

IDSC 4444 (004)

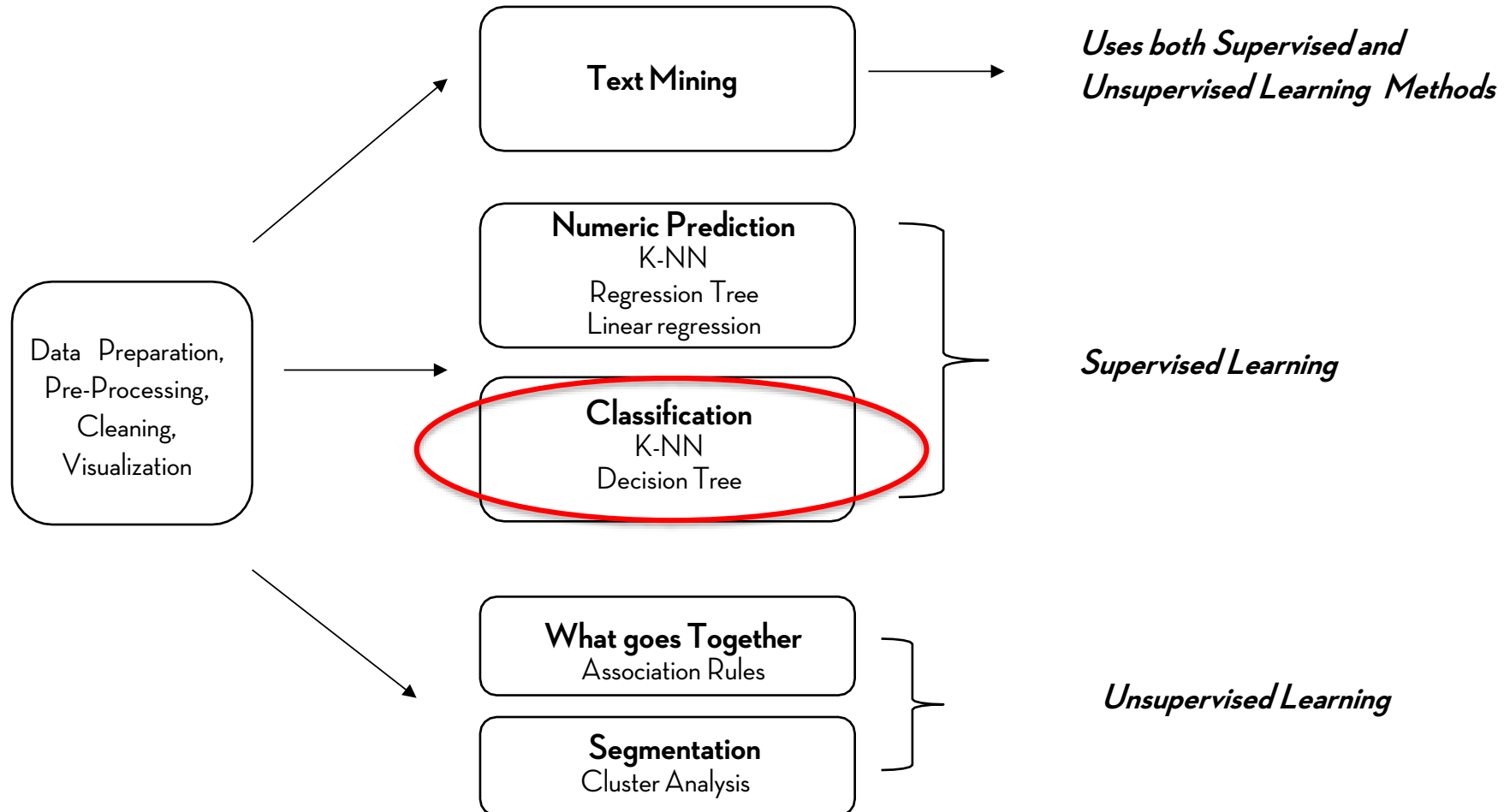
Predictive Analytics: Classification

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Agenda

- ❑ Classification Definitions and Steps
- ❑ Classifiers
 - k-NN
 - Decision Tree
- ❑ Evaluating Performance
 - Confusion Matrix

