More on Supervised Learning

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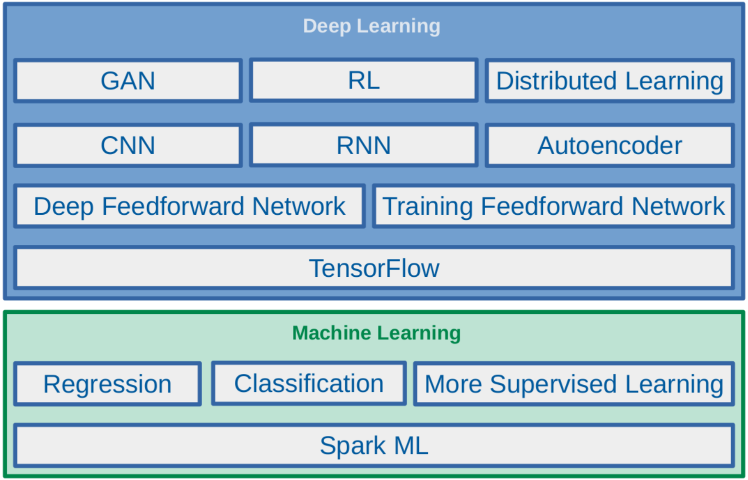
The Course Web Page

`https://id2223kth.github.io`

Where Are We?


Deep Learning
GAN
RL
Distributed Learning
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Spark ML

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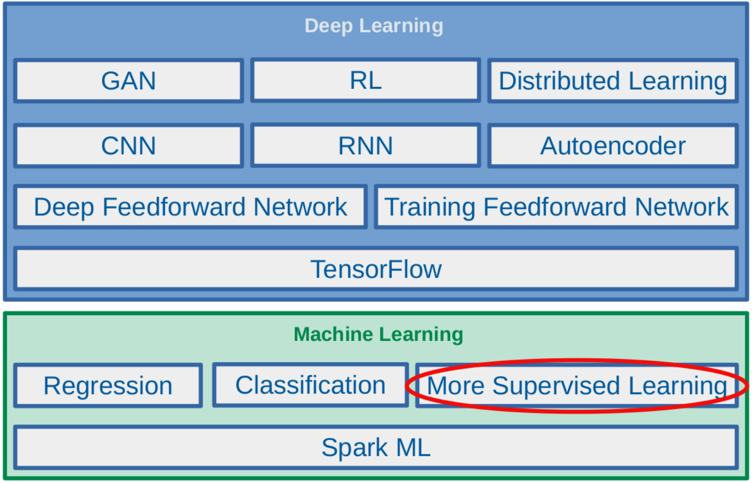
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Let's Start with an Example

Buying Computer Example (1/3)

- Given the dataset of `m` people.

id	age	income	student	credit rating	buys computer
1	youth	high	no	fair	no
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- Predict if a new person buys a computer?
- Given an instance $\mathbf{x}^{(i)}$, e.g., $x_1^{(i)} = \mathtt{senior}$, $x_2^{(i)} = \mathtt{medium}$, $x_3^{(i)} = \mathtt{no}$, and $x_4^{(i)} = \mathtt{fair}$, then $y^{(i)} = ?$

Buying Computer Example (2/3)

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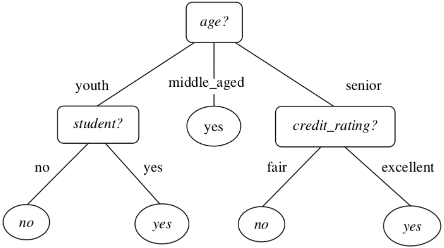

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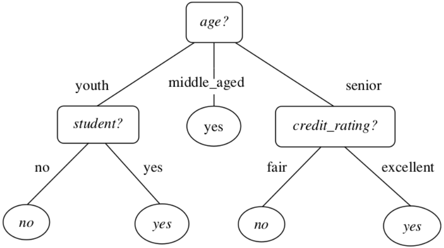

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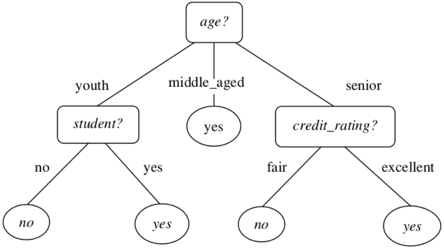

