



More on Supervised Learning

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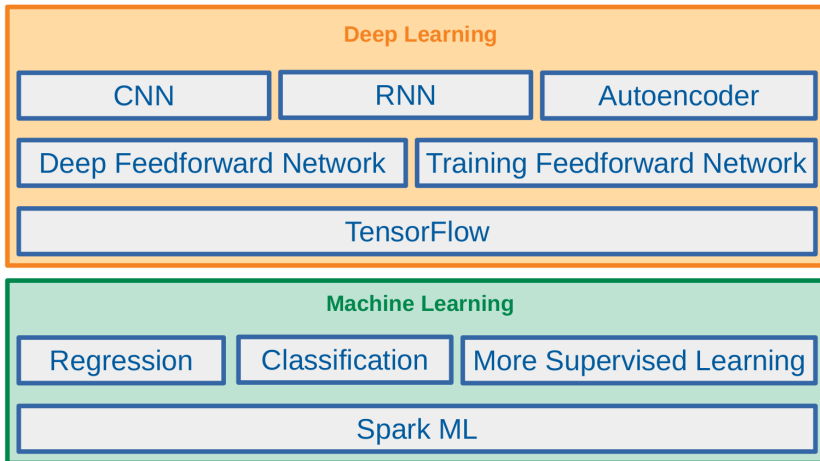


The Course Web Page

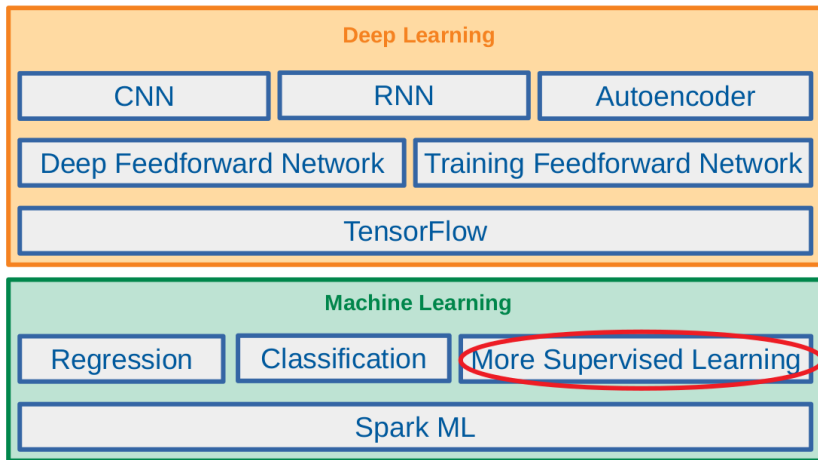
`https://id2223kth.github.io`



Where Are We?



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Let's Start with an Example



Buying Computer Example (1/3)

- ▶ Given the dataset of m people.

id	age	income	student	credit rating	buys computer
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- ▶ Predict if a new person buys a computer?

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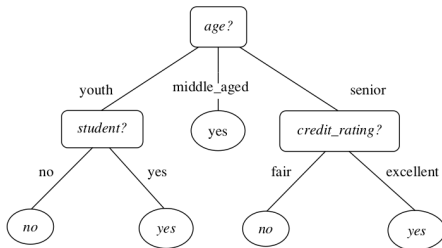
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- ▶ **Predict** if a new person **buys a computer**?
- ▶ Given an instance $\mathbf{x}^{(i)}$, e.g., $x_1^{(i)} = \text{senior}$, $x_2^{(i)} = \text{medium}$, $x_3^{(i)} = \text{no}$, and $x_4^{(i)} = \text{fair}$, then $y^{(i)} = ?$

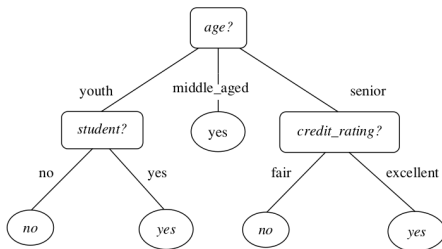
Buying Computer Example (2/3)