An Overview



Predictive Data Mining

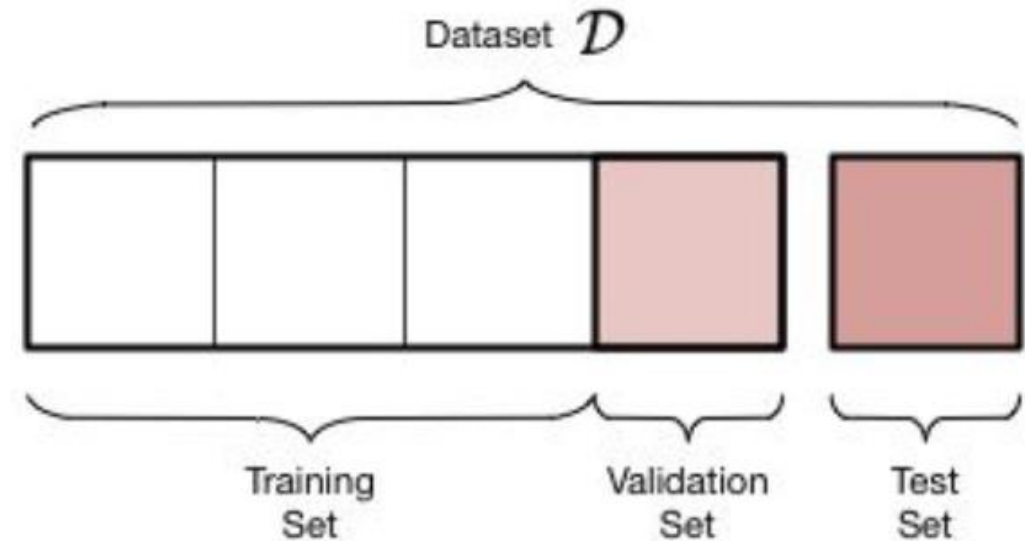
- ❑ Unlike exploratory data analytics (Association Rules, Cluster Analysis), in predictive analytics we know exactly what you are looking for
 - We are trying to predict certain well-defined outcome using existing data
 - Among the attributes we have in the data, we have to specify **dependent (outcome) variables** and **independent variables (attributes/features)**
- ❑ **Classification:** predict categorical values of the outcome variable using other available attributes, e.g.
 - Techniques: **k-NN (Nearest-Neighbors)**, **Decision Trees**, etc.
- ❑ **Numeric Prediction:** predicts continuous/numeric values of an outcome variable, e.g.
 - Techniques: **K-Nearest-Neighbors**, **Regression Trees**, etc

Classification: Some Definitions

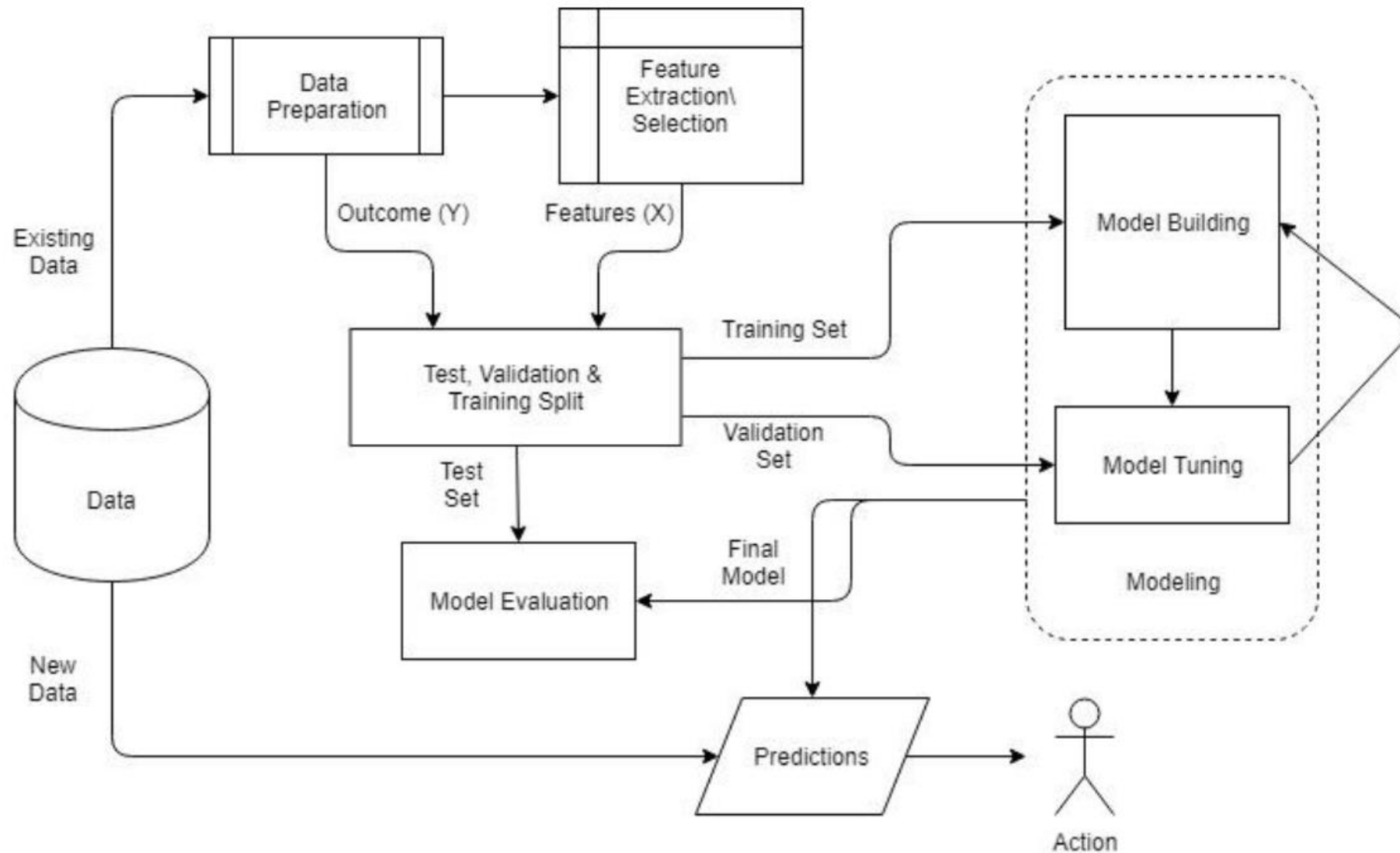
- ❑ **Observation/Record: our unit of observation** (example, a customer), defined by the collection of available attributes (variables)
- ❑ **The attributes** that refer to a given observation, are now divided into:
 - **One dependent variable (Y) / Outcome Variable, Class variable:**
 - ✓ This variable represents the outcome we want to predict
 - **Independent Variables (X) /Predictors, Covariates:**
 - ✓ The attributes of an observation used to predict the outcome variable Y
 - ✓ Collectively known as **Features vector** or **Covariates vector**