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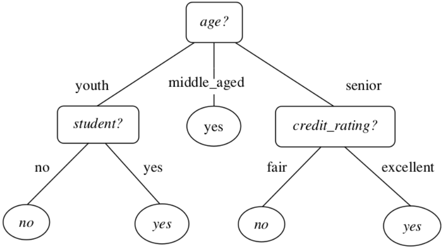

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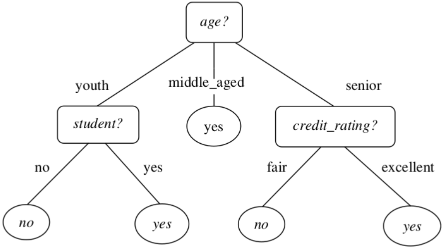
- E.g., input $\mathbf{x}^{(i)}$ with $x_1^{(i)} = \texttt{senior}$, $x_2^{(i)} = \texttt{medium}$, $x_3^{(i)} = \texttt{no}$, and $x_4^{(i)} = \texttt{fair}$.



Decision Tree

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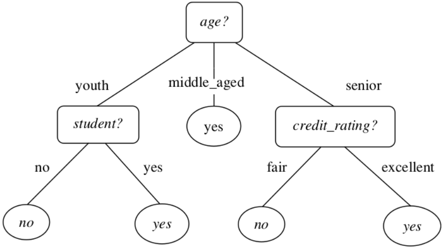

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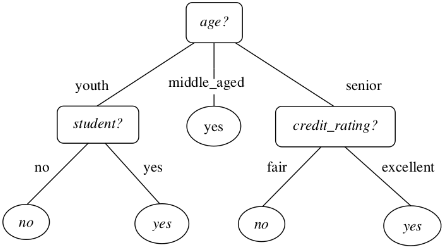

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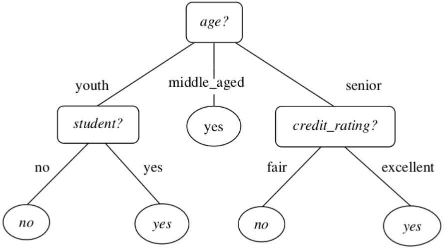

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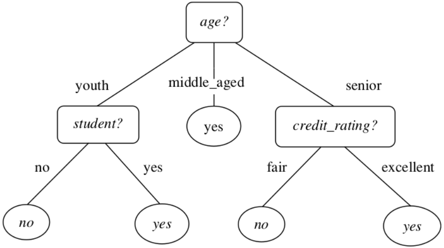

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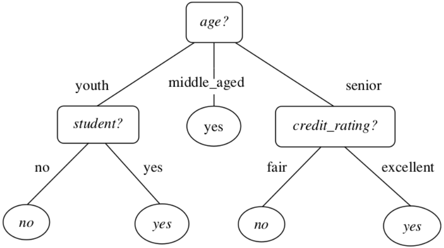

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- 4. The algorithm repeats the same process recursively to form a decision tree.

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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)

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- Three possibilities to partition instances in `D` based on the feature `A`.
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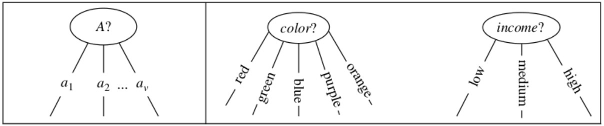

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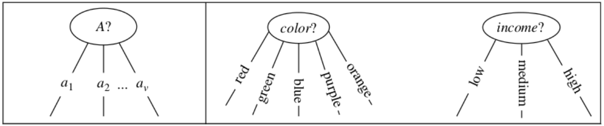

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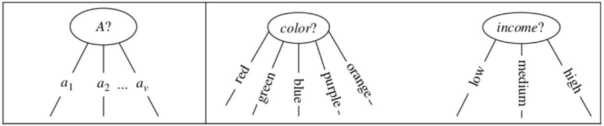
    - Partition D_j is the subset of tuples in D having value a_j of A.



