# COMP809 Data Mining and Machine Learning

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SCHOOL OF ENGINEERING, COMPUTER AND MATHEMATICAL SCIENCES

Classification Basic Concept- Decision Tree (1)

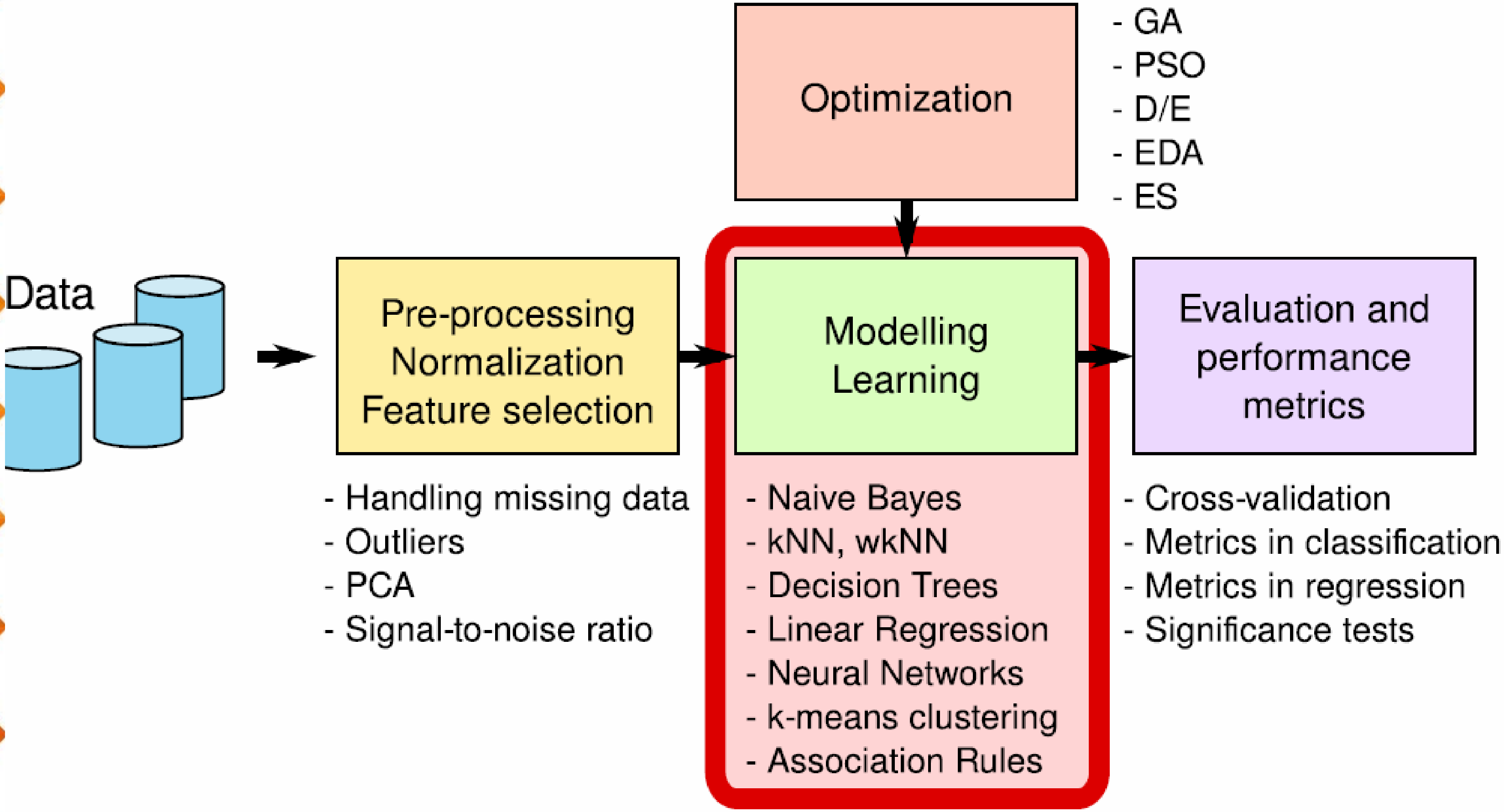
## Weekly Learning Outcomes

- Classification Basic Concept
- Classification Algorithms
- Decision Tree

# Prediction Problems

- Classification
  - *predicts* categorical class labels *(discrete or nominal)*
  - *classifies data (constructs a model) based on the training set and the values (class labels) in a classifying attribute and uses it in classifying new data*

- Numeric Prediction
  - *models continuous-valued functions, i.e., predicts unknown or missing values*



Optimization

- GA
- PSO
- D/E
- EDA
- ES

Data

Pre-processing
Normalization
Feature selection

- Handling missing data
- Outliers
- PCA
- Signal-to-noise ratio

Modelling
Learning

- Naive Bayes
- kNN, wkNN
- Decision Trees
- Linear Regression
- Neural Networks
- k-means clustering
- Association Rules

Evaluation and
performance
metrics

- Cross-validation
- Metrics in classification
- Metrics in regression
- Significance tests

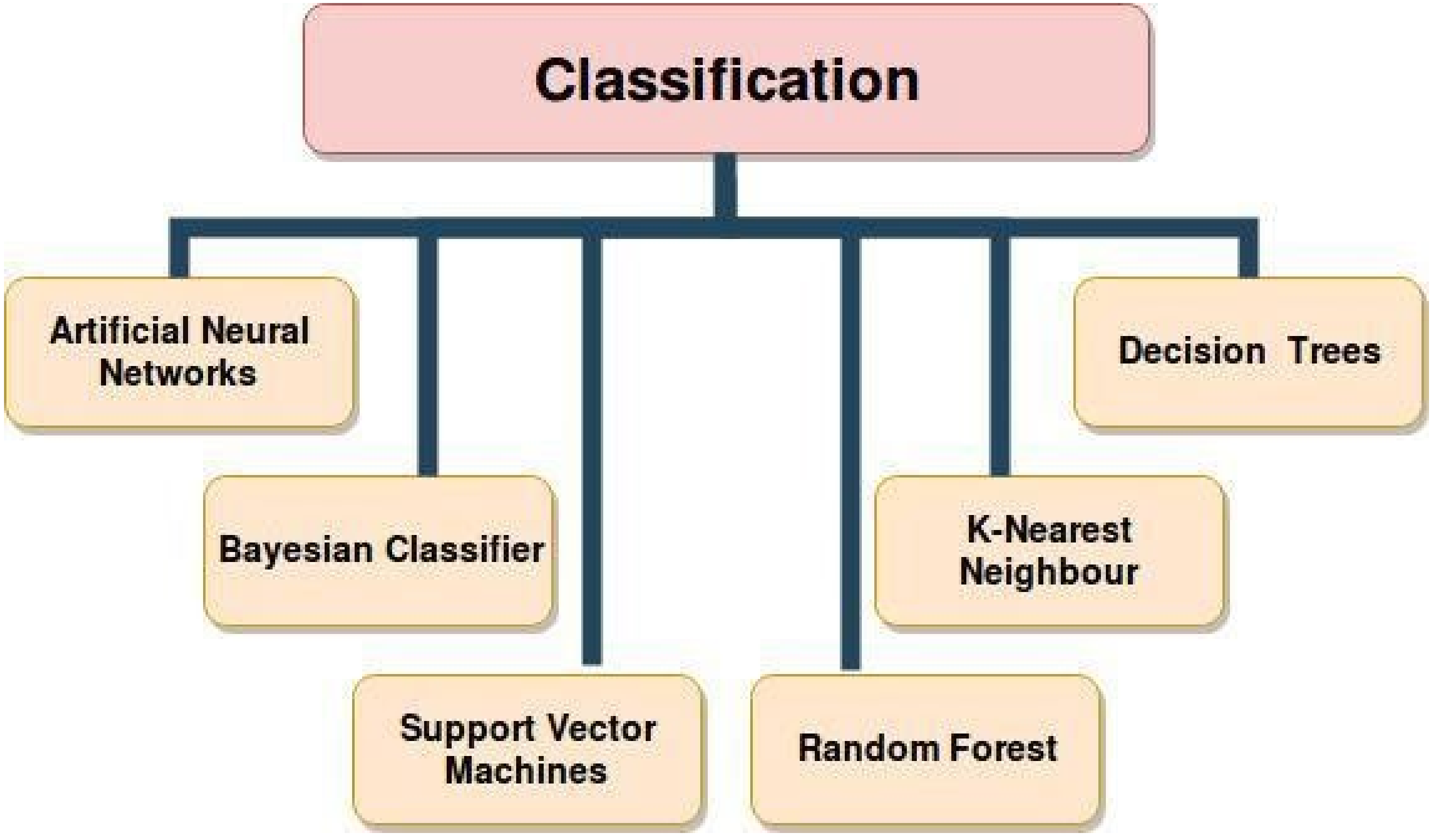
# Supervised vs. Unsupervised Learning

- Supervised learning (classification)
  - *Supervision: The training data (observations, measurements, etc.) are accompanied by **labels** indicating the class of the observations*
  - *New data is classified based on the training set*
- Unsupervised learning (clustering)
  - *The class labels of training data is unknown*
  - *Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data*

# Classification: Definition

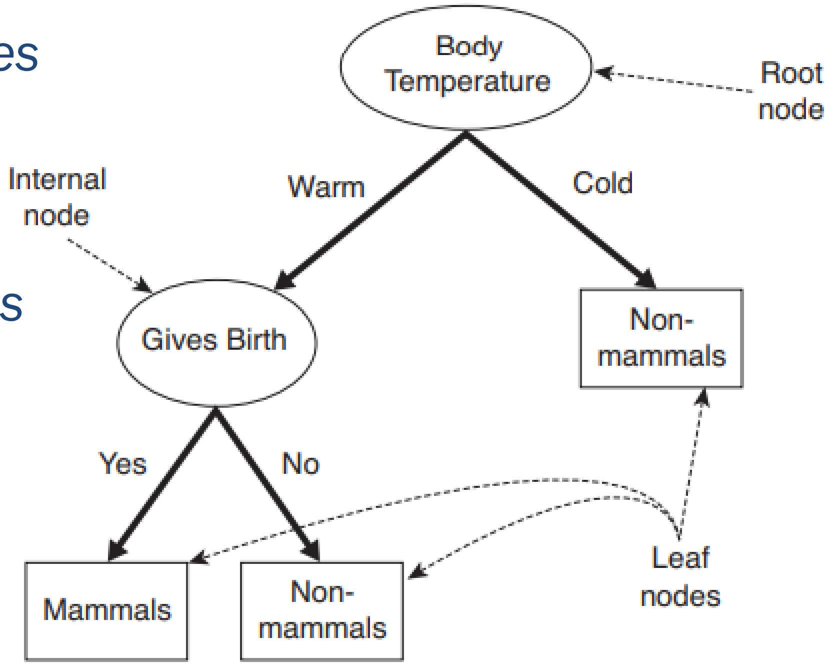
- Given a collection of records (*training set* )
  - *Each record contains a set of attributes, one of the attributes is the class.*
- Find a *model* for class attribute as a function of the values of other attributes.
- Goal: previously unseen records should be assigned a class as accurately as possible.
  - *A test set is used to determine the accuracy of the model.*
  - *Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it.*

# Classification Algorithms



# Mammals Classification

- Root node
  - *No incoming edges*
  - *Zoro or more outgoing edges*
- Internal Node
  - *One incoming edge*
  - *Two or more outgoing edges*
- Leaf/Terminal Node
  - *One incoming edges*
  - *No outgoing edges*



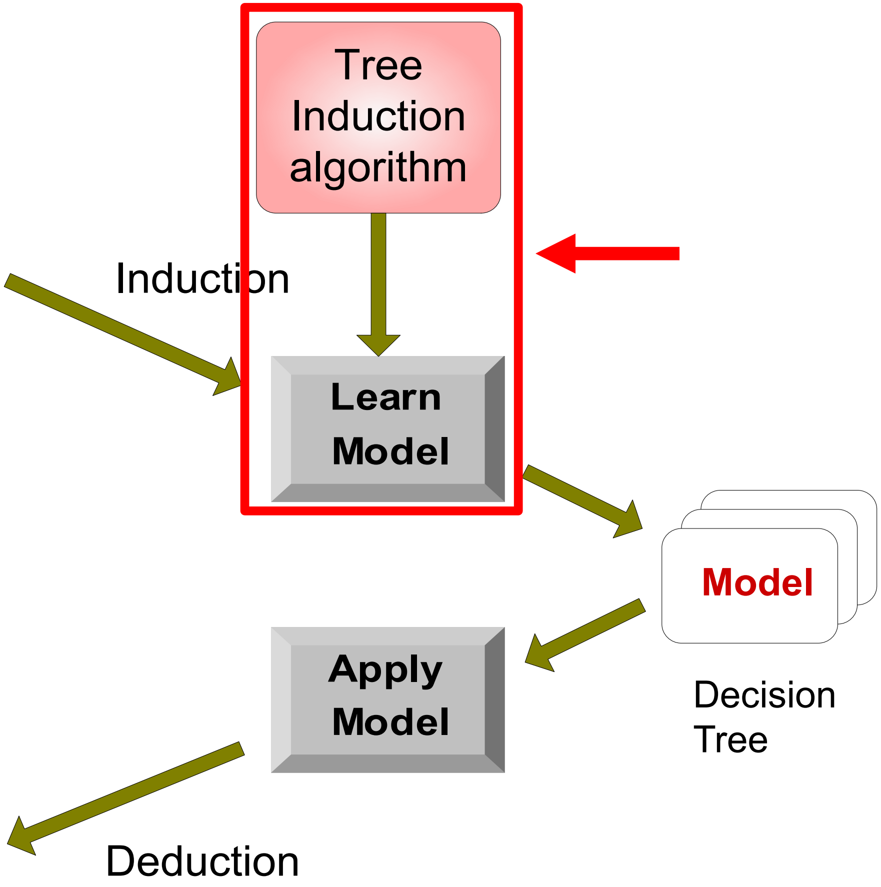
# Decision Tree Classification Task

| *Tid* | Attrib1 | Attrib2 | Attrib3 | Class |
|---|---|---|---|---|
| 1 | Yes | Large | 125K | No |
| 2 | No | Medium | 100K | No |
| 3 | No | Small | 70K | No |
| 4 | Yes | Medium | 120K | No |
| 5 | No | Large | 95K | Yes |
| 6 | No | Medium | 60K | No |
| 7 | Yes | Large | 220K | No |
| 8 | No | Small | 85K | Yes |
| 9 | No | Medium | 75K | No |
| 10 | No | Small | 90K | Yes |

