

# Advanced Business Data Mining

## MSIS 522 – Lesson 2

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# Course Overview

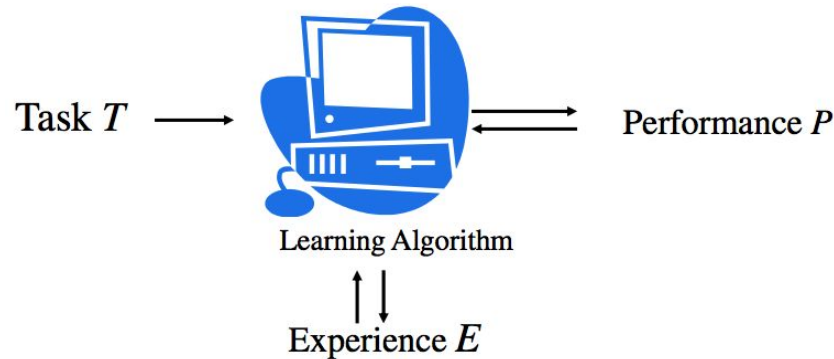
- Lecture 1 - Fundamentals of Machine Learning
- **Lecture 2 - Decision Tree**
- Lecture 3 - Ensemble Learning
- Lecture 4 - Clustering
- Lecture 5 - Recommendation Systems

# Recap of Lesson 1

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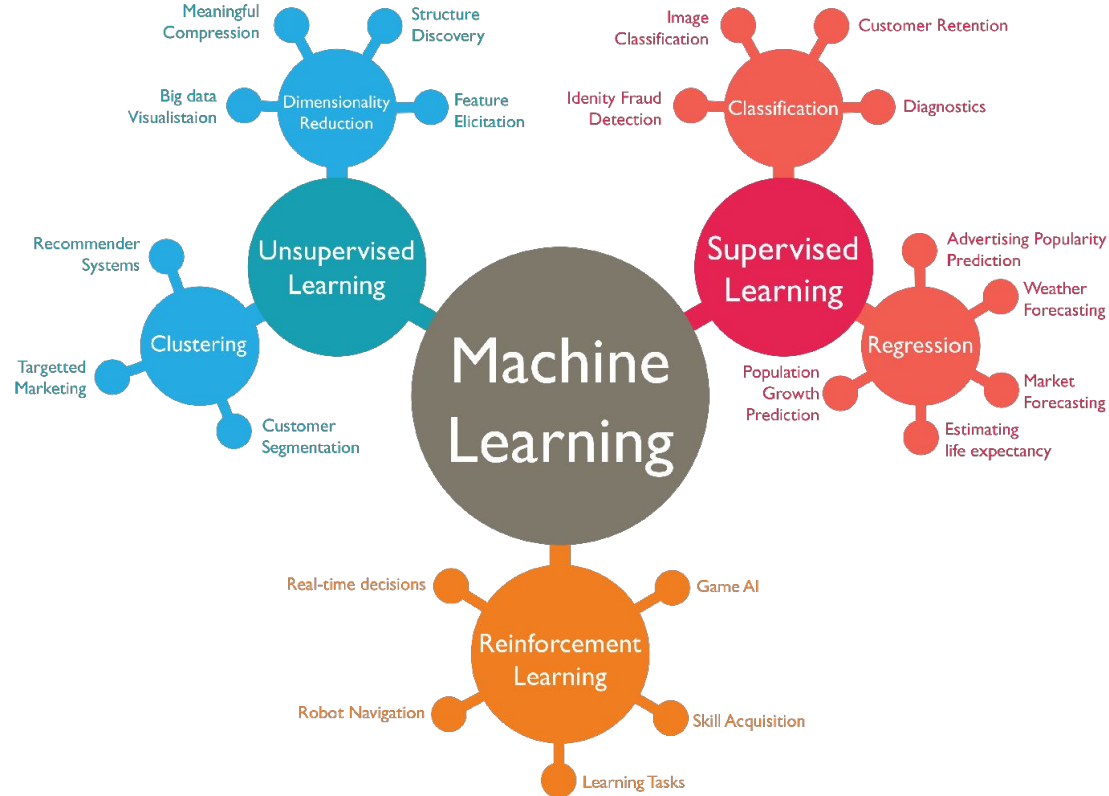
# What is Machine Learning?

A computer program is said to learn from **experience**  $E$  with respect to some class of **tasks**  $T$  and **performance measure**  $P$  if its performance at tasks in  $T$ , as measured by  $P$ , improves with experience  $E$ . -- Tom Mitchell



Improving *performance*  $P$  with *experience*  $E$  at some *task*  $T$ .

# 3 Types of Machine Learning Algorithms



# Supervised Learning

- **Regression:** A regression model predicts **continuous values**. For example, regression models make predictions that answer questions like the following:
  - What is the value of a house in California?
  - What is the demand of a product on Amazon next month?
- **Classification:** A classification model predicts **discrete values**. For example, classification models make predictions that answer questions like the following:
  - Is a given email message spam or not spam?
  - Is this an image of a dog, a cat, or a hamster?

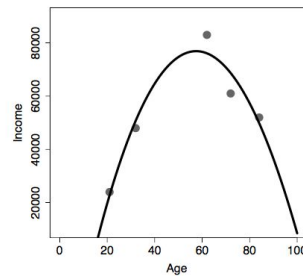
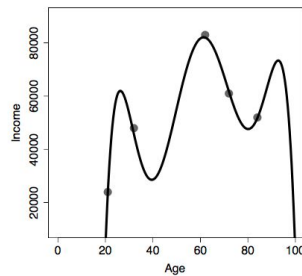
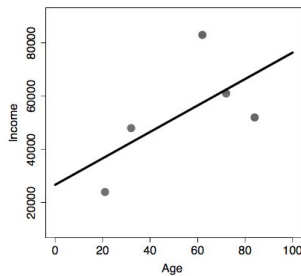
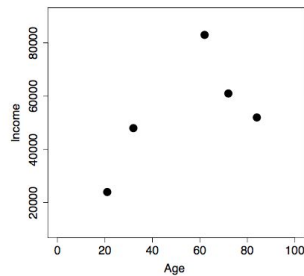
# Generalization

Machine Learning is all about **generalization** to future unseen data points.

- **Underfitting** – a model is too simple and can not capture the underlying patterns within the data, thus does not perform well on new data.
- **Overfitting** – a model tries to fit the training data so closely that it does not generalize well to new data.

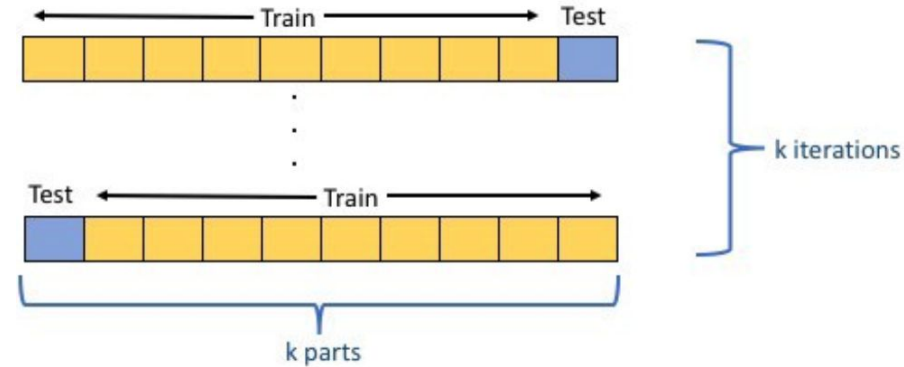
**Table:** The age-income dataset.

ID	AGE	INCOME
1	21	24,000
2	32	48,000
3	62	83,000
4	72	61,000
5	84	52,000



# K-fold Cross-validation

1. Divide the training data into  $K$  parts.
2. Use  $K-1$  of the parts for training and 1 for testing.
3. Repeat the procedure  $K$  times, rotating the test set.
4. Determine the performance based on the results across all  $K$  iterations.