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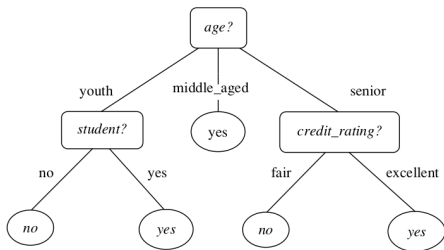
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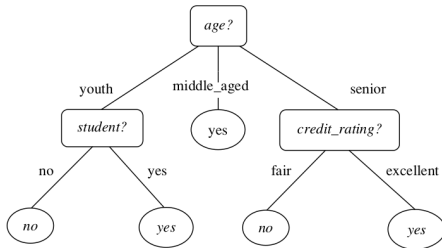
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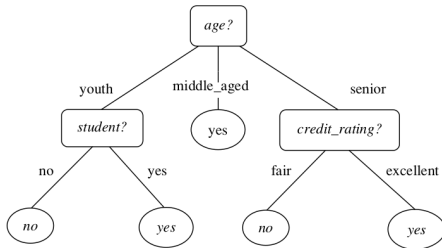
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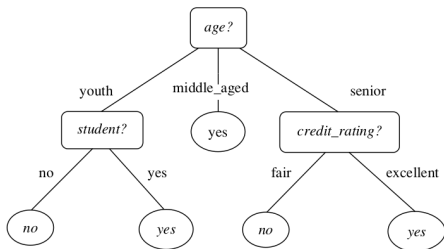
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- ▶ E.g., input $\mathbf{x}^{(i)}$ with $x_1^{(i)} = \text{senior}$, $x_2^{(i)} = \text{medium}$, $x_3^{(i)} = \text{no}$, and $x_4^{(i)} = \text{fair}$.



Decision Tree

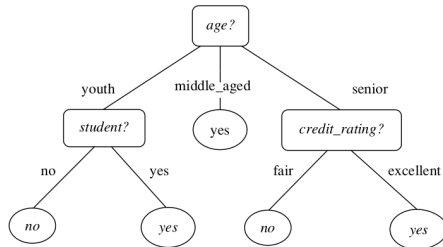
Decision Tree

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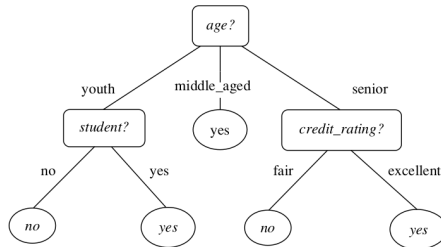
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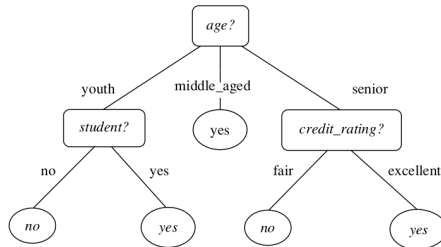
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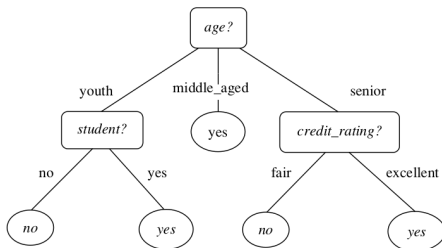
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 - Each **leaf**: holds a **class label**





Training Algorithm (1/2)

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 - Feature selection method: determines the splitting criterion.



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- ▶ 4. The algorithm repeats the same process **recursively** to form a decision tree.



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- ▶ In **conditions 2 and 3**:
 - Convert node N into a **leaf**.
 - Label it either with the **most common class** in D .
 - Or, the **class distribution** of the node tuples may be stored.