Training Set

| *Tid* | Attrib1 | Attrib2 | Attrib3 | Class |
|---|---|---|---|---|
| 11 | No | Small | 55K | ? |
| 12 | Yes | Medium | 80K | ? |
| 13 | Yes | Large | 110K | ? |
| 14 | No | Small | 95K | ? |
| 15 | No | Large | 67K | ? |

Test Set



# Example of a Decision Tree

categorical categorical continuous class

| ID | Home Owner | Marital Status | Annual Income | Defaulted Borrower |
|---|---|---|---|---|
| 1 | Yes | Single | 125K | No |
| 2 | No | Married | 100K | No |
| 3 | No | Single | 70K | No |
| 4 | Yes | Married | 120K | No |
| 5 | No | Divorced | 95K | Yes |
| 6 | No | Married | 60K | No |
| 7 | Yes | Divorced | 220K | No |
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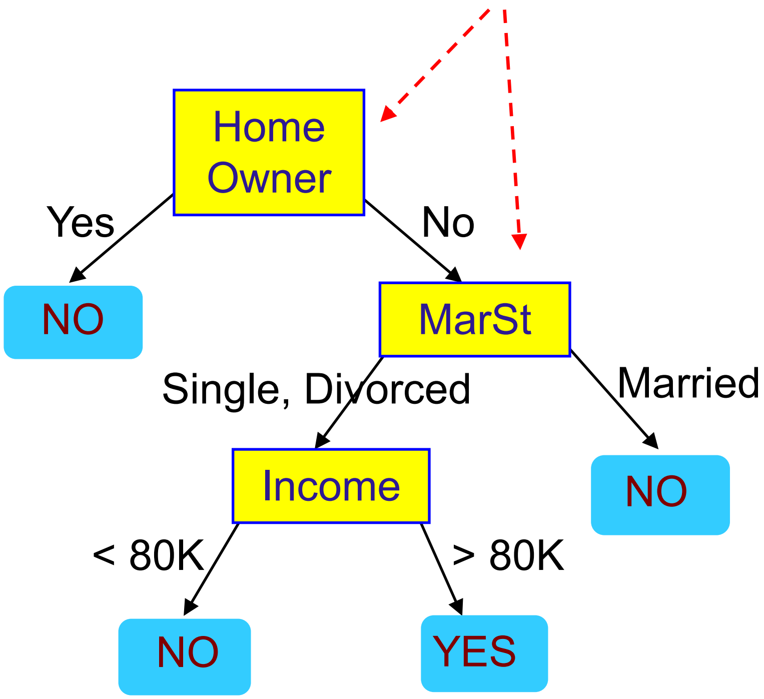
Training Data

*Splitting Attributes*



Model: Decision Tree

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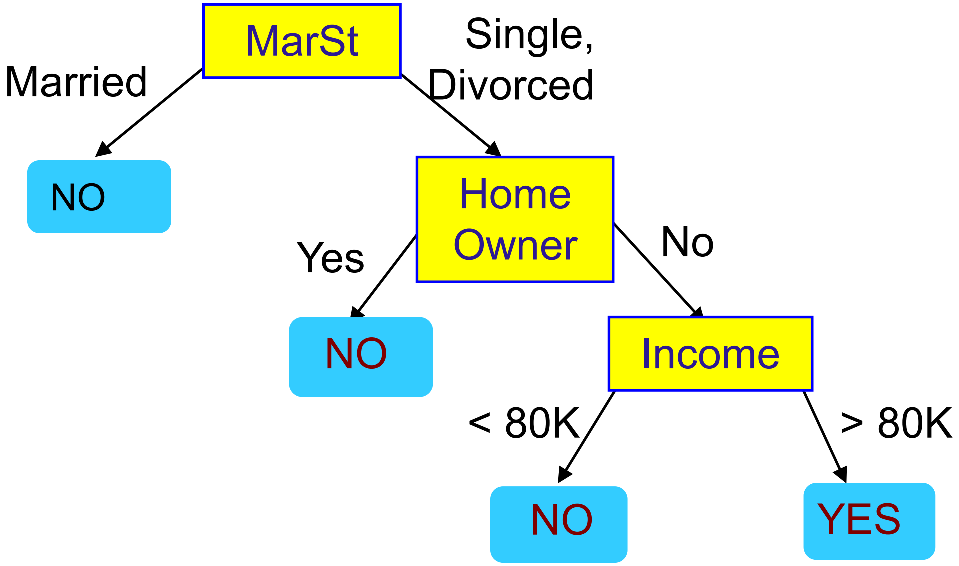
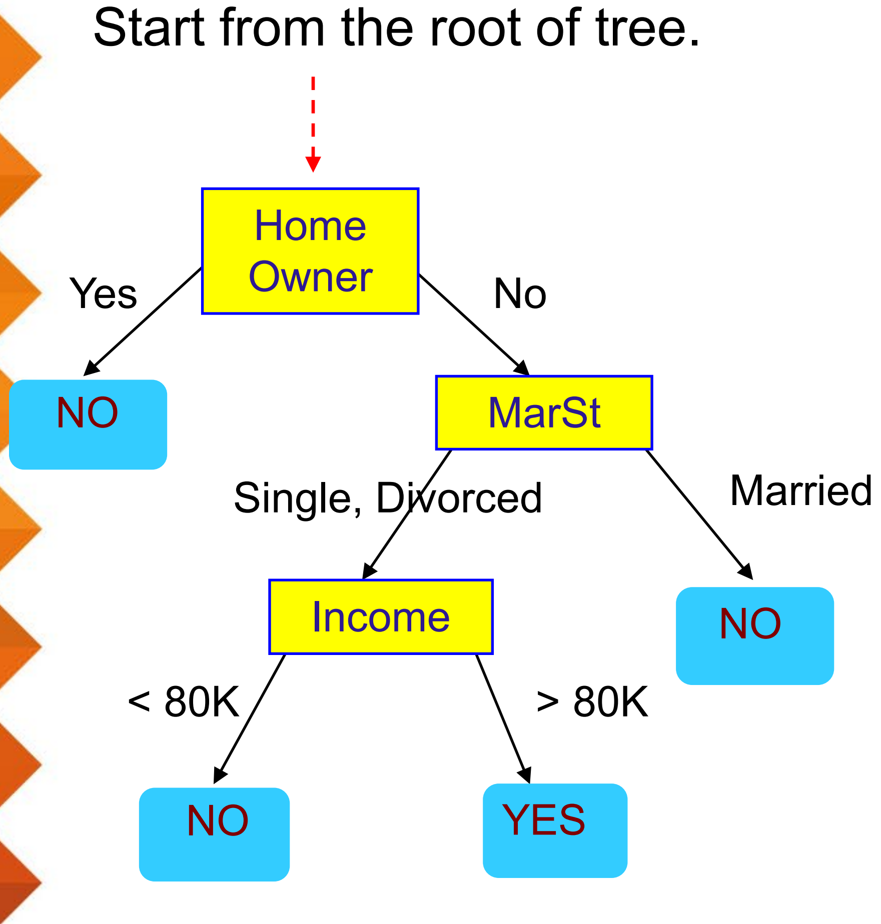
Training Data



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

# Apply Model to Test Data

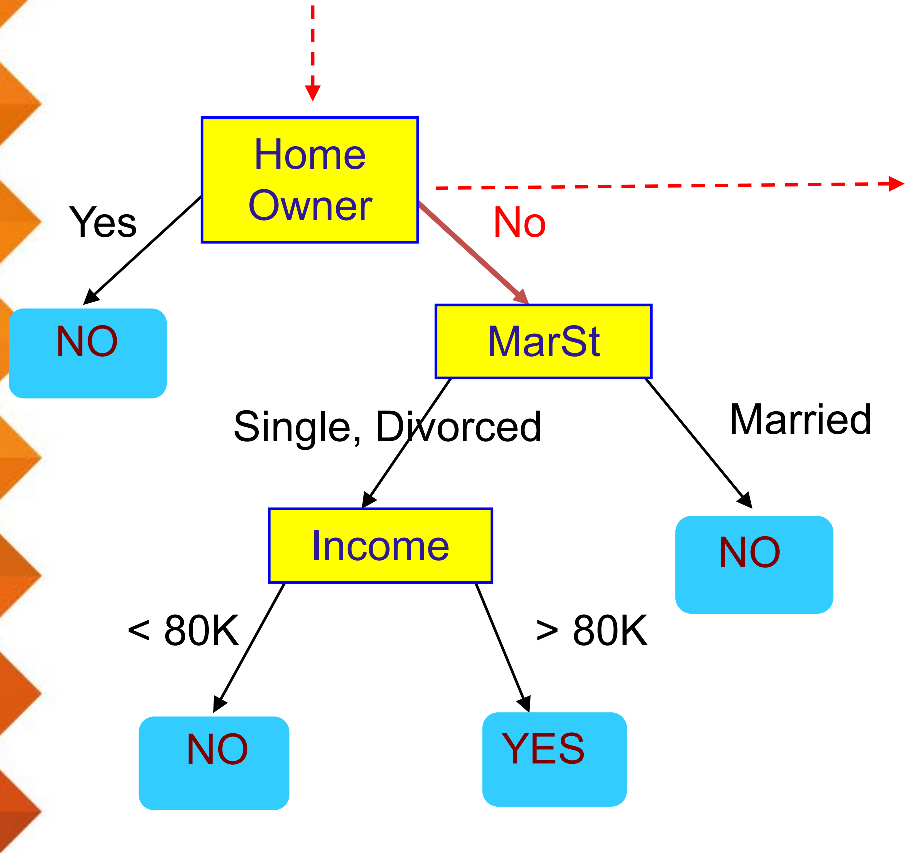

Start from the root of tree.

Test Data

| Home Owner | Marital Status | Annual Income | Defaulted Borrower |
|---|---|---|---|
| No | Married | 80K | ? |

# Apply Model to Test Data

Start from the root of tree.



Test Data

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# Apply Model to Test Data

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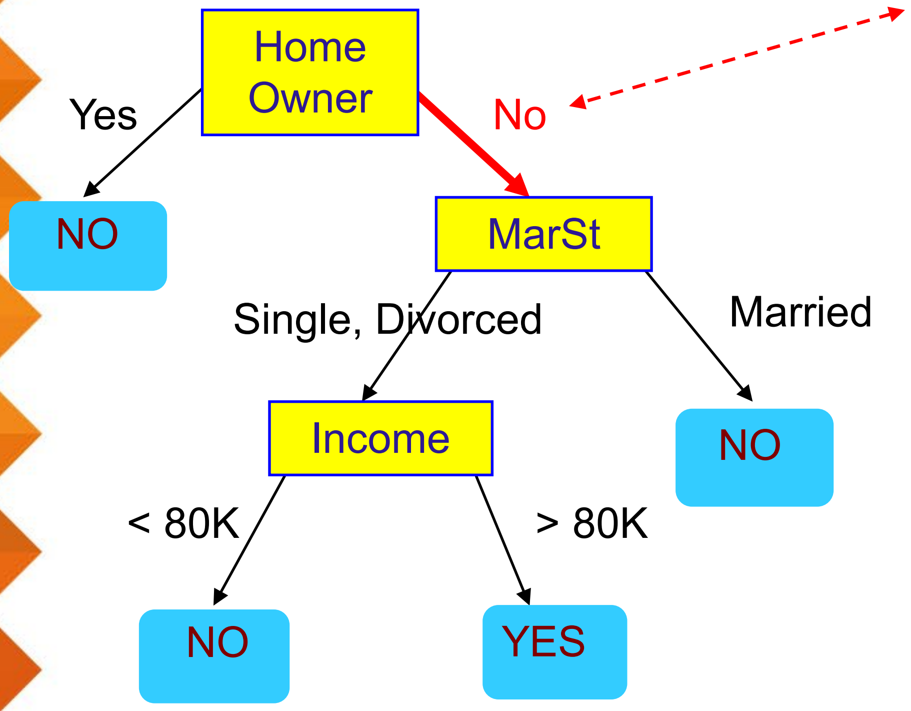