**Leave-one-out Cross-validation** is the extreme case of K-fold Cross-Validation where we keep only one data point in the test set.



# Outline

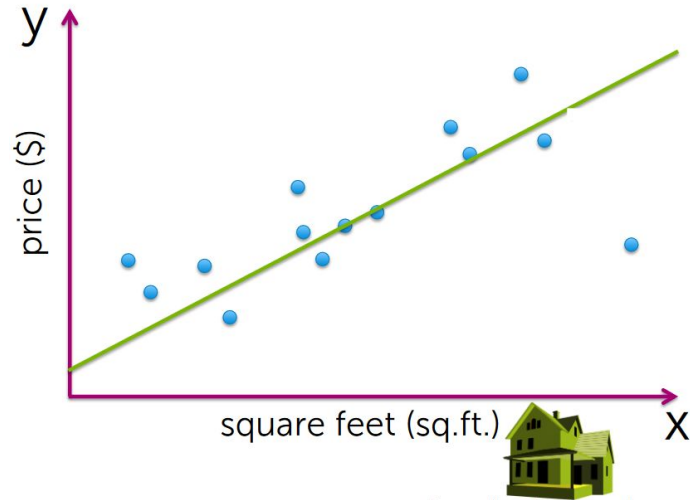
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- Linear Model and Its Limitation
- Decision Tree
- Hyper-parameter Tuning
- One-hot Encoding
- Lab

# Linear Model and Its Limitation

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# Linear Model



## Linear Regression

Predict continuous values, e.g. house price

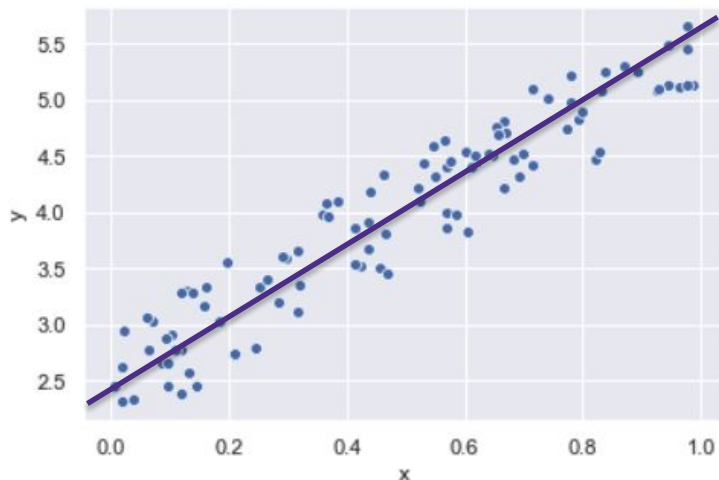


## Logistic Regression

Predict discrete values, e.g. email spam

# Linear Regression

$$h_w(x) = w_0 + w_1 x$$

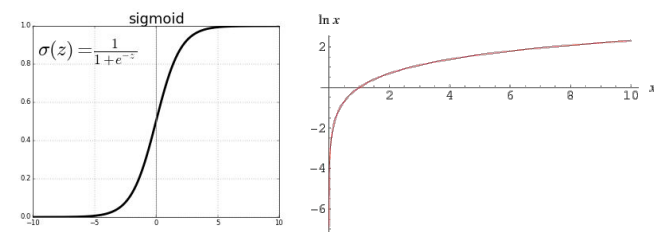


- > **Mean Squared Error (MSE):** the average squared difference between the actual and predicted values.

$$\mathcal{L}(w) = \frac{1}{N} \sum_{i=1}^N (y_i - h_w(x_i))^2$$

- > Find parameters  $w = \{w_0, w_1\}$  that minimize MSE over the training dataset.

# Logistic Regression



$$h_w(x) = \sigma(w_0 + w_1 x)$$



Decision Boundary

- > **Cross Entropy (aka log-loss)** measures the performance of a classification model based on its probabilistic output.

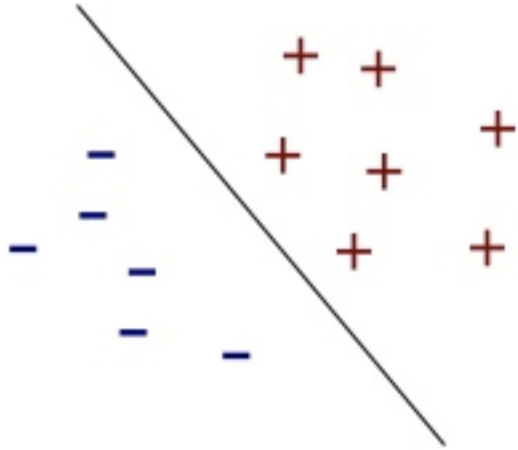
$$\mathcal{L}(w) = -\frac{1}{N} \sum_{i=1}^N [y_i \log(h_w(x_i)) + (1 - y_i) \log(1 - h_w(x_i))]$$

$$\log(h_w(x_i)) \quad \text{if } y_i = 1$$

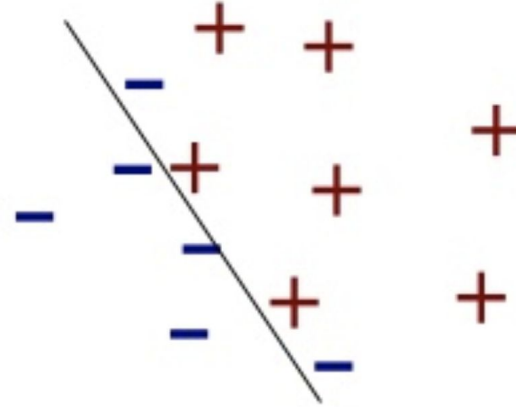
$$\log(1 - h_w(x_i)) \quad \text{if } y_i = 0$$

- > Find parameters  $w = \{w_0, w_1\}$  that minimize the cross entropy over the training dataset.