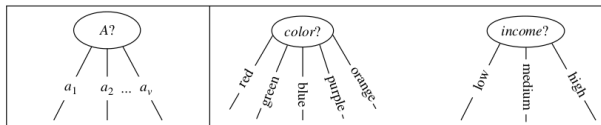


Training Algorithm - Partitioning Instances (1/3)

- ▶ Assume A is the **splitting feature**
- ▶ **Three** possibilities to **partition instances** in D based on the feature A .
- ▶ 1. A is **discrete-valued**

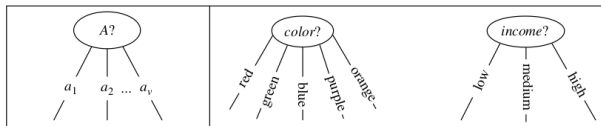
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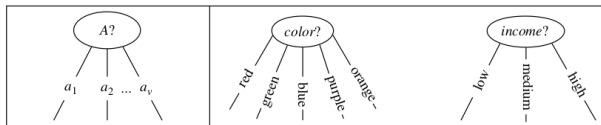
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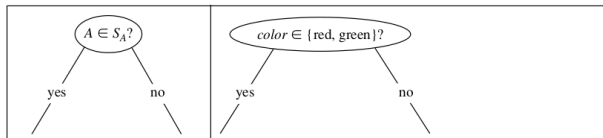
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 - Partition D_j is the **subset of tuples** in D having value a_j of A .



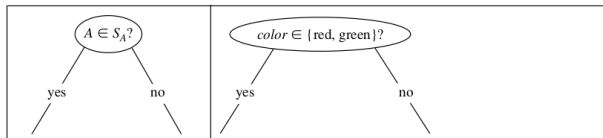
Training Algorithm - Partitioning Instances (2/3)

- ▶ 2. A is discrete-valued



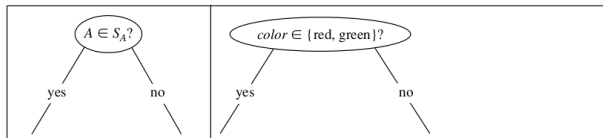
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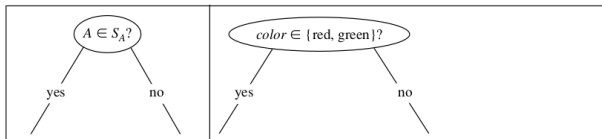
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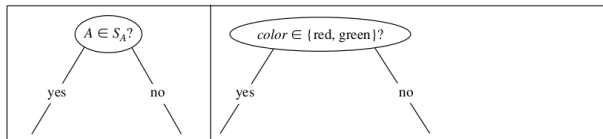
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 - The **right branch** out of N corresponds to the **instances in D that do not satisfy the test**.



Training Algorithm - Partitioning Instances (3/3)



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 - Two branches are labeled according to the previous outcomes.





Training Algorithm - Feature Selection Measures (1/2)

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- ▶ Pure partition: if all instances in a partition belong to the same class.
- ▶ The best splitting criterion is the one that most closely results in a pure scenario.



Training Algorithm - Feature Selection Measures (2/2)

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- ▶ Two popular feature selection measures are:
 - Information gain (ID3 and C4.5)
 - Gini index (CART)

Information Gain (Entropy)



ID3 (1/8)

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- ▶ The information gain is based on the decrease in entropy after a dataset is split on a feature.



ID3 (2/8)

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- ▶ D 's entropy is zero when it contains instances of only one class (pure partition).

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label = buys_computer $\Rightarrow m = 2$

$$\text{entropy}(D) = - \frac{9}{14} \log_2\left(\frac{9}{14}\right) - \frac{5}{14} \log_2\left(\frac{5}{14}\right) = 0.94$$



ID3 (4/8)