Training - Validation - Test

- ❑ Randomly split your labeled data into three parts:
 - **Training data:** to build your model
 - **Validation data:** to tune the performance of your model
 - **Test data:** to test the performance of your model
- ❑ It works because your model, built on training data, has not “seen” the validation data
 - If your models perform well on validation data, it is likely to also perform well for new, unseen data when you actually deploy it.
 - Sometimes, Validation might be skipped



The Prediction Process



k-NN (k- Nearest Neighbors)

- ❑ Do not confuse with k-Means in Clustering!
- ❑ **Main idea:** For a given observation, identify “nearby” (similar) observations
 - Use distance metrics seen in Clustering (Euclidian is the favorite)
- ❑ k-NN will classify the observation according to the predominant class among the identified nearest neighbors observations
 - We need to decide k, how many neighbors we want to consider.

	(Age)	(Income)	(Gender)	Purchase/Not Purchase Product
A	25	55000	M	No Purchase
B	32	120000	M	Purchase
C	43	150000	F	Purchase

Labeled Data:
We know the Y
("class")

Euclidian Distance

d(D,A)	2.8489
d(D,B)	1.9545
d(D, C)	0.5285

K = 1, ?

K = 3, ?

New observation
to classify →

D	40	130000	F	???
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k-NN Procedure

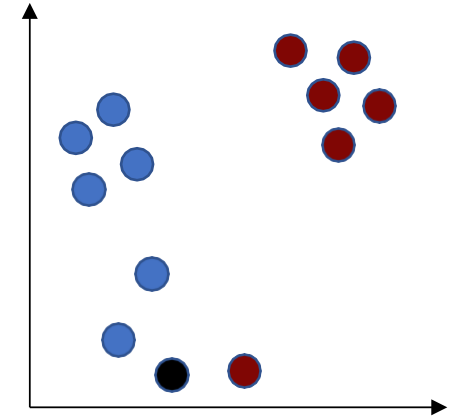
- ❑ Choose a specific k and a distance measure (usually, Euclidian)
 - Remember, in this case, k is the number of neighbors you want to look at
- ❑ Normalize data if needed
- ❑ For every unlabeled observation, identify the k -nearest existing labeled observations
- ❑ Classify the unlabeled observation as the majority class among the k -nearest
- ❑ In case of a tie, randomly choose a class
 - E.g., if k is an even number

Choosing k value

- ❑ k is the number of neighbors considered when classifying a new observation
- ❑ Usually, choose k that has lowest error rate in validation data (or, equivalently, the greatest accuracy)
 - **Error:** classifying an observation as belonging to one class when it belongs to another
 - **Error rate:** % of misclassified observations out of the total number of observations in the validation data
 - **Accuracy:** $1 - \text{error rate}$

k-NN Summary

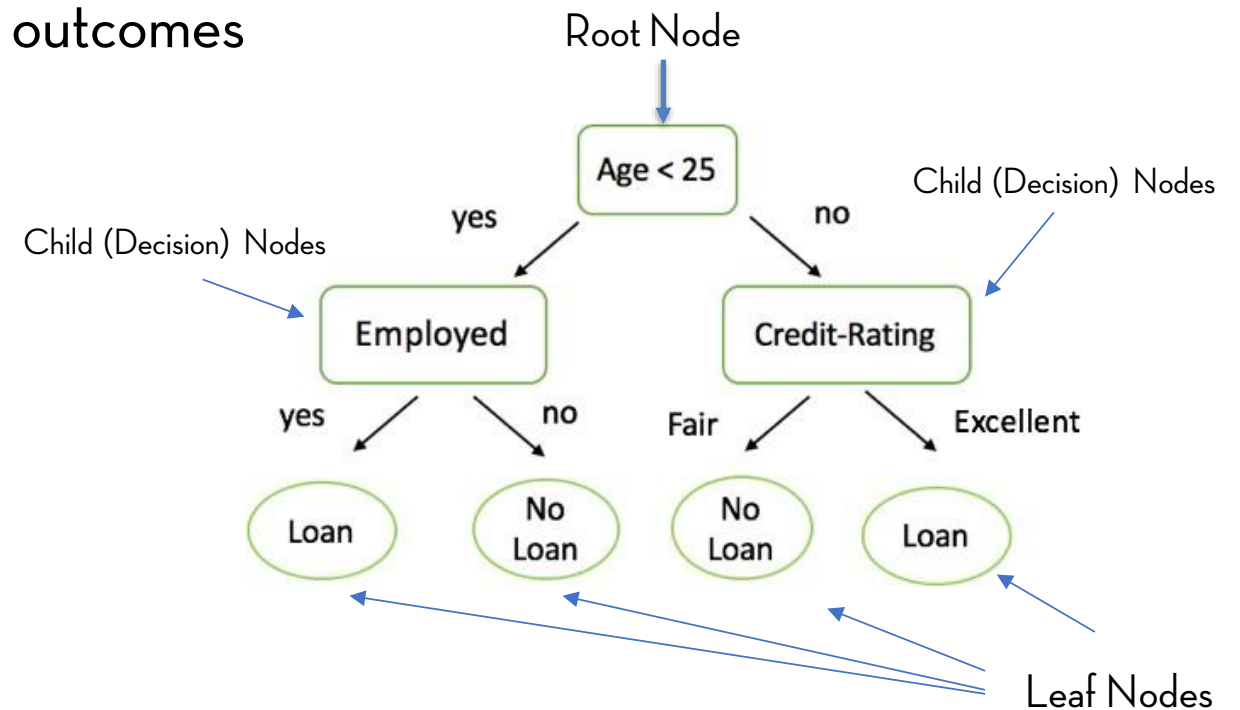
- ❑ k-NN is known as a type of “Lazy” classifier
 - No “real” model building – your labeled data is your model
- ❑ Enhancement:
 - **Weighted distance**, e.g., give more importance (weight) to closer neighbors
- ❑ **Strengths:**
 - Easy to implement and use
 - Do not make assumptions about statistical/distributional characteristics of the data (other methods do)
- ❑ **Weakness:** bad for big dataset
 - Slower learner, cannot be used for real-time prediction.