# Linear Separable



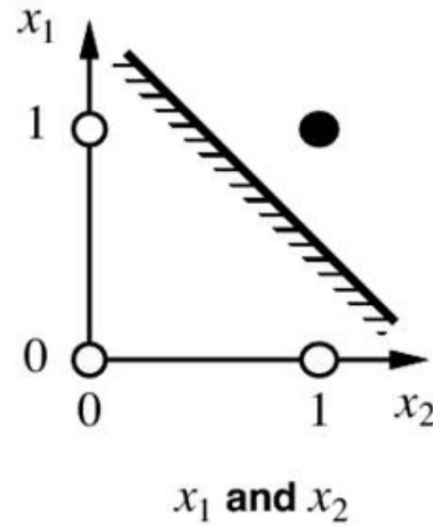
Linear Separable



Not Linear Separable

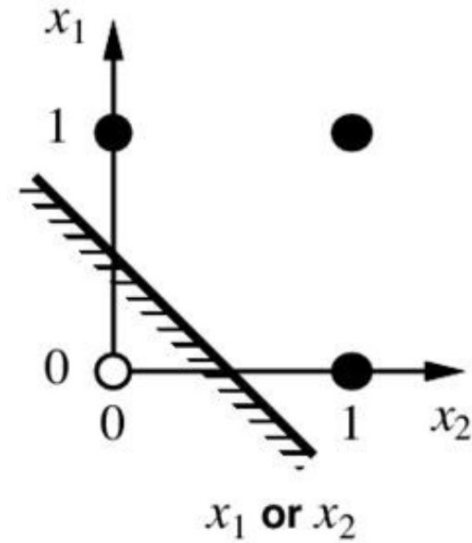
# Logical AND

X1	X2	Y
1	1	1
1	0	0
0	1	0
0	0	0



# Logical OR

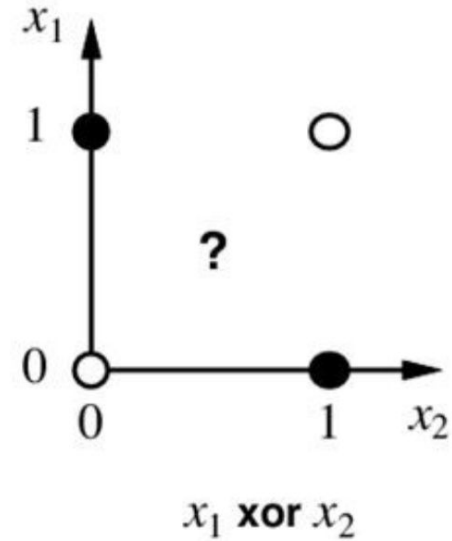
X1	X2	Y
1	1	1
1	0	0
0	1	0
0	0	0





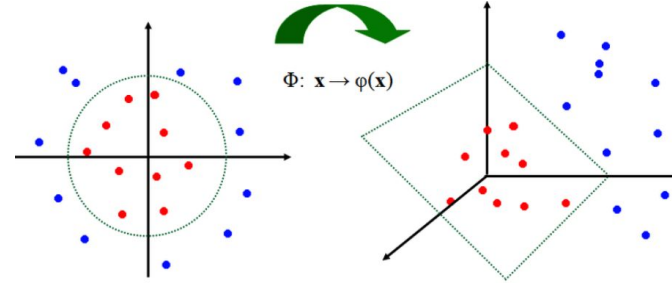
# Logical XOR

X1	X2	Y
1	1	0
1	0	1
0	1	1
0	0	0

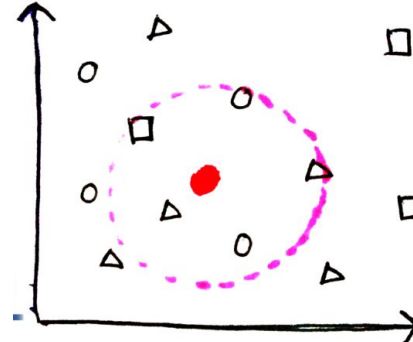
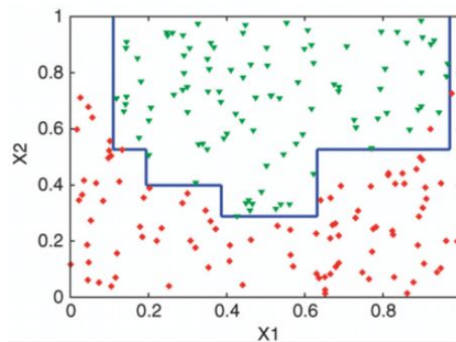


# Handle Nonlinear Separable Data

- Project existing data into other dimensional space so that data becomes linear separable in that space and then apply a linear model.



- Use a more powerful model which can model non-linearity in the data by itself.

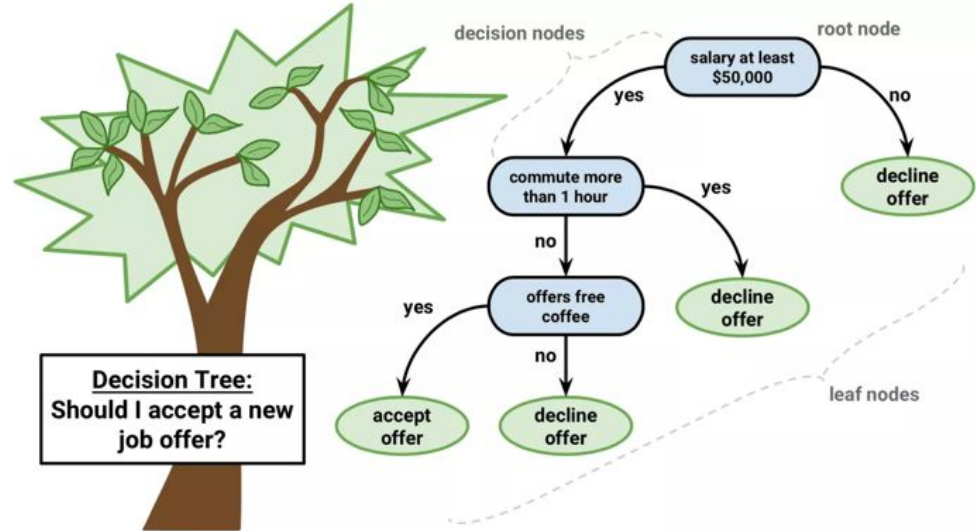


# Decision Tree



# Decision Tree Basics

- **Decision nodes (blue):** each node represents a test on a particular attribute.
- **Leaf nodes (green):** each node represents a prediction.

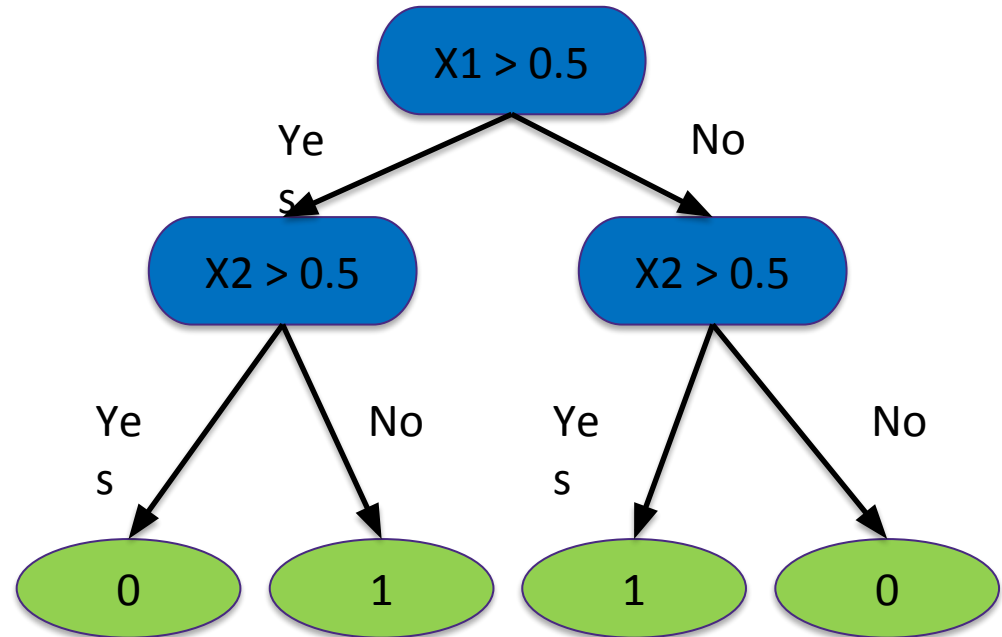


- Read down the tree to derive rules.
- # of leaf nodes equals # of rules encoded in a decision tree.