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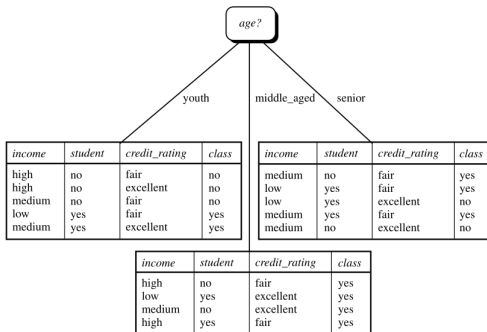
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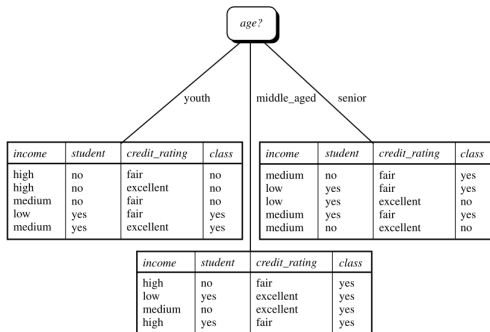
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- ▶ $\frac{|D_j|}{|D|}$ is the **weight** of the j th partition.
- ▶ The **smaller** the **expected information** required, the **greater** the **purity** of the partitions.

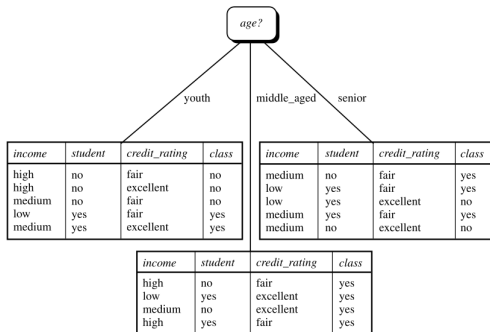


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$$\text{entropy}(\text{age}, D) = \frac{5}{14} \left(-\frac{2}{5} \log_2\left(\frac{2}{5}\right) - \frac{3}{5} \log_2\left(\frac{3}{5}\right) \right) + \frac{4}{14} \left(-\frac{4}{4} \log_2\left(\frac{4}{4}\right) \right) + \frac{5}{14} \left(-\frac{3}{5} \log_2\left(\frac{3}{5}\right) - \frac{2}{5} \log_2\left(\frac{2}{5}\right) \right) = 0.694$$



ID3 (6/8)

- ▶ The information gain $\text{Gain}(A, D)$ is defined as:

$$\text{Gain}(A, D) = \text{entropy}(D) - \text{entropy}(A, D)$$



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- ▶ It shows how much would be gained by branching on A .
- ▶ The feature A with the highest $\text{Gain}(A, D)$ is chosen as the splitting feature at node N .



ID3 (7/8)

- ▶ Now, we can compute the information gain $\text{Gain}(A)$ for the feature $A = \text{age}$.

$$\text{Gain}(\text{age}, D) = \text{entropy}(D) - \text{entropy}(\text{age}, D) = 0.940 - 0.694 = 0.246$$



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- ▶ Similarly we have:
 - $\text{Gain}(\text{income}, D) = 0.029$
 - $\text{Gain}(\text{student}, D) = 0.151$
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- ▶ The **age** has the highest information gain among the attributes, it is selected as the **splitting feature**.



ID3 (8/8)

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3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
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- ▶ For example, a split on **RID** would result in a **large number of partitions**.
 - Each partition is **pure**.
 - Info product $\text{entropy}(\text{RID}, D) = 0$, thus, the **information gained** by partitioning on this feature is **maximal**.

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 - Each partition is **pure**.
 - Info product $\text{entropy}(\text{RID}, D) = 0$, thus, the **information gained** by partitioning on this feature is **maximal**.
- ▶ Clearly, such a partitioning is **useless** for classification.



C4.5 (1/2)

- ▶ C4.5 is a successor of ID3 that overcomes its bias problem.
- ▶ It normalizes the information gain using a split information value:

$$\text{SplitInfo}(A, D) = - \sum_{j=1}^v \frac{|D_j|}{|D|} \log_2 \left(\frac{|D_j|}{|D|} \right)$$

$$\text{GainRatio}(A, D) = \frac{\text{Gain}(A, D)}{\text{SplitInfo}(A, D)}$$

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$$\text{SplitInfo}(\text{income}, D) = - \frac{4}{14} \log_2 \left(\frac{4}{14} \right) - \frac{6}{14} \log_2 \left(\frac{6}{14} \right) - \frac{4}{14} \log_2 \left(\frac{4}{14} \right) = 1.557$$

► $\text{Gain}(\text{income}, D) = 0.029$, therefore $\text{GainRatio}(\text{income}, D) = \frac{0.029}{1.557} = 0.019$.

