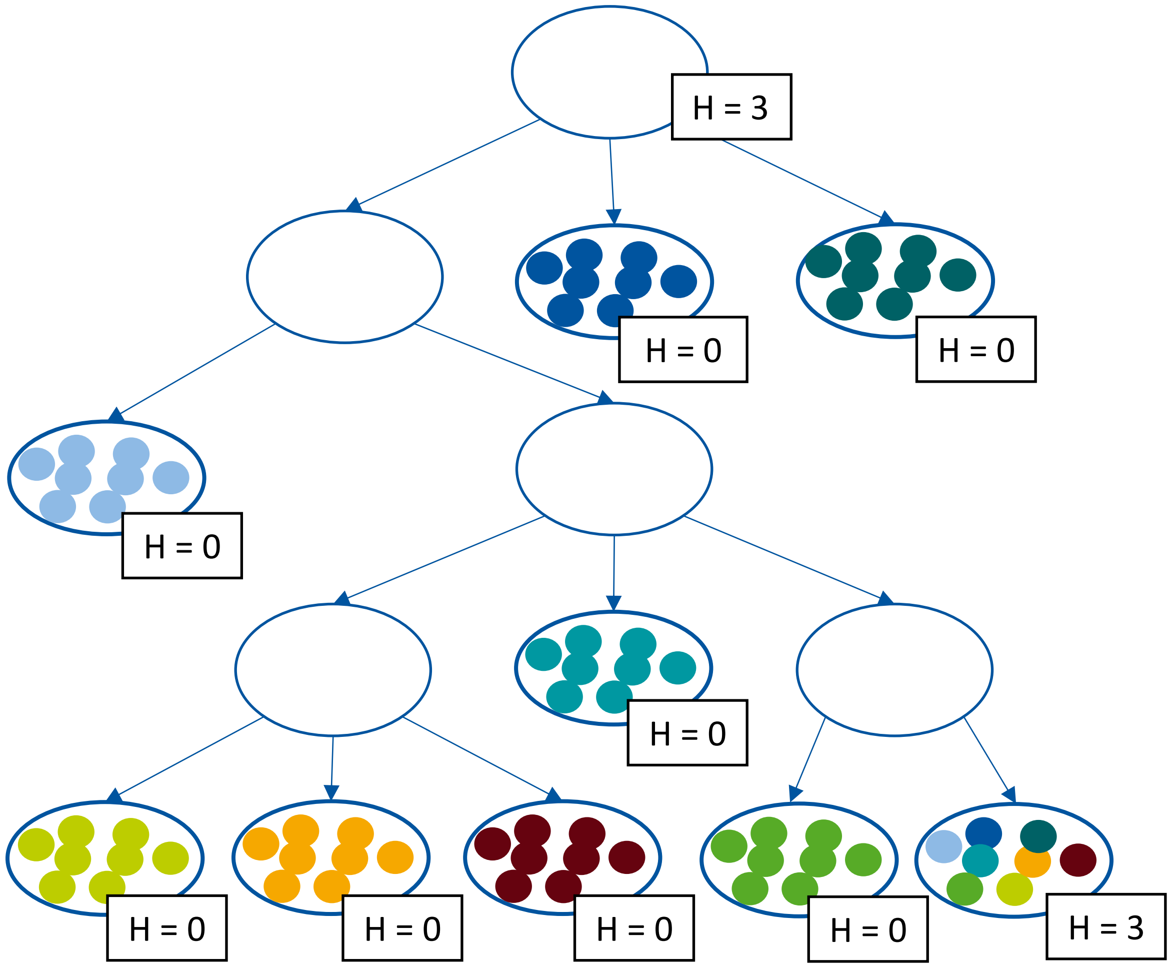
Information Gain



$$H_W(color) = 3$$

information loss
≈ 2.66

information gain
≈ 2.66

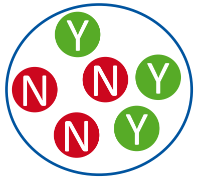
$$H_W(color) \approx 0.33$$

Information Gain – Another Flight Example

Entropy before splitting

$$H(\text{delayed}) = 1$$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	No	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	Yes	**No**
Clear	No	No	**No**

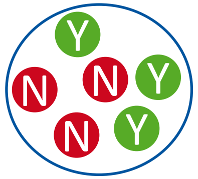


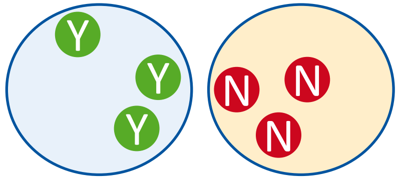
Information Gain – Another Flight Example

$$H(\text{delayed}) = 1$$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	No	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	Yes	**No**
Clear	No	No	**No**

Weather	Flight delayed
Cloudy	**Yes**
Cloudy	**Yes**
Cloudy	**Yes**
Clear	**No**
Clear	**No**
Clear	**No**





Information Gain – Another Flight Example

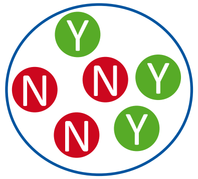
$$H^{cloudy}(\text{delayed}) = 0$$
$$H^{clear}(\text{delayed}) = 0$$

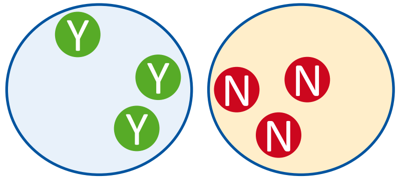
Single leaf entropies after splitting based on *weather*

$$H(\text{delayed}) = 1$$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	No	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	Yes	**No**
Clear	No	No	**No**

Weather	Flight delayed
Cloudy	**Yes**
Cloudy	**Yes**
Cloudy	**Yes**
Clear	**No**
Clear	**No**
Clear	**No**

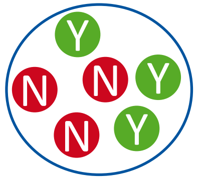




Information Gain – Another Flight Example

$$H(\text{delayed}) = 1$$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	No	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	Yes	**No**
Clear	No	No	**No**

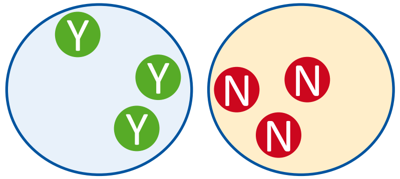


$$H^{cloudy}(\text{delayed}) = 0$$
$$H^{clear}(\text{delayed}) = 0$$

$$H_W^{weather}(\text{delayed}) = 0$$

Weighted entropy after splitting based on *weather*

Weather	Flight delayed
Cloudy	**Yes**
Cloudy	**Yes**
Cloudy	**Yes**
Clear	**No**
Clear	**No**
Clear	**No**



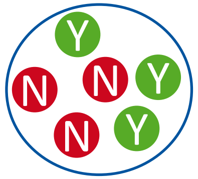
Information Gain – Another Flight Example

$$H^{cloudy}(\text{delayed}) = 0$$
$$H^{clear}(\text{delayed}) = 0$$

$$H^{traffic\_yes}(\text{delayed}) = 0.92$$
$$H^{traffic\_no}(\text{delayed}) = 0.92$$

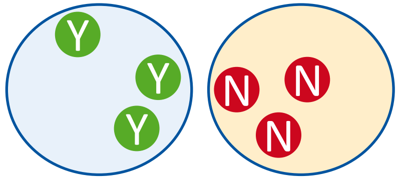
$$H(\text{delayed}) = 1$$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	No	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	Yes	**No**
Clear	No	No	**No**



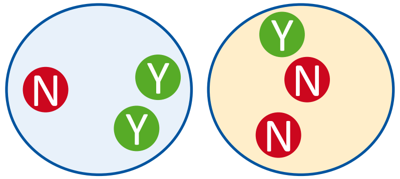
$$H_W^{weather}(\text{delayed}) = 0$$

Weather	Flight delayed
Cloudy	**Yes**
Cloudy	**Yes**
Cloudy	**Yes**
Clear	**No**
Clear	**No**
Clear	**No**



$$H_W^{traffic}(\text{delayed}) = 0.92$$

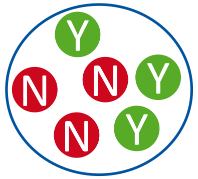
Traffic	Flight delayed
No	**Yes**
Yes	**Yes**
Yes	**Yes**
Yes	**No**
No	**No**
No	**No**



Information Gain – Another Flight Example

$$H(\text{delayed}) = 1$$

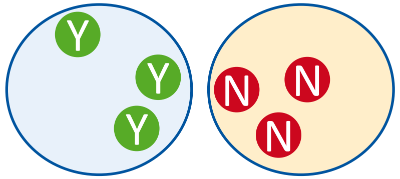
Weather	Traffic	Night flight	Flight delayed
Cloudy	No	No	**Yes**
Cloudy	Yes	No	**Yes**
Cloudy	Yes	No	**Yes**
Clear	Yes	Yes	**No**
Clear	No	Yes	**No**
Clear	No	No	**No**



$$H^{cloudy}(\text{delayed}) = 0$$
$$H^{clear}(\text{delayed}) = 0$$

$$H_W^{weather}(\text{delayed}) = 0$$

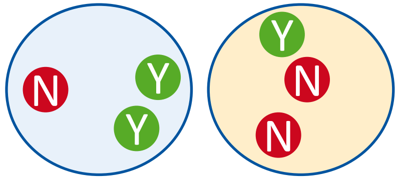
Weather	Flight delayed
Cloudy	**Yes**
Cloudy	**Yes**
Cloudy	**Yes**
Clear	**No**
Clear	**No**
Clear	**No**



$$H^{traffic\_yes}(\text{delayed}) = 0.92$$
$$H^{traffic\_no}(\text{delayed}) = 0.92$$

$$H_W^{traffic}(\text{delayed}) = 0.92$$

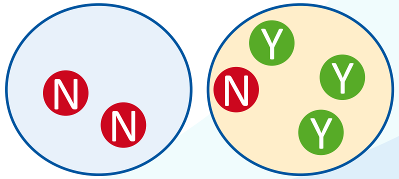
Traffic	Flight delayed
No	**Yes**
Yes	**Yes**
Yes	**Yes**
Yes	**No**
No	**No**
No	**No**



$$H^{night\_yes}(\text{delayed}) = 0$$
$$H^{night\_no}(\text{delayed}) \approx 0.81$$

$$H_W^{night\_flight}(\text{delayed}) \approx 0.54$$

Night flight	Flight delayed
No	**Yes**
No	**Yes**
No	**Yes**
Yes	**No**
Yes	**No**
No	**No**



Information Gain – Another Flight Example

$H(\text{delayed}) = 1$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	No	**Yes**
...	...	...	**...**

$H^{cloudy}(\text{delayed}) = 0$
$H^{clear}(\text{delayed}) = 0$

$H_W^{weather}(\text{delayed}) = 0$

Weather	Flight delayed
Cloudy	**Yes**
...	**...**

$H^{traffic\_yes}(\text{delayed}) = 0.92$
$H^{traffic\_no}(\text{delayed}) = 0.92$

$H_W^{traffic}(\text{delayed}) = 0.92$

Traffic	Flight delayed
No	**Yes**
...	**...**

$H^{night\_yes}(\text{delayed}) = 0$
$H^{night\_no}(\text{delayed}) \approx 0.81$

$H_W^{night\_flight}(\text{delayed}) \approx 0.54$

Night flight	Flight delayed
No	**No**
...	**...**

$$IG(weather) = H(delayed) - H_W^{weather}(delayed) = 1 - 0 = 1$$

Information Gain – Another Flight Example

$H(\text{delayed}) = 1$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	Yes	**Yes**
...	...	...	**...**

$H^{cloudy}(\text{delayed}) = 0$
$H^{clear}(\text{delayed}) = 0$

$H_W^{weather}(\text{delayed}) = 0$

Weather	Flight delayed
Cloudy	**Yes**
...	**...**

$H^{traffic\_yes}(\text{delayed}) = 0.92$
$H^{traffic\_no}(\text{delayed}) = 0.92$

$H_W^{traffic}(\text{delayed}) = 0.92$

Traffic	Flight delayed
No	**Yes**
...	**...**

$H^{night\_yes}(\text{delayed}) = 0$
$H^{night\_no}(\text{delayed}) \approx 0.81$

$H_W^{night\_flight}(\text{delayed}) \approx 0.54$

Night flight	Flight delayed
Yes	**No**
...	**...**

$$IG(weather) = H(delayed) - H_W^{weather}(delayed) = 1 - 0 = 1$$

$$IG(traffic) = H(delayed) - H_W^{traffic}(delayed) = 1 - 0.92 = 0.08$$

Information Gain – Another Flight Example

$$H(\text{delayed}) = 1$$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	Yes	**Yes**
…	…	…	**…**

$$H^{cloudy}(\text{delayed}) = 0$$
$$H^{clear}(\text{delayed}) = 0$$

$$H_W^{weather}(\text{delayed}) = 0$$

Weather	Flight delayed
Cloudy	**Yes**
…	**…**

$$H^{traffic\_yes}(\text{delayed}) = 0.92$$
$$H^{traffic\_no}(\text{delayed}) = 0.92$$

$$H_W^{traffic}(\text{delayed}) = 0.92$$

Traffic	Flight delayed
No	**Yes**
…	**…**

$$H^{night\_yes}(\text{delayed}) = 0$$
$$H^{night\_no}(\text{delayed}) \approx 0.81$$

$$H_W^{night\_flight}(\text{delayed}) \approx 0.54$$

Night flight	Flight delayed
Yes	**No**
…	**…**

$$IG(weather) = H(delayed) - H_W^{weather}(delayed) = 1 - 0 = 1$$

$$IG(traffic) = H(delayed) - H_W^{traffic}(delayed) = 1 - 0.92 = 0.08$$

$$IG(night\_flight) = H(delayed) - H_W^{night\_flight}(delayed) = 1 - 0.54 = 0.46$$

Information Gain – Another Flight Example

$H(\text{delayed}) = 1$

Weather	Traffic	Night flight	Flight delayed
Cloudy	No	Yes	**Yes**
...	...	...	**...**

$H^{cloudy}(\text{delayed}) = 0$
$H^{clear}(\text{delayed}) = 0$

$H_W^{weather}(\text{delayed}) = 0$

Weather	Flight delayed
Cloudy	**Yes**
...	**...**

$H^{traffic\_yes}(\text{delayed}) = 0.92$
$H^{traffic\_no}(\text{delayed}) = 0.92$

$H_W^{traffic}(\text{delayed}) = 0.92$

Traffic	Flight delayed
No	**Yes**
...	**...**

$H^{night\_yes}(\text{delayed}) = 0$
$H^{night\_no}(\text{delayed}) \approx 0.81$

$H_W^{night\_flight}(\text{delayed}) \approx 0.54$

Night flight	Flight delayed
Yes	**No**
...	**...**

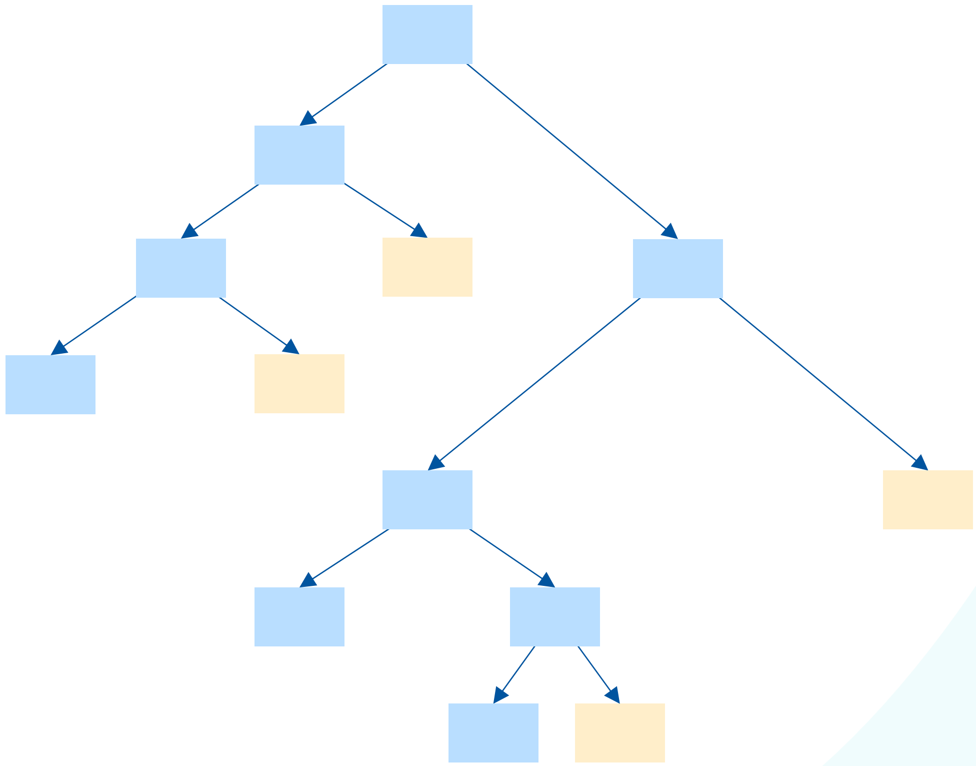
$$IG(weather) = H(delayed) - H_W^{weather}(delayed) = 1 - 0 = 1$$ **best**

$$IG(traffic) = H(delayed) - H_W^{traffic}(delayed) = 1 - 0.92 = 0.08$$ **worst**

$$IG(night\_flight) = H(delayed) - H_W^{night\_flight}(delayed) = 1 - 0.54 = 0.46$$ **intermediate**

Decision Trees

1. Introduction to Decision Trees
2. Entropy and Information Gain
3. **ID3 Algorithm**
4. Quantifying Information Gain
5. Pruning
6. Continuous Data
7. Ensembles



ID3 (Iterative Dichotomiser 3) - Key Idea

Approach

1. For each candidate feature: calculate the resulting entropy splitting the dataset $\mathcal{X}$ using the selected feature.
2. Split the set $\mathcal{X}$ into subsets using the feature for which the resulting entropy (after splitting) is minimal (equivalently, information gain is maximal)
3. Create new decision tree leaf nodes based on that feature
4. Recurse on these subsets using remaining features (until stopping criteria are reached)

When to Stop?