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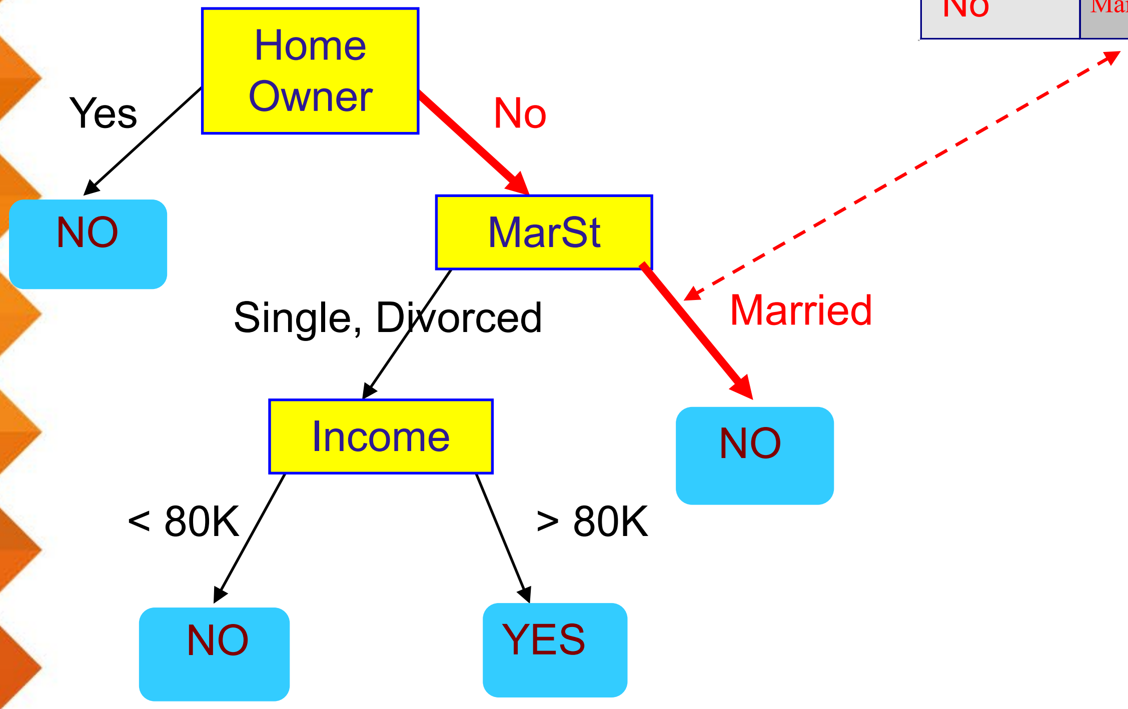

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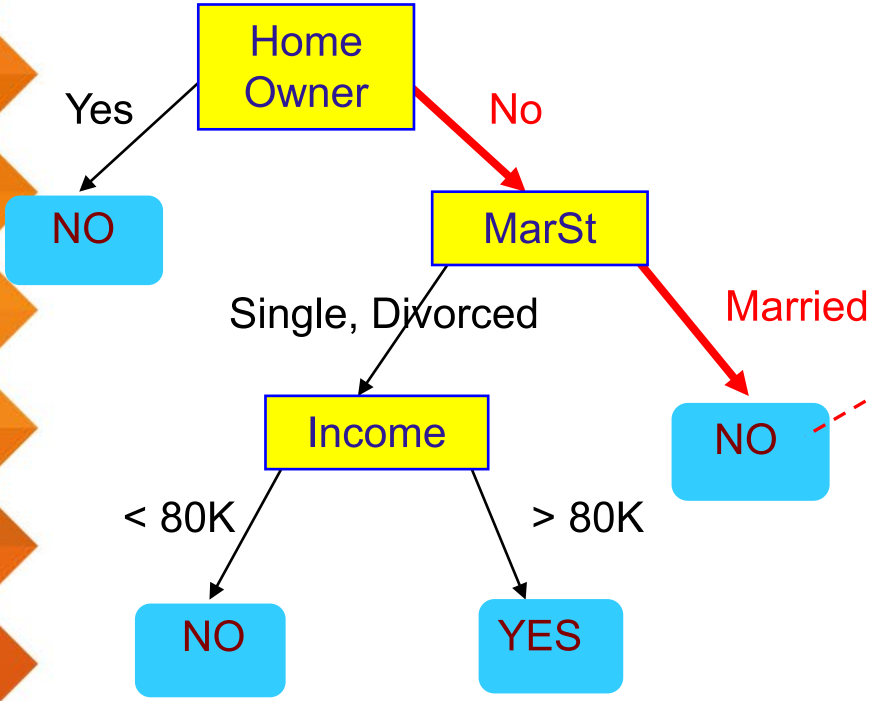

Home Owner

Yes

No

NO

MarSt

Single, Divorced

Married

Income

NO

< 80K

> 80K

NO

YES

Test Data

| Home Owner | Marital Status | Annual Income | Defaulted Borrower |
|---|---|---|---|
| No | Married | 80K | ? |

Assign Defaulted to “No”

# Decision Tree Induction

- Many Algorithms:
  - *Hunt's Algorithm (one of the earliest)*
  - *CART*
  - *ID3, C4.5*
  - *SLIQ,SPRINT*

# Predict if John will play tennis

- Hard to guess
- Try to understand when John plays
- Divide & conquer:
  - *split into subsets*
  - *are they pure? (all yes or all no)*
  - *if yes: stop*
  - *if not: repeat*
- See which subset
  - *New data falls into*

**Training examples: 9 yes/ 5 no**

| Day | Outlook | Humidity | Wind | Play |
|---|---|---|---|---|
| D1 | Sunny | High | Weak | No |
| D2 | Sunny | High | Strong | No |
| D3 | Overcast | High | Weak | Yes |
| D4 | Rain | High | Weak | Yes |
| D5 | Rain | Normal | Weak | Yes |
| D6 | Rain | Normal | Strong | No |
| D7 | Overcast | Normal | Weak | Yes |
| D8 | Sunny | High | Weak | No |
| D9 | Sunny | Normal | Weak | Yes |
| D10 | Rain | Normal | Strong | Yes |
| D11 | Sunny | Normal | Strong | Yes |
| D12 | Overcast | High | Strong | Yes |
| D13 | Overcast | Normal | Weak | Yes |
| D14 | Rain | High | Strong | No |
| New data: | | | | |
| D15 | Rain | High | Weak | ? |

# Predict if John will play tennis

- Hard to guess
- Try to understand when John plays
- Divide & conquer:
  - *split into subsets*
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| D6 | Rain | Normal | Strong | No |
| D7 | Overcast | Normal | Weak | Yes |
| D8 | Sunny | High | Weak | No |
| D9 | Sunny | Normal | Weak | Yes |
| D10 | Rain | Normal | Weak | Yes |
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| New data: | | | | |
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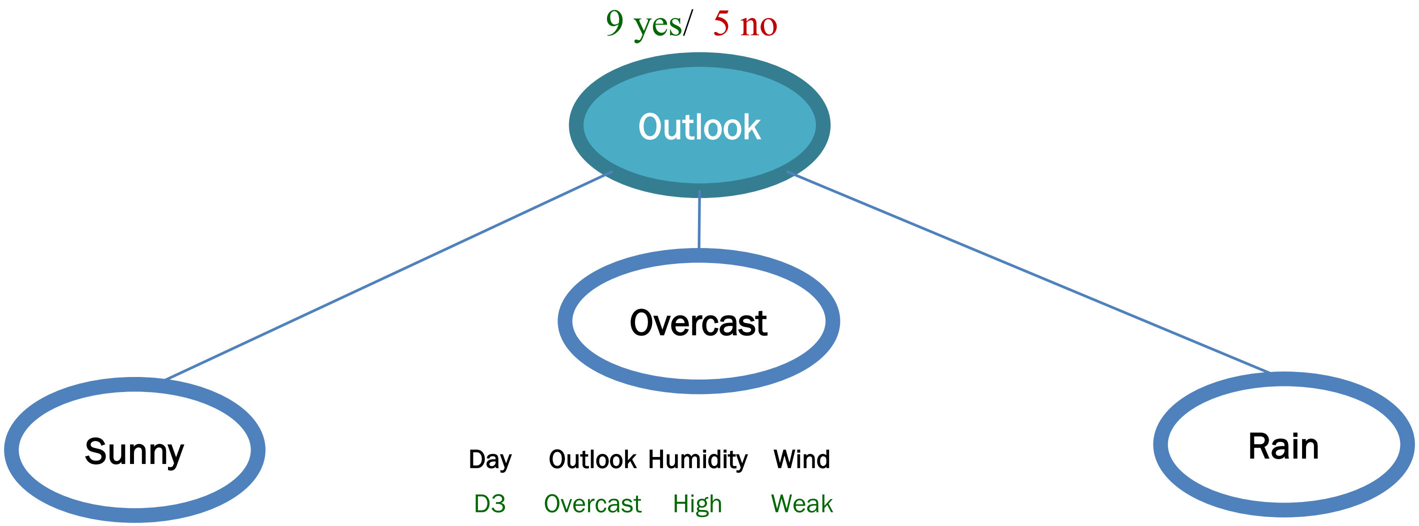

9 yes/ 5 no

Outlook

Overcast

Sunny

Rain

| Day | Outlook | Humidity | Wind |
|---|---|---|---|
| D1 | Sunny | High | Weak |
| D2 | Sunny | High | Strong |
| D8 | Sunny | High | Weak |
| D9 | Sunny | Normal | Weak |
| D11 | Sunny | Normal | Strong |

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|---|---|---|---|
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| D12 | Overcast | High | Strong |
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| Day | Outlook | Humidity | Wind |
|---|---|---|---|
| D4 | Rain | High | Weak |
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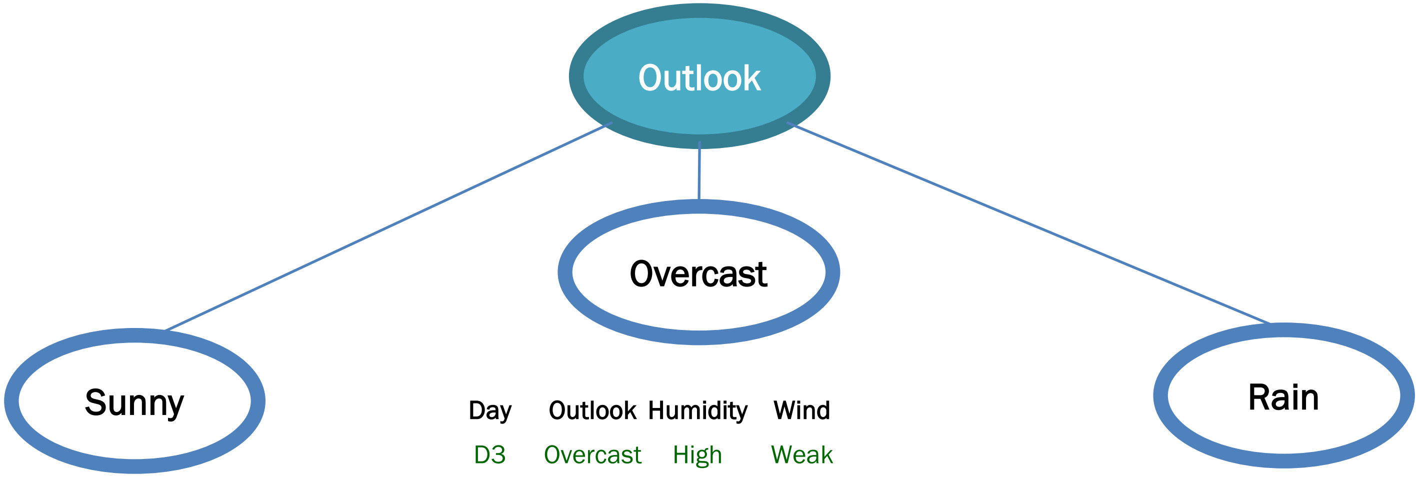
9 yes/ 5 no



Outlook

Overcast

Sunny

Rain

| Day | Outlook | Humidity | Wind |
|---|---|---|---|
| D1 | Sunny | High | Weak |
| D2 | Sunny | High | Strong |
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| D9 | Sunny | Normal | Weak |
| D11 | Sunny | Normal | Strong |

2 yes/ 3 no

Split further

| Day | Outlook | Humidity | Wind |
|---|---|---|---|
| D3 | Overcast | High | Weak |
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| D12 | Overcast | High | Strong |
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4 yes/ 0 no

pure subset

| Day | Outlook | Humidity | Wind |
|---|---|---|---|
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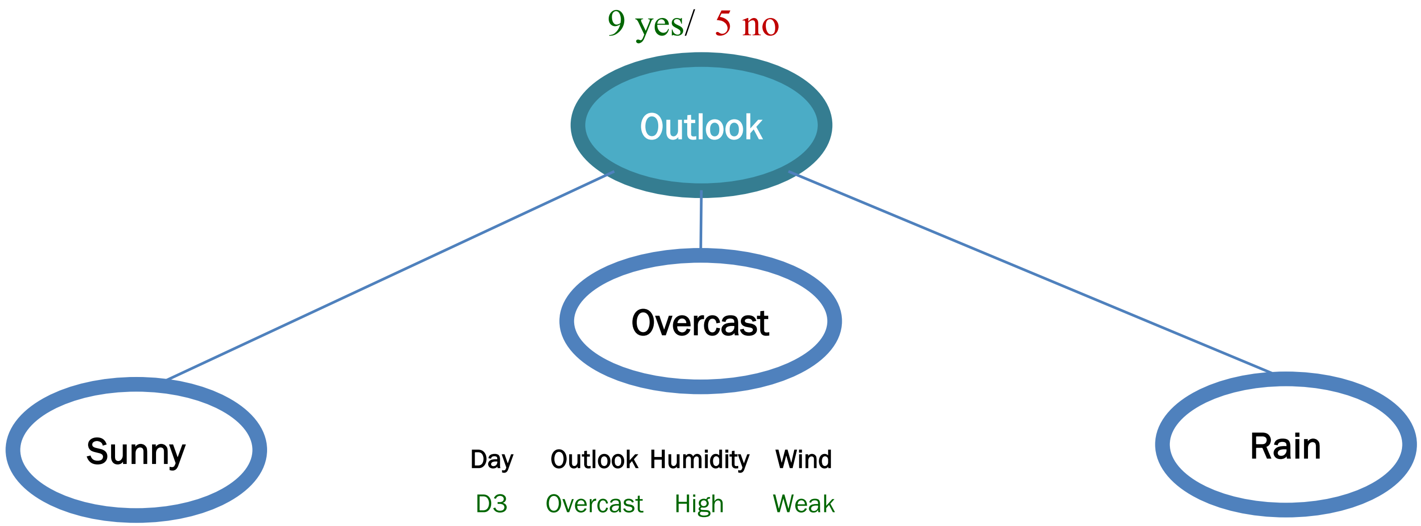
3 yes/ 2 no