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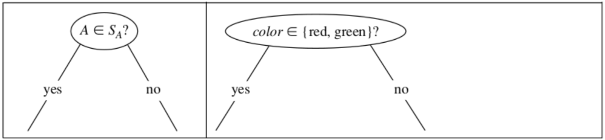

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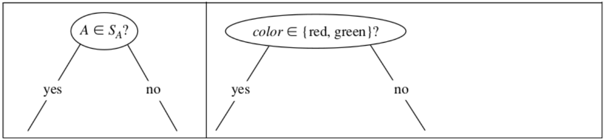

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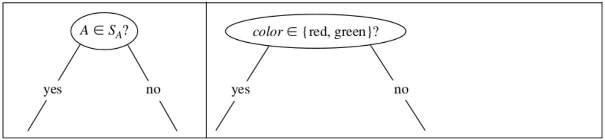

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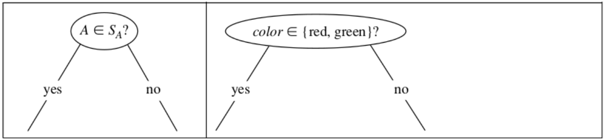

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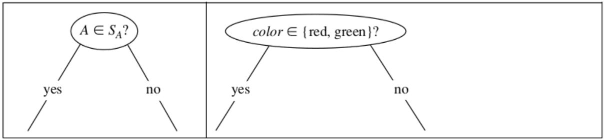

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  - Two branches are labeled according to the previous outcomes.

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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.

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- Two popular feature selection measures are:
  - Information gain (ID3)
  - Gini index (CART)

Information Gain (Entropy)

ID3 (1/7)

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- The feature with the highest information gain is chosen as the splitting feature for node `N`.
- The information gain is based on the decrease in entropy after a dataset is split on a feature.

ID3 (2/7)

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$$\text{entropy}(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

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

ID3 (3/7)

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1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle_aged	high	no	fair	yes
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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
14	senior	medium	no	excellent	no

$$\mathtt{entropy}(\mathtt{D}) = -\sum_{\mathtt{i}=1}^{\mathtt{m}} \mathtt{p_i} \log_2(\mathtt{p_i})$$

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$$\mathtt{entropy}(\mathtt{D}) = -\sum_{\mathtt{i}=1}^{\mathtt{m}} \mathtt{p_i} \log_2(\mathtt{p_i})$$

$$\text{label} = \mathtt{buys\_computer} \Rightarrow \mathtt{m} = 2$$

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

ID3 (4/7)

- Suppose we want to partition instances in $\mathtt{D}$ on some feature $\mathtt{A}$ with $\mathtt{v}$ distinct values, $\{\mathtt{a}_1, \mathtt{a}_2, \cdots, \mathtt{a}_\mathtt{v}\}$.

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- Suppose we want to partition instances in D on some feature A with v distinct values, $\{a_1, a_2, \cdots, a_v\}$.
- A can split D into v partitions $\{D_1, D_2, \cdots, D_v\}$.

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- The expected information required to classify an instance from $\mathtt{D}$ based on the partitioning by $\mathtt{A}$ is:

$$\mathtt{entropy}(\mathtt{A}, \mathtt{D}) = \sum_{\mathtt{j}=1}^{\mathtt{v}} \frac{|\mathtt{D}_\mathtt{j}|}{|\mathtt{D}|} \mathtt{entropy}(\mathtt{D}_\mathtt{j})$$

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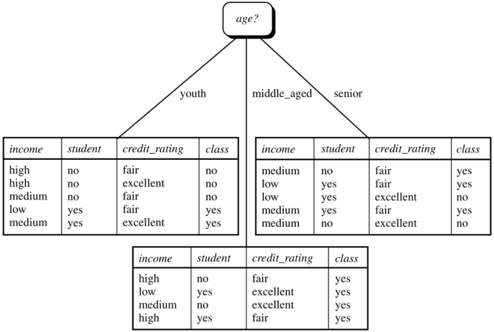
- $\frac{|\mathtt{D}_\mathtt{j}|}{\mathtt{D}}$ is the weight of the $\mathtt{j}$th partition.
- The smaller the expected information required, the greater the purity of the partitions.