Three stopping criteria

- When all of the instances have the same classification (label = consensus value)
- When there are no features left (label = majority value)
- When the dataset is empty (label = majority parent)

ID3 Algorithm

ID3 algorithm:

1. **if** all the instances in X have the same classification
   (a) **return** a decision tree with one leaf node with consensus value as a label
2. **else if** there are no features left
   (a) **return** a decision tree with one leaf node with majority value as a label
3. **else if** the dataset is empty
   (a) **return** a decision tree with one leaf node with majority parent value as a label

three stopping criteria

4. **else**
   (a) pick a feature that maximizes information gain
   (b) once a feature is picked along a path from the root, it cannot be used again
   (c) create subproblems based on the selected feature

recursively constructing the tree

Example

ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	Basic
2	Yes	High school	Unemployed	Premium
3	Yes	Bachelor	Self-employed	Premium
4	No	Bachelor	Self-employed	Basic
5	No	Master	Employed	Economy
6	Yes	Bachelor	Retired	Economy
7	Yes	High school	Employed	Premium

$$H(\text{Customer})$$
$$= -\left(\frac{2}{7} \cdot log_2\left(\frac{2}{7}\right) + \frac{3}{7} \cdot log_2\left(\frac{3}{7}\right) + \frac{2}{7} \cdot log_2\left(\frac{2}{7}\right)\right)$$
$$= 1.5567$$

Example

$$H(\text{Customer}) = 1.5567$$

ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	**Basic**
2	Yes	High school	Unemployed	**Premium**
3	Yes	Bachelor	Self-employed	**Premium**
4	No	Bachelor	Self-employed	**Basic**
5	No	Master	Employed	**Economy**
6	Yes	Bachelor	Retired	**Economy**
7	Yes	High school	Employed	**Premium**

Split by feature	Possible Values	Instance Distribution	Entropy	Overall Entropy	Information Gain
Insurance	No	**4, 5**	1	1.265	1.5567 – 1.265 = **0.2917**
	Yes	**1, 2, 3, 6, 7**	1.3710		
Education	High school	**2, 7**	0	0.8571	1.5567 – 0.8571 = **0.6996**
	Master	**5**	0		
	Bachelor	**1, 3, 4, 6**	1.5		
Employment	Employed	**1, 5, 7**	1.5850	0.9650	1.5567 – 0.9650= **0.5917**
	Unemployed	**2**	0		
	Self-employed	**3, 4**	1		
	Retired	**6**	0		

Example

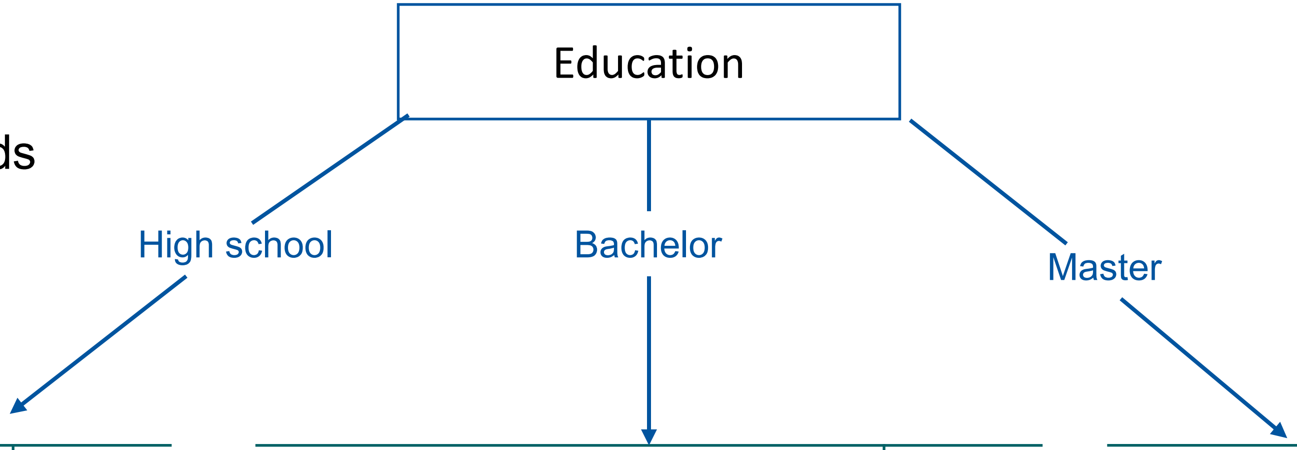
ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	Basic
2	Yes	High school	Unemployed	Premium
3	Yes	Bachelor	Self-employed	Premium
4	No	Bachelor	Self-employed	Basic
5	No	Master	Employed	Economy
6	Yes	Bachelor	Retired	Economy
7	Yes	High school	Employed	Premium

$$H(\text{Customer}) = 1.5567$$

Split by feature	Possible Values	Instances	Entropy	Overall Entropy	Information Gain
Insurance	No	4, 5	1	1.265	1.5567 – 1.265 = **0.2917**
	Yes	1, 2, 3, 6, 7	1.3710		
Education	High school	2, 7	0	0.8571	1.5567 – 0.8571 = **0.6996**
	Master	5	0		
	Bachelor	1, 3, 4, 6	1.5		
Employment	Employed	1, 5, 7	1.5850	0.9650	1.5567 – 0.9650= **0.5917**
	Unemployed	2	0		
	Self-employed	3, 4	1		
	Retired	6	0		

Example

Recursion until
stopping criteria holds



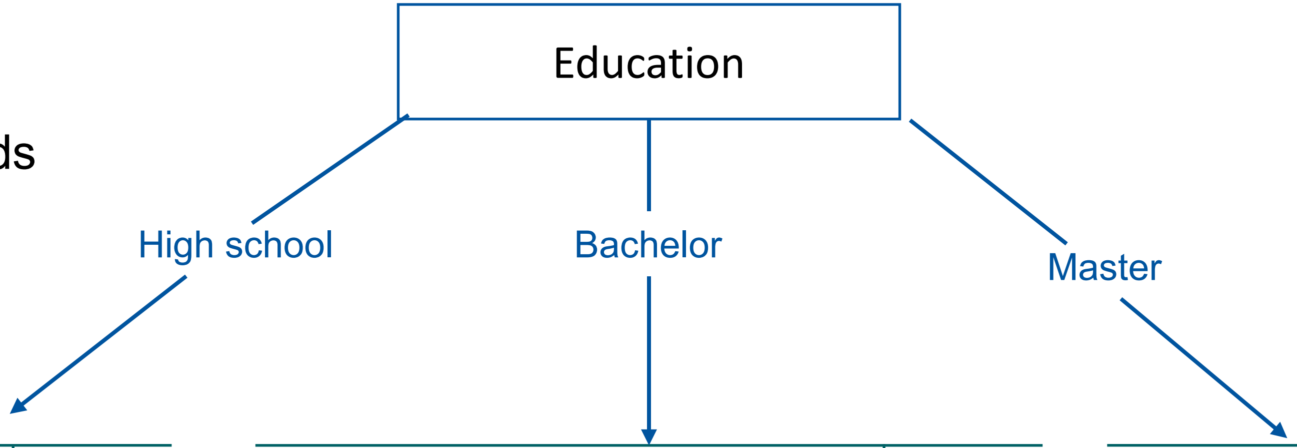
ID	Insurance	Education	Employment	Customer
2	Yes	High school	Unemployed	Premium
7	Yes	High school	Employed	Premium

ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	Basic
3	Yes	Bachelor	Self-employed	Premium
4	No	Bachelor	Self-employed	Basic
6	Yes	Bachelor	Retired	Economy

ID	Insurance	Education	Employment	Customer
5	No	Master	Employed	Economy

Example

Recursion until
stopping criteria holds



ID	Insurance	Education	Employment	Customer
2	Yes	High school	Unemployed	Premium
7	Yes	High school	Employed	Premium

consensus

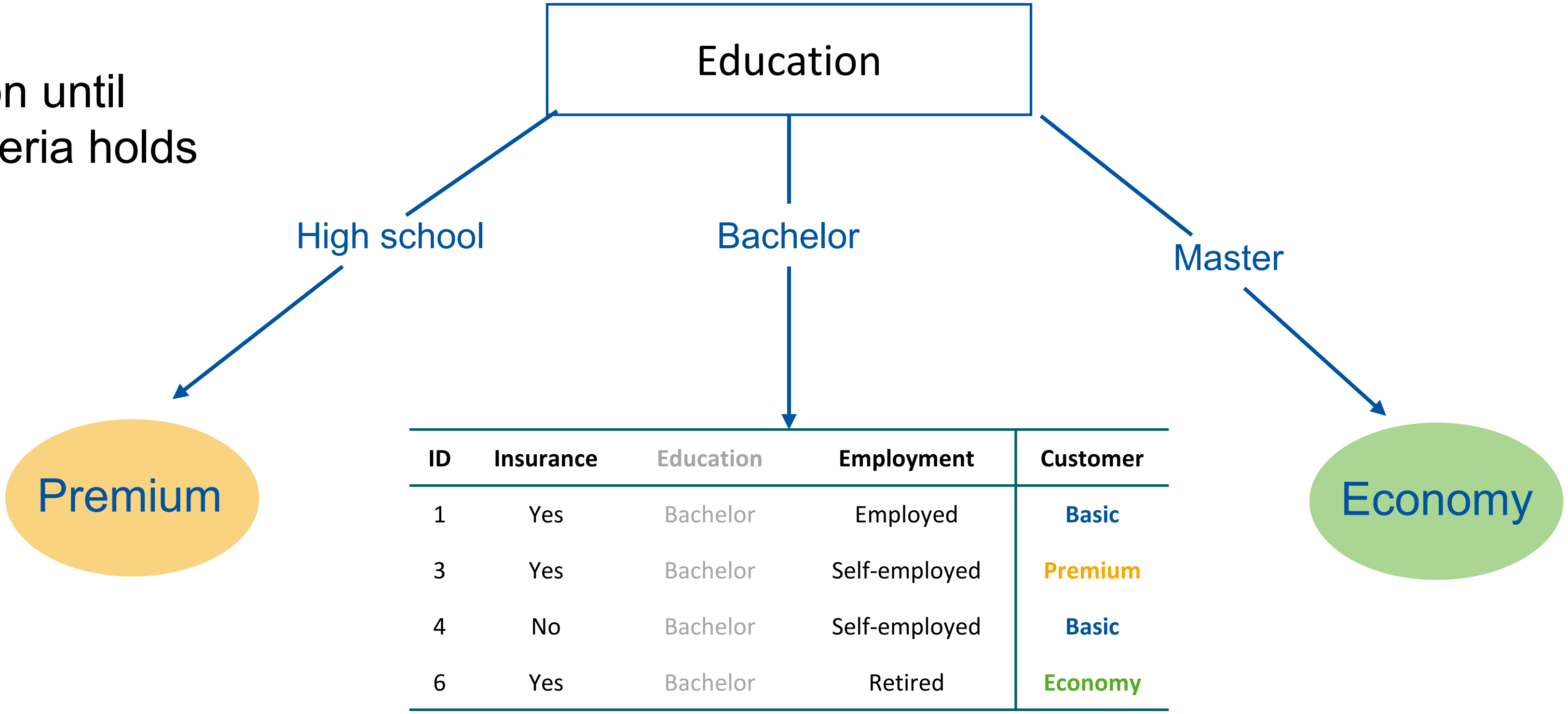
ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	Basic
3	Yes	Bachelor	Self-employed	Premium
4	No	Bachelor	Self-employed	Basic
6	Yes	Bachelor	Retired	Economy

ID	Insurance	Education	Employment	Customer
5	No	Master	Employed	Economy

consensus

Example

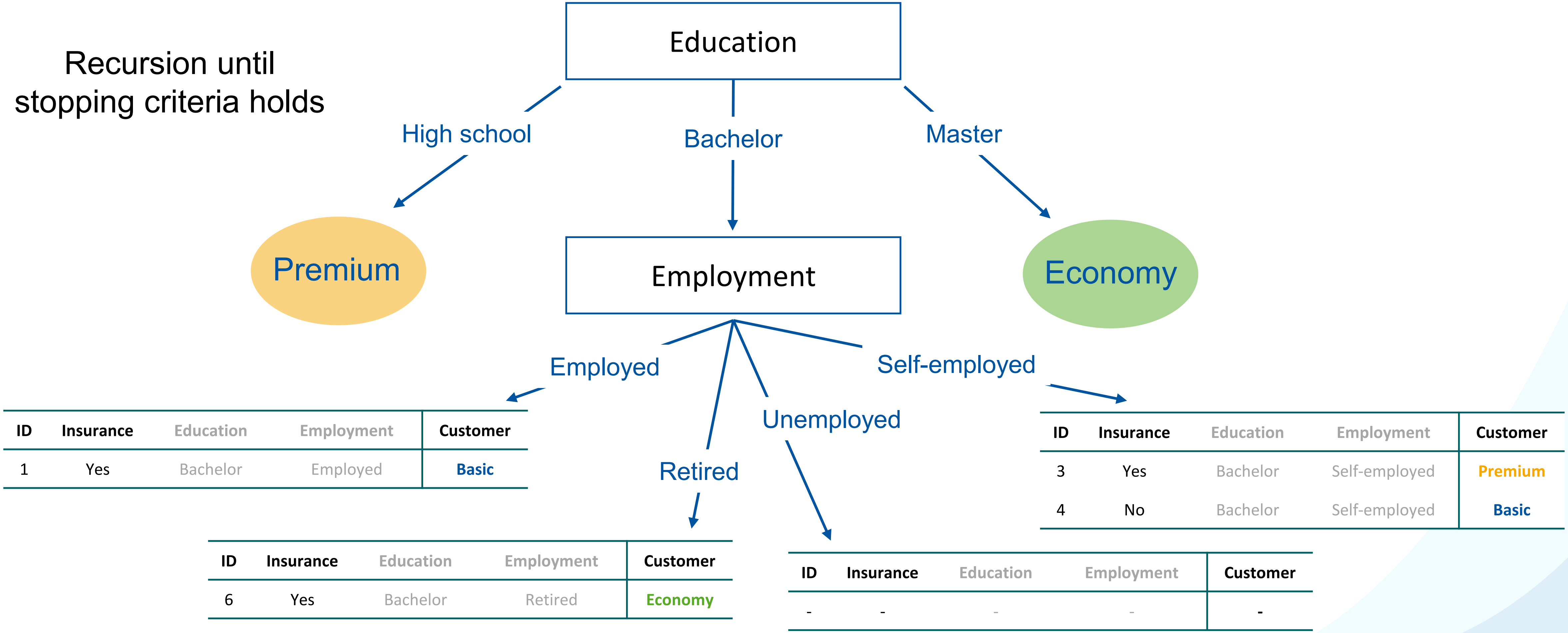
Recursion until stopping criteria holds



ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	**Basic**
3	Yes	Bachelor	Self-employed	**Premium**
4	No	Bachelor	Self-employed	**Basic**
6	Yes	Bachelor	Retired	**Economy**