Decision Trees

- ❑ Also known as *Classification* Trees
- ❑ Goal: To classify data into predefined classes based on attributes
 - The output is a Decision Tree which is a set of decision rules organized as a tree.
- ❑ Nodes indicate decisions, leaves indicate outcomes

Ind.	Age	Employed	Credit-rating	Loan
A	23	Yes	Fair	Yes
B	28	No	Excellent	Yes
C	22	No	Fair	No
D	35	No	Fair	No
E	21	Yes	Fair	No
F	22	Yes	Fair	Yes
G	33	No	Excellent	Yes



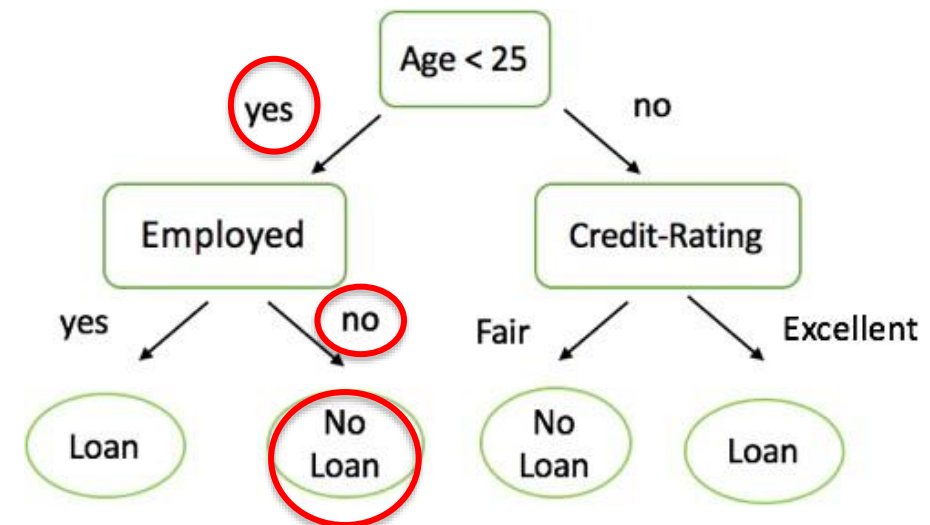
Decision Trees

❑ To classify a new record, the attributes are tested against the decision tree

❑ Example:

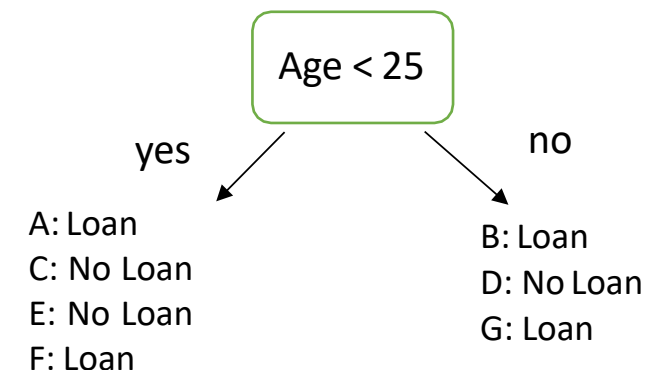
Ind.	Age	Employed	Credit-rating	Loan
ZZ	23	No	Fair	??