# Decision Tree to the Rescue

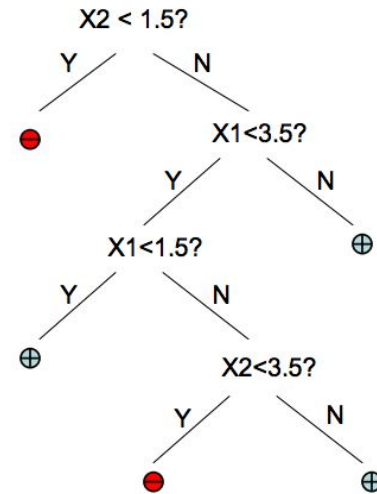
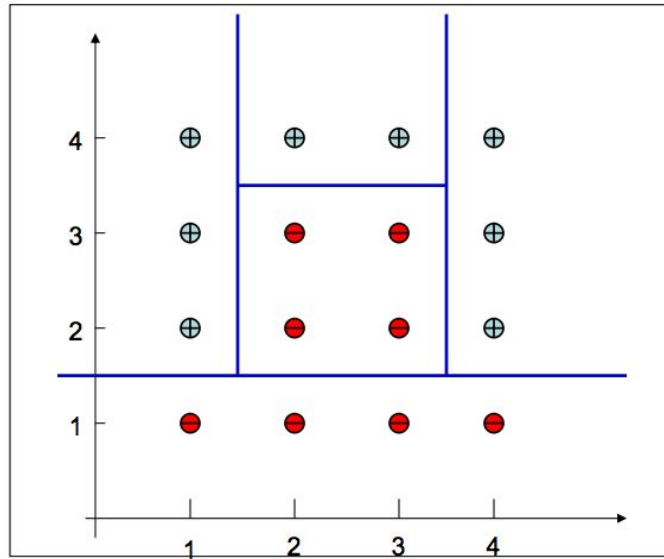
Logical XOR

X1	X2	Y
1	1	0
1	0	1
0	1	1
0	0	0

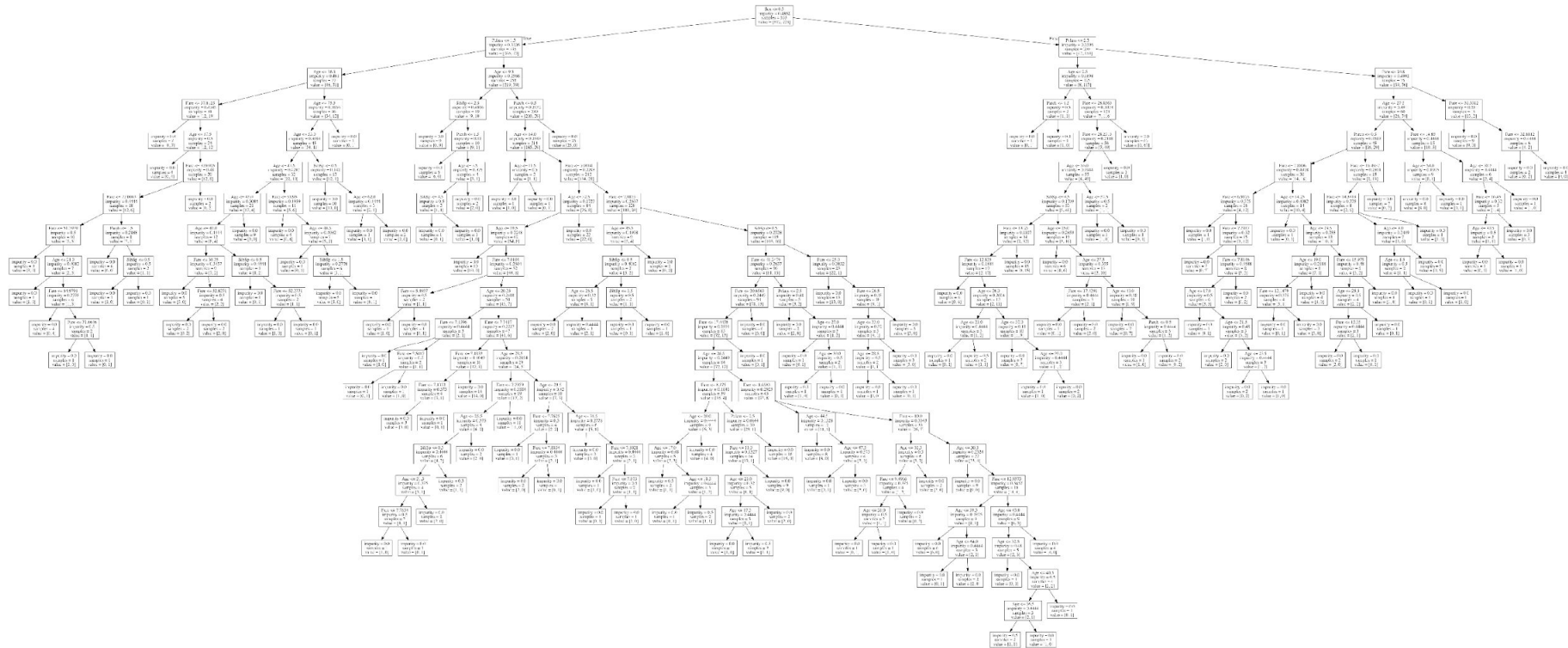


# Decision Boundaries

Decision Tree divides the input space into **axis-parallel** rectangles and label each rectangle with the class with most data in it.



# A More Realistic Decision Tree



# Classification And Regression Trees (CART)

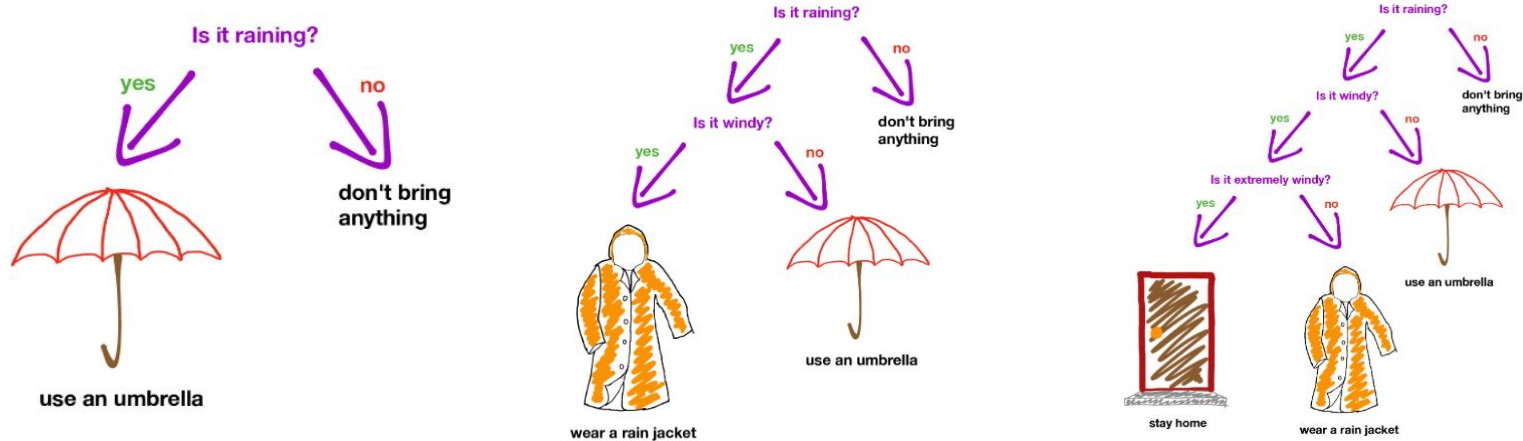
- **Classification Trees** - predict categorical variable.
- **Regression Trees** - predict continuous variable.





# How to construct a Decision Tree?

- Choose an attribute (i.e. a feature) for root.
- Split data using chosen attribute into disjoint subsets.
- Recursive partitioning for each subset.



# Split of a Categorical Variable

- Examine all possible ways in which the categories can be split into two groups.

- E.g. categories A, B, C can be split 3 ways.

- {A} and {B, C}
- {B} and {A, C}
- {C} and {A, B}

- In theory, we have an exponential number of different splits.

- In practice, we often use one vs the rest.