Example

Recursion until
stopping criteria holds



ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	**Basic**

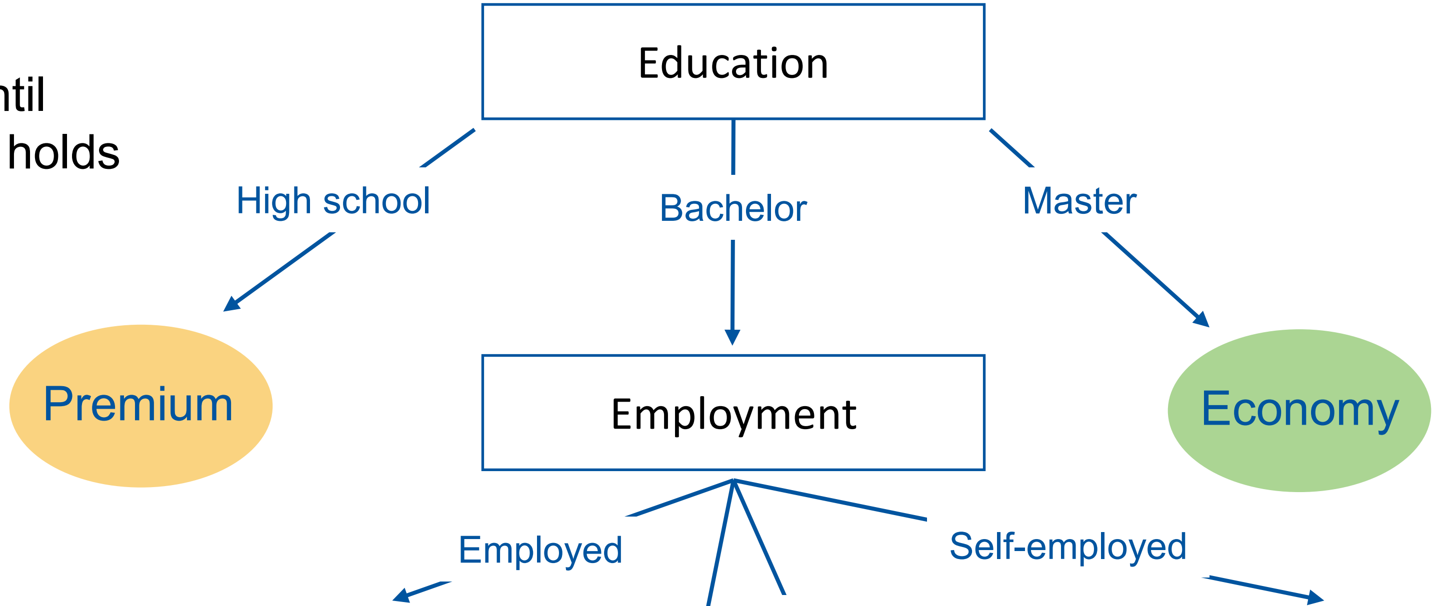
ID	Insurance	Education	Employment	Customer
6	Yes	Bachelor	Retired	**Economy**

ID	Insurance	Education	Employment	Customer
-	-	-	-	-

ID	Insurance	Education	Employment	Customer
3	Yes	Bachelor	Self-employed	**Premium**
4	No	Bachelor	Self-employed	**Basic**

Example

Recursion until stopping criteria holds



ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	**Basic**

consensus

ID	Insurance	Education	Employment	Customer
6	Yes	Bachelor	Retired	**Economy**

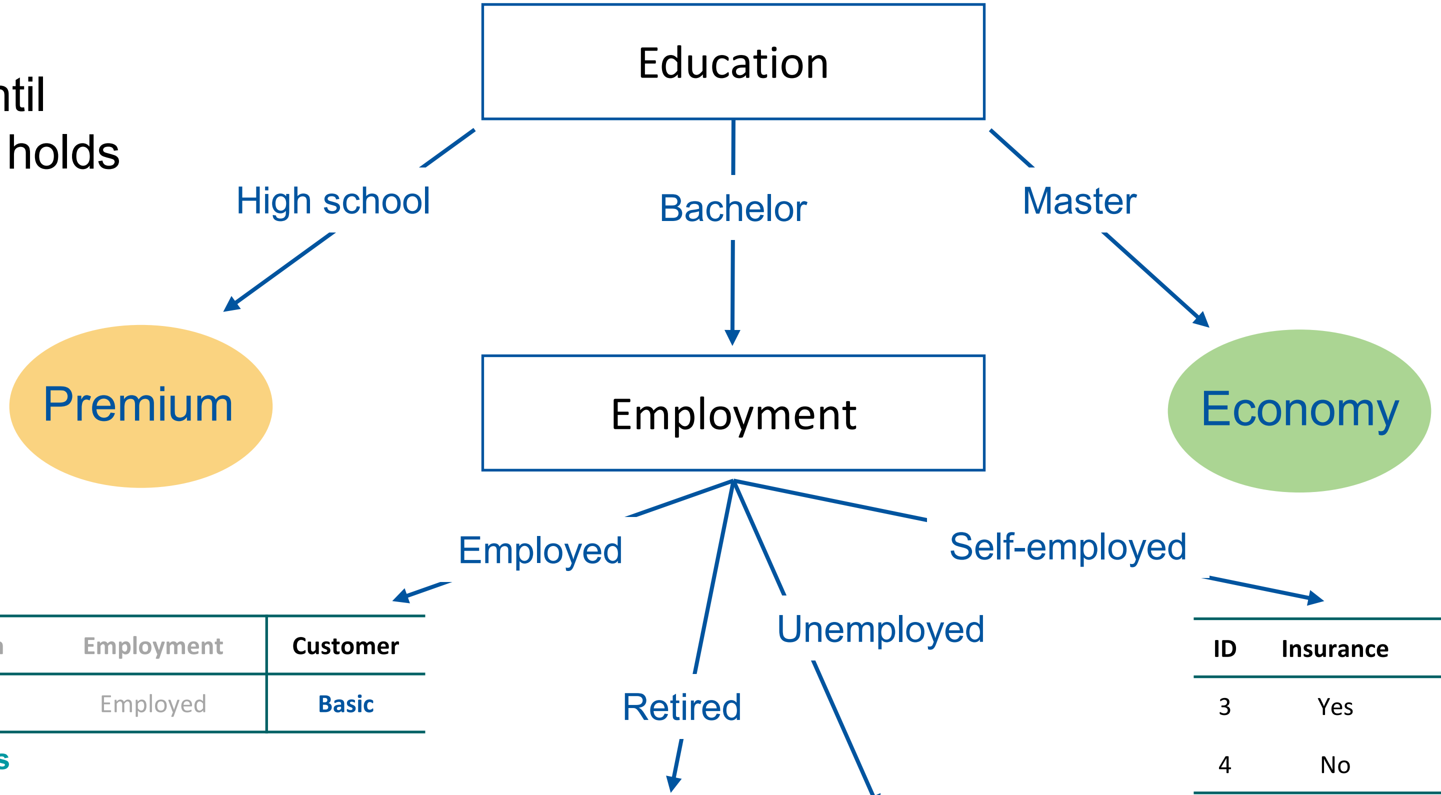
consensus

ID	Insurance	Education	Employment	Customer
-	-	-	-	-

ID	Insurance	Education	Employment	Customer
3	Yes	Bachelor	Self-employed	**Premium**
4	No	Bachelor	Self-employed	**Basic**

Example

Recursion until stopping criteria holds



Employed:

ID	Insurance	Education	Employment	Customer
1	Yes	Bachelor	Employed	**Basic**

consensus

Retired:

ID	Insurance	Education	Employment	Customer
6	Yes	Bachelor	Retired	**Economy**

consensus

Unemployed:

ID	Insurance	Education	Employment	Customer
-	-	-	-	-

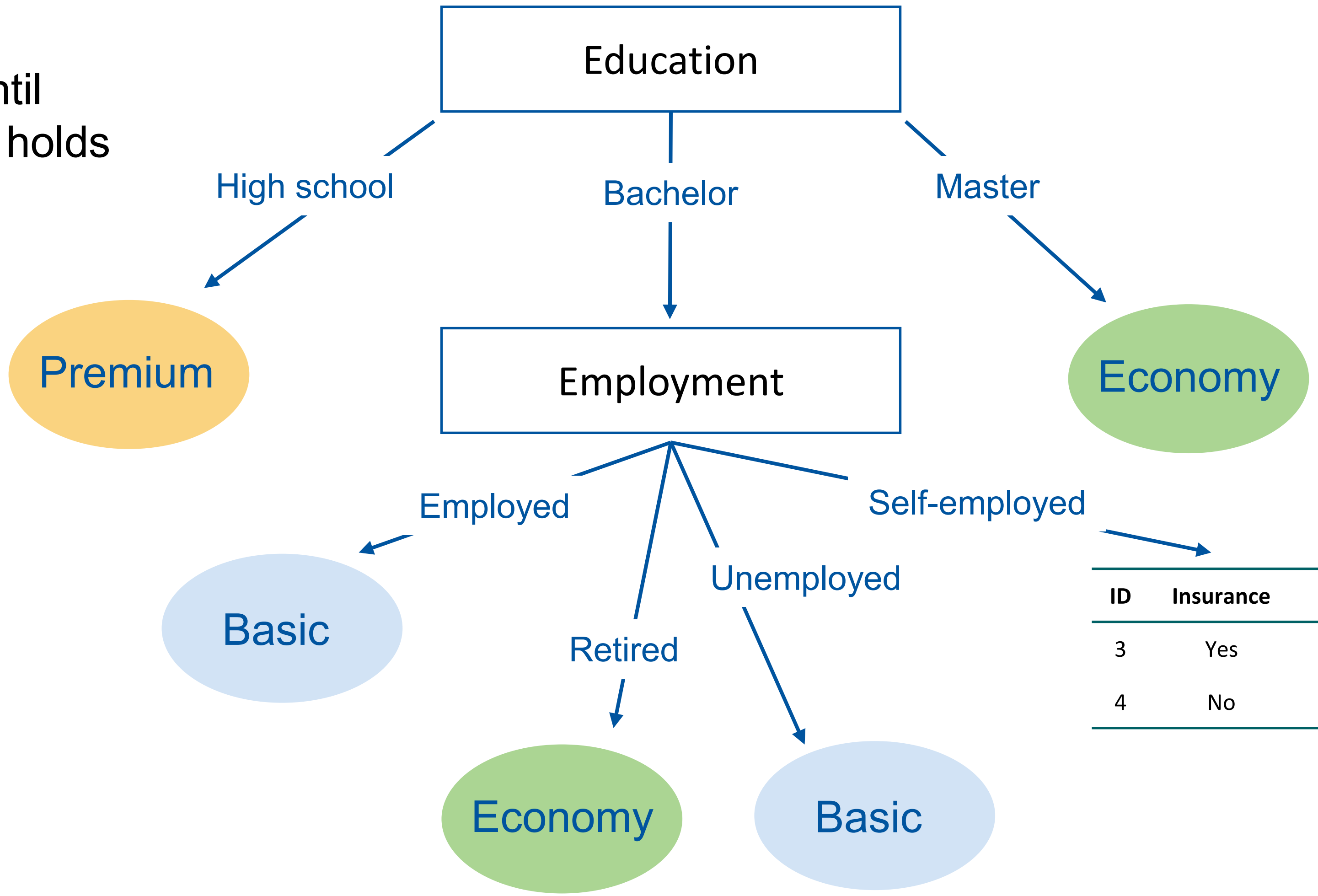
empty (label parent majority = Basic)

Self-employed:

ID	Insurance	Education	Employment	Customer
3	Yes	Bachelor	Self-employed	**Premium**
4	No	Bachelor	Self-employed	**Basic**

Example

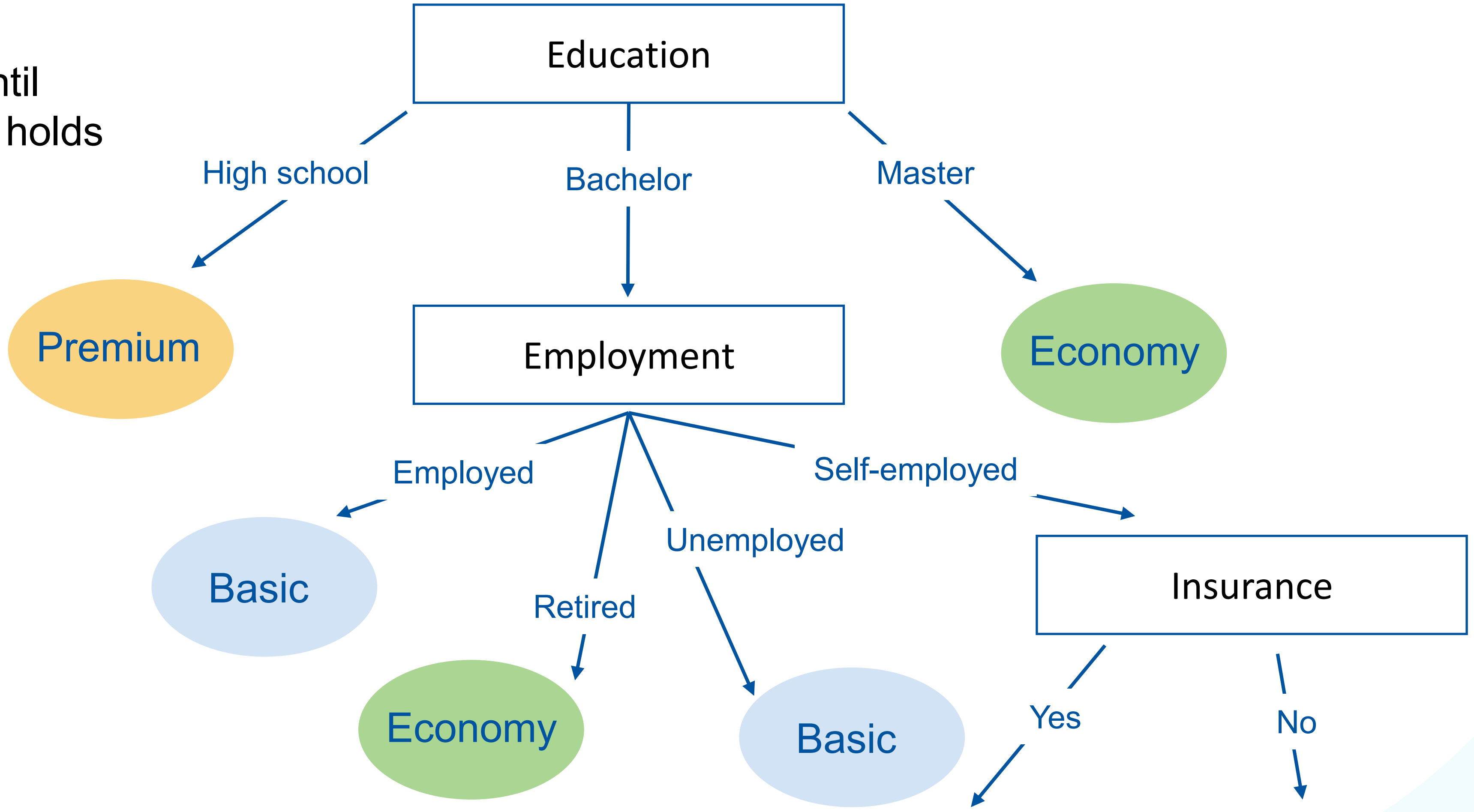
Recursion until stopping criteria holds



ID	Insurance	Education	Employment	Customer
3	Yes	Bachelor	Self-employed	Premium
4	No	Bachelor	Self-employed	Basic

Example

Recursion until stopping criteria holds



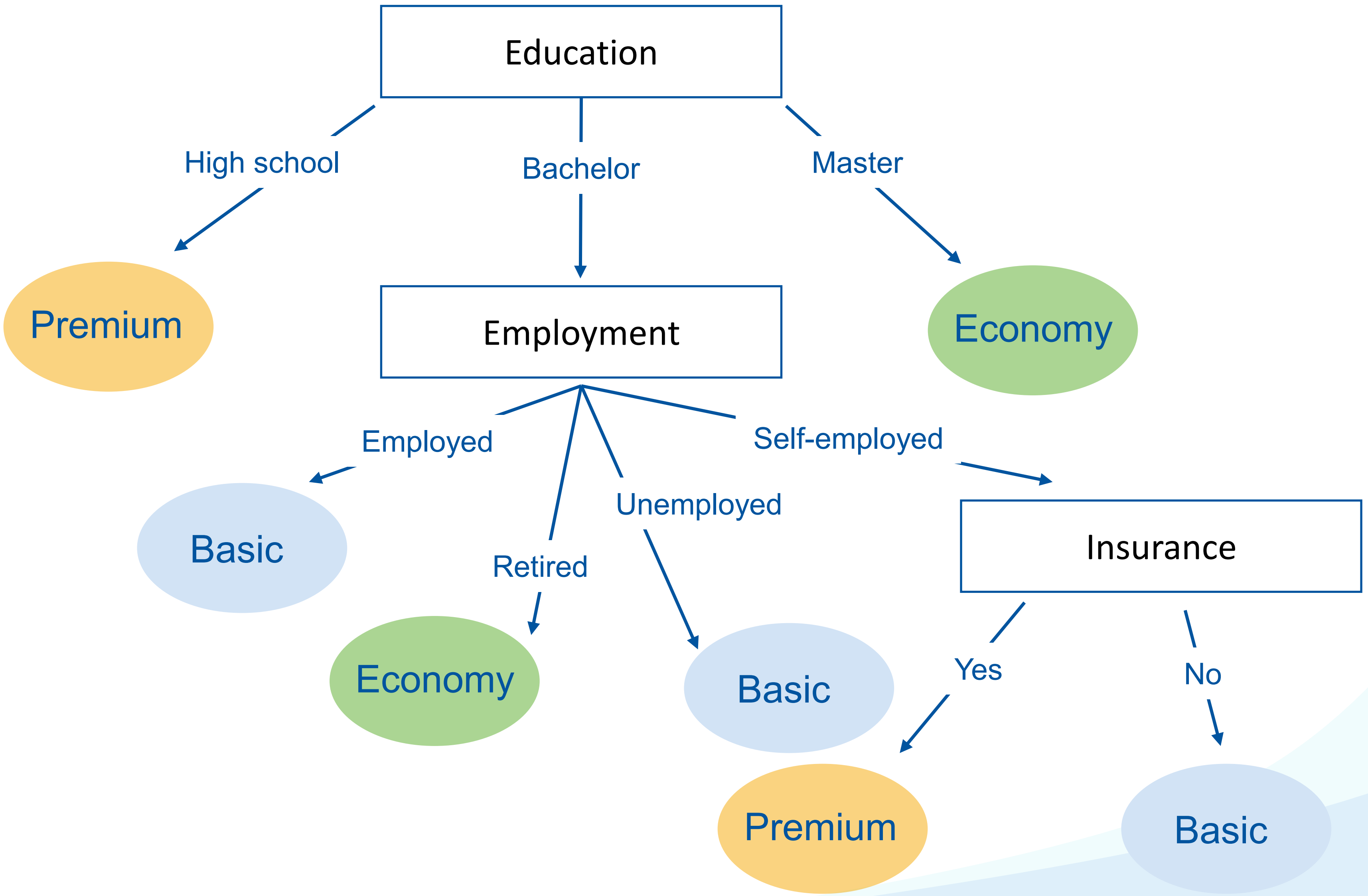
ID	Insurance	Education	Employment	Customer
3	Yes	Bachelor	Self-employed	**Premium**

consensus

ID	Insurance	Education	Employment	Customer
4	No	Bachelor	Self-employed	**Basic**

consensus

Example



(no feature exhaustion in this small example)