- Test on Age: Age < 25: Yes
- Test on Employed: No
- Reach Leaf node (class): No Loan
- Customer ZZ is unlikely to get a Loan



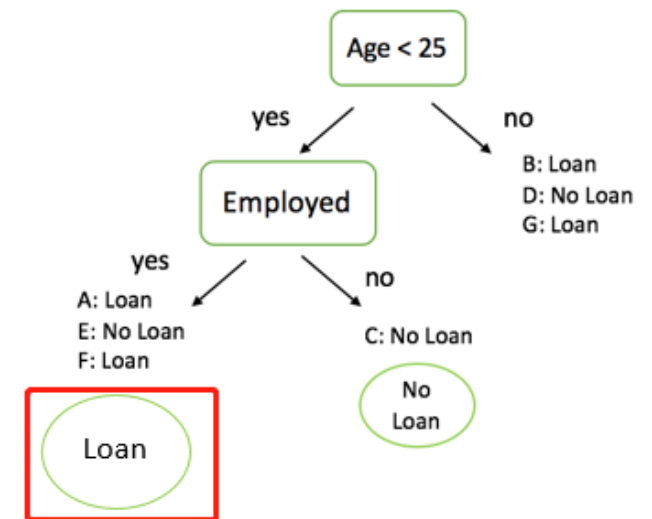
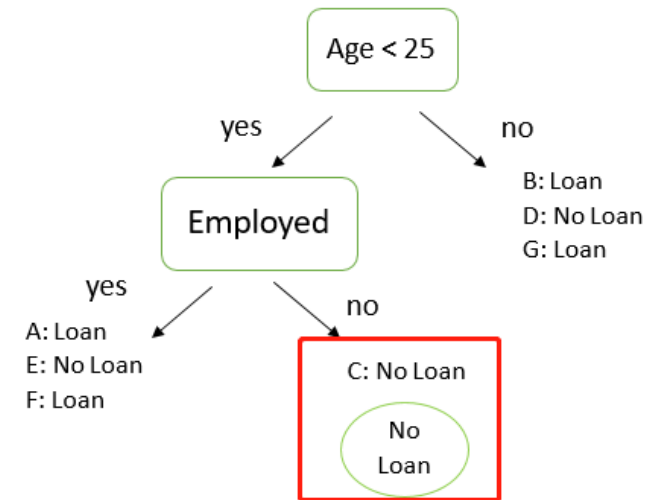
How is Decision Tree Built?

- ❑ The decision tree is built (trained) from the training data
- ❑ Data are split (partitioned) based on the attributes/predictor variables
- ❑ **Recursive Partitioning**
 - Pick one of the **attributes**, X_i , e.g., Age
 - Pick a **value** of X_i (let us call it S_i) that divides the training data into portions (not necessarily equal), one with $X_i \geq S_i$ and the other with $X_i < S_i$
 - Measure **how “pure”** each of the resulting proportion is
 - ✓ “Pure” means the partition contains records of mostly one class
 - Repeat the process until find X_i and S_i to **maximize purity of the partitions**



When do We Stop?

- ❑ Stopping criteria (when to stop splitting nodes?)
 - All data points associated with a node are from the same class
 - ✓ The node becomes a leaf node of that class
 - There are no remaining attributes to further split the data
 - ✓ E.g., no attribute further increases “purity” much
 - ✓ Use “majority vote” to label that node

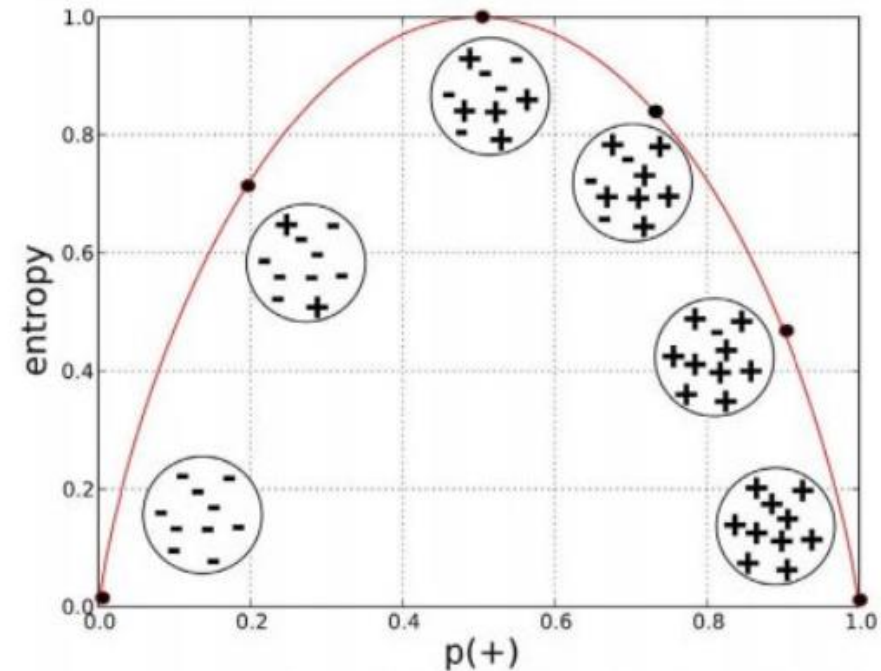


Choose Attributes to Split on (Entropy)

