Scalable Decision Trees and Ensembles

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COM6012 Scalable Machine Learning

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Contents

What is a decision tree

- Decision tree is a machine learning algorithm that tries to build predictive models **<u>using the most informative features</u>**

- An informative feature is a **<u>descriptive feature</u>** whose values split the instances in the dataset into **<u>homogeneous sets</u>** with respect to the target value

- More information can be found in the MLAI module and resources provided at the end

- APIs used in `spark.ml` are very similar to the ones used in `scikit-learn`

Advantages of decision trees

- ❑ Easy to interpret
- ❑ Can handle categorical features well
- ❑ Extends to the multiclass classification setting
- ❑ Do not require feature scaling
- ❑ Able to capture non-linearities and feature interactions

Contents

Nodes in a decision tree

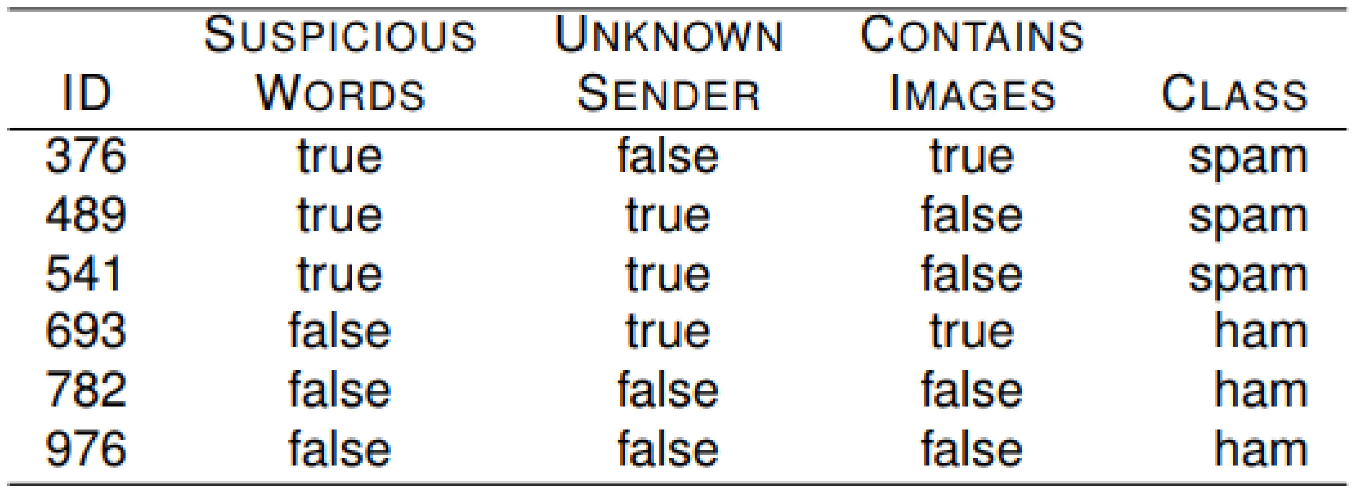
- A decision tree consists of:
  - A root node (or starting node)
  - Interior nodes
  - Leaf nodes (or terminating nodes)

- Each of the non-leaf nodes (root and interior) in the tree specifies a test to be carried out on one of the query's descriptive features

- Each of the leaf nodes specifies a predicted classification or predicted regression value for the query