Decision Trees

1. Introduction to Decision Trees
2. Entropy and Information Gain
3. ID3 Algorithm
4. **Quantifying Information Gain**
5. Pruning
6. Continuous Data
7. Ensembles

$$H(t) = -\sum_{k=1}^{K}(P(t=k) \cdot log_s(P(t=k)))$$

$$H_W^d(t) = \sum_{node \in nodes(d)}(\frac{|node|}{N} \cdot H_{node}(t))$$

$$IG(d) = H(t) - H_W^d(t)$$

Alternative Information Gain Notions

- Information gain aims to measure the improvement in purity / predictability / compressibility

- Example approaches:
  - Entropy-based information gain (IG)
  - Information gain ratio (GR)
  - Gini index (Gini)
  - Chi-square (χ^2)

Alternative Information Gain Notions

- Information gain aims to measure the improvement in purity / predictability / compressibility

- Example approaches:
  - **Entropy-based information gain (IG)**
  - Information gain ratio (GR)
  - Gini index (Gini)
  - Chi-square (χ^2)

Seen before:

Entropy of target feature *t* before splitting

$$H(t) = -\sum_{k=1}^{K}(P(t=k) \cdot log_s(P(t=k)))$$

$$H_W^d(t) = \sum_{node \in nodes(d)}(\frac{|node|}{N} \cdot H_{node}(t))$$

Weighted entropy of target feature *t* after splitting based on *d*

$$IG(d) = H(t) - H_W^d(t)$$

Alternative Information Gain Notions

- Information gain aims to measure the improvement in purity / predictability / compressibility

- Example approaches:
  - Entropy-based information gain (IG)
  - **Information gain ratio (GR)**
  - ~~**Gini index (Gini)**~~
  - ~~**Chi-square (χ^2)**~~

not covered in this lecture

Information Gain Ratio

- Entropy-based information gain favors features with many different values (split in many subsets decreases entropy)
- Information gain ratio addresses this issue

Consider the extreme case:
A descriptive feature with a unique value for each instance
→ Entropy after splitting will be 0
→ Maximal information gain
→ Little insight to be gained from the resulting decision tree!

Information Gain Ratio

- Entropy-based information gain favors features with many different values (split in many subsets decreases entropy)
- Information gain ratio addresses this issue:

Information gain when splitting based on descriptive feature *d*

$$GR(d) = \frac{IG(d)}{H(d)}$$

Entropy of descriptive feature *d*

→ we can think of it as making an absolute value relative

Information Gain Ratio

- Entropy-based information gain favors features with many different values (split in many subsets decreases entropy)
- Information gain ratio addresses this issue:

Information gain when splitting based on descriptive feature *d*

Entropy of target feature *t*

Overall entropy of target feature *t* after splitting based on *d*

$$GR(d) = \frac{IG(d)}{H(d)} = \frac{H(t) - H_W^d(t)}{-\sum_{k=1}^{K}(P(d=k) \cdot log_2(P(d=k)))}$$

Entropy of descriptive feature *d*

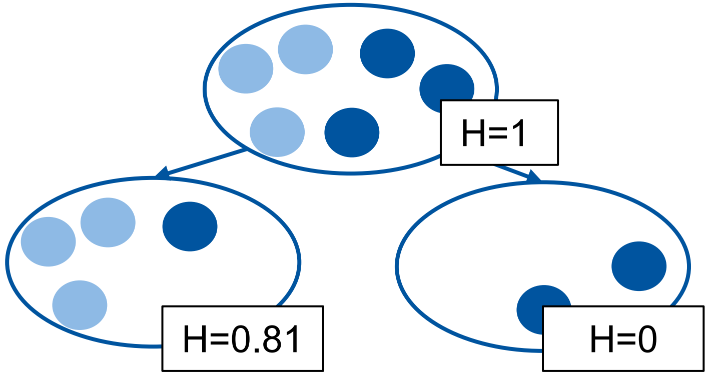
d can take *K* possible values

Probability of *d* taking the *k*th possible value

→ we can think of it as making an absolute value relative

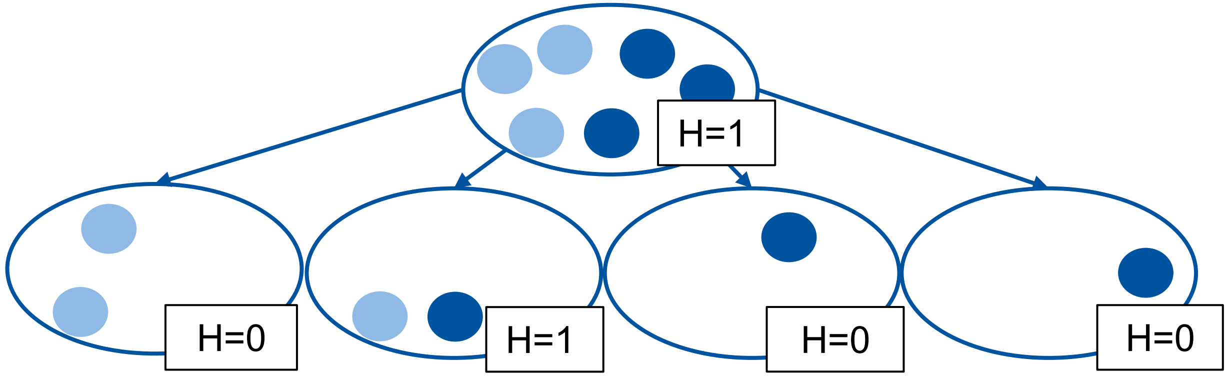
Information Gain Ratio - Example

split based on feature *d*



$$H_W^d(color) = \frac{4}{6} \cdot 0.81 + \frac{2}{6} \cdot 0 = 0.54$$
$$IG(d) = 0.46$$

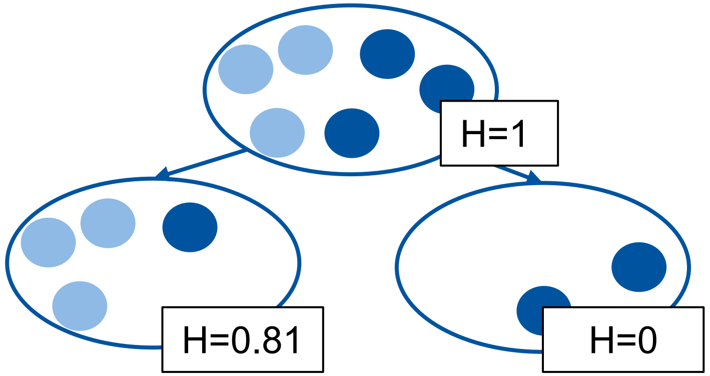
split based on feature *d'*



$$H_W^{d'}(color) = \frac{2}{6} \cdot 0 + \frac{2}{6} \cdot 1\frac{1}{6} \cdot 0 + \frac{1}{6} \cdot 0 = 0.33$$
$$IG(d') = 0.67$$

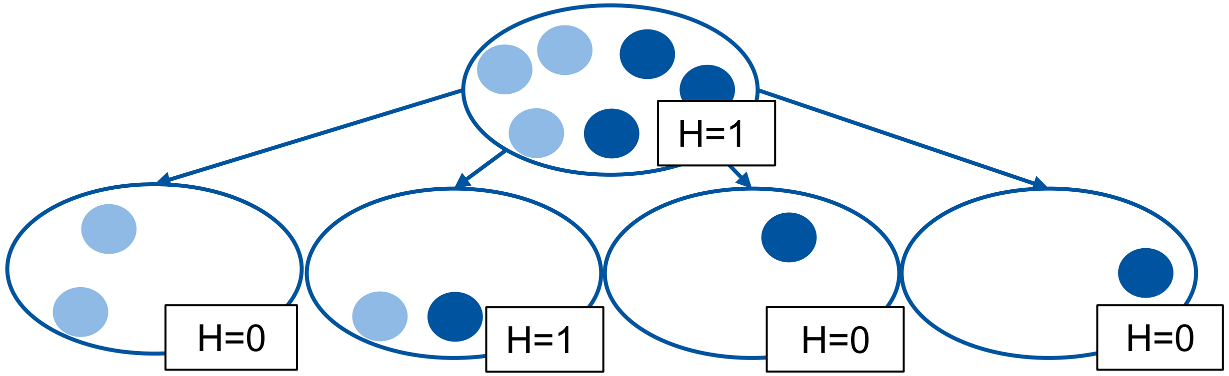
Information Gain Ratio - Example

split based on feature *d*



$IG(d) = 0.46$

split based on feature *d’*

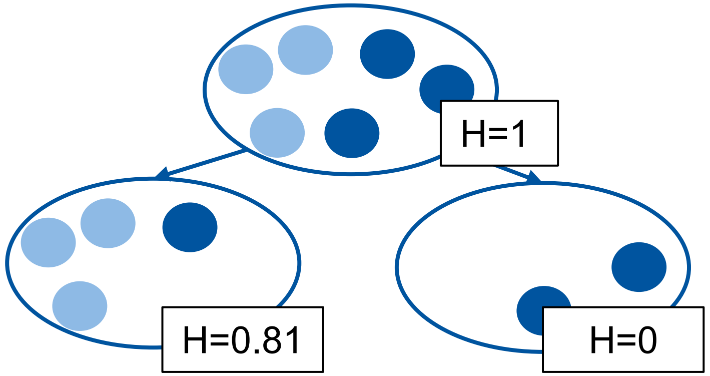


$IG(d') = 0.67$

$$GR(d) = \frac{IG(d)}{H(d)} = \frac{H(t) - H_W^d(t)}{-\sum_{k=1}^{K}(P(d=k) \cdot log_2(P(d=k)))}$$

Information Gain Ratio - Example

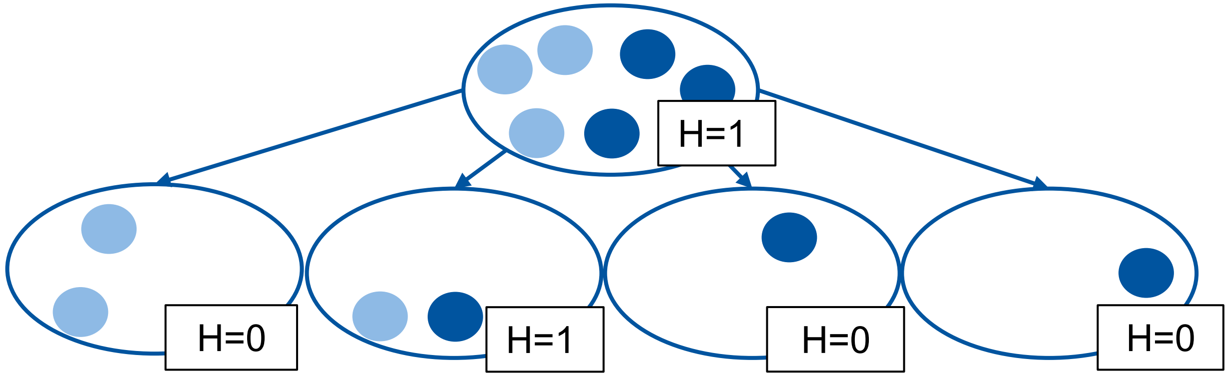
split based on feature *d*



$$IG(d) = 0.46$$

$$GR(d) = \frac{0.46}{-(\frac{4}{6} \cdot \log_2(\frac{4}{6}) + \frac{2}{6} \cdot \log_2(\frac{2}{6}))} = \frac{0.46}{0.92} = 0.5$$

split based on feature *d'*



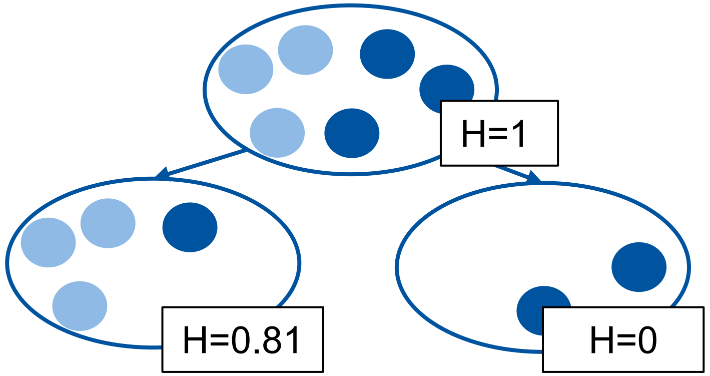
$$IG(d') = 0.67$$

Feature d splits the 6 instances into one partition of size 4 and one partition of size 2

$$GR(d) = \frac{IG(d)}{H(d)} = \frac{H(t) - H_W^d(t)}{-\sum_{k=1}^{K}(P(d=k) \cdot log_2(P(d=k)))}$$

Information Gain Ratio - Example

split based on feature *d*



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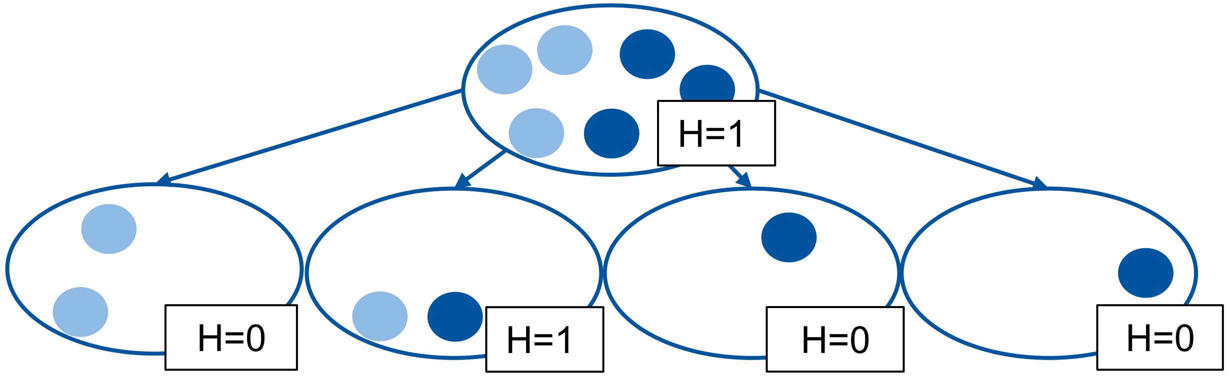
split based on feature *d'*



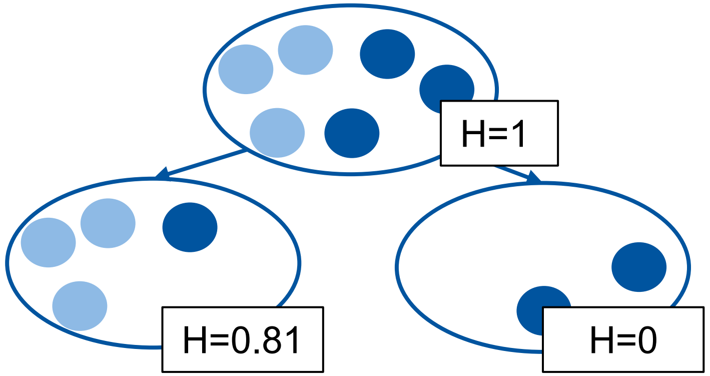
$$IG(d') = 0.67$$

$$GR(d') = \frac{0.67}{-(\frac{2}{6}\cdot\log_2(\frac{2}{6}) + \frac{2}{6}\cdot\log_2(\frac{2}{6}) + \frac{1}{6}\cdot\log_2(\frac{1}{6}) + \frac{1}{6}\cdot\log_2(\frac{1}{6}))} = \frac{0.67}{1.92} = 0.35$$

$$\boxed{GR(d) = \frac{IG(d)}{H(d)} = \frac{H(t) - H_W^d(t)}{-\sum_{k=1}^{K}(P(d=k)\cdot log_2(P(d=k)))}}$$