Split further

9 yes/ 5 no



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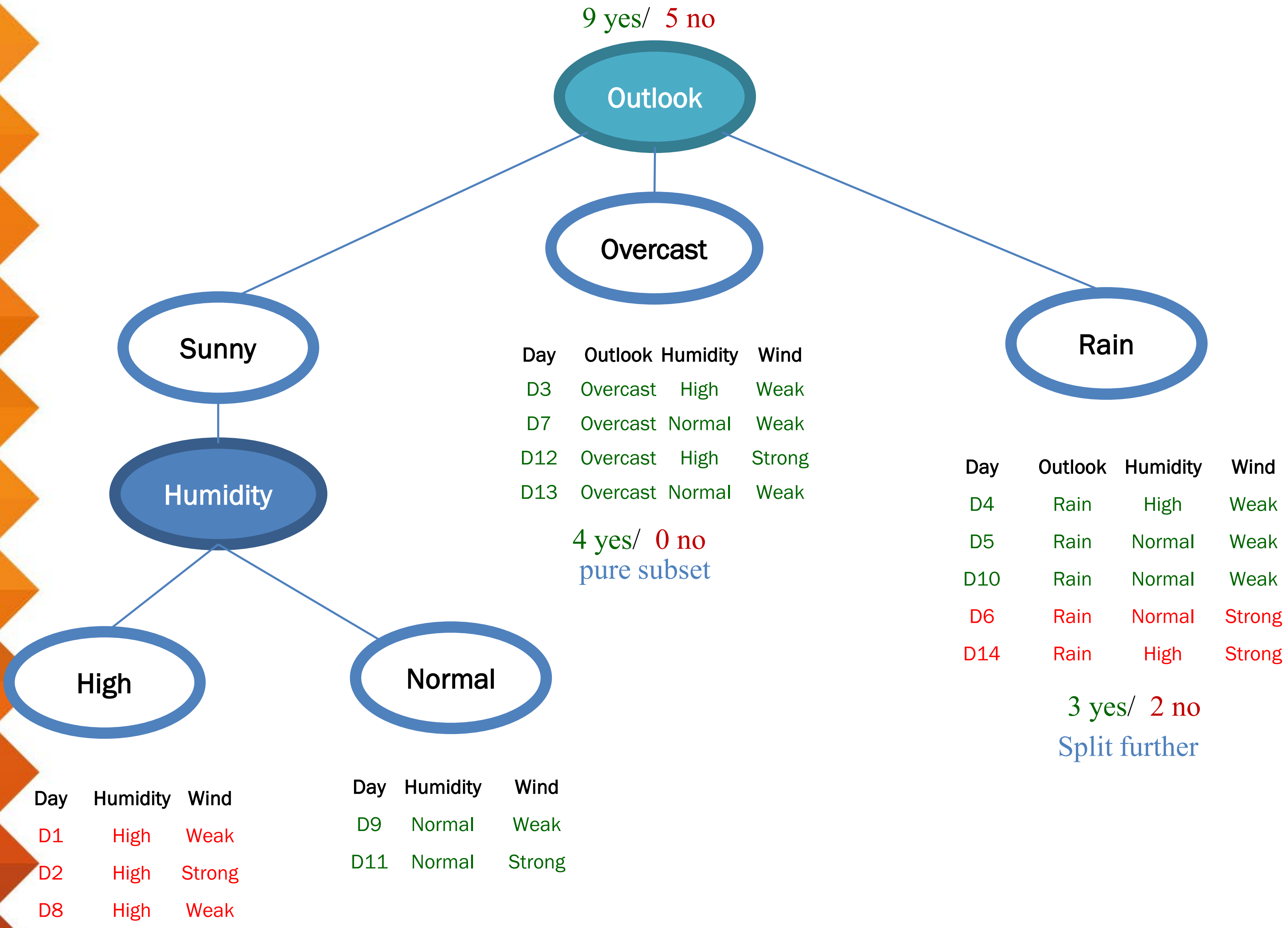

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Split further

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| Day | Humidity | Wind |
|---|---|---|
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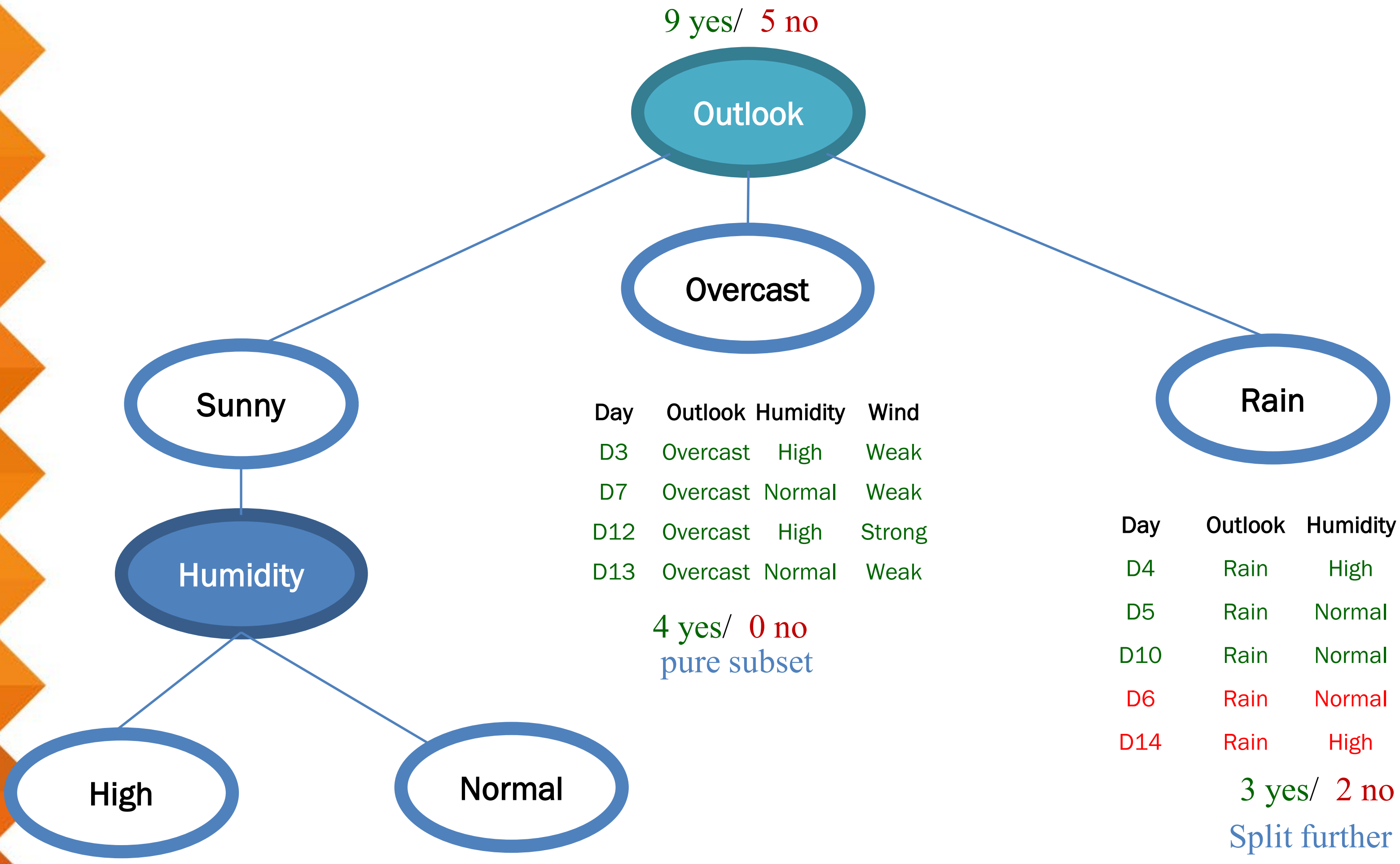

9 yes/ 5 no

Outlook

Sunny

Overcast

Rain

Humidity

High

Normal

| Day | Outlook | Humidity | Wind |
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Split further

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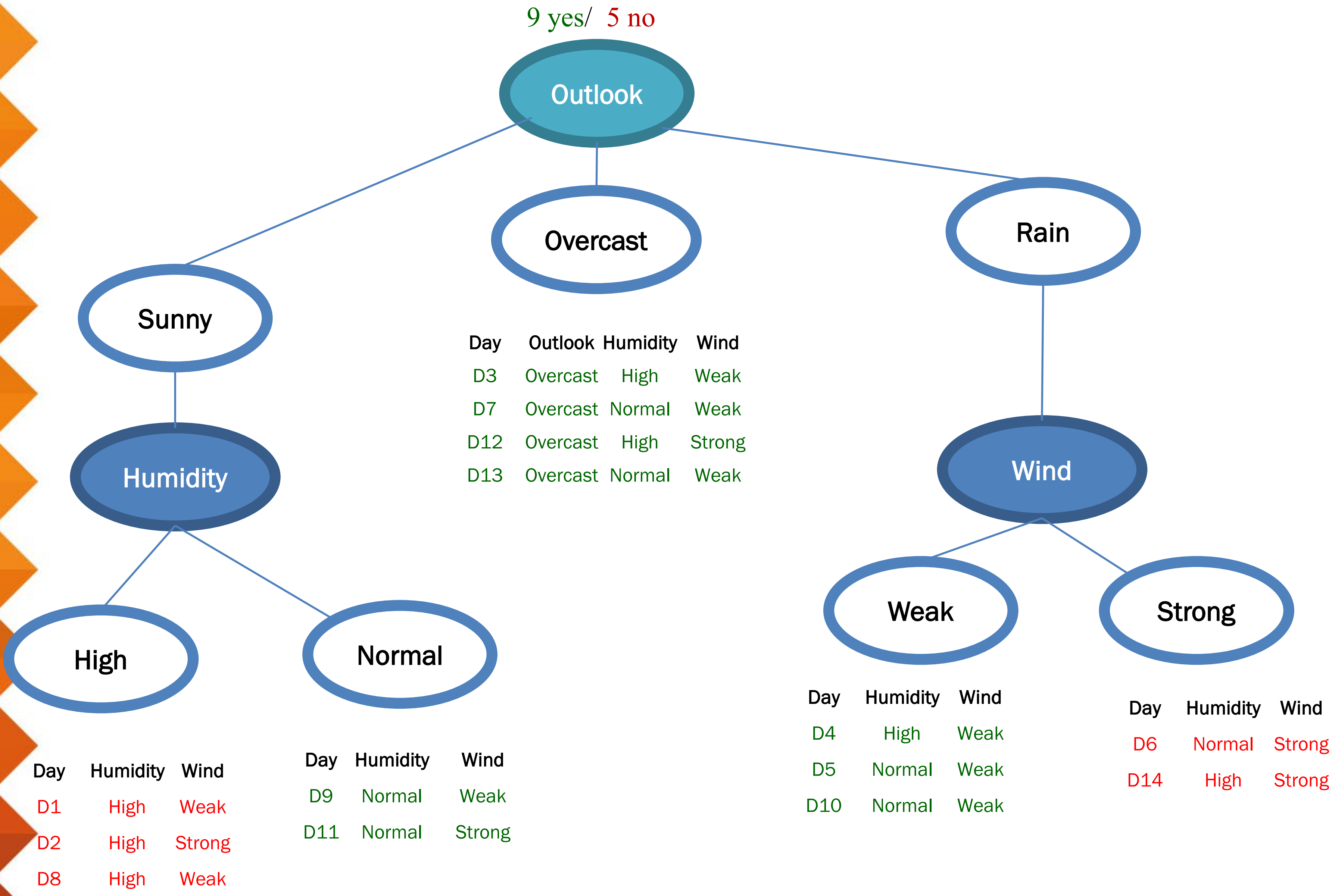