ID3 (5/7)



youth

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medium	yes	excellent	yes

middle_aged

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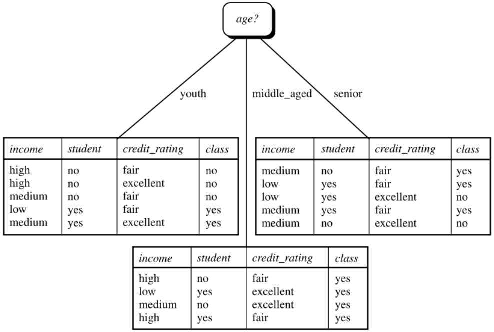
high	yes	fair	yes

senior

income	*student*	*credit_rating*	*class*
medium	no	fair	yes
low	yes	fair	yes
low	yes	excellent	no
medium	yes	fair	yes
medium	no	excellent	no

$$\mathtt{entropy}(\mathtt{A},\mathtt{D}) = \sum_{\mathtt{j}=1}^{\mathtt{v}} \frac{|\mathtt{D}_\mathtt{j}|}{|\mathtt{D}|}\mathtt{entropy}(\mathtt{D}_\mathtt{j})$$

ID3 (5/7)



youth:

income	*student*	*credit_rating*	*class*
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medium	no	fair	no
low	yes	fair	yes
medium	yes	excellent	yes

middle_aged:

income	*student*	*credit_rating*	*class*
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low	yes	excellent	yes
medium	no	excellent	yes
high	yes	fair	yes

senior:

income	*student*	*credit_rating*	*class*
medium	no	fair	yes
low	yes	fair	yes
low	yes	excellent	no
medium	yes	fair	yes
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$$\mathtt{entropy}(\mathtt{A},\mathtt{D}) = \sum_{j=1}^{v} \frac{|\mathtt{D}_j|}{|\mathtt{D}|}\mathtt{entropy}(\mathtt{D}_j)$$

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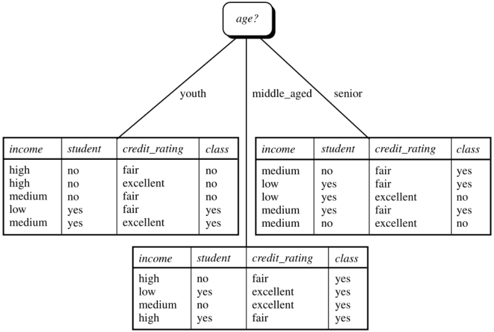

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ID3 (6/7)

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

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- The feature $\texttt{A}$ with the highest $\texttt{Gain}(\texttt{A}, \texttt{D})$ is chosen as the splitting feature at node $\texttt{N}$.

ID3 (7/7)

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

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

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- Similarly we have:
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  - $\texttt{Gain}(\texttt{student}, \texttt{D}) = 0.151$
  - $\texttt{Gain}(\texttt{credit\_rating}, \texttt{D}) = 0.048$

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- The age has the highest information gain among the attributes, it is selected as the splitting feature.

Gini Impurity

CART (1/8)

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

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

CART (2/8)

- Assume $\mathtt{A}$ is a discrete-valued feature with $\mathtt{v}$ distinct values, $\{\mathtt{a}_1, \mathtt{a}_2, \cdots, \mathtt{a}_\mathtt{v}\}$, occurring in $\mathtt{D}$.

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  - E.g., $\mathtt{A} = \mathtt{income} = \{\mathtt{low}, \mathtt{medium}, \mathtt{high}\}$
  - $\mathtt{S}_\mathtt{A} = \{\{\mathtt{low}, \mathtt{medium}, \mathtt{high}\}, \{\mathtt{low}, \mathtt{medium}\}, \{\mathtt{medium}, \mathtt{high}\}, \{\mathtt{low}, \mathtt{high}\}, \{\mathtt{low}\}, \{\mathtt{medium}\}, \{\mathtt{high}\}, \{\}\}$

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

CART (3/8)

RID	age	income	student	credit_rating	Class: buys_computer
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
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
14	senior	medium	no	excellent	no

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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
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14	senior	medium	no	excellent	no

$$\mathtt{Gini}(\mathtt{D}) = 1 - \sum_{\mathtt{i}=1}^{\mathtt{m}} \mathtt{p}_\mathtt{i}^2$$

$$\text{label} = \mathtt{buys\_computer} \Rightarrow \mathtt{m} = 2$$

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

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:

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

CART (4/8)

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

CART (5/8)

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CART (5/8)