# How to Construct a Decision Tree

Training Set: 3 features and 2 classes

X	Y	Z	C
1	1	1	I
1	1	0	I
0	0	1	II
1	0	0	II

**How do we build a Decision Tree to distinguish class I from II?**

# Classification Impurity Measure: Entropy

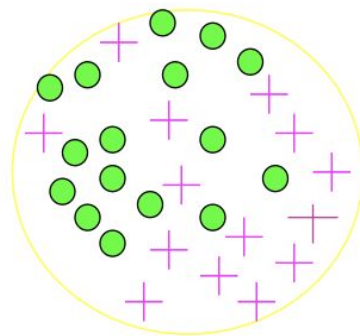
- Entropy measures the level of impurity in a group of examples.

$$H(x) = - \sum_i p_i \log(p_i)$$

16/30 are green circles; 14/30 are pink crosses

$\log_2(16/30) = -.9$ ;  $\log_2(14/30) = -1.1$

Entropy =  $-(16/30)(-.9) - (14/30)(-1.1) = .99$



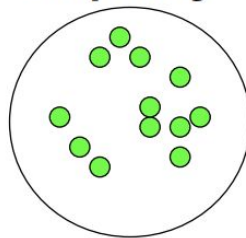
## Entropy for 2-class Cases

- What is the entropy of a group in which all examples belong to the same class?

–  $\text{entropy} = -1 \log_2 1 = 0$

not a good training set for learning

Minimum  
impurity

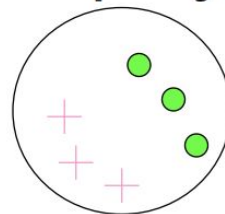


- What is the entropy of a group with 50% in either class?

–  $\text{entropy} = -0.5 \log_2 0.5 - 0.5 \log_2 0.5 = 1$

good training set for learning

Maximum  
impurity



## Quiz: Andrew Moore's Entropy in a Nutshell



Low Entropy



High Entropy

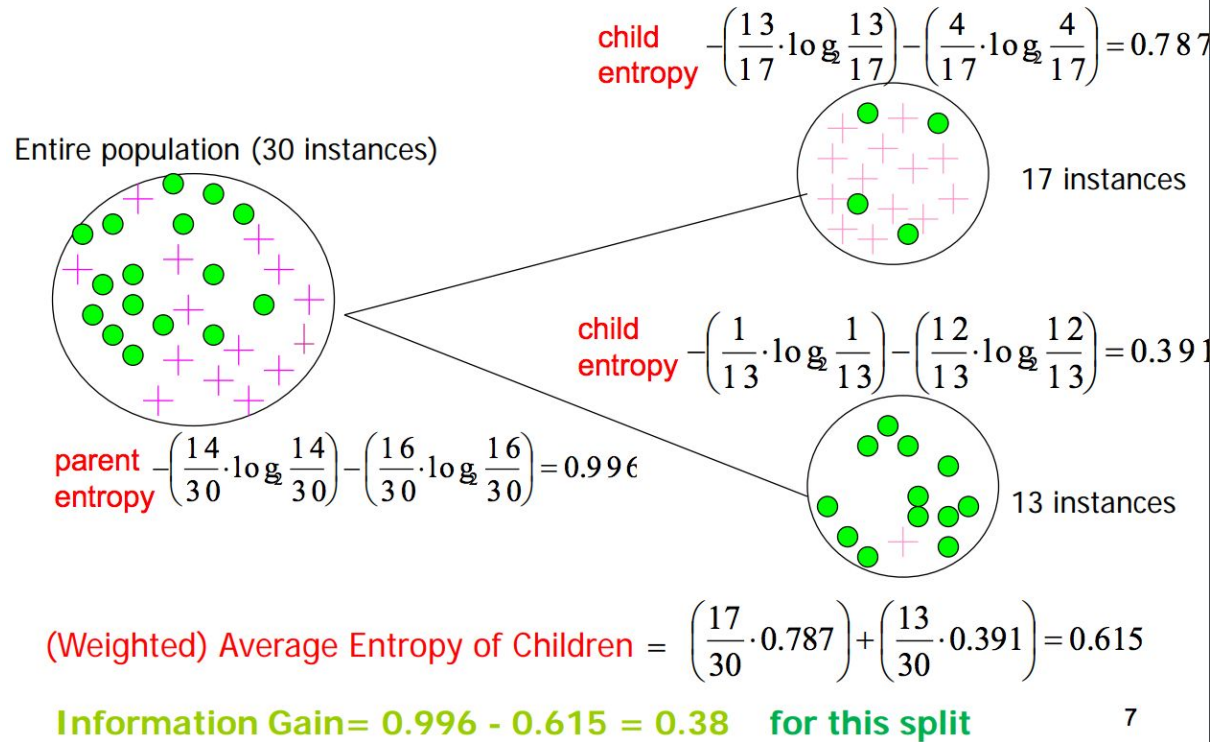
# Information Gain

- Determine **which attribute** in a given set of training features is most useful for discriminating between the classes.
- **Information Gain** tells us how important a given attribute is in discriminating between the classes.
- Choose the attribute and split that maximize the information gain.

$$\text{Information Gain} = \text{entropy}(\text{parent}) - [\text{average entropy}(\text{children})]$$

# Information Gain Example

**Information Gain** = entropy(parent) – [average entropy(children)]





# Quiz

Training Set: 3 features and 2 classes

X	Y	Z	C
1	1	1	I
1	1	0	I
0	0	1	II
1	0	0	II

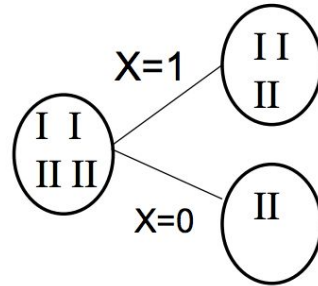
**How do we build a Decision Tree to distinguish class I from II?**

## Quiz: Split on attribute X

X	Y	Z	C
1	1	1	I
1	1	0	I
0	0	1	II
1	0	0	II

Split on attribute X

If X is the best attribute,  
this node would be further split.



$$\begin{aligned} E_{\text{child1}} &= -(1/3)\log_2(1/3) - (2/3)\log_2(2/3) \\ &= .5284 + .39 \\ &= .9184 \end{aligned}$$

$$E_{\text{child2}} = 0$$

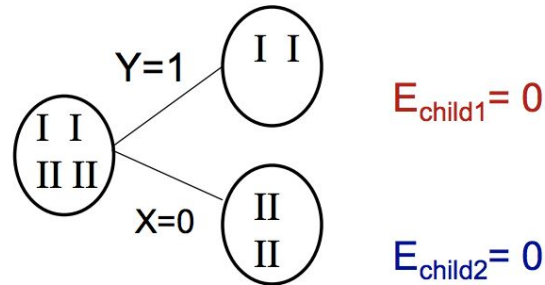
$$E_{\text{parent}} = 1$$

$$\text{GAIN} = 1 - (3/4)(.9184) - (1/4)(0) = .3112$$

## Quiz: Split on attribute Y

X	Y	Z	C
1	1	1	I
1	1	0	I
0	0	1	II
1	0	0	II

Split on attribute Y



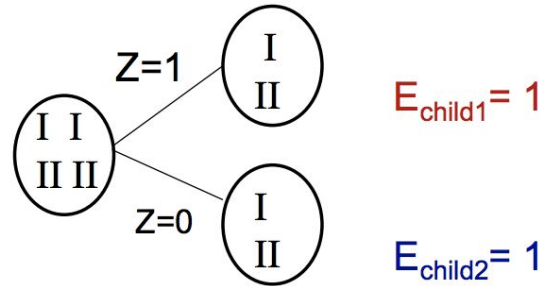
$$E_{\text{parent}} = 1$$

$$\text{GAIN} = 1 - (1/2)0 - (1/2)0 = 1; \text{ BEST ONE}$$

## Quiz: Split on attribute Z

X	Y	Z	C
1	1	1	I
1	1	0	I
0	0	1	II
1	0	0	II

Split on attribute Z



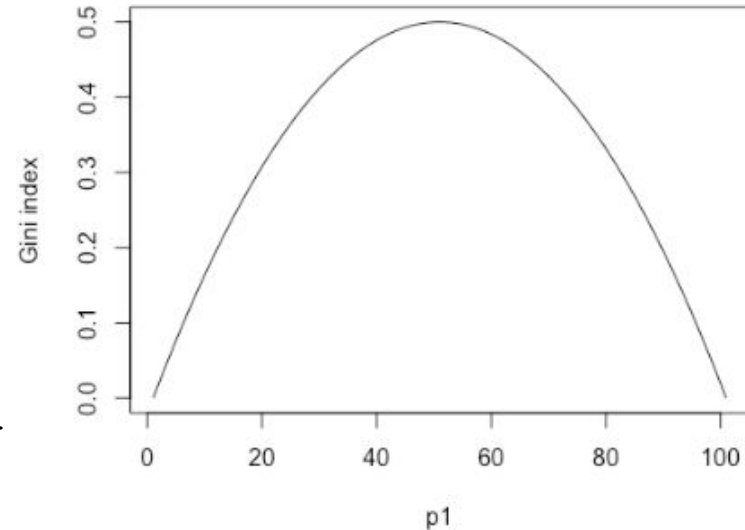
$$E_{\text{parent}} = 1$$

$$\text{GAIN} = 1 - \left( \frac{1}{2} \right)(1) - \left( \frac{1}{2} \right)(1) = 0 \quad \text{ie. NO GAIN; WORST}$$