Gini Impurity



CART (1/8)

- ▶ CART (Classification And Regression Tree) considers a **binary split** for each **feature**.



CART (1/8)

- ▶ CART (Classification And Regression Tree) considers a binary split for each feature.
- ▶ It uses the Gini index to measure the misclassification (impurity of D).

$$\text{Gini}(D) = 1 - \sum_{i=1}^m p_i^2$$



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- ▶ We need to determine the splitting criterion: splitting feature + splitting subset.



CART (2/8)

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 - E.g., $A = \text{income} = \{\text{low}, \text{medium}, \text{high}\}$
 - $S_A = \{\{\text{low}, \text{medium}, \text{high}\}, \{\text{low}, \text{medium}\}, \{\text{medium}, \text{high}\}, \{\text{low}, \text{high}\}, \{\text{low}\}, \{\text{medium}\}, \{\text{high}\}, \{\}\}$



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 - The **test** is of the form $D_1 \in s_A?$, where s_A is a subset of S_A , e.g., $s_A = \{\text{low}, \text{high}\}$.

CART (3/8)

<i>RID</i>	<i>age</i>	<i>income</i>	<i>student</i>	<i>credit_rating</i>	<i>Class: buys_computer</i>
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
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4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
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$$\text{Gini}(D) = 1 - \sum_{i=1}^m p_i^2$$

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$$\text{Gini}(D) = 1 - \sum_{i=1}^m p_i^2$$

label = buys_computer $\Rightarrow m = 2$

$$\text{Gini}(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$



CART (4/8)

- ▶ If a binary split on A partitions D into D_1 and D_2 , the **Gini index** of D given that partitioning is:

$$\text{Gini}(A, D) = \frac{|D_1|}{D} \text{Gini}(D_1) + \frac{|D_2|}{D} \text{Gini}(D_2)$$



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- ▶ The subset that gives the **minimum Gini index** is selected as its **splitting subset**.



CART (5/8)

- ▶ For a feature $A = \text{income}$, we consider each of the possible **splitting subsets**.



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 - $S_A = \{\{\text{low}, \text{medium}, \text{high}\}, \{\text{low}, \text{medium}\}, \{\text{medium}, \text{high}\}, \{\text{low}, \text{high}\}, \{\text{low}\}, \{\text{medium}\}, \{\text{high}\}, \{\}\}$



CART (5/8)

- ▶ For a feature $A = \text{income}$, we consider each of the possible **splitting subsets**.
 - $S_A = \{\{\text{low, medium, high}\}, \{\text{low, medium}\}, \{\text{medium, high}\}, \{\text{low, high}\}, \{\text{low}\}, \{\text{medium}\}, \{\text{high}\}, \{\}\}$
- ▶ Assume, we choose the **splitting subset** $s_A = \{\text{low, medium}\}$.

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- ▶ Assume, we choose the **splitting subset** $s_A = \{\text{low, medium}\}$.
- ▶ Consider partition D_1 satisfies the condition $D_1 \in s_A$, and D_2 does not.

$$\begin{aligned} \text{Gini}_{\text{income} \in \{\text{low, medium}\}}(A, D) &= \frac{10}{14} \text{Gini}(D_1) + \frac{4}{14} \text{Gini}(D_2) \\ &= \frac{10}{14} \text{Gini}\left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14} \left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right) = 0.443 \end{aligned}$$



CART (6/8)

- ▶ Similarly, we calculate the **Gini index** values for splits on the **remaining subsets**.

$$\text{Gini}_{\text{income} \in \{\text{low}, \text{medium}\}}(A, D) = \text{Gini}_{\text{income} \in \{\text{high}\}}(A, D) = 0.443$$

$$\text{Gini}_{\text{income} \in \{\text{low}, \text{high}\}}(A, D) = \text{Gini}_{\text{income} \in \{\text{medium}\}}(A, D) = 0.458$$

$$\text{Gini}_{\text{income} \in \{\text{medium}, \text{high}\}}(A, D) = \text{Gini}_{\text{income} \in \{\text{low}\}}(A, D) = 0.450$$

- ▶ Similarly, we calculate the **Gini index** values for splits on the **remaining subsets**.