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

$$\mathtt{Gini}_{\mathtt{income}\in\{\mathtt{low},\mathtt{medium}\}}(\mathtt{A}, \mathtt{D}) = \frac{10}{14}\mathtt{Gini}(\mathtt{D_1}) + \frac{4}{14}\mathtt{Gini}(\mathtt{D_2})$$

$$= \frac{10}{14}\mathtt{Gini}(1 - (\frac{7}{10})^2 - (\frac{3}{10})^2) + \frac{4}{14}(1 - (\frac{2}{4})^2 - (\frac{2}{4})^2) = 0.443$$

CART (6/8)

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

$$\mathtt{Gini}_{\mathtt{income}\in\{\mathtt{low},\mathtt{medium}\}}(\mathtt{A},\mathtt{D}) = \mathtt{Gini}_{\mathtt{income}\in\{\mathtt{high}\}}(\mathtt{A},\mathtt{D}) = 0.443$$
$$\mathtt{Gini}_{\mathtt{income}\in\{\mathtt{low},\mathtt{high}\}}(\mathtt{A},\mathtt{D}) = \mathtt{Gini}_{\mathtt{income}\in\{\mathtt{medium}\}}(\mathtt{A},\mathtt{D}) = 0.458$$
$$\mathtt{Gini}_{\mathtt{income}\in\{\mathtt{medium},\mathtt{high}\}}(\mathtt{A},\mathtt{D}) = \mathtt{Gini}_{\mathtt{income}\in\{\mathtt{low}\}}(\mathtt{A},\mathtt{D}) = 0.450$$

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- The best binary split for attribute $\texttt{A} = \texttt{income}$ is on $\texttt{s}_\texttt{A} = \{\texttt{low},\texttt{medium}\}$ because it minimizes the Gini index.

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CART (8/8)

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

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  - $\Delta\texttt{Gini}(\texttt{credit\_rating}) = 0.459 - 0.429 = 0.03$
- The feature $\texttt{A} = \texttt{age}$ and splitting subset $\texttt{s}_\texttt{A} = \{\texttt{youth}, \texttt{senior}\}$ 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)
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Decision Tree in Spark (3/4)

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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)

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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)
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Ensemble Methods

Wisdom of the Crowd

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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.

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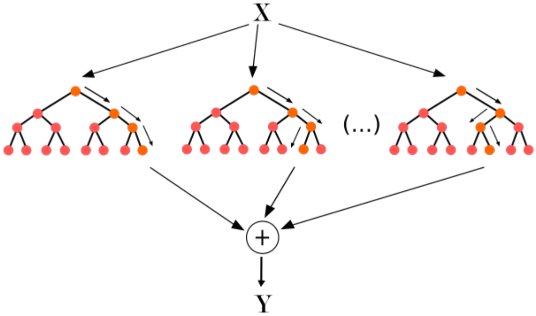
- Boosting
  - Train estimators sequentially, each trying to correct its predecessor.
  - E.g., adaboost and gradient boosting

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.

- `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.
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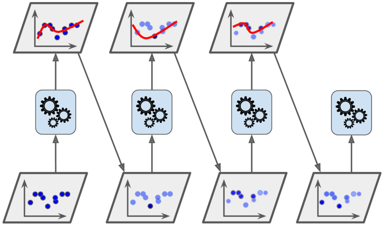
- `featureSubsetStrategy`: number of features to use as candidates for splitting at each tree node, as a fraction of the total number of features.
  - Possible values: `auto`, `all`, `onethird`, `sqrt`, `log2`, `n`

AdaBoost

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



AdaBoost

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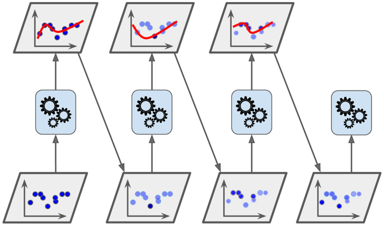
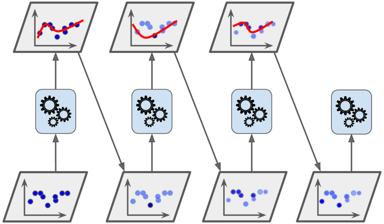
- Each estimator is trained on a random subset of the total training set.



AdaBoost

- 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.



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

- 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

- 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)
```

- 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?