Information Gain Ratio - Example

split based on feature *d*



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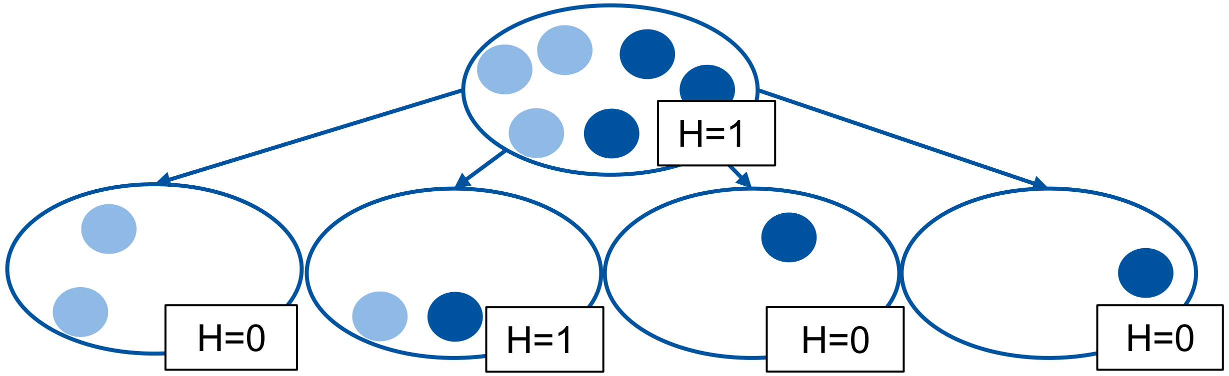
split based on feature *d'*



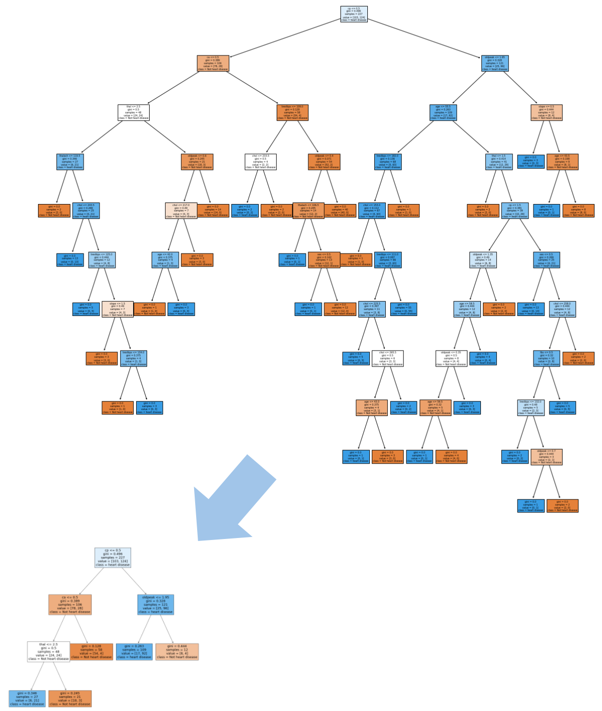
$IG(d') = 0.67$

$$GR(d') = \frac{0.67}{-(\frac{2}{6} \cdot \log_2(\frac{2}{6}) + \frac{2}{6} \cdot \log_2(\frac{2}{6}) + \frac{1}{6} \cdot \log_2(\frac{1}{6}) + \frac{1}{6} \cdot \log_2(\frac{1}{6}))} = \frac{0.67}{1.92} = 0.35$$

$$\boxed{GR(d) = \frac{IG(d)}{H(d)} = \frac{H(t) - H_W^d(t)}{-\sum_{k=1}^{K}(P(d=k) \cdot log_2(P(d=k)))}}$$

Decision Trees

1. Introduction to Decision Trees
2. Entropy and Information Gain
3. ID3 Algorithm
4. Quantifying Information Gain
5. **Pruning**
6. Continuous Data
7. Ensembles

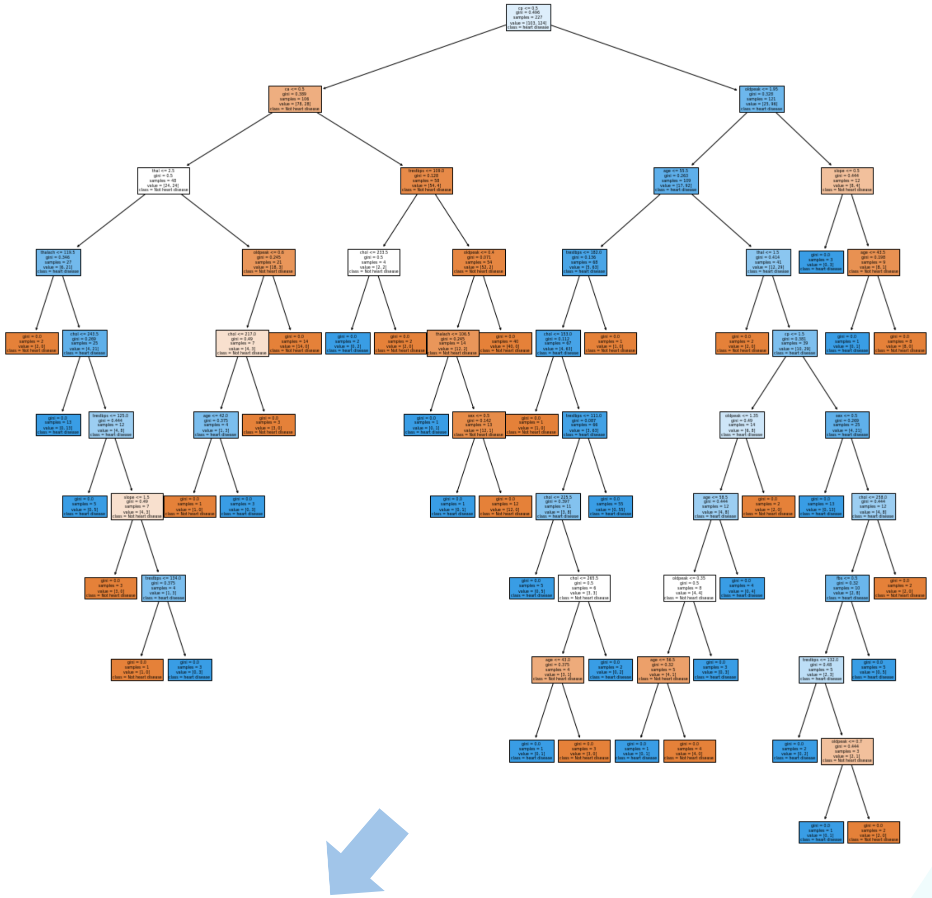


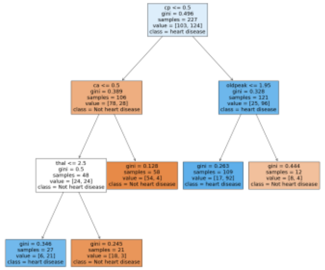
Pruning Decision Trees

- Possible problems:
  - Decision tree is overfitting the data
  - Decision tree is too complex or too deep

- Two solution directions:
  - Pre-pruning (early stopping/forward)
  - Post-pruning (reduced error/backward)

- To generalize and avoid overfitting





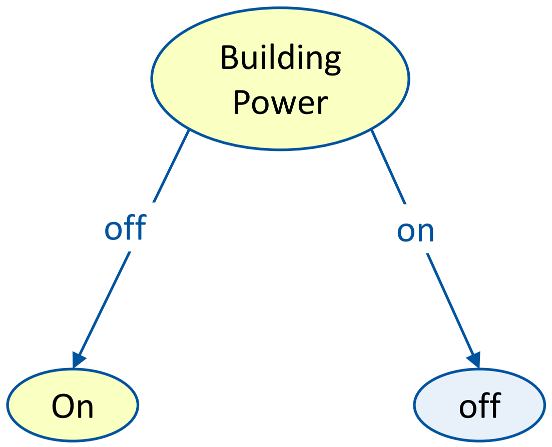
[arunmohan_003, kaggle]

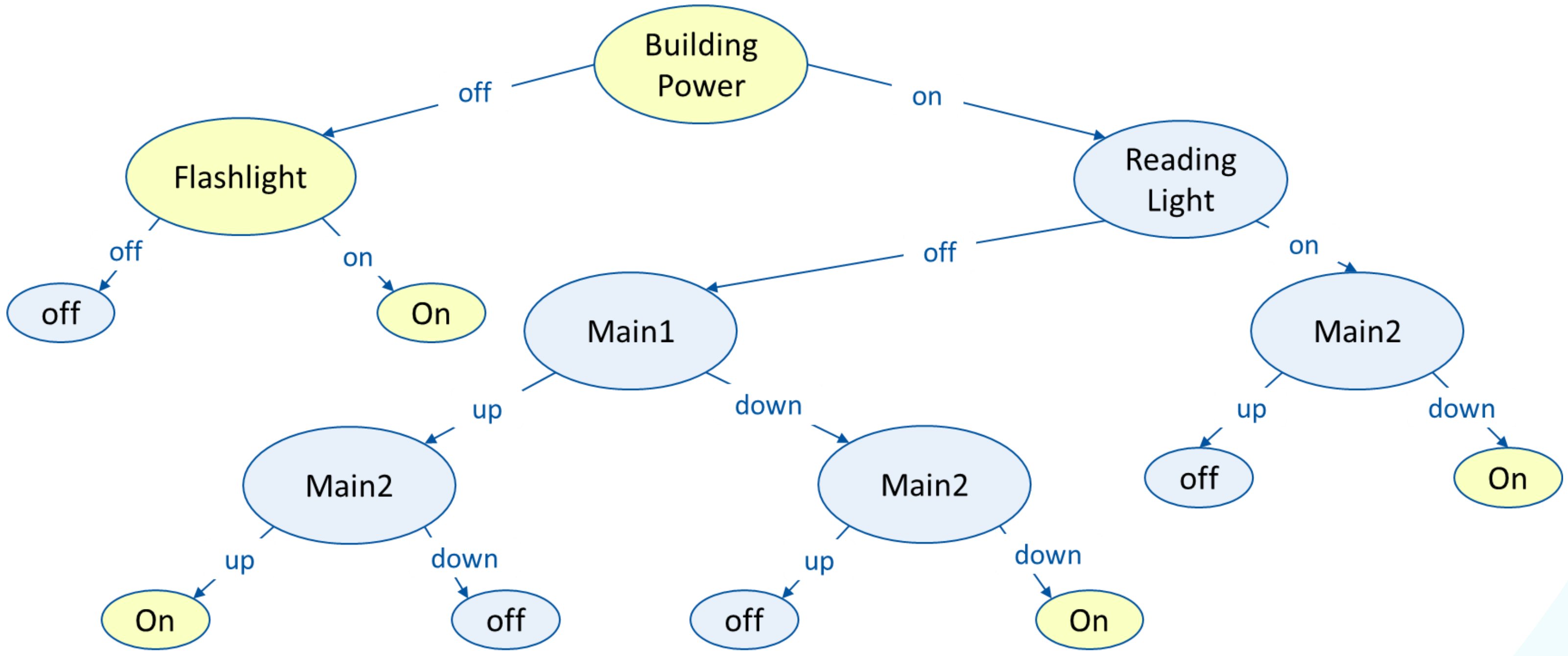
Pre-pruning

- Idea: Stop creating subtrees and use majority vote to determine the label
- Many possible stopping criteria:
  - maximum tree depth
  - lower bound for number of instances before split
  - Lower bound for number of instances after split
  - lower bound for information gain
  - …
- May create trees that are not consistent with respect to the data

Pre-pruning – Enlightening Example

Building the tree with pre-pruning



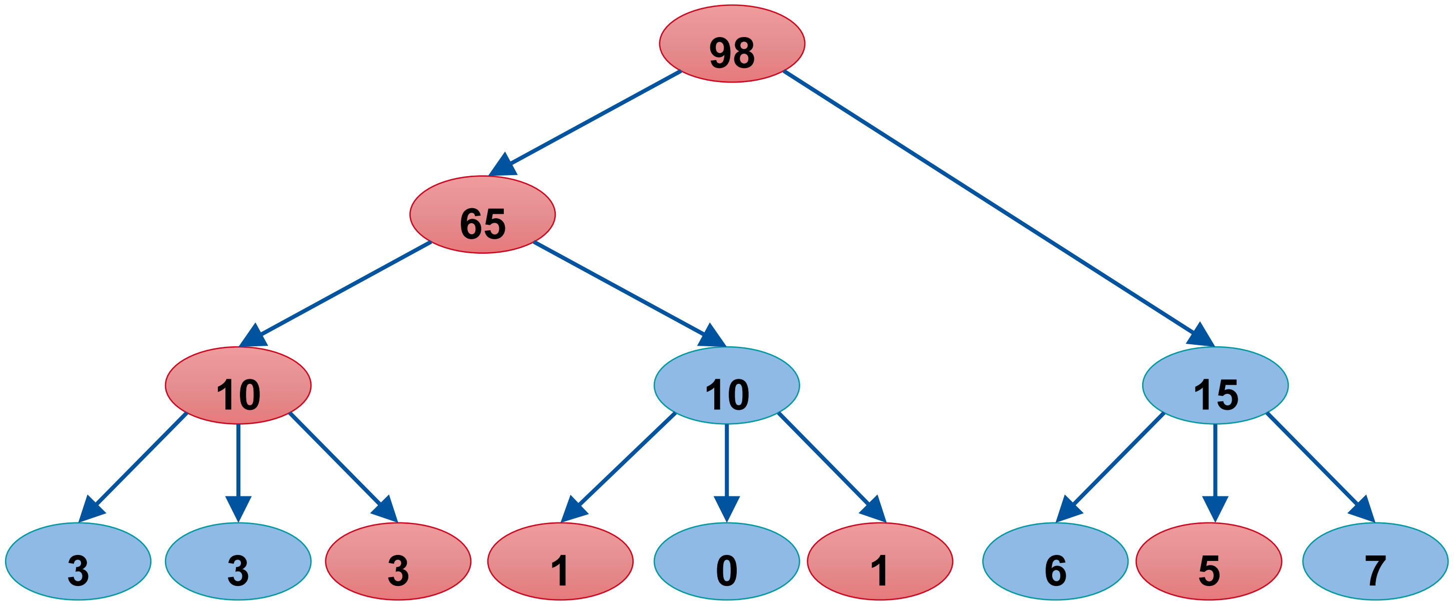


Pre-pruning is efficient, but we may miss interesting dependencies at lower levels of the tree

Post-pruning

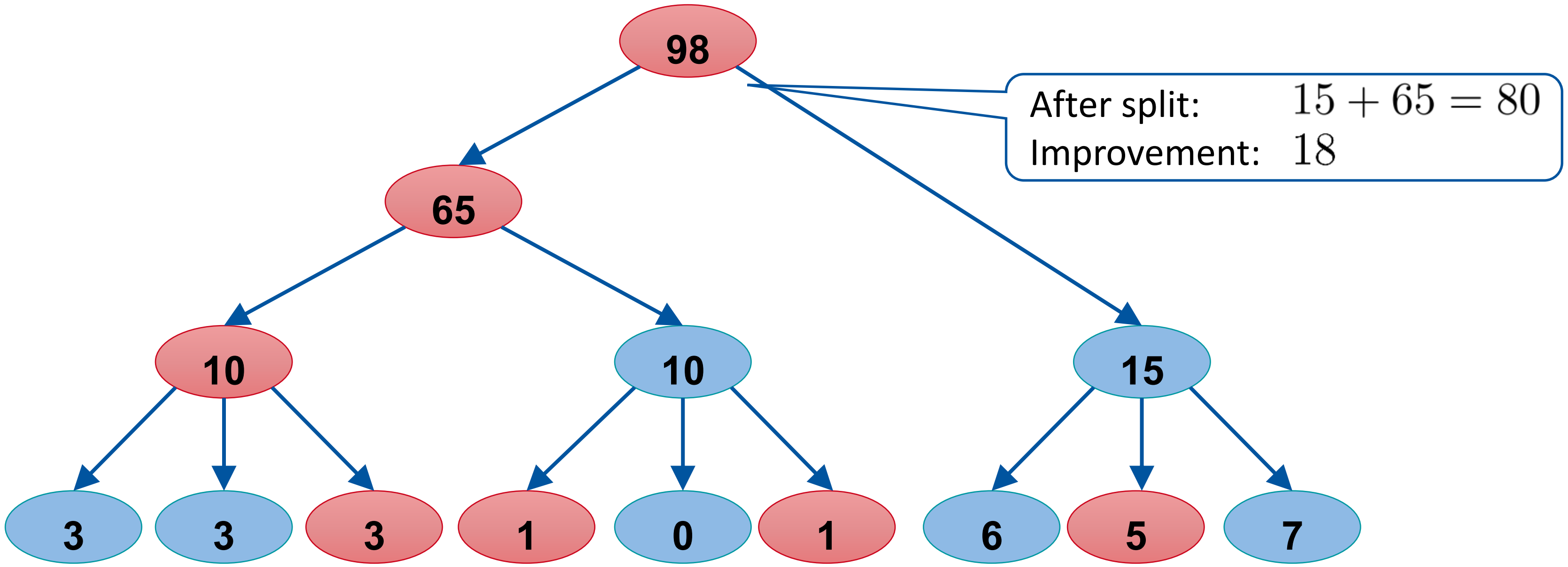
- First, build the whole decision tree; then cut off branches that do not add (much)
- Common approach is to split the data into a training set and a validation/test set
- Measure the performance of splits based on a validation/test set