9 yes/ 5 no

Outlook

Sunny

Overcast

Rain

Humidity

Wind

High

Normal

Weak

Strong

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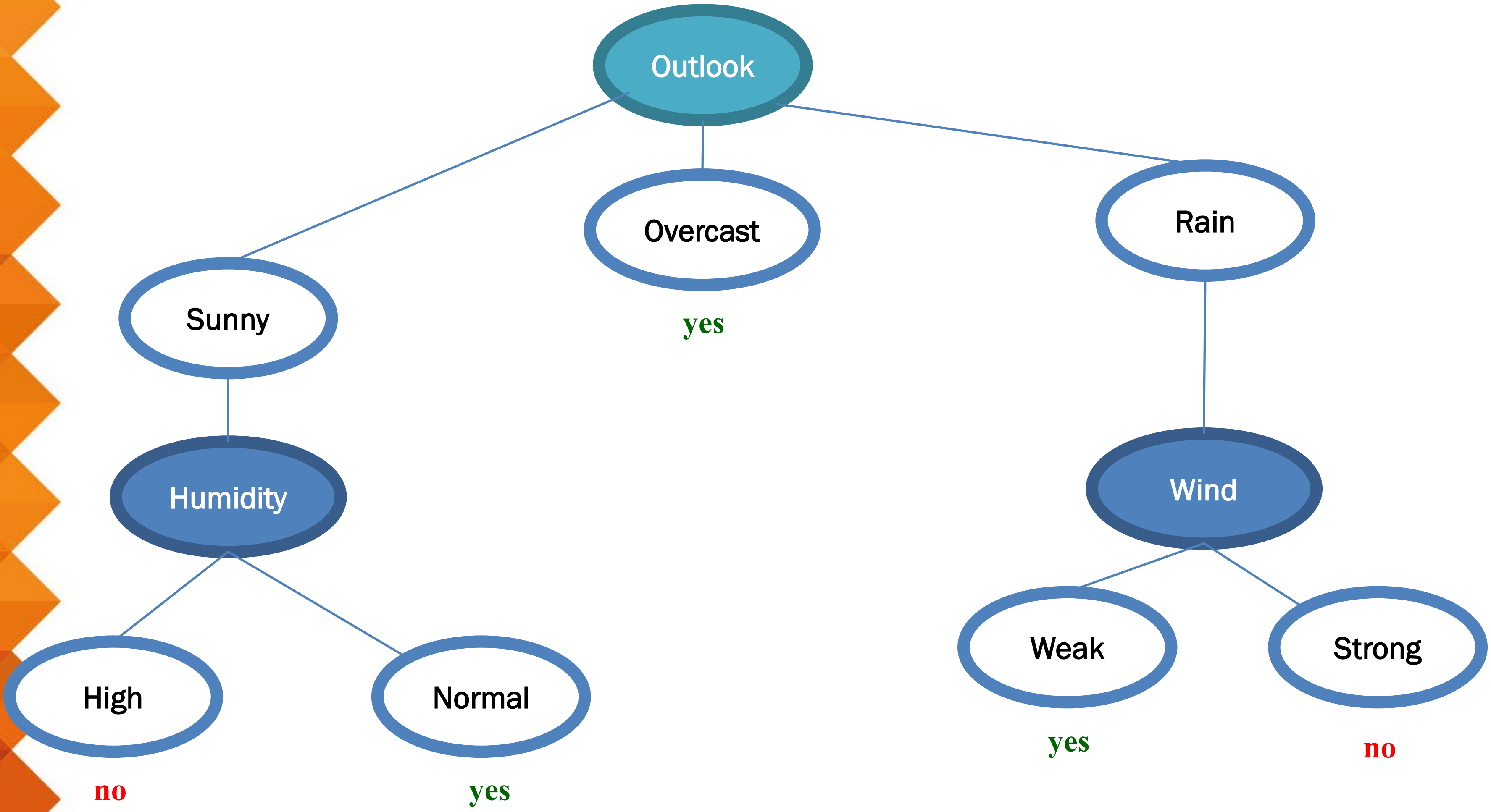
Outlook
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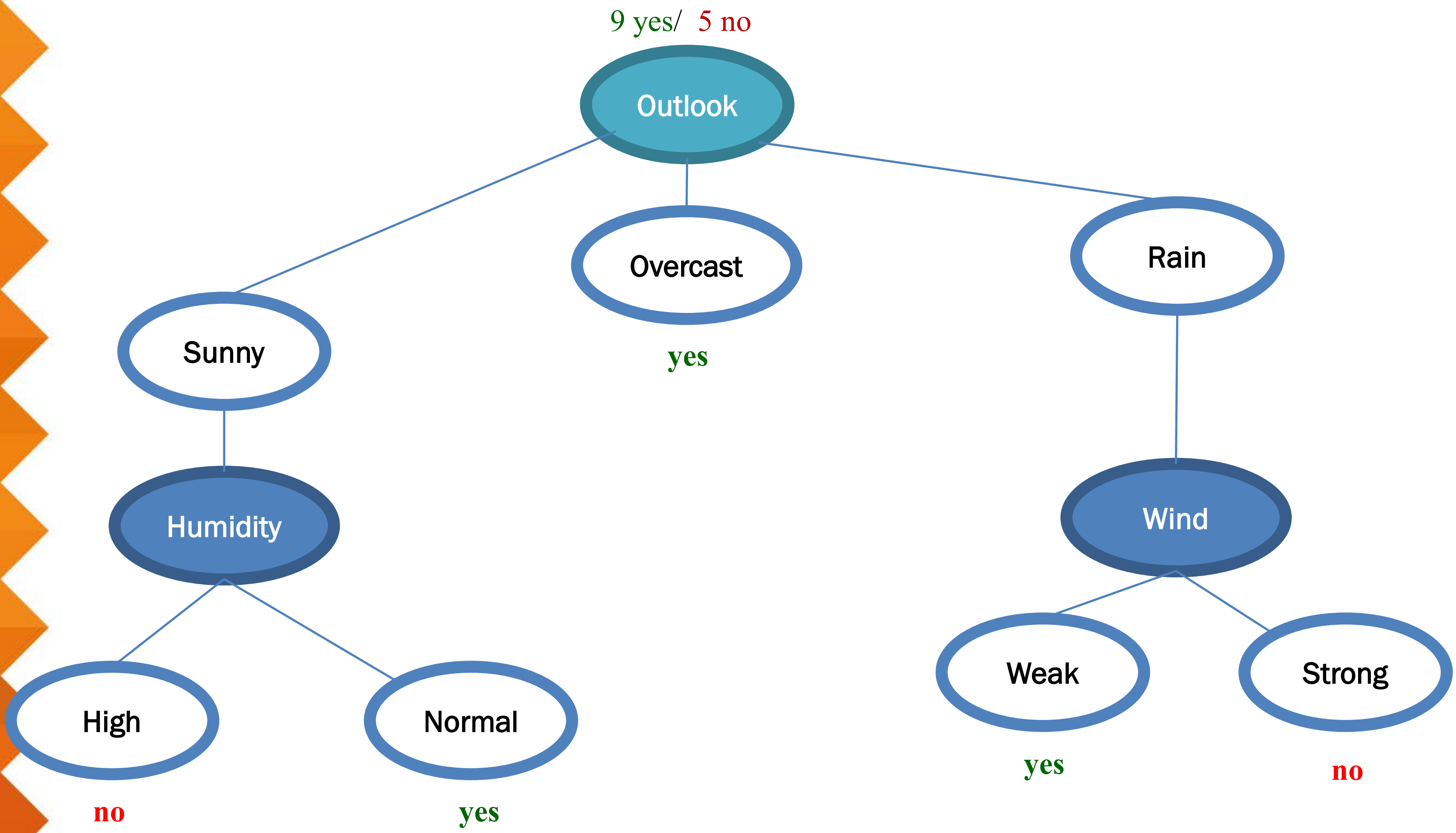
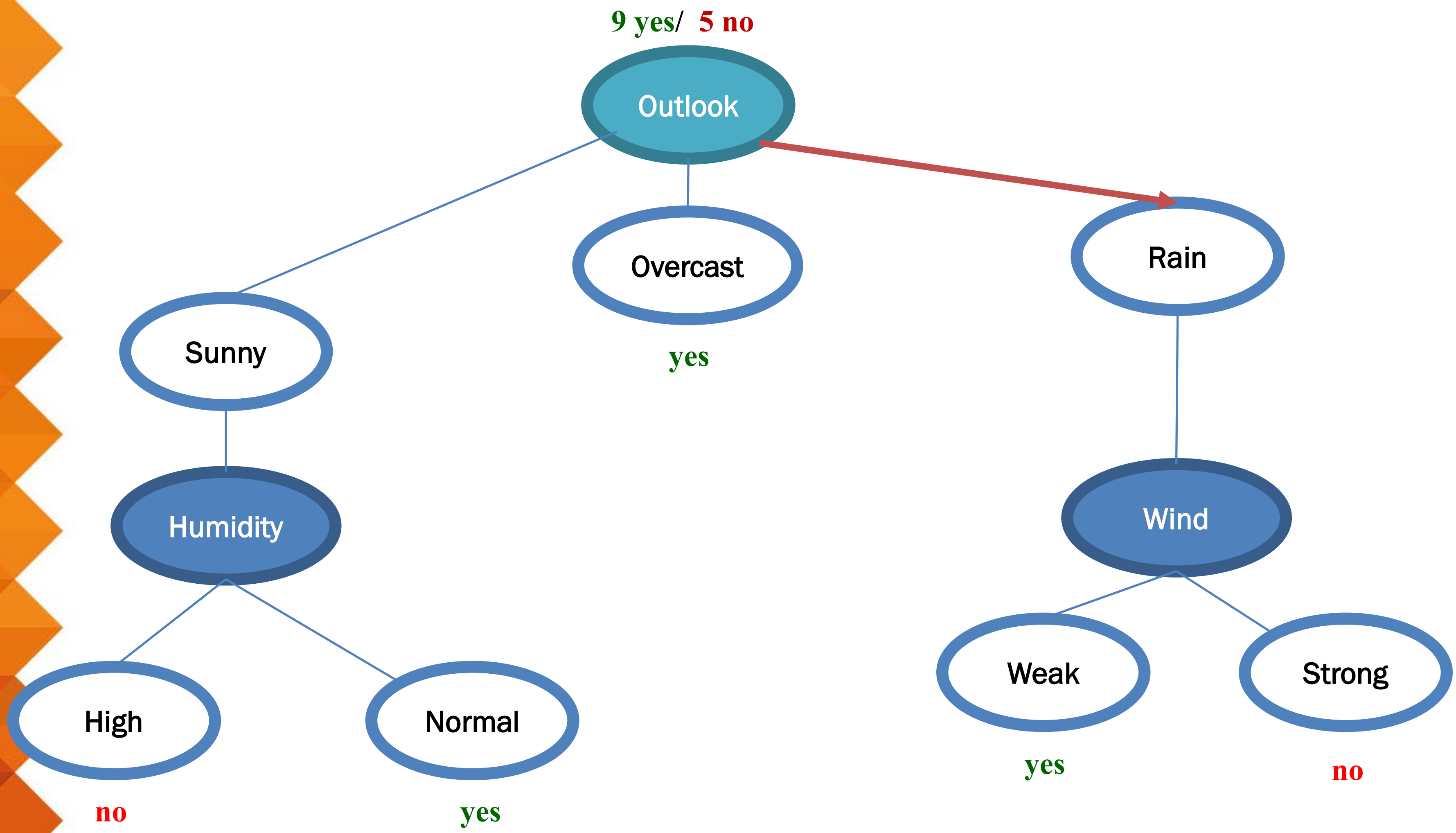


**New data:**

| Day | Outlook | Humidity | Wind | **Play** |
|---|---|---|---|---|
| D15 | Rain | High | Weak | ? |



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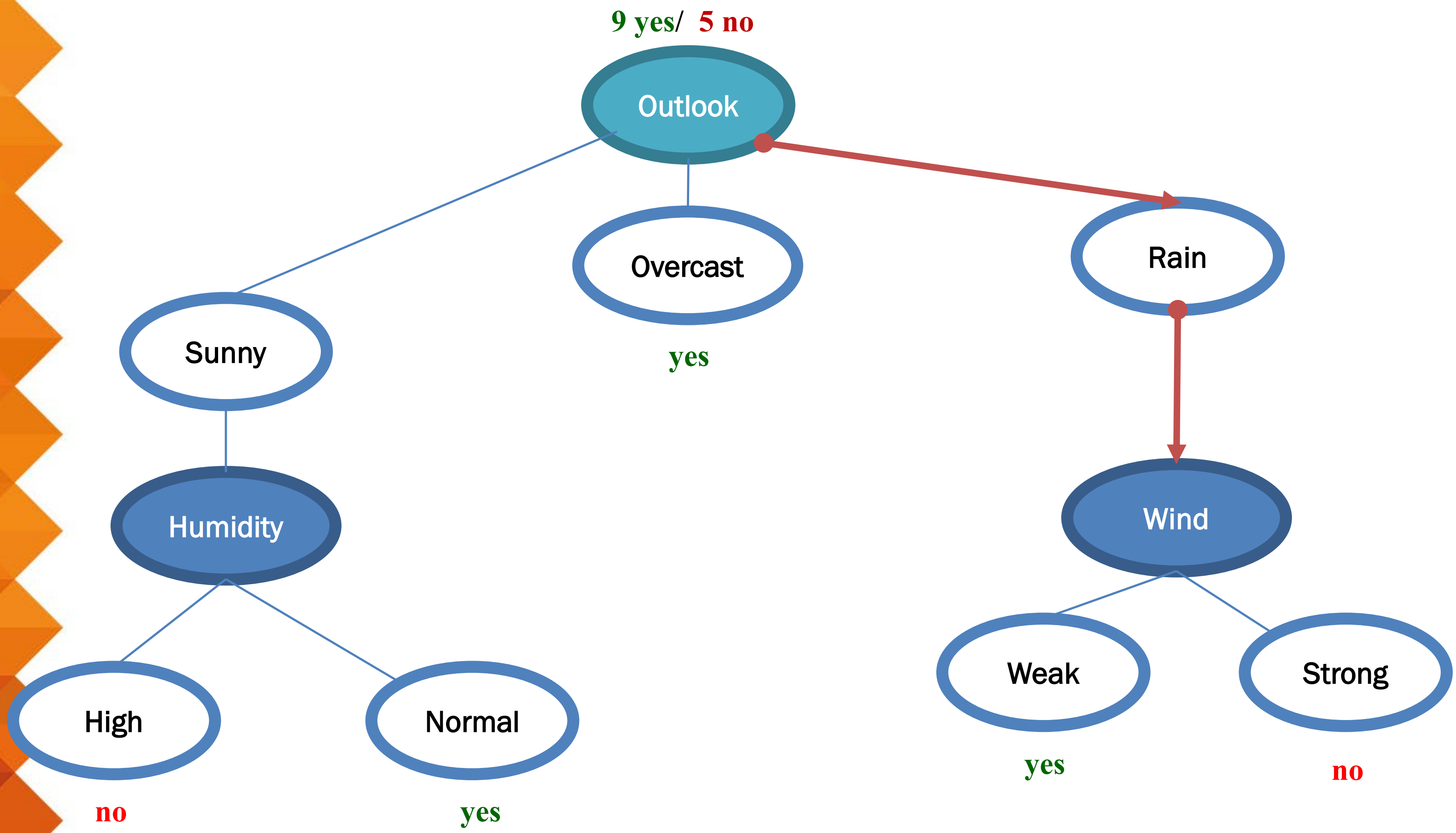