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$$\text{Gini}_{\text{income} \in \{\text{medium}, \text{high}\}}(A, D) = \text{Gini}_{\text{income} \in \{\text{low}\}}(A, D) = 0.450$$

- ▶ The best binary split for attribute $A = \text{income}$ is on $s_A = \{\text{low}, \text{medium}\}$ because it **minimizes the Gini index**.



CART (7/8)

- ▶ But, which feature?



CART (7/8)

- ▶ But, **which feature?**
- ▶ The **reduction in impurity** that would be incurred by a binary split on feature **A** is:

$$\Delta\text{Gini}(A) = \text{Gini}(D) - \text{Gini}(A,D)$$



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- ▶ The feature that **maximizes the reduction in impurity** (has the **minimum Gini index**) is selected as the **splitting feature**.



CART (8/8)

- Now, we can compute the **information gain** $\text{Gain}(A)$ for different features.
- $\Delta\text{Gini}(\text{income}) = 0.459 - 0.443 = 0.016$
 - $\Delta\text{Gini}(\text{age}) = 0.459 - 0.357 = 0.102$
 - $\Delta\text{Gini}(\text{student}) = 0.459 - 0.367 = 0.092$
 - $\Delta\text{Gini}(\text{credit_rating}) = 0.459 - 0.429 = 0.03$



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 - $\Delta\text{Gini}(\text{credit_rating}) = 0.459 - 0.429 = 0.03$
- ▶ The feature $A = \text{age}$ and splitting subset $s_A = \{\text{youth}, \text{senior}\}$ gives the **minimum Gini index** overall.



Decision Tree in Spark (1/4)

- ▶ Two classes in `spark.ml`.
- ▶ Regression: `DecisionTreeRegressor`

```
val dt_regressor = new DecisionTreeRegressor().setLabelCol("label").setFeaturesCol("features")
val model = dt_regressor.fit(trainingData)
val predictions = model.transform(testData)
predictions.select("prediction", "rawPrediction", "probability", "label", "features").show(5)
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Decision Tree in Spark (2/4)

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- ▶ `probabilityCol` is a **vector** of length of number of classes equal to `rawPrediction` **normalized to a multinomial distribution**.



Decision Tree in Spark (3/4)

- ▶ Tunable parameters



Decision Tree in Spark (3/4)

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- ▶ `maxBins`: number of bins used when discretizing continuous features.



Decision Tree in Spark (3/4)

- ▶ Tunable parameters
- ▶ `maxBins`: number of bins used when discretizing continuous features.
- ▶ `impurity`: impurity measure used to choose between candidate splits, e.g., `entropy` and `gini`.

```
val maxBins = ...  
val dt_classifier = new DecisionTreeClassifier().setMaxBins(maxBins).setImpurity("gini")
```



Decision Tree in Spark (4/4)

- ▶ **Stopping criteria** that determines when the tree stops building.



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- ▶ **maxDepth**: **maximum depth** of a tree.



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Decision Tree in Spark (4/4)

- ▶ **Stopping criteria** that determines when the tree stops building.
- ▶ **maxDepth**: **maximum depth** of a tree.
- ▶ **minInstancesPerNode**: for a node to be split further, each of its **children** must receive **at least this number of training instances**.
- ▶ **minInfoGain**: for a node to be split further, the split must **improve** at least this much (in terms of **information gain**).