Post-pruning



- Decision tree learned on a training set
- Numbers indicate misclassifications based on a validation set

Post-pruning



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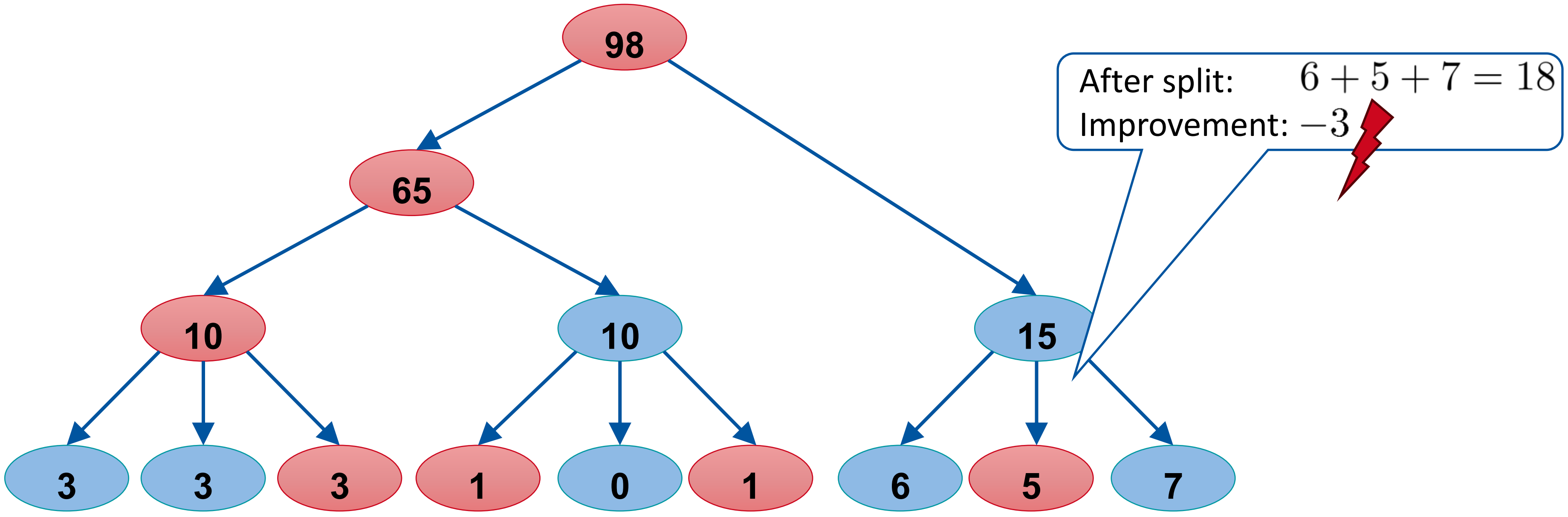
Post-pruning



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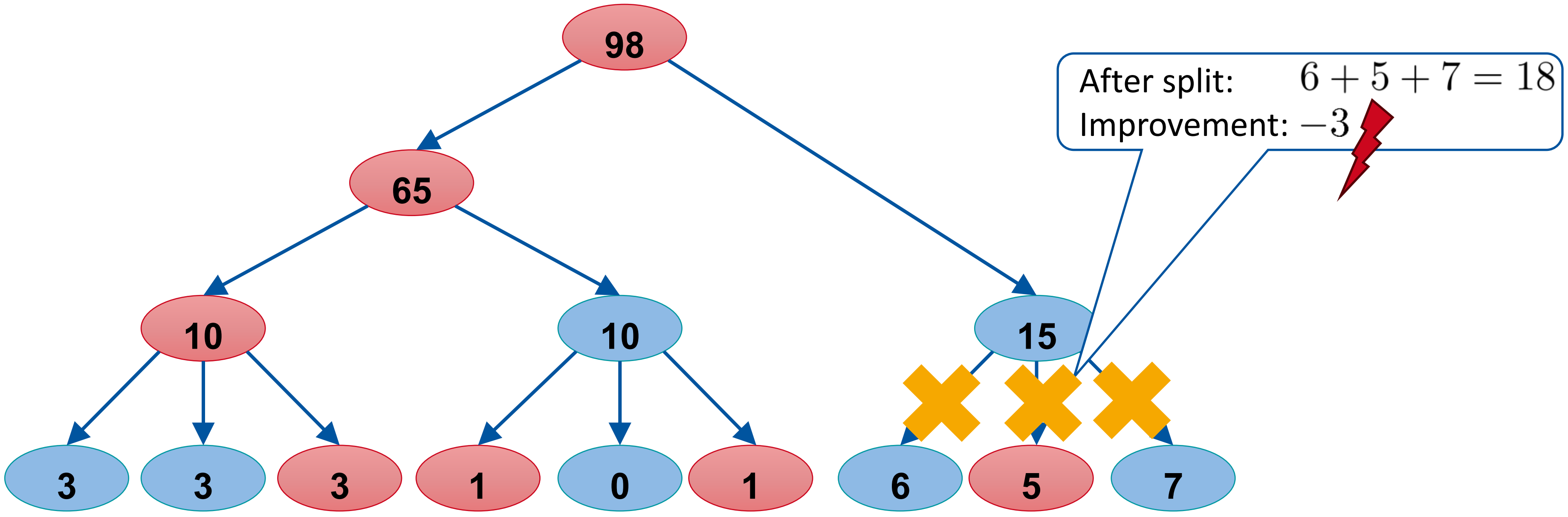

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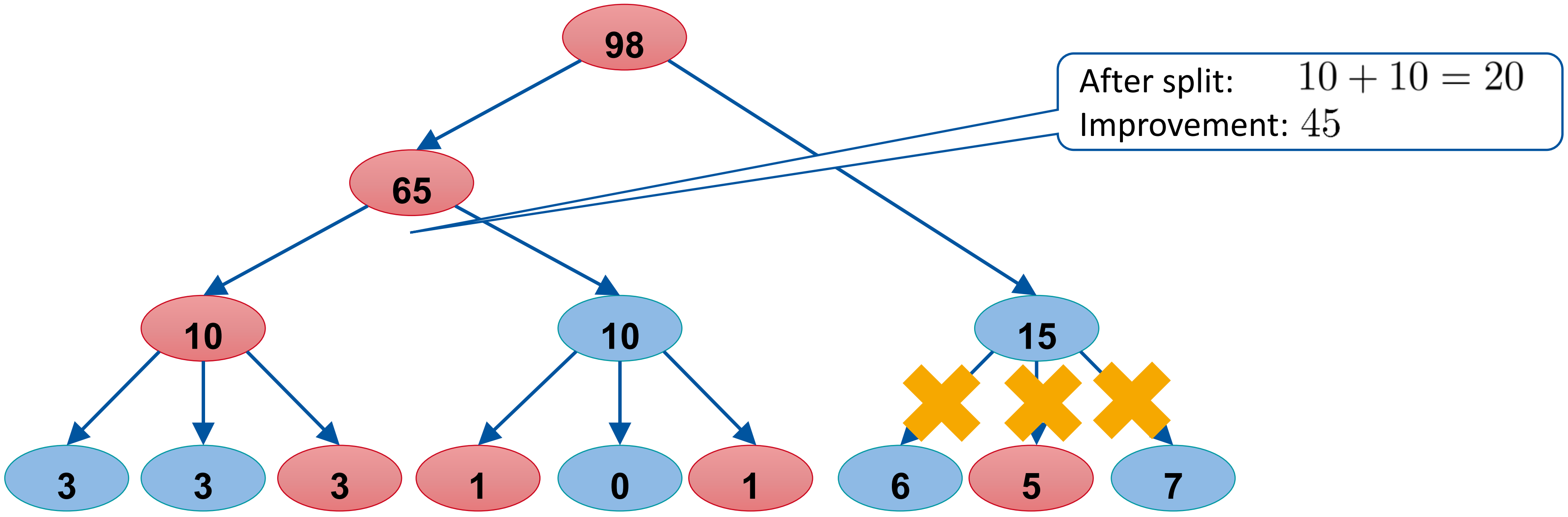
Post-pruning



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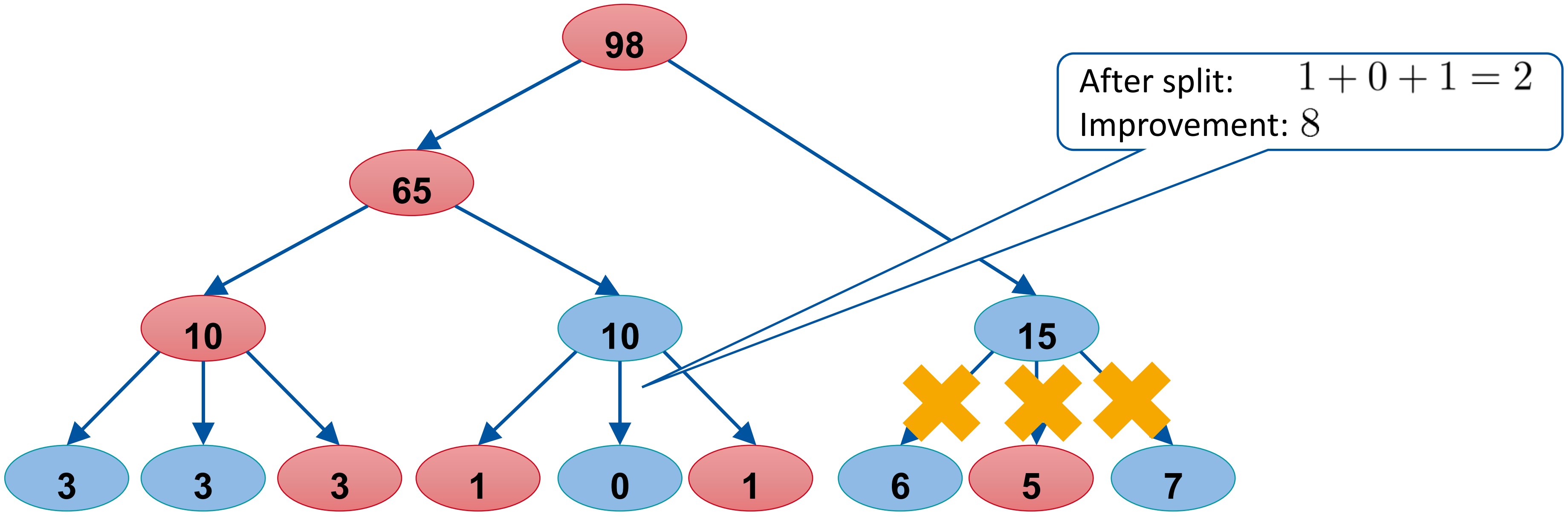

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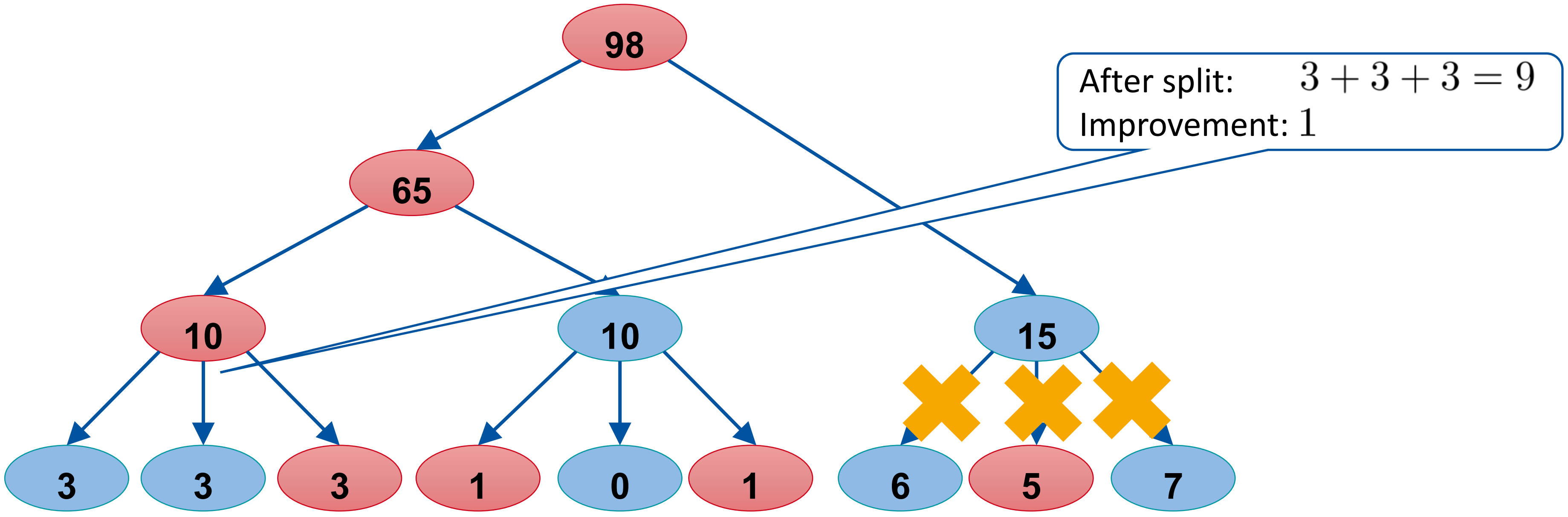
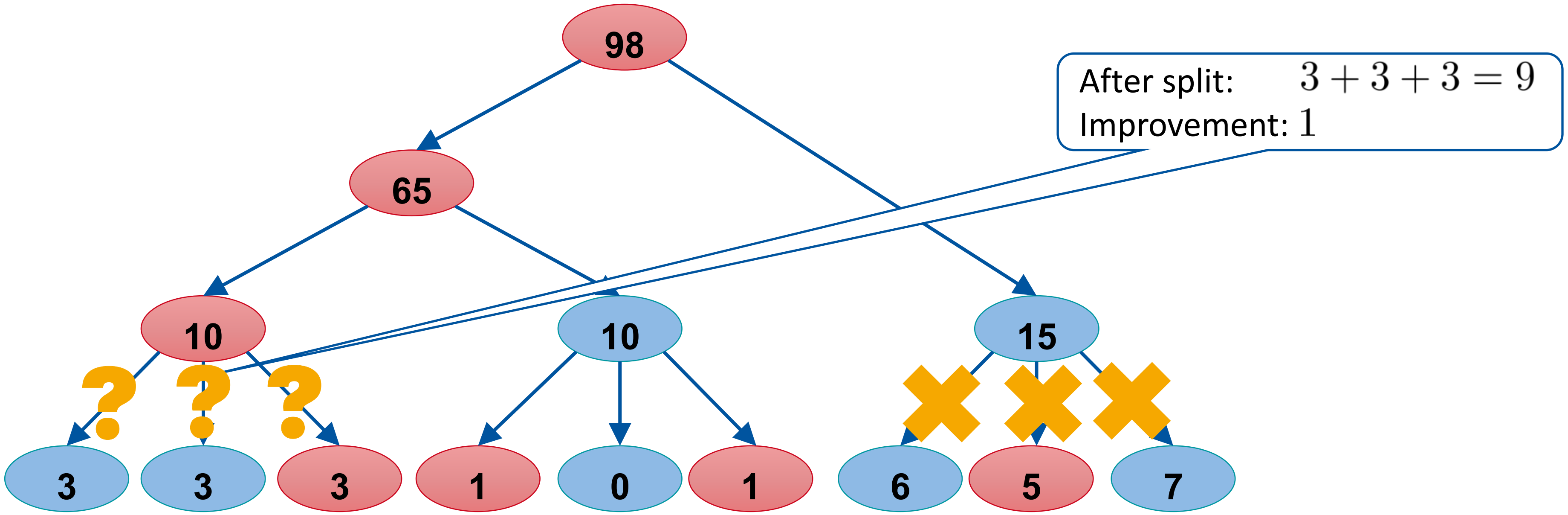
Post-pruning



- Decision tree learned on a training set
- Numbers indicate misclassifications based on a validation set

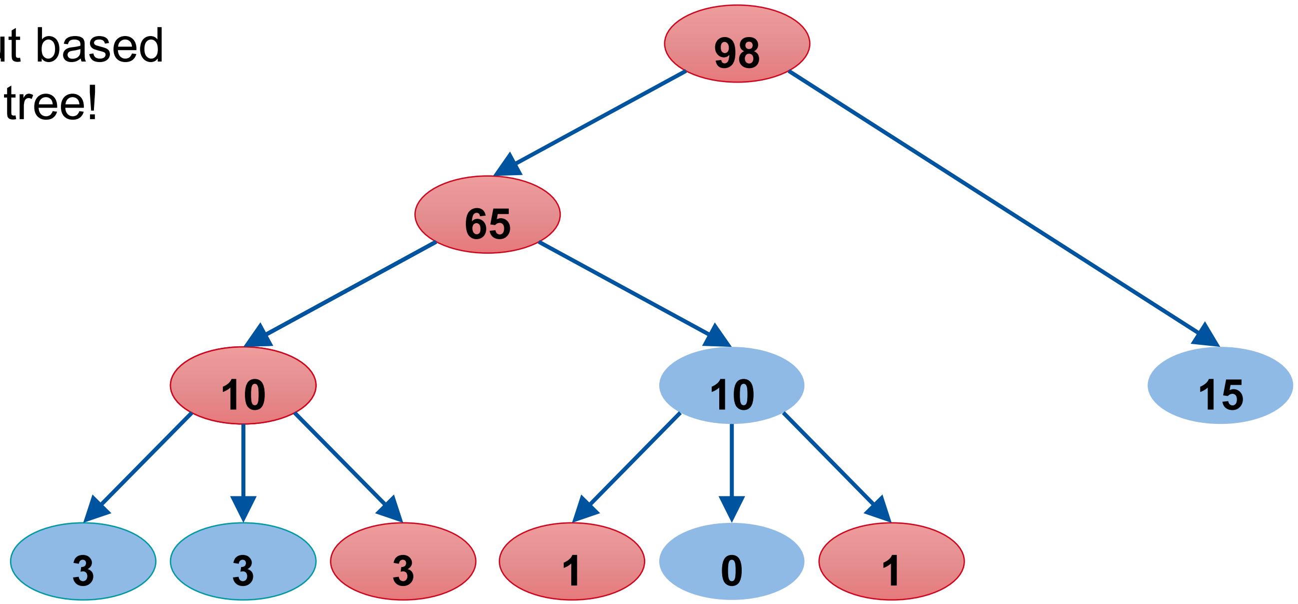
Post-pruning



- Decision tree learned on a training set
- Numbers indicate misclassifications based on a validation set

Post-pruning

Less efficient, but based on the complete tree!