- ❑ Intuition: pick the attribute that **maximizes the purity** of the resulting split
- ❑ We measure “purity” through **Entropy**:

$$Entropy = - \sum_{k=1}^m p_k \log_2(p_k)$$

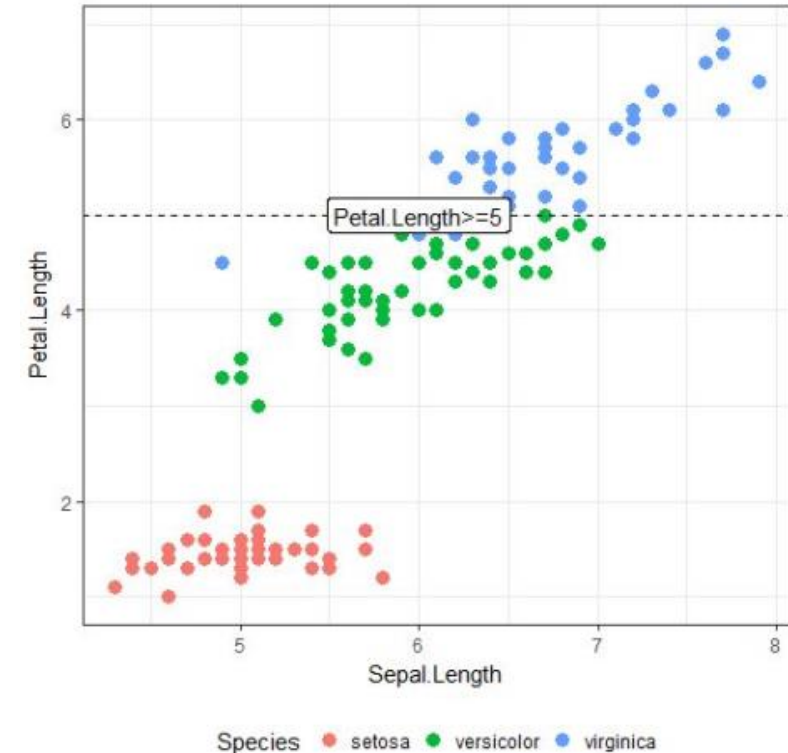
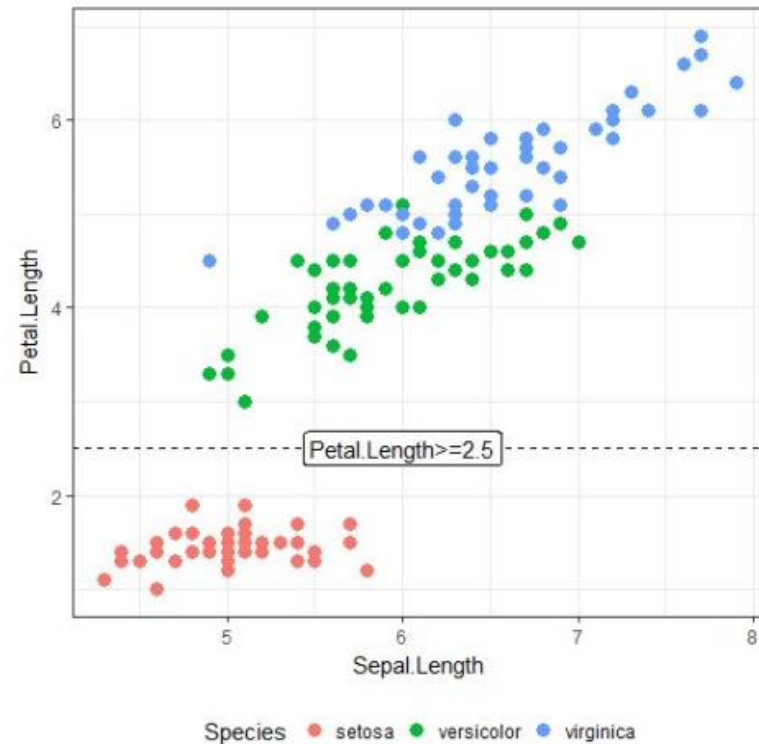
- where m = number of classes, p_k is the prob. of the class in a given partition
- Between $[0, \log_2(m)]$
- 0, most pure, all records belong to the same class



Source: "Data Science for Business" by Provost & Fawcett, 2013

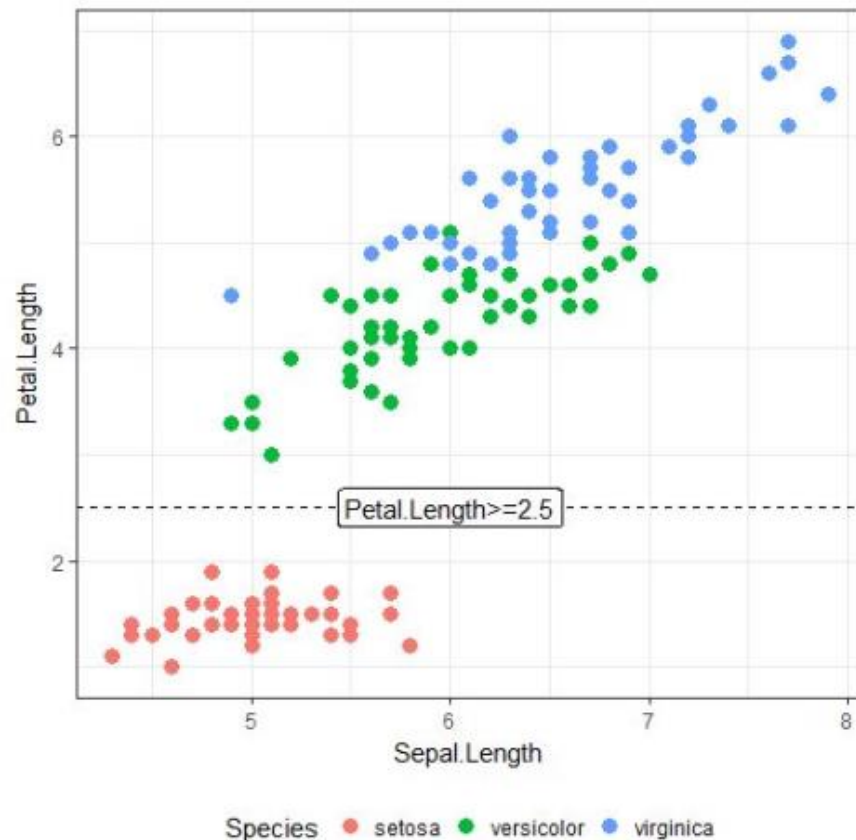
- ❑ E.g., if the data contains 70% of Class A and 30% of Class B then:
 - Entropy = $- [0.7 \cdot \log_2(0.7) + 0.3 \cdot \log_2(0.3)] \sim 0.88$
- ❑ Higher the entropy, more impure the data.
 - Highest (2 classes) = $- [0.5 \cdot \log_2(0.5) + 0.5 \cdot \log_2(0.5)] = 1$