# Classification Impurity Measure: Gini Impurity

$$I_G = 1 - \sum_{j=1}^c p_j^2$$

- **Gini impurity/index** is a measure to quantify the level of impurity in a group of examples.
  - $I(A) = 0$  when all cases belong to the same class.
  - Max value when all classes are equally represented.



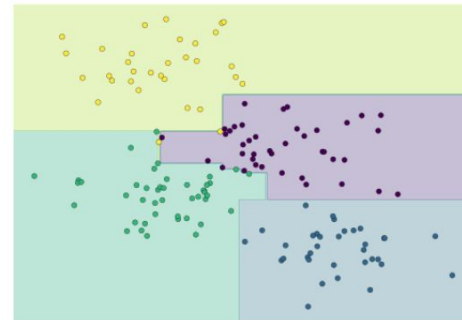
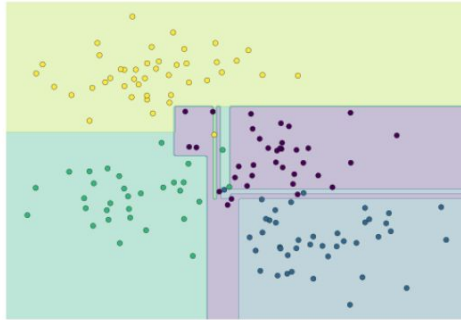
# Split of a Numerical Variable

- For each numerical attribute:
  - Sort the attribute from the smallest to the largest.
  - Linearly scan these values and choose the split position leading to the maximum impurity reduction (i.e. information gain).

		Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
		Taxable Income										
Sorted Values	→	60	70	75	85	90	95	100	120	125	220	
Split Positions	→	55	65	72	80	87	92	97	110	122	172	230
		≤ >	≤ >	≤ >	≤ >	≤ >	≤ >	≤ >	≤ >	≤ >	≤ >	≤ >
Yes		0 3	0 3	0 3	0 3	1 2	2 1	3 0	3 0	3 0	3 0	3 0
No		0 7	1 6	2 5	3 4	3 4	3 4	3 4	4 3	5 2	6 1	7 0
Gini		0.420	0.400	0.375	0.343	0.417	0.400	0.300	0.343	0.375	0.400	0.420

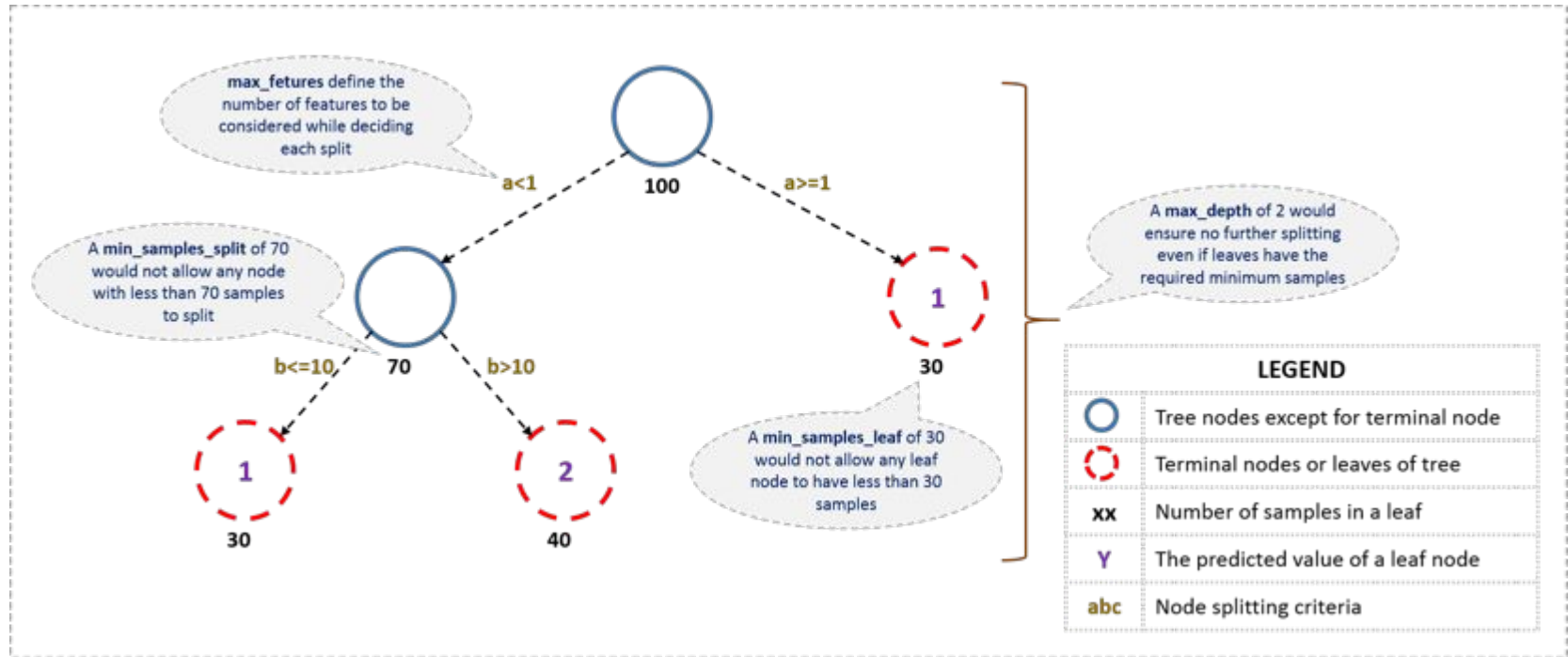
# How to avoid overfitting in Decision Tree?

- Decision tree is very powerful in modeling complex patterns within the data.
- As the nodes increase, we can represent arbitrarily complex decision boundaries.



- Two major ways to prevent overfitting:
  - Set constraints on the tree size.
  - True pruning.