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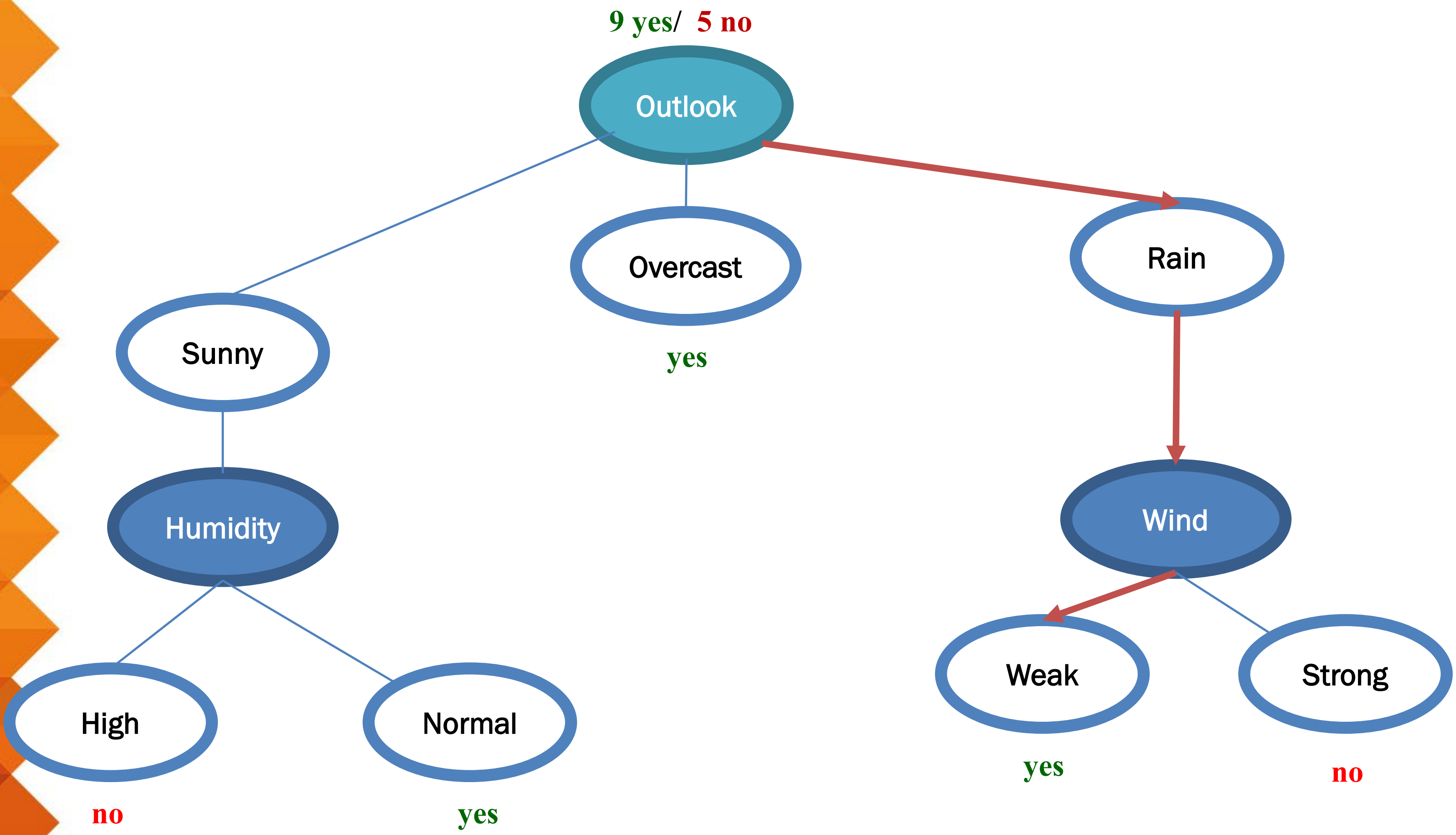

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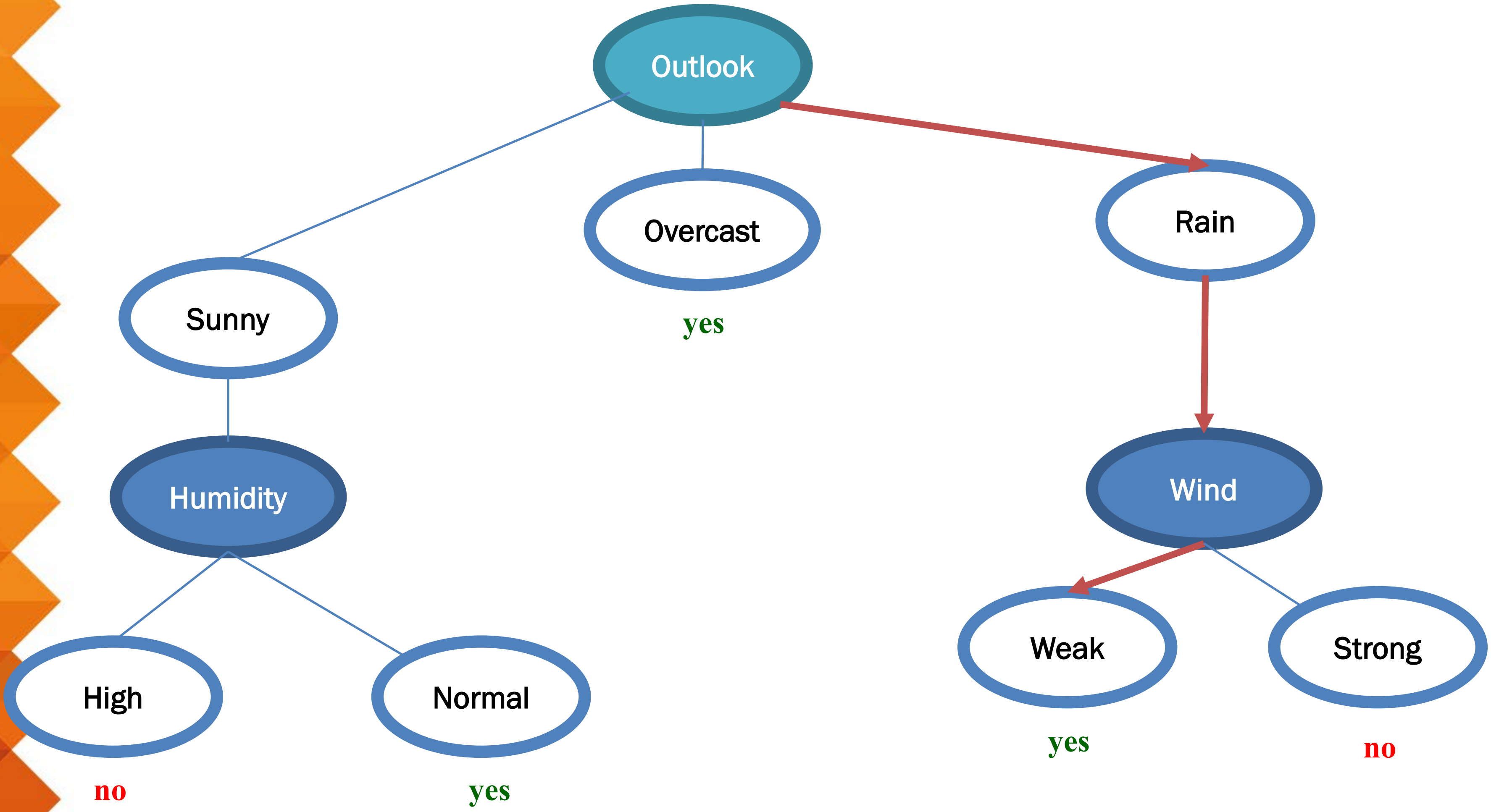

**New data:**

| Day | Outlook | Humidity | Wind | **Play** |
|---|---|---|---|---|
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# Tree Induction

- Greedy strategy.
  - *Split the records based on an attribute test that optimizes certain criterion.*

- Issues
  - *Determine how to split the records*
    - How to specify the attribute test condition?
    - How to determine the best split?
  - *Determine when to stop splitting*

# Tree Induction

- Greedy strategy.
  - *Split the records based on an attribute test that optimizes certain criterion.*

- Issues
  - *Determine how to split the records*
    - How to specify the attribute test condition?
    - How to determine the best split?
  - *Determine when to stop splitting*

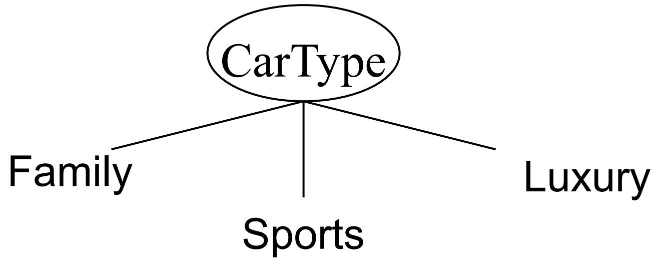
# How to Specify Test Condition?

- Depends on attribute types
  - *Nominal*
  - *Ordinal*
  - *Continuous*

- Depends on number of ways to split
  - *2-way split*
  - *Multi-way split*

# Splitting Based on Nominal Attributes

- Multi-way split: Use as many partitions as distinct values.



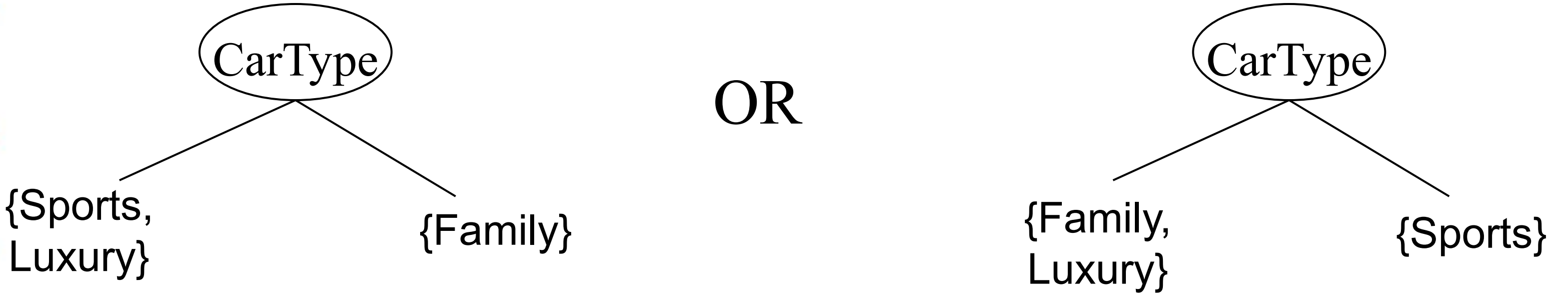
CarType

Family

Sports

Luxury

- Binary split: Divides values into two subsets.
  Need to find optimal partitioning.



CarType

{Sports, Luxury}

{Family}

OR

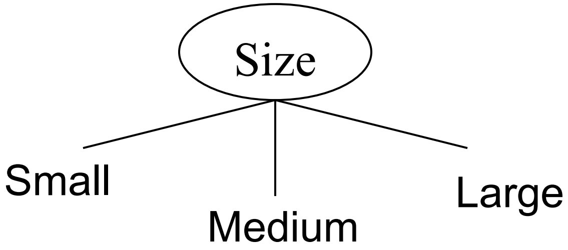
CarType

{Family, Luxury}

{Sports}

# Splitting Based on Ordinal Attributes

- Multi-way split: Use as many partitions as distinct values.



Size

Small

Medium

Large

- Binary split: Divides values into two subsets.
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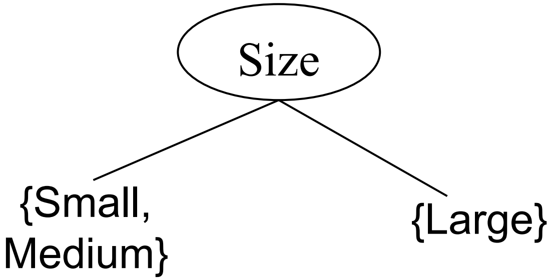
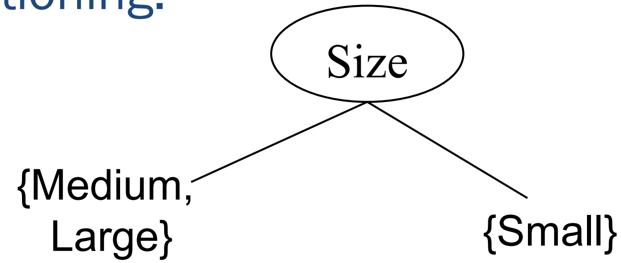


Size

{Small, Medium}

{Large}

OR

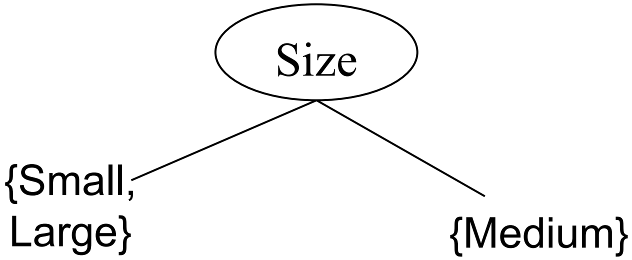


Size

{Medium, Large}

{Small}

- What about this split?