- Many variants
  - Bottom up instead of top-down
  - Quantification of Performance (e.g., normalize misclassifications)
  - Various pruning thresholds (in this lecture, subtrees are pruned when misclassification increases)
  - …

Decision Trees

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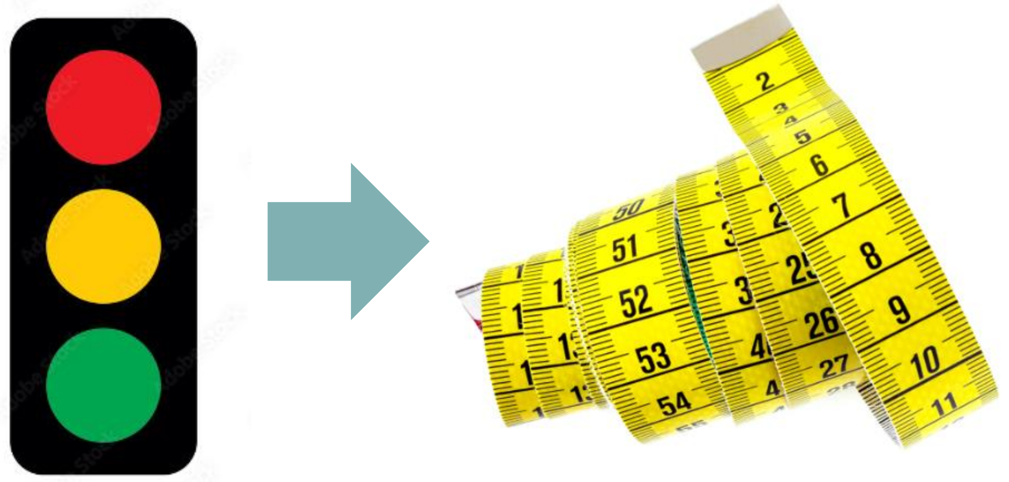
6. **Continuous Data**
7. Ensembles



Dealing with Continuous Variables

- So far we assumed features were categorical
- We can use binning to make continuous features categorical

continuous target feature

features

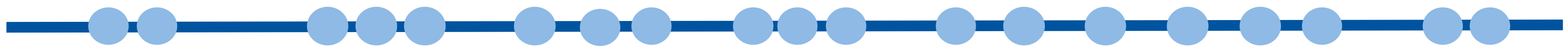
f_1	f_2	…	f_D	class
high	88		59.99	**5043**
high	76		50.00	**4598**
low	32		39.50	**3248**
low	89		49.99	**5466**
high	21		59.99	**7682**

instances

continuous descriptive features

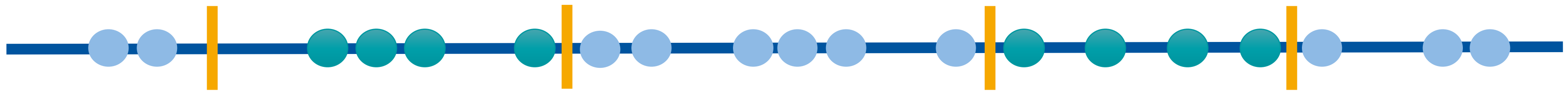
Continuous Descriptive Features

- Challenge: determine suitable boundaries (infinite number of thresholds is possible)



Continuous Descriptive Features

- Challenge: determine suitable boundaries (infinite number of thresholds is possible)
- Idea:
  - sort instances based on the continuous descriptive feature
  - look for changes in target feature labels
- Change points are candidate thresholds
- Select the threshold with the highest information gain



Continuous Descriptive Features - Example

ID	Insurance	Income	Employment	Customer
1	Yes	3500	Employed	**Basic**
2	Yes	0	Unemployed	**Premium**
3	Yes	1000	Self-employed	**Premium**
4	No	2000	Self-employed	**Basic**
5	No	5000	Employed	**Economy**
6	Yes	5100	Retired	**Economy**
7	Yes	3000	Employed	**Premium**

sort

Continuous Descriptive Features - Example

ID	Insurance	Income	Employment	Customer
2	Yes	0	Unemployed	Premium
3	Yes	1000	Self-employed	Premium
4	No	2000	Self-employed	Basic
7	Yes	3000	Employed	Premium
1	Yes	3500	Employed	Basic
5	No	5000	Employed	Economy
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sort

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5	No	5000	Employed	Economy
6	Yes	5100	Retired	Economy

1500

Change in target feature: candidate threshold

Continuous Descriptive Features - Example

ID	Insurance	Income	Employment	Customer
2	Yes	0	Unemployed	Premium
3	Yes	1000	Self-employed	Premium
4	No	2000	Self-employed	Basic
7	Yes	3000	Employed	Premium
1	Yes	3500	Employed	Basic
5	No	5000	Employed	Economy
6	Yes	5100	Retired	Economy

1500

Change in target feature: candidate threshold

Thresholds: middle values of continuous feature in between changed target features

Continuous Descriptive Features - Example

ID	Insurance	Income	Employment	Customer
2	Yes	0	Unemployed	Premium
3	Yes	1000	Self-employed	Premium
		1500		
4	No	2000	Self-employed	Basic
		2500		
7	Yes	3000	Employed	Premium
1	Yes	3500	Employed	Basic
5	No	5000	Employed	Economy
6	Yes	5100	Retired	Economy

Change in target feature:
candidate threshold

Thresholds: middle values of continuous feature in between changed target features

Continuous Descriptive Features - Example

ID	Insurance	Income	Employment	Customer
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1	Yes	3500	Employed	Basic
5	No	5000	Employed	Economy
6	Yes	5100	Retired	Economy

1500

2500

3250

4250

Four candidate thresholds

Thresholds: middle values of continuous feature in between changed target features

Continuous Descriptive Features - Example

Threshold	Instances
≥1500	2, 3 1, 4, 5, 6, 7
≥2500	2, 3, 4 1, 5, 6, 7
≥3250	2, 3, 4, 7 1, 5, 6
≥4250	1, 2, 3, 4, 7 5, 6

Continuous Descriptive Features - Example

Threshold	Instances	Partition Entropy	Overall Entropy	Information Gain
≥1500	2, 3 1, 4, 5, 6, 7	0 1.5219	1.0871	0.1981
≥2500	2, 3, 4 1, 5, 6, 7	0.9183 1.5	1.2507	0.306
≥3250	2, 3, 4, 7 1, 5, 6	0.8113 0.9183	0.8572	0.6995
≥4250	1, 2, 3, 4, 7 5, 6	0.9710 0	0.6935	0.8631

Compute as usual

Continuous Descriptive Features - Example

Threshold	Instances	Partition Entropy	Overall Entropy	Information Gain
≥1500	2, 3 1, 4, 5, 6, 7	0 1.5219	1.0871	0.1981
≥2500	2, 3, 4 1, 5, 6, 7	0.9183 1.5	1.2507	0.306
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≥4250	1, 2, 3, 4, 7 5, 6	0.9710 0	0.6935	0.8631

best

Continuous Descriptive Features - Example

Resulting decision tree:

Income

<4250

≥4250

Economy

ID	Insurance	Income	Employment	Customer
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3	Yes	1000	Self-employed	Premium
4	No	2000	Self-employed	Basic
7	Yes	3000	Employed	Premium
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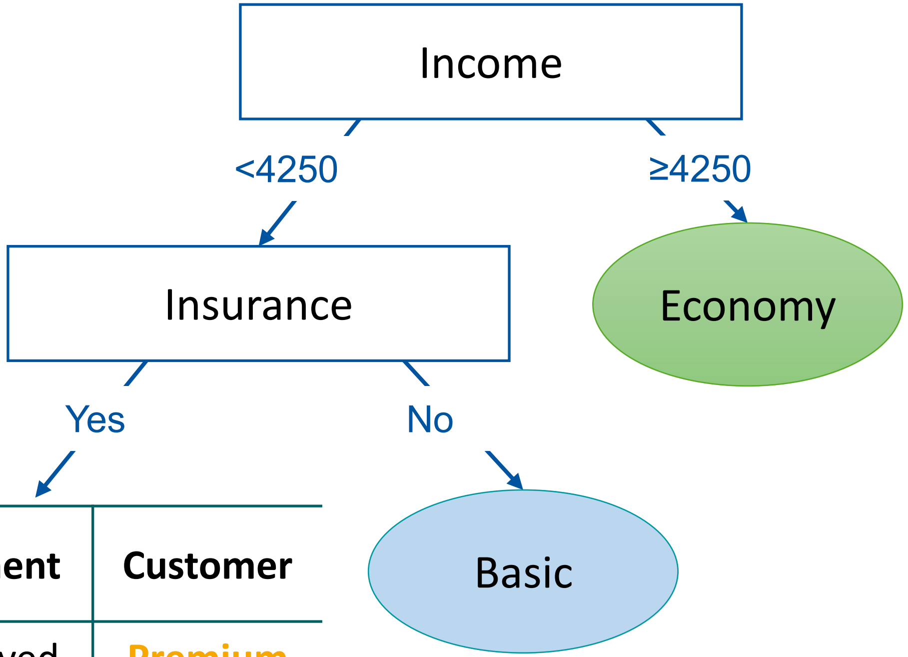
Continuous Descriptive Features - Example

Resulting decision tree:



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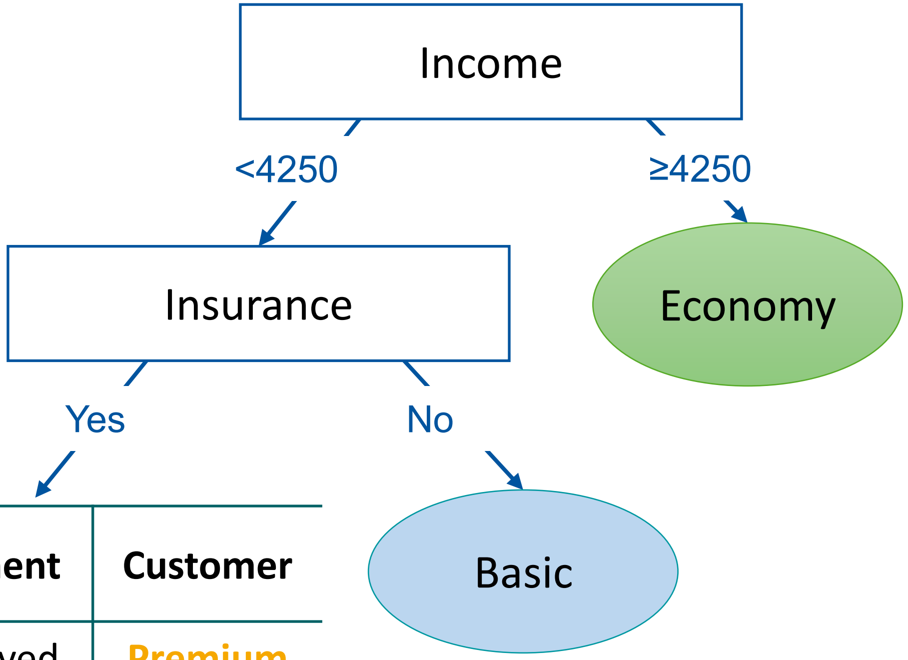
Continuous Descriptive Features - Example

Resulting decision tree:



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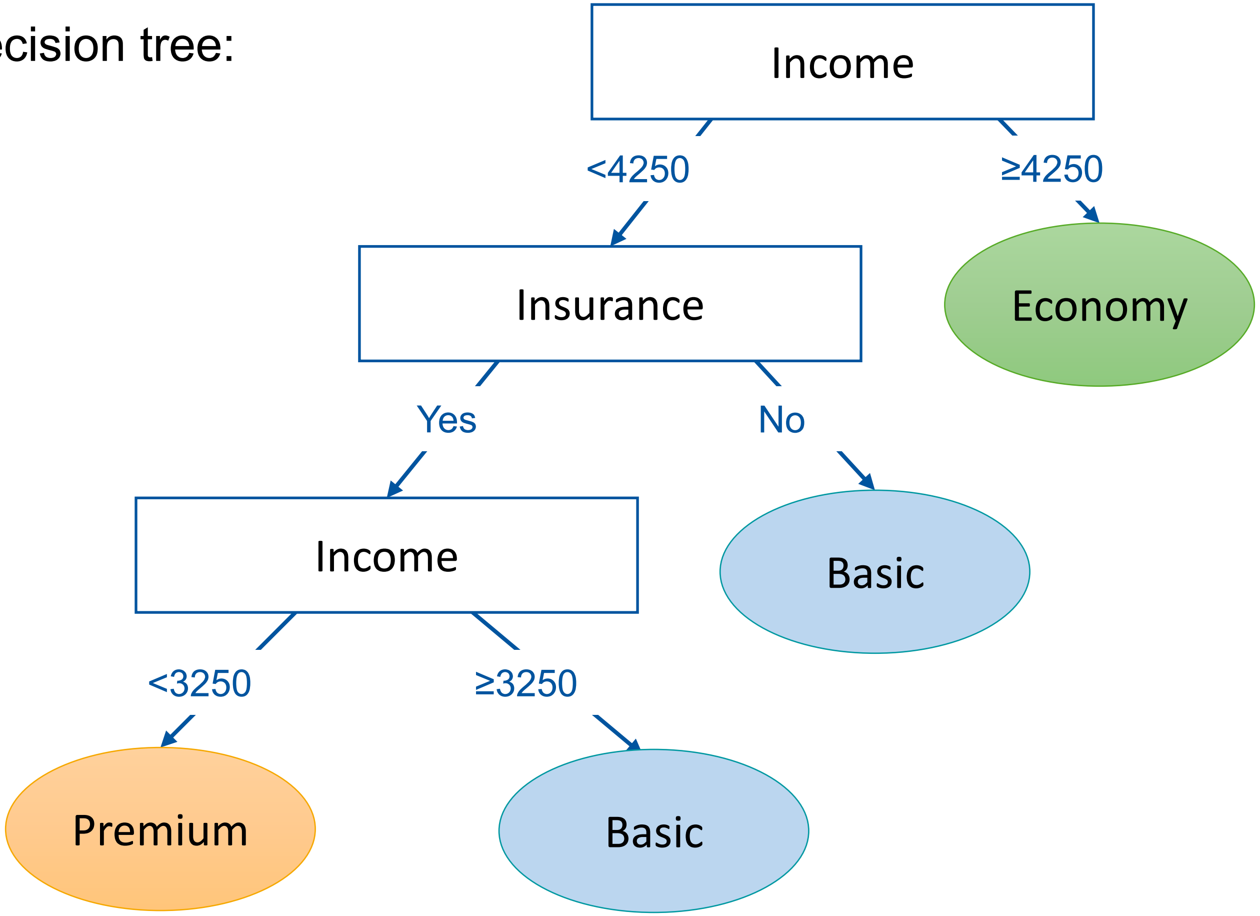
The same continuous feature can now be used multiple times!

Continuous Descriptive Features - Example

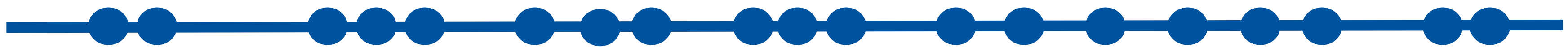
Resulting decision tree:



The same continuous feature can now be used multiple times!