```
val maxDepth = ...
val minInstancesPerNode = ...
val minInfoGain = ...
val dt_classifier = new DecisionTreeClassifier()
                    .setMaxDepth(maxDepth)
                    .setMinInstancesPerNode(minInstancesPerNode)
                    .setMinInfoGain(minInfoGain)
```



Ensemble Methods



Wisdom of the Crowd

- ▶ Ask a **complex question** to **thousands of random people**, then aggregate their answers.
- ▶ In many cases, this **aggregated answer** is **better** than an **expert's answer**.



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- ▶ In many cases, this **aggregated answer** is **better** than an **expert's answer**.
- ▶ This is called the **wisdom of the crowd**.
- ▶ Similarly, the aggregated estimations of a **group of estimators** (e.g., **classifiers or regressors**), often gets **better estimations** than with the best individual estimator.
- ▶ A **group of estimators** is an **ensemble**, and this technique is called **Ensemble Learning**.



Ensemble Learning

- ▶ Two main categories of **ensemble learning** algorithms.



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- ▶ **Bagging**
 - Use the **same training algorithm** for **every estimator**, but to train them on **different random subsets** of the training set.
 - E.g., **random forest**

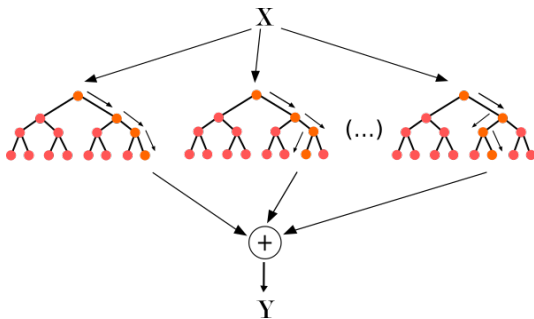


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- ▶ **Boosting**
 - Train estimators **sequentially**, each trying to **correct its predecessor**.
 - E.g., **adaboost** and **gradient boosting**

Random Forest

- ▶ **Random forest** builds **multiple decision trees** that are most of the time trained with the **bagging** method.
- ▶ It, then, merges the trees together to get a more **accurate and stable prediction**.





Random Forest in Spark (1/2)

- ▶ Two classes in `spark.ml`.
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val rf_regressor = new RandomForestRegressor().setLabelCol("label")  
                                                    .setFeaturesCol("features").setNumTrees(10)  
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Random Forest in Spark (2/2)

- ▶ `numTrees`: number of trees in the forest.



Random Forest in Spark (2/2)

- ▶ `numTrees`: **number of trees** in the forest.
- ▶ `subsamplingRate`: specifies the **size of the dataset** used for training each tree in the forest, as a **fraction of the size of the original dataset**.
 - Default is 1.0 and decreasing it can speed up training.

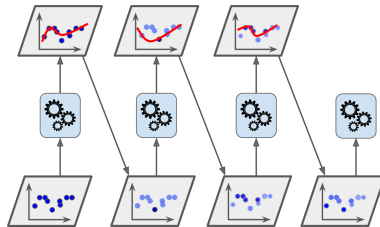


Random Forest in Spark (2/2)

- ▶ `numTrees`: **number of trees** in the forest.
- ▶ `subsamplingRate`: specifies the **size of the dataset** used for training each tree in the forest, as a **fraction of the size of the original dataset**.
 - Default is 1.0 and decreasing it can speed up training.
- ▶ `featureSubsetStrategy`: **number of features** to use as candidates for splitting at each tree node, as a **fraction of the total number of features**.
 - Possible values: `auto`, `all`, `onethird`, `sqrt`, `log2`, `n`

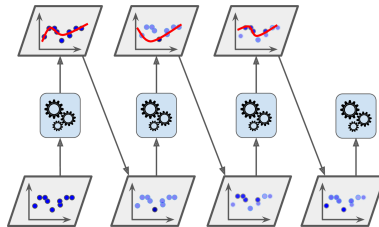
AdaBoost (1/3)

- ▶ **AdaBoost**: train a **new estimator** by paying more attention to the training instances that the **predecessor underfitted**.



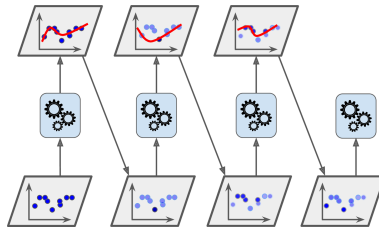
AdaBoost (1/3)

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- ▶ Each **estimator** is trained on a **random subset** of the **total training set**.



AdaBoost (1/3)

- ▶ **AdaBoost**: train a **new estimator** by paying more attention to the training instances that the **predecessor underfitted**.
- ▶ Each **estimator** is trained on a **random subset** of the **total training set**.
- ▶ AdaBoost assigns a **weight** to each **training instance**, which determines the **probability** that each instance should **appear in the training set**.





AdaBoost (2/3)

- ▶ Each instance weight $h^{(i)}$ is initially set to $\frac{1}{m}$ for m instances.



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- ▶ The j th **estimator's weight** α_j is then computed as follows:

$$\alpha_j = \eta \frac{1 - r_j}{r_j}$$



AdaBoost (3/3)

- ▶ Next the **instance weights** are updated:

$$h^{(i)} = \begin{cases} h^{(i)} & \text{if } \hat{y}_j^{(i)} = y_j^{(i)} \\ h^{(i)} e^{\alpha_j} & \text{if } \hat{y}_j^{(i)} \neq y_j^{(i)} \end{cases}$$



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- ▶ Then, a **new estimator** is trained using the **updated weights**, and the whole process is repeated.
- ▶ To make **predictions**, AdaBoost computes the **predictions** of all the estimators and **weighs** them using the estimator weights α_j .



Gradient Boosting (1/3)

- ▶ Just like AdaBoost, **Gradient Boosting** works by **sequentially** adding **estimators to an ensemble**, each one **correcting its predecessor**.
- ▶ However, instead of tweaking the instance weights at every iteration, this method **tries to fit the new estimator** to the **residual errors** made by the previous estimator.



Gradient Boosting (2/3)

- ▶ Let's go through a regression example using **Gradient Boosted Regression Trees**.
- ▶ Fit the **first estimator** on the **training set**.