Size

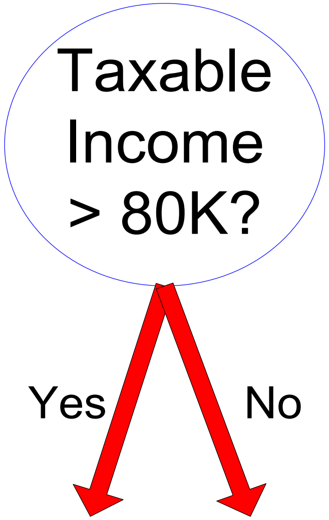
{Small, Large}

{Medium}

# Splitting Based on Continuous Attributes

- Different ways of handling
  - *Discretization to form an ordinal categorical attribute*
    - Static – discretize once at the beginning
    - Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - *Binary Decision: (A < v) or (A ≥ v)*
    - consider all possible splits and finds the best cut
    - can be more computationally intensive

# Splitting Based on Continuous Attributes

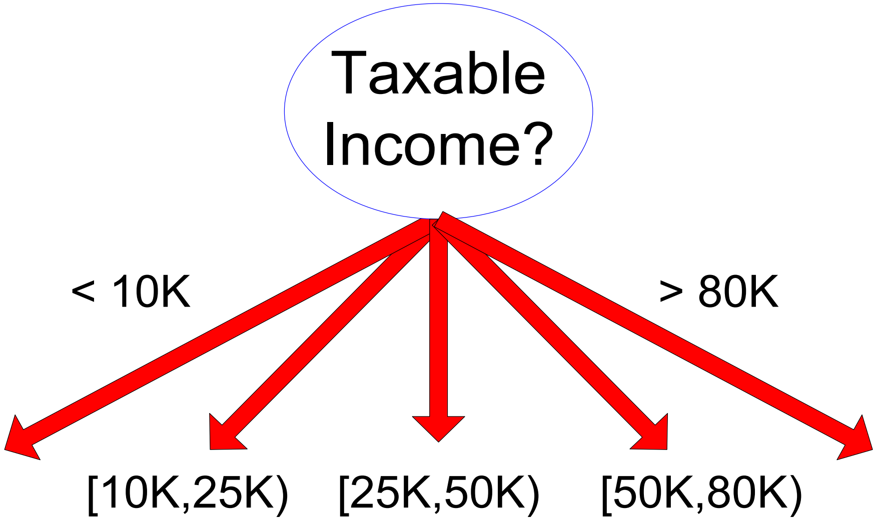


Taxable Income > 80K?

Yes

No

(i) Binary split



Taxable Income?

< 10K

[10K,25K)

[25K,50K)

[50K,80K)

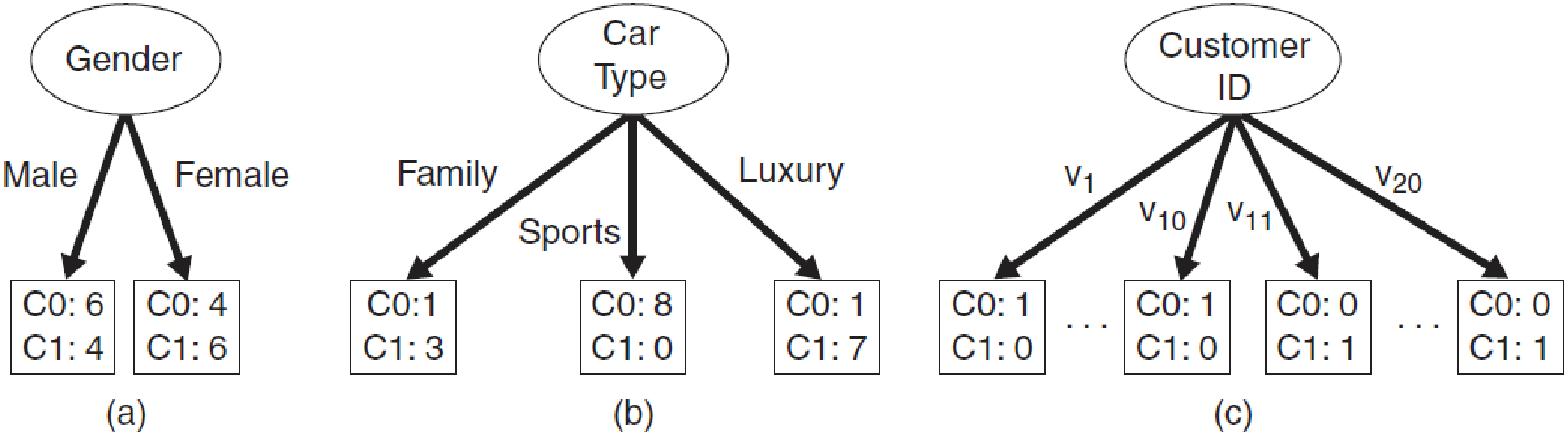
> 80K

(ii) Multi-way split

# How to determine the Best Split?

**Before Splitting: 10 records of class 0,**
**10 records of class 1**

C0: 10
C1: 10



**Which test condition is the best?**

# How to determine the Best Split?

- Greedy approach:
  - *Nodes with homogeneous class distribution are preferred*
- Need a measure of node impurity:

C0: 5
C1: 5

**Non-homogeneous,**

**High degree of impurity**

C0: 9
C1: 1

**Homogeneous,**

**Low degree of impurity**

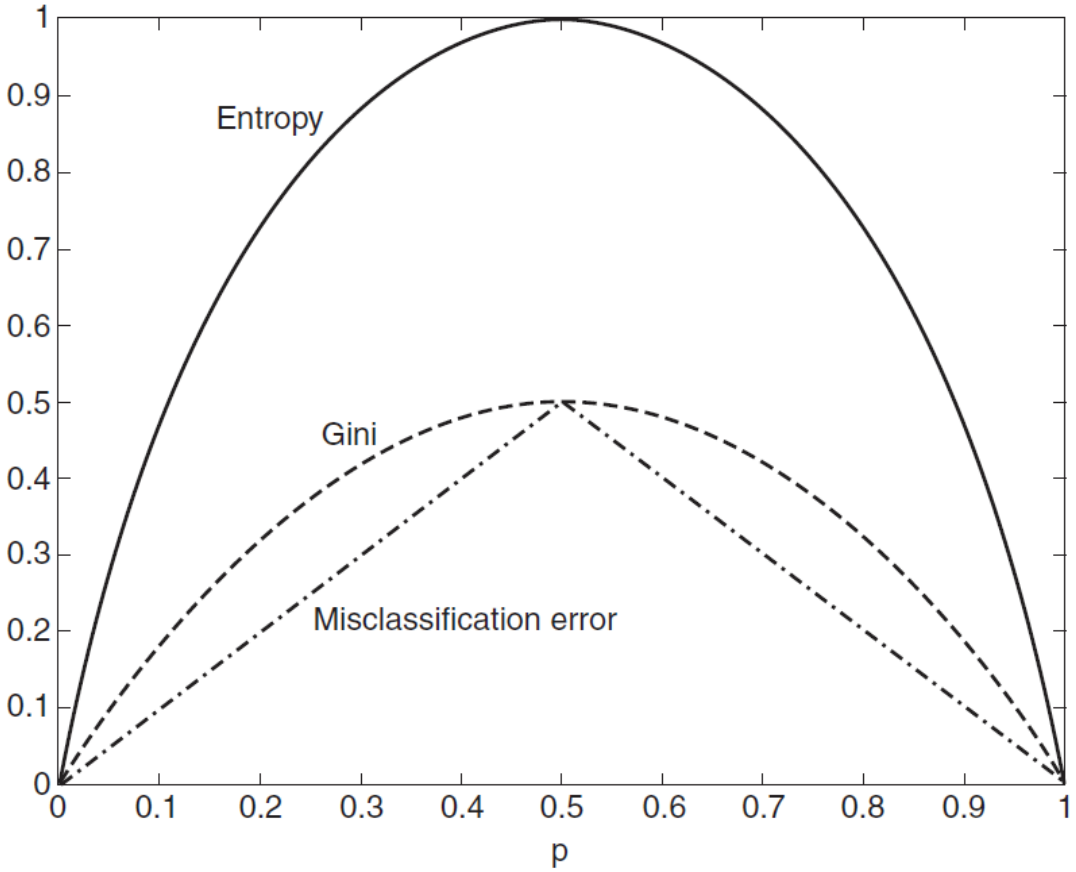
# Measures of Node Impurity

p(i|t): fraction of records associated with node **t** belonging to class **i**

$$\begin{aligned} \text{Entropy}(t) &= -\sum_{i=0}^{c-1} p(i|t)\log_2 p(i|t), \\ \text{Gini}(t) &= 1-\sum_{i=0}^{c-1}[p(i|t)]^2, \\ \text{Classification error}(t) &= 1-\max_i[p(i|t)], \end{aligned}$$

# Comparison

- For a 2-class problem:
  - *Probability of the majority class p is always > .5*



# Splitting Criteria based on Classification Error

- Classification error at a node t :

$$\boxed{Error(t) = 1 - \max_i P(i \mid t)}$$

- Measures misclassification error made by a node.
  - Maximum (1 - 1/$n_c$) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0.0) when all records belong to one class, implying most interesting information

# Computing Error of a Single Node

$$\boxed{Error(t) = 1 - \max_i P(i \mid t)}$$

| | |
|---|---|
| C1 | **0** |
| C2 | **6** |

P(C1) = 0/6 = 0     P(C2) = 6/6 = 1

Error = 1 – max (0, 1) = 1 – 1 = 0

| | |
|---|---|
| C1 | **1** |
| C2 | **5** |

P(C1) = 1/6     P(C2) = 5/6

Error = 1 – max (1/6, 5/6) = 1 – 5/6 = 1/6

| | |
|---|---|
| C1 | **2** |
| C2 | **4** |

P(C1) = 2/6     P(C2) = 4/6

Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

# Example

| | |
|---|---|
| C1 | **0** |
| C2 | **6** |

P(C1) = 0/6 = 0     P(C2) = 6/6 = 1

Entropy = – 0 log 0 – 1 log 1 = – 0 – 0 = 0

Error = 1 – max (0, 1) = 1 – 1 = 0

| | |
|---|---|
| C1 | **1** |
| C2 | **5** |

P(C1) = 1/6          P(C2) = 5/6

Entropy = – (1/6) $\log_2$ (1/6) – (5/6) $\log_2$ (1/6) = 0.65

Error = 1 – max (1/6, 5/6) = 1 – 5/6 = 1/6 = 0.16

| | |
|---|---|
| C1 | **2** |
| C2 | **4** |

P(C1) = 2/6          P(C2) = 4/6

Entropy = – (2/6) $\log_2$ (2/6) – (4/6) $\log_2$ (4/6) = 0.92

Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3 = 0.33

# Impurity measures

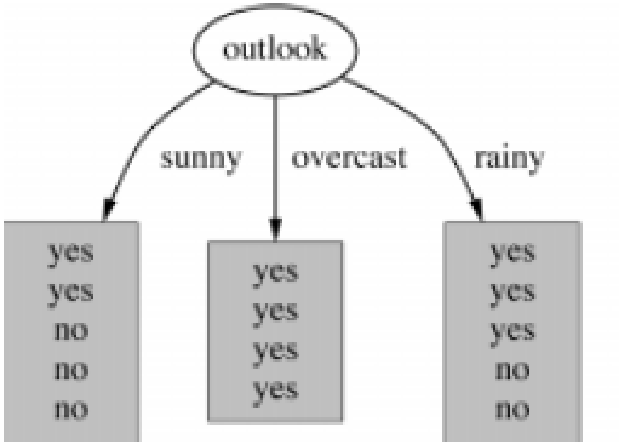
- All of the impurity measures take value zero (minimum) for the case of a pure node where a single value has probability 1

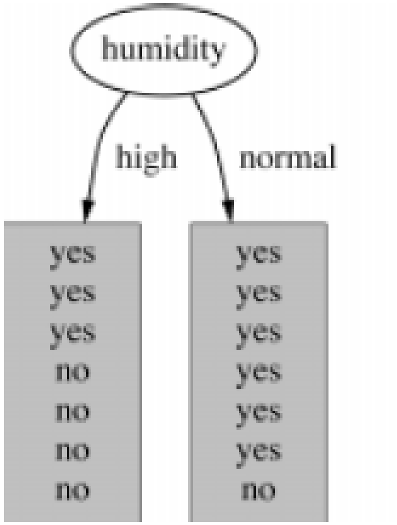
- All of the impurity measures take maximum value when the class distribution in a node is uniform.