Choose Attributes to Split on



- ❑ **Information Gain** : Compare shift from original entropy. **(Higher the better)**
 - Information Gain = Entropy(Parent) – Weighted Avg (Entropy(Children))

Choose Attributes to Split on



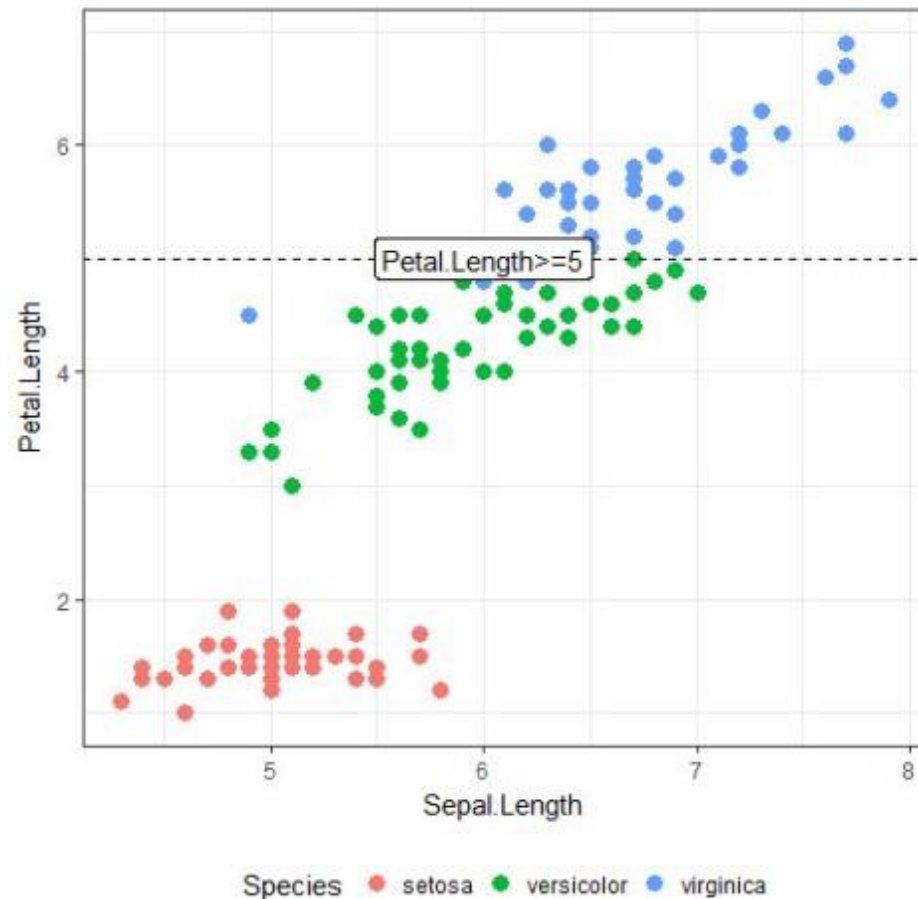
- ❑ Calculate the entropies of the two partitions
 - **Petal.Length < 2.5:** $-1 * \log_2(1) = 0$
 - **Petal.Length >= 2.5:** $-[0.5 * \log_2(0.5) + 0.5 * \log_2(0.5)] = 1$
 - **Weighted Entropy:** $0 * (50/150) + 1 * (100/150) = \mathbf{0.67}$

- ❑ Calculate the entropy of the parent (in this case, all the data points together, before initial split)
 - $-[0.33 * \log_2(0.33) + 0.33 * \log_2(0.33) + 0.33 * \log_2(0.33)] = \mathbf{1.58}$

- ❑ **Information Gain: $1.58 - 0.67 = 0.91$**

The data: 150 points in total, 50 red, 50 green, 50 blue

Choose Attributes to Split on



Above the line, you have 43 points (41 blue and 2 green)

Below the line, you have 107 points (50 red, 9 blue and 48 green)