Continuous Target Features

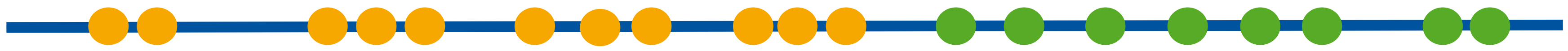
- Goal: find descriptive features that ‘nicely’ partition the target feature axis
- Impurity = Variance within a partition
- We cannot use the target feature itself
- We ‘color the dots’ based on a selected descriptive feature



Continuous Target Features

- Goal: find descriptive features that ‘nicely’ partition the target feature axis
- Impurity = Variance within a partition
- We cannot use the target feature itself
- We ‘color the dots’ based on a selected descriptive feature

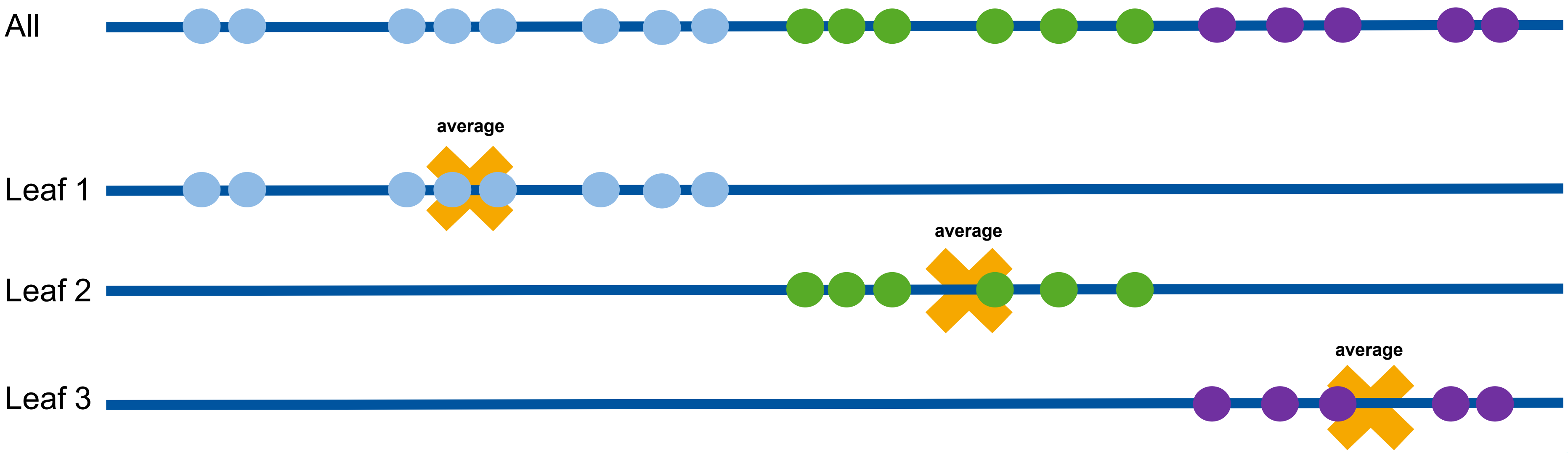
Intuition: instances described as green are predicted to have a value in this range



Continuous Target Features

Good Classification

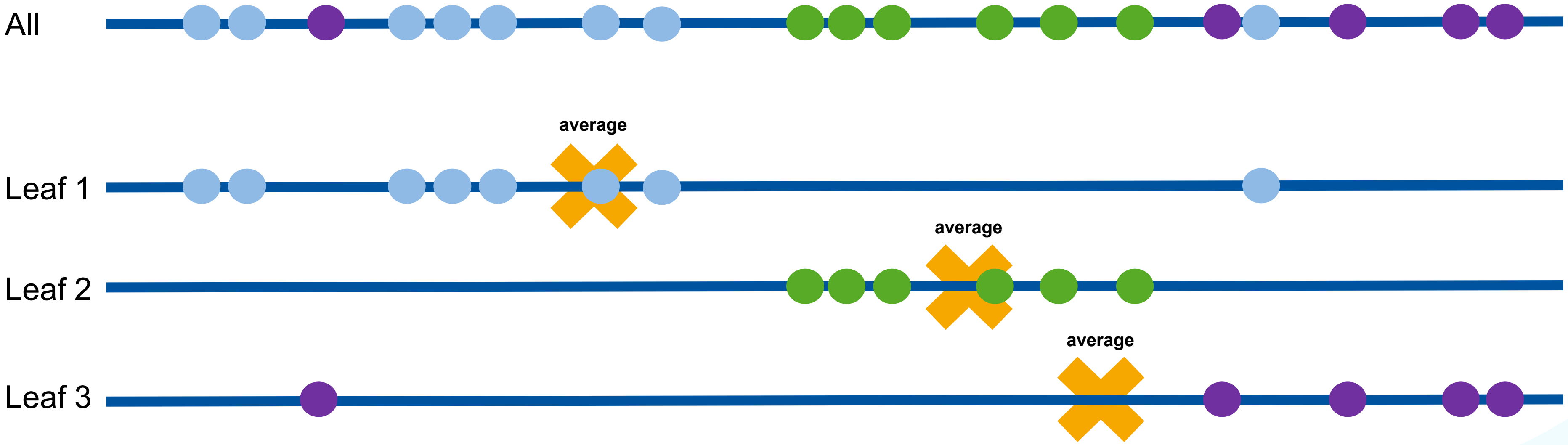
- Three leaves (purple, green, blue show mapping based on descriptive feature)
- Impurity as measure of quality: variance within a leaf of the decision tree



Continuous Target Features

Reasonable Classification

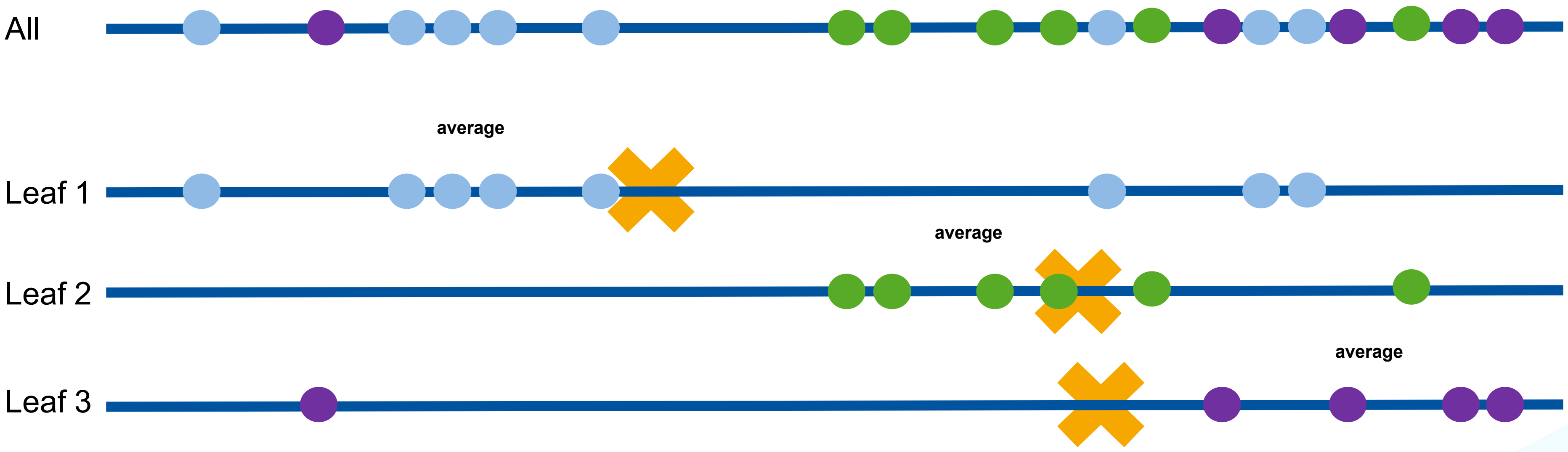
Variance within Leaf 1 and Leaf 3 increased with respect to the ‘good classification’



Continuous Target Features

Poor Classification

Variance within all leaves is high compared to the ‘good classification’



Impurity

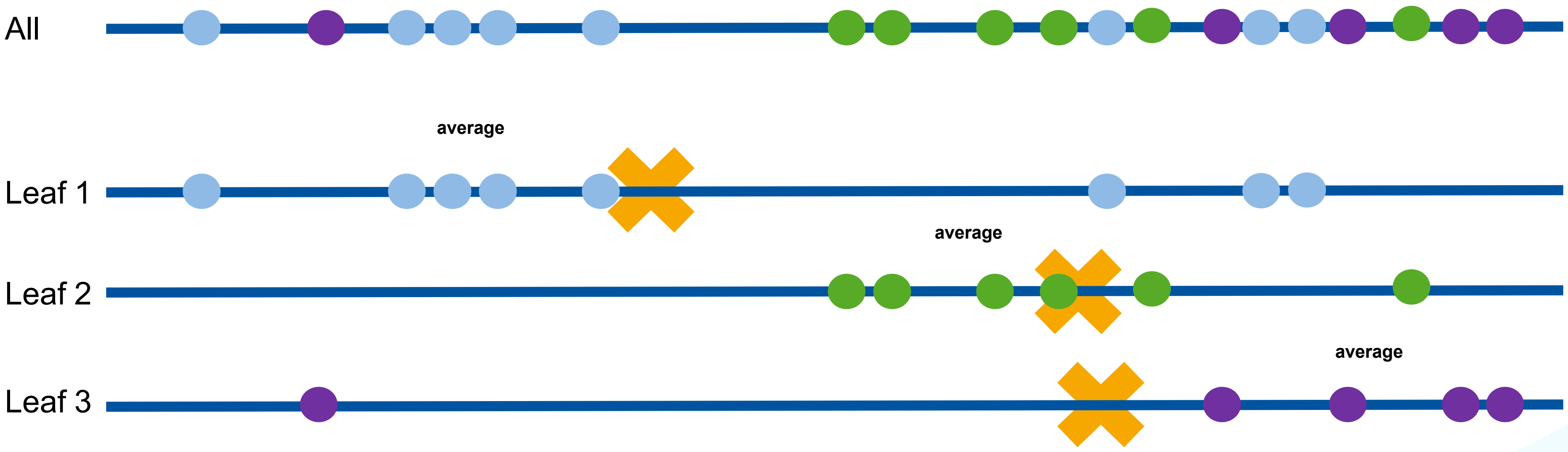
Variance in a Node/Leaf

Number of instances

Target value of instance *i*

Mean of target values

$$Var(t) = \frac{\sum_{i=1}^{N}(t_i - \bar{t})^2}{N-1}$$



Adapting the ID3 Algorithm

ID3 algorithm:

1. **if** all the instances in the dataset have the same classification
   (a) **return** a decision tree with one leaf node with consensus value as a label
2. **else if** there are no features left
   (a) **return** a decision tree with one leaf node with majority value as a label
3. **else if** the dataset is empty
   (a) **return** a decision tree with one leaf node with majority parent value as a label
4. **else**
   (a) pick a feature that lowers the weighted variance most within the subtrees
   (b) once a feature is picked along a path from the root, it cannot be used again
   (c) create subproblems based on the selected feature

Stopping criteria (as before)

Instead of maximizing information gain

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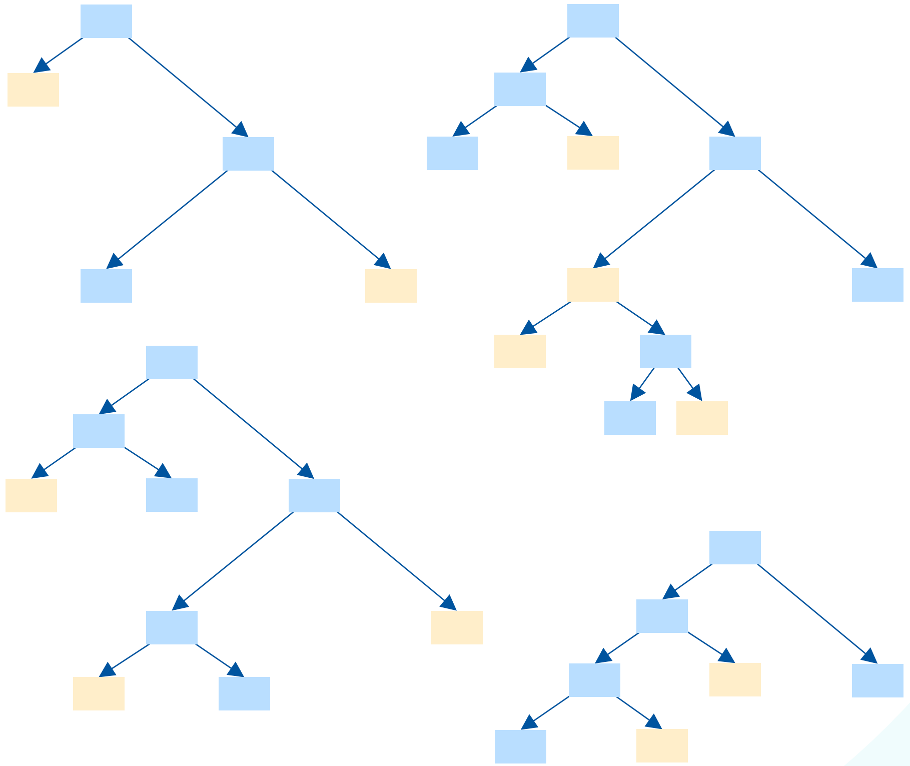
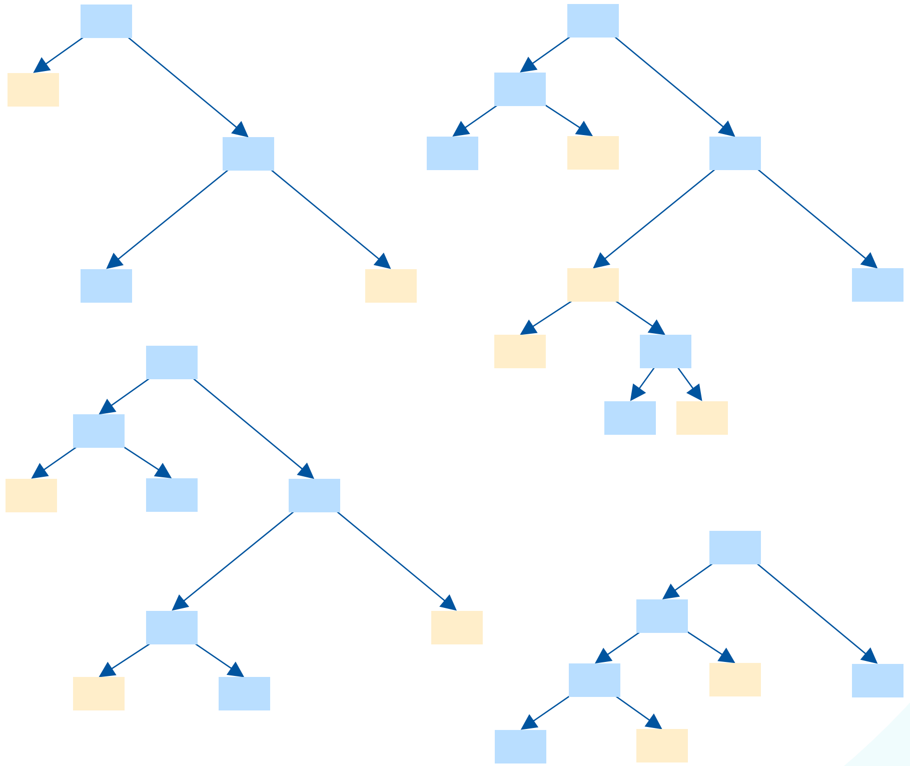


Ensembles: Main Idea

- Rather than creating a single decision tree, we aim to create a set of trees (called a model ensemble)
- Models should complement each other
- Different models can ”vote” on the label (votes may be weighted)
- Multiple trees may give different answers (select the most frequent value or the average)
- Many variations of the same idea…



Ensembles: From one to multiple

- **Bagging** (sample instances): Trees focus on subsets of instances (i.e., rows)
- **Subspace sampling** (sample features): Trees focus on subsets of features (i.e., columns)
- **Random forest** (combine bagging and subspace sampling): Trees focus on subsets of instances and features
- **Boosting** (focus on errors): Create additional trees giving more weight to incorrectly classified instances.

One glimpse into the toolbox…

- Not one specific ‘decision tree algorithm’
- Any variations are possible by combining ideas
- There is no best solution, it all depends on your data and goal

Performance on unseen test data is what counts

- Avoid overfitting the data!
- Split data into training and test data
- Evaluation methods such as accuracy and confusion matrix will be discussed later

Decision Trees - Conclusion

- Supervised learning aims to explain the target feature in terms of descriptive features
- Decision trees are easy to understand and interpret
- Focus on categorical variables but extensions to continuous data are possible
- Many variations based on the basic ID3 algorithm
  - Pruning
  - Ensembles
  - Information gain definitions
  - …
- You have seen conceptual examples – implementations will differ in design choices, e.g., how to handle border cases, pick thresholds…