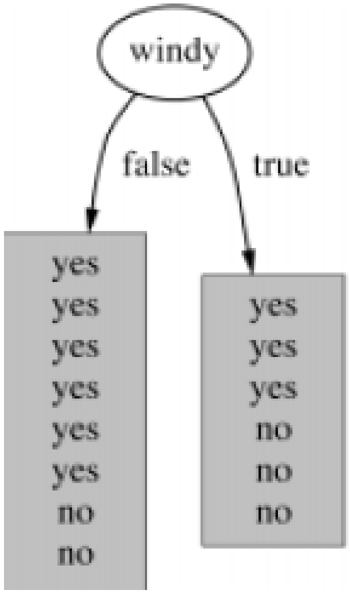
# Decision Trees Classifiers

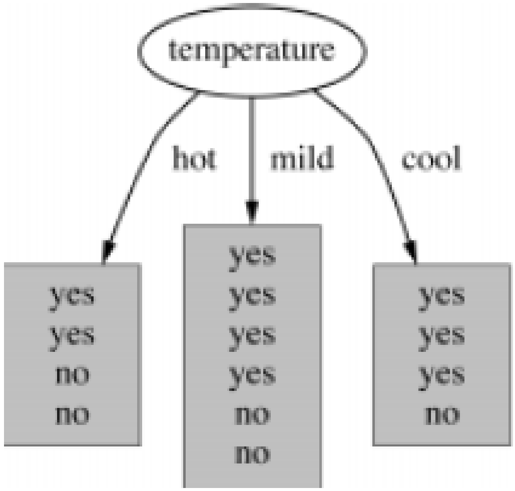
- Normal procedure: top down in recursive divide and conquer fashion
- First: attribute is selected for root node and branch is created for each possible attribute value
- Then: the instances are split into subsets (one for each branch extending from the node)
- Finally: procedure is repeated recursively for each branch, using only instances that reach the branch
- Process stops if all instances have the same class

# Decision Trees: which attribute to select?









# Criterion for attribute selection

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

# Computing Information Gain

- Information is measured in bits
  - *Given a probability distribution, the info required to predict an event is the distribution's entropy*
  - *Entropy gives the information required in bits (this can involve fractions of bits!)*
- Formula for computing the entropy:

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

Where $p_1$, $p_2$, …., $p_n$ denote the probability of occurrence of outcomes for class 1, 2, …, n respectively

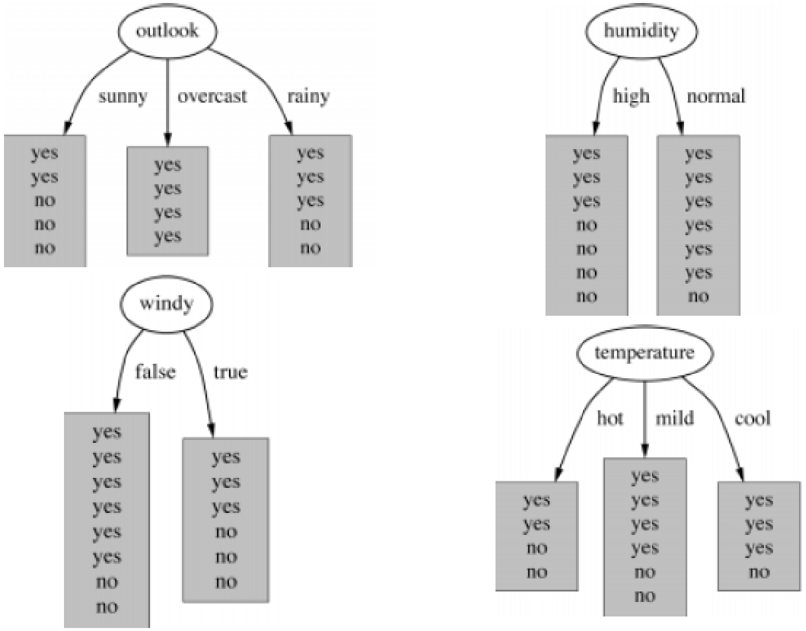
# Example: Attribute Outlook

- "Outlook" = "Sunny":

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

- "Outlook" = "Overcast":

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



# Example: Attribute Outlook

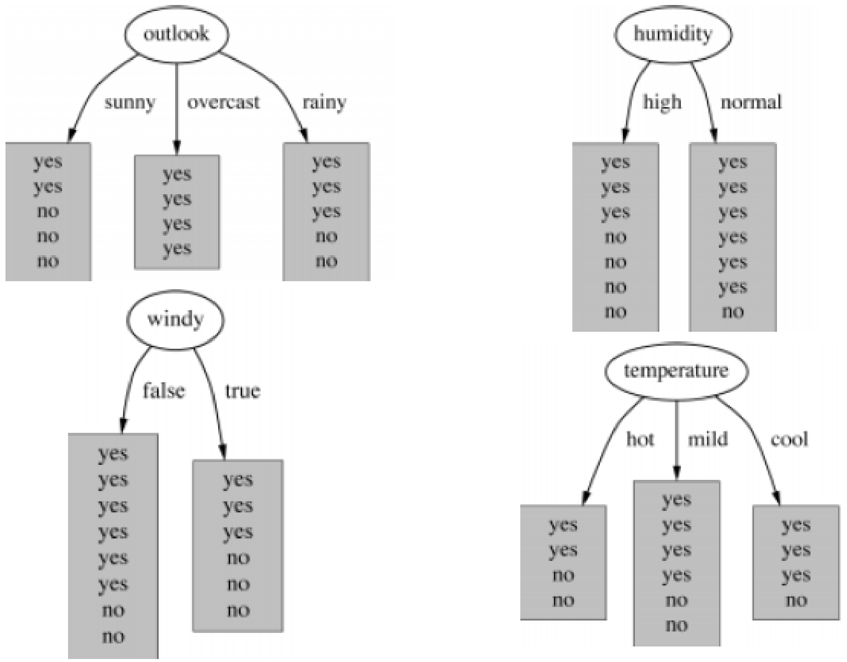
- “Outlook” = “Rainy”:

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

- Expected information for attribute:

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

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



# Computing Gain

- Information gain: information before splitting – information after splitting

gain(“Outlook”) = info([9,5]) – info([3,2],[4,0],[3,2])

= 0.940 - 0.693

= 0.247 bits

- Information gain for attributes from weather data:

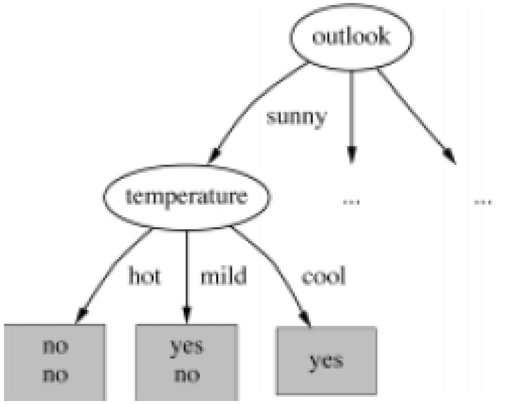
$$\text{gain}(\text{"Outlook"}) = 0.247 \text{ bits}$$

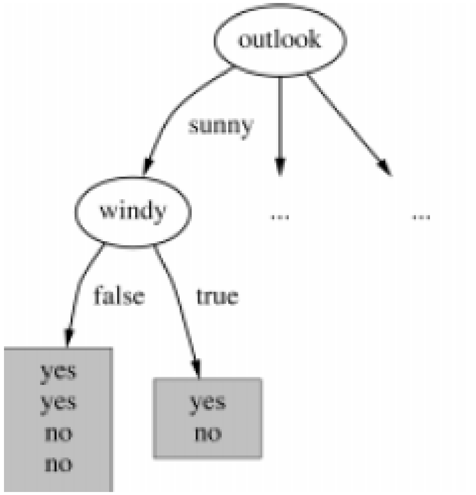
$$\text{gain}(\text{"Temperature"}) = 0.029 \text{ bits}$$

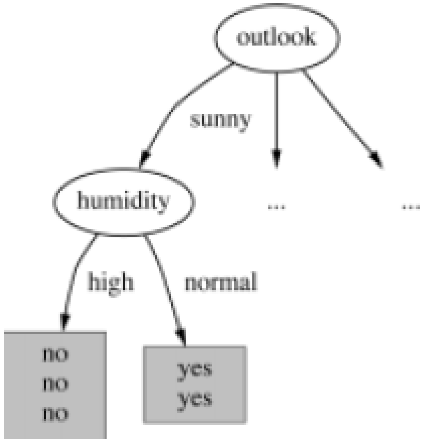
$$\text{gain}(\text{"Humidity"}) = 0.152 \text{ bits}$$

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

# Continuing the split







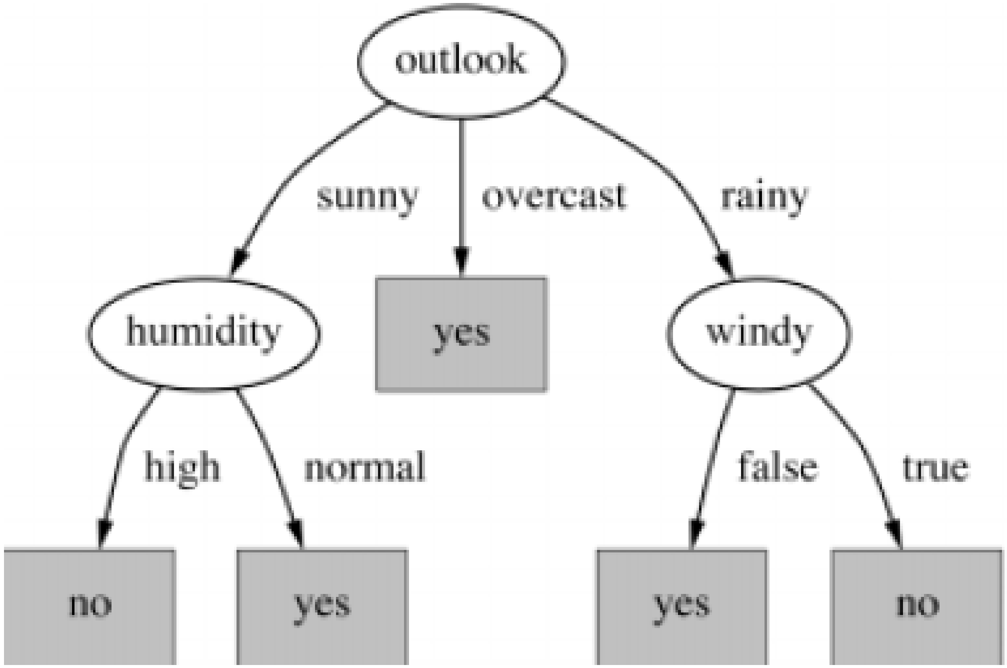
$$\text{gain}(\text{"Temperature"}) = 0.571\,\text{bits}$$

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

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

# The final tree

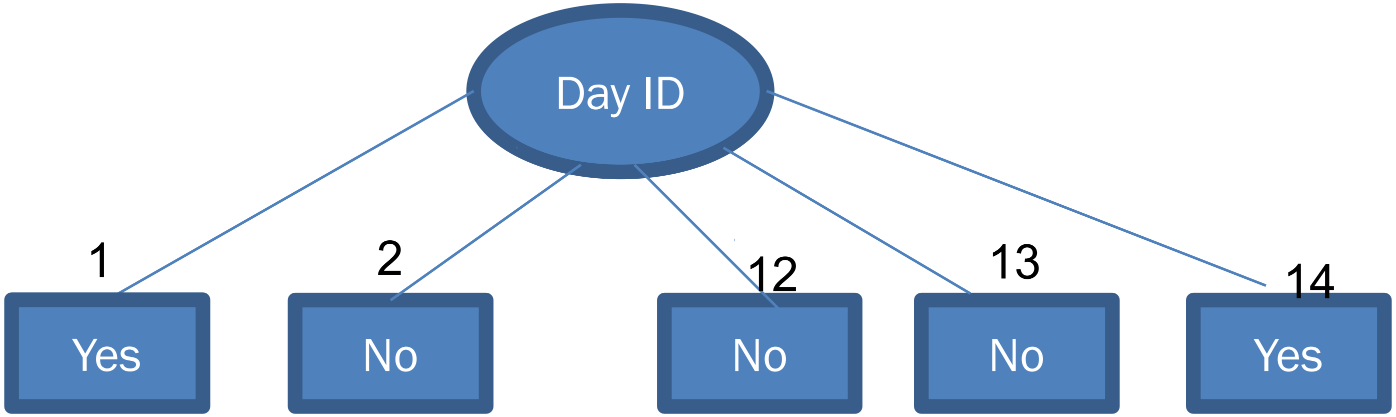
- Note: not all leaves need to be pure
- Some leaf nodes will have instances belonging to more than one class – in this case the leaf node is labelled with the *majority* class
- Splitting stops when data can't be split any further – when we run out of attributes to split on or the number of instances at the node to be split is less than a specified minimum number.



# Getting rid of bias introduced by Information Gain (IG)

- IG is a good method of identifying splits in the tree but it can cause problems for features with high cardinality
- In the weather example the Day ID perfectly correlates to the right play decision in *historical data*
- This means that Day ID has the highest IG value
- However, it has no power whatsoever to predict decisions, hence no generalization capability!
- The solution in this case is to use Gain Ratio

# Problem with highly branching features



- Remember there were 9 playing days and 5 non playing days and so:

  info([0,1]) + info([0,1]) + info([1,0])+ ….. + info([1,0])+ info([0,1])

- Thus it follows that Day ID has the maximum information gain (=0.94)

(See Weka Book 2011: pp105-108)

# Intrinsic Information

- The problem occurs due to the high intrinsic information held by highly branching features
- Intrinsic Information contained by a split S created by a feature F is given by:

I(F,S)$=-\sum_i \frac{|B_i|}{|B|} \log\left(\frac{|B_i|}{B}\right)$ where $|B_i$ is the number of data instances on branch i and $|B|$ is the total number across all branches (size of training dataset)

- For day ID, I$=14\left(-\frac{1}{14} log\left(\frac{1}{14}\right)\right)=3.807$ which is the highest out of all the features

# Gain Ratio

- We are now in a better position to get rid of troublesome features
  - We define Gain Ratio (GR) as the ratio of Information Gain (IG) to Intrinsic Information (IS)

$$GR(F,S) = \frac{IG(F,S)}{I(F,S)}$$ where F is the feature and S is the split

| Feature\Measure | Information Gain | Gain Ratio |
|---|---|---|
| Outlook | 0.247 | 0.157 |
| Humidity | 0.152 | 0.152 |
| Windy | 0.029 | 0.049 |
| Temperature | 0.048 | 0.019 |
| Day ID | **0.940** | 0.246 |

# Gain Ratio vs Information Gain

- Thus it can be seen that GR has narrowed the gap between Day ID and Outlook
- However, Day ID *still wins* as it has the highest Gain Ratio
- The lesson here is that the data miner *has to use his/her judgement and not rely totally on automated tools*
- It is easy for the human data miner to identify that Day ID is not suitable as it has no predictive power (generalizability).

# References

1. *Data Mining: Practical Machine Learning Tools and Techniques (3rd edition)* / Ian Witten, Eibe Frank; Elsevier, 2011, Chapter 4