```
tree_reg1 = DecisionTreeRegressor(max_depth=2)
tree_reg1.fit(X, y)
```

- ▶ Now train the **second estimator** on the **residual errors** made by the **first estimator**.

```
y2 = y - tree_reg1.predict(X)
tree_reg2 = DecisionTreeRegressor(max_depth=2)
tree_reg2.fit(X, y2)
```



Gradient Boosting (3/3)

- ▶ Then we train the **third estimator** on the **residual errors** made by the **second estimator**.

```
y3 = y2 - tree_reg2.predict(X)
tree_reg3 = DecisionTreeRegressor(max_depth=2)
tree_reg3.fit(X, y3)
```

- ▶ Now we have an **ensemble containing three trees**.
- ▶ It can **make predictions** on a new instance simply by adding up the predictions of all the trees.

```
y_pred = sum(tree.predict(X_new) for tree in (tree_reg1, tree_reg2, tree_reg3))
```



Gradient Boosting in Spark (1/2)

- ▶ Two classes in `spark.ml`.
- ▶ Regression: `GBTRegressor`

```
val gbt = new GBTRegressor().setLabelCol("label").setFeaturesCol("features")
    .setMaxIter(10).setFeatureSubsetStrategy("auto")

val model = gbt.fit(trainingData)
val predictions = model.transform(testData)
```



Gradient Boosting in Spark (1/2)

- ▶ Two classes in `spark.ml`.
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```

- ▶ Classifier: `GBTClassifier`

```
val gbt = new GBTClassifier().setLabelCol("label").setFeaturesCol("features")
    .setMaxIter(10).setFeatureSubsetStrategy("auto")

val model = gbt.fit(trainingData)
val predictions = model.transform(testData)
```

Summary



Summary

- ▶ Decision tree
 - Top-down training algorithm
 - Termination condition
 - Feature selection: entropy, gini

- ▶ Ensemble models
 - Bagging: random forest
 - Boosting: AdaBoost, Gradient Boosting



Reference

- ▶ Aurélien Géron, Hands-On Machine Learning (Ch. 5, 6, 7)
- ▶ Matei Zaharia et al., Spark - The Definitive Guide (Ch. 27)

Questions?