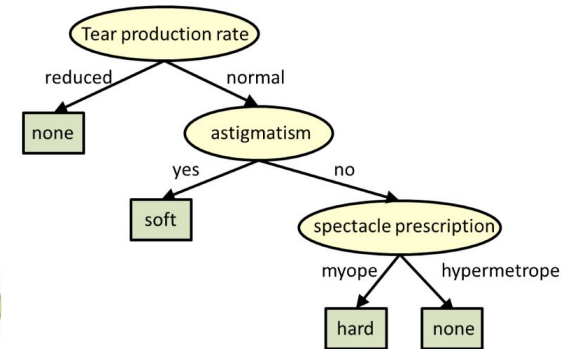
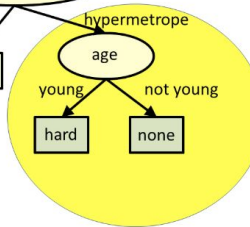
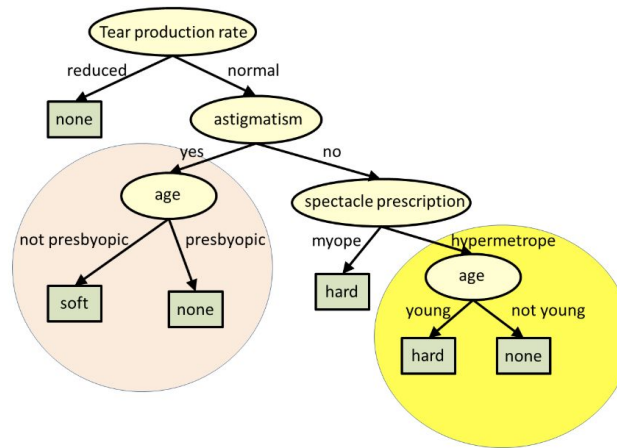
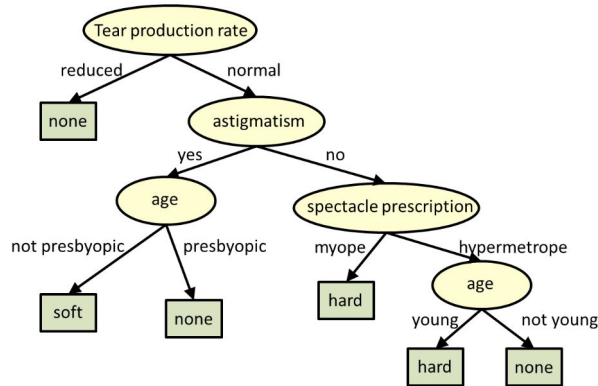
# Setting Constraints on Tree Size





# Pruning Decision Tree

- Grow the decision tree to a large depth.
- Start at the bottom and start removing leaves which are giving us negative returns based on a validation dataset.



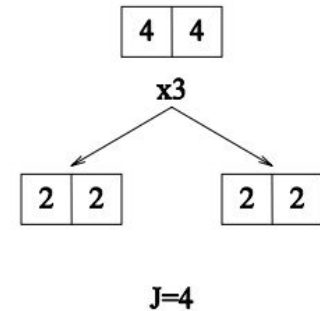
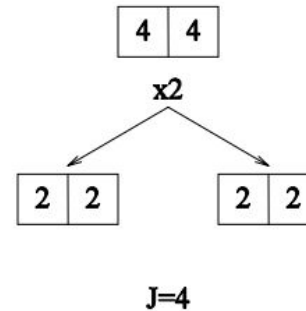
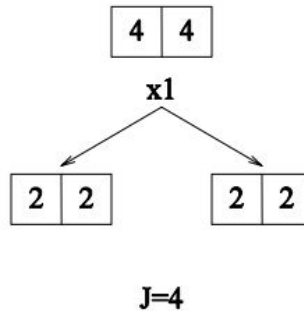
# Pros and Cons of Decision Tree

- Pros:
  - Easy to interpret.
  - Model nonlinear decision boundary.
  - Works well out of the box.
- Cons:
  - Tend to overfit if not properly tuned on validation data.
  - Sensitive to feature space rotation due to axis parallel decision boundaries.

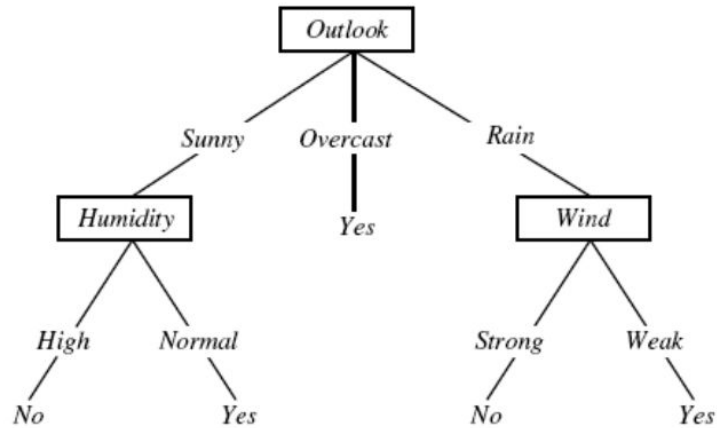
# Learning Optimal Decision Tree is NP-complete

- **Optimal Decision Tree** finds the best partition of the data to achieve the global minimum error.
- Greedy learning in constructing a Decision Tree does not guarantee optimality.

$x_1$	$x_2$	$x_3$	$y$
0	0	0	0
0	0	1	0
0	1	0	1
0	1	1	1
1	0	0	1
1	0	1	1
1	1	0	0
1	1	1	0

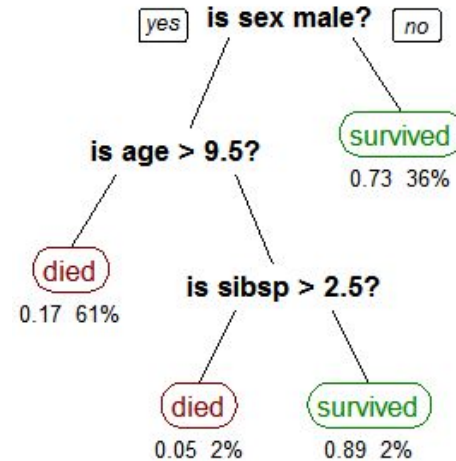


# Decision Tree Variants



## C4.5

- Multiple way split
- Error based Pruning



## CART

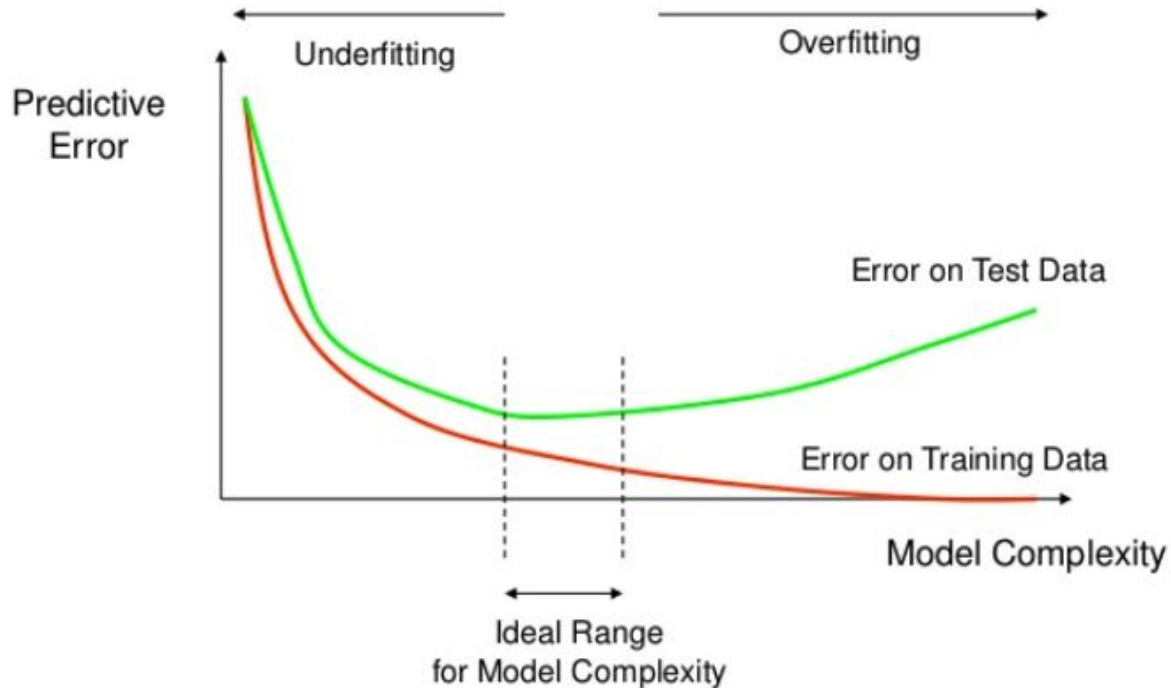
- Binary split
- Cost-Complexity Pruning