❑ Calculate the entropies of the two partitions

○ **Petal.Length <5:**

$$-[0.47 * \log_2(0.47) + 0.45 * \log_2(0.45) + 0.08 * \log_2(0.08)] = 1.31$$

○ **Petal.Length >=5:**

$$-[0.95 * \log_2(0.95) + 0.05 * \log_2(0.05)] = 0.28$$

○ **Weighted Entropy:**

$$1.31 * (107/150) + 0.28 * (43/150) = 1.01$$

❑ The entropy of the parent

$$-[0.33 * \log_2(0.33) + 0.33 * \log_2(0.33) + 0.33 * \log_2(0.33)] = 1.58$$

❑ Information Gain: $1.58 - 1.01 = 0.57$

**Splitting on Petal.Length at 2.5 is better as the
Information Gain is higher**

Decision Trees: Procedure Recap

- ❑ Final tree is constructed as follows:
 - Start with the attribute-split for **the root node**: this is going to be the attribute-split that leads to the **largest information gain**, compared to all the others
 - From there, the algorithm proceeds looking at the information gain of subsequent splits on different attributes-values, conditional on the previous one
 - Note:
 - ✓ **The same attribute can be used again**, as long as the partitions/splits are not overlapping
 - ✓ Not all the attributes available in the dataset need to be used in the tree

Classification Probabilities and Cutoffs

- ❑ Many classifiers (including k-NN, Decision Trees) not only produce a class prediction, but they also produce a **probability** that the data point belongs to that class
 - k-NN: % of a class among k-neighbors
 - Decision tree: % of a class in a leaf node
- ❑ Predictions can then generated based on a **cutoff** value:
 - Default cutoff is 0.5 (50%) (majority rule):
 - ✓ If probability of belonging to class “A” is >50%, then classify as belonging to class “A”
 - ✓ Otherwise, classify as class “B”
 - Different cutoffs can be set and can lead to different classification results

Evaluating Model Performance

- ❑ In classification, performance is evaluated using a **confusion matrix**

		Actual Class	
		Yes (Pos.)	No (Neg.)
Predicted Class	Yes (Pos.)	True Positive	False positive (Type I error)
	No (Neg.)	False Negative (Type II error)	True Negative

- ❑ For each cell, e.g., True Positive (TP), **the number of cases** for which we predict Yes, and the actual class is Yes

- ❑ In classification, a **Confusion matrix** is created to calculate:

- **Accuracy (error rate):** overall performance
 - ✓ Not good in unbalanced dataset
 - ✓ E.g., 95 “Yes, Loan”, 5 “No Loan”
- **Precision:** class specific
- **Recall:** class specific
- **F-measure:** class specific

Intuition Behind Each Measure

- ❑ **Accuracy:** Among all predictions, how many did the model get right?

$$\text{Accuracy} = (TP + TN) / (TP + TN + FP + FN)$$

- ❑ **Precision:** For each class, how many did the model get right?

- Precision_pos. = positive predictive value (**PPV**) = $TP / (TP + FP)$
- Precision_neg. = negative predictive value (**NPV**) = $TN / (TN + FN)$

- ❑ **Recall:** How many per each class were recovered?

- Recall_pos. = **Sensitivity** = $TP / (TP + FN)$
- Recall_neg. = **Specificity** = $TN / (TN + FP)$

- ❑ **F-measure:** the harmonic mean of precision and recall

- $F1_score = 2 * ((\text{recall} * \text{precision}) / (\text{recall} + \text{precision}))$
- It is a more reliable measure than accuracy when your data is unbalanced
- The higher the F1 score, the better the classification model

		Actual Class	
		Yes (Pos.)	No (Neg.)
Predicted Class	Yes (Pos.)	True Positive	False positive (Type I error)
	No (Neg.)	False Negative (Type II error)	True Negative

TP: True Positive

TN: True Negative

FP: False Positive

FN: False Negative

Example

- ❑ Accuracy: $0.7 = 70\%$
- ❑ Recall (Sensitivity) for class **Non-Fraud**: $=0.75 = 75\%$
- ❑ Recall (Specificity) for class **Fraud**: $=0.5 = 50\%$
- ❑ Precision (PPV) for class **Non-Fraud**: $=0.86 = 86\%$
- ❑ Precision (NPV) for class **Fraud**: $=0.33 = 33\%$

		Actual Class	
		Non-Fraud	Fraud
Predicted Class	Non-Fraud	60	10
	Fraud	20	10

- F1_Score for **Non-Fraud**: $2 * ((0.75 * 0.86) / (0.75 + 0.86)) = 0.80$
- F1_Score for **Fraud**: $2 * ((0.5 * 0.33) / (0.5 + 0.33)) = 0.40$
- In this example, the overall accuracy of the model is about 70%. Nevertheless, if we look at the F1 scores, we see that for the class **Fraud**, F1 score is about 40%.
- Since this dataset is unbalanced (there are way more cases of **Non-Fraud** than **Fraud**), F1 scores is a more appropriate measure.

Differing Misclassification Costs

- ❑ In many real-world applications, different types of mistakes in classification are not equally important
 - E.g., missing a fraud transaction is very costly, classify a non-fraud as fraud is not as detrimental
- ❑ Instead of maximizing accuracy, sometimes we want to **minimize misclassification cost**
- ❑ One way to minimize misclassification cost is to **adjust the cutoff value**
 - E.g., if misclassifying “Fraud” as “Non-Fraud” is far more costly than the other way around, we want to **reduce cutoff** for classifying a transaction as Fraud.

Cost Matrix		Actual	
		+	-
Predicted	+	TP (P1)	FN (C1)
	-	FP (C2)	TN (P2)

$$\text{Avg Misclassification cost} = (C2 * FP + C1 * FN) / \text{All}$$

Questions?