# Hyper-parameter Tuning

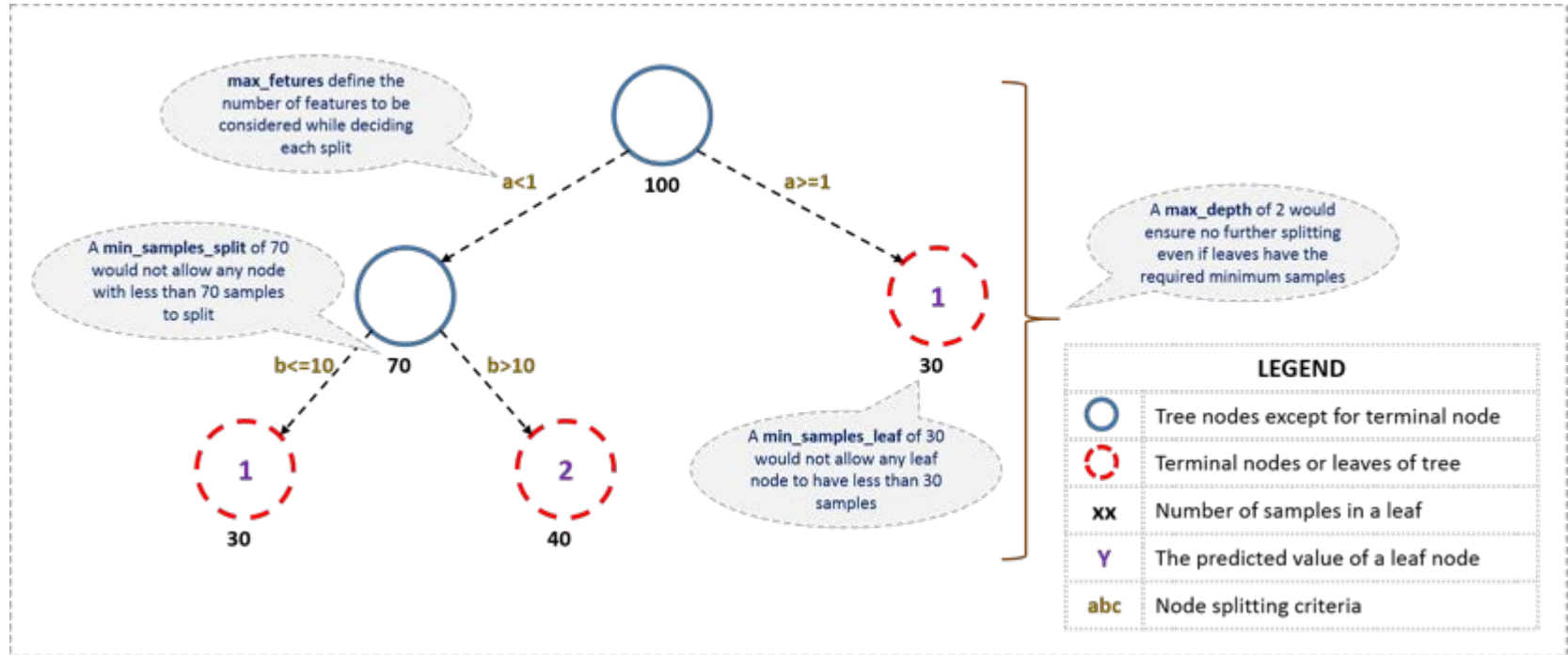


# Generalization

Machine Learning is all about **generalization** to future unseen data points.

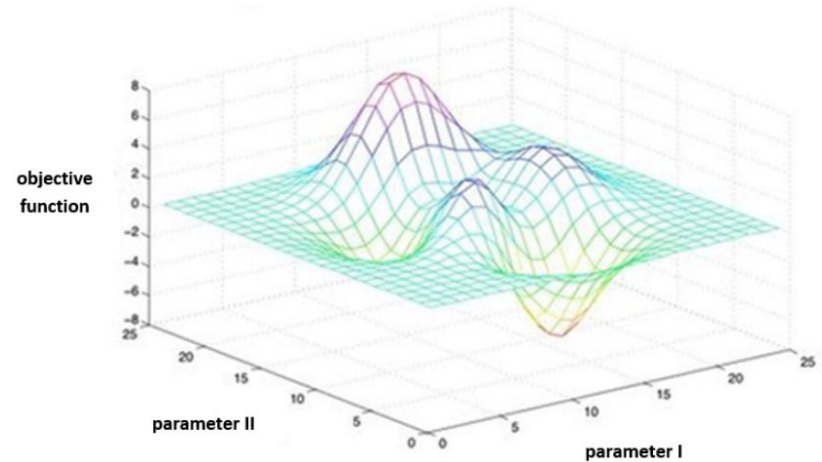
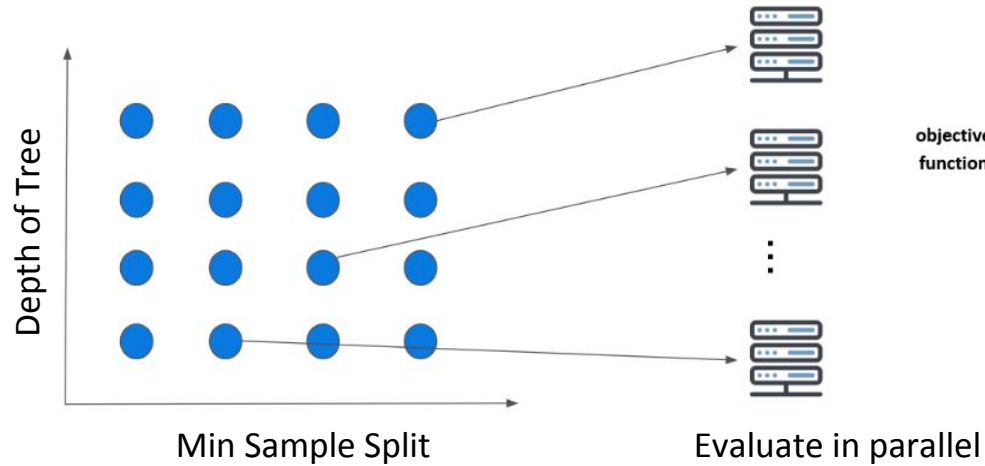


# Hyper-parameters of Decision Tree



# Grid Search

Find the best configuration for the hyper-parameters used in a ML model.





# One-hot Encoding



# What's One-hot Encoding?

- Categorical variables cannot be easily handled for most of the machine learning algorithms, e.g. linear regression, support vector machine and neural networks.

Food Name	Categorical #	Calories
Apple	1	95
Chicken	2	231
Broccoli	3	50

$$2 \text{ Chickens} \stackrel{?}{=} 1 \text{ Apple} + 1 \text{ Broccoli}$$

- One-hot encoding is a process by which **categorical variables** are converted into a form that could be provided to ML algorithms to do a better job in prediction.

# One-hot Encoding Example

Label Encoding

Food Name	Categorical #	Calories
Apple	1	95
Chicken	2	231
Broccoli	3	50



One Hot Encoding

Apple	Chicken	Broccoli	Calories
1	0	0	95
0	1	0	231
0	0	1	50

# Deal with Categorical Features of High Cardinality

For categorical features of high cardinality, one-hot encoding could potentially create a huge sparse feature vector, making it hard for ML to learn.

- Solution 1: one-hot encode a subset of the most common values of that variable and encode the rest as one value.
- Solution 2: substitute the value with the average of the target variable for each value in the training set.



# Lab