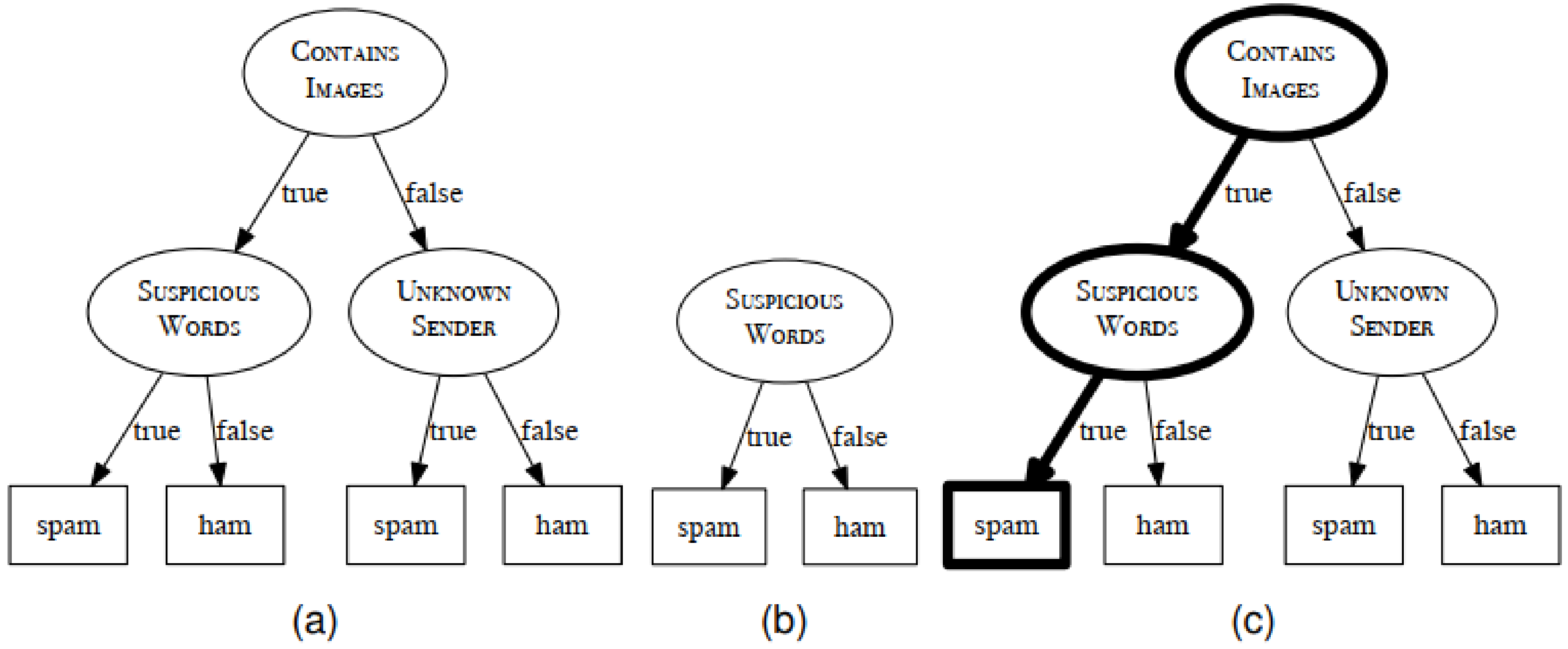
Binary classification: spam prediction

An email spam prediction dataset.



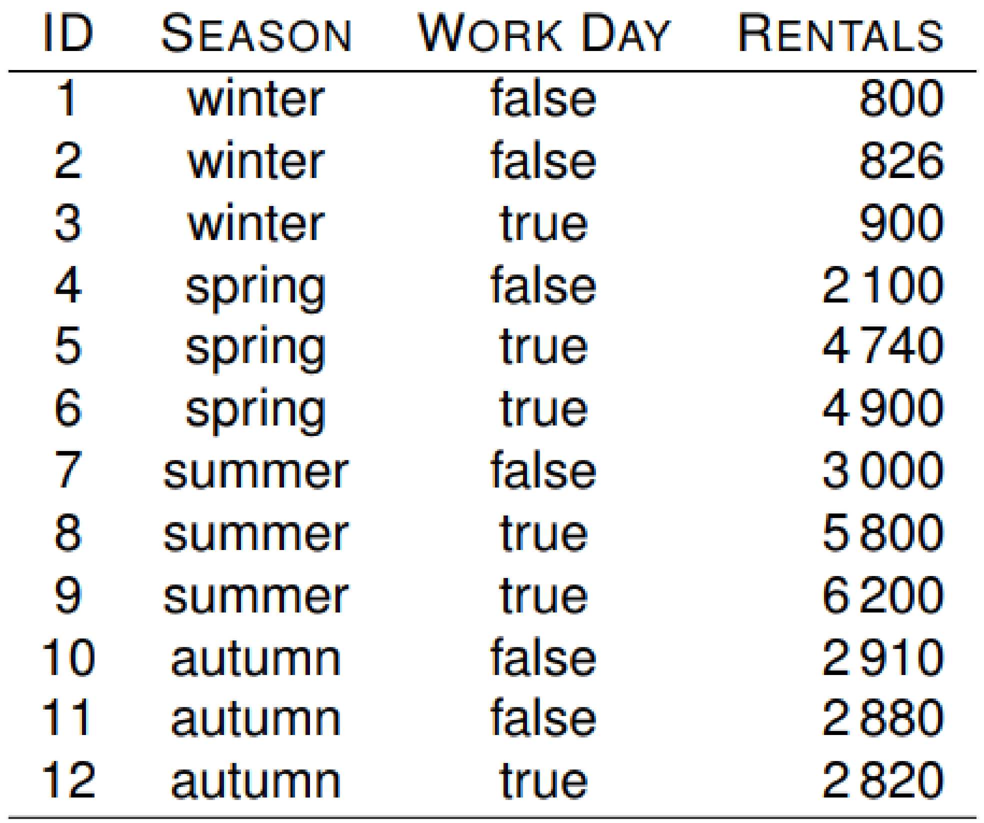
ID	Suspicious Words	Unknown Sender	Contains Images	Class
376	true	false	true	spam
489	true	true	false	spam
541	true	true	false	spam
693	false	true	true	ham
782	false	false	false	ham
976	false	false	false	ham

Two decision trees and a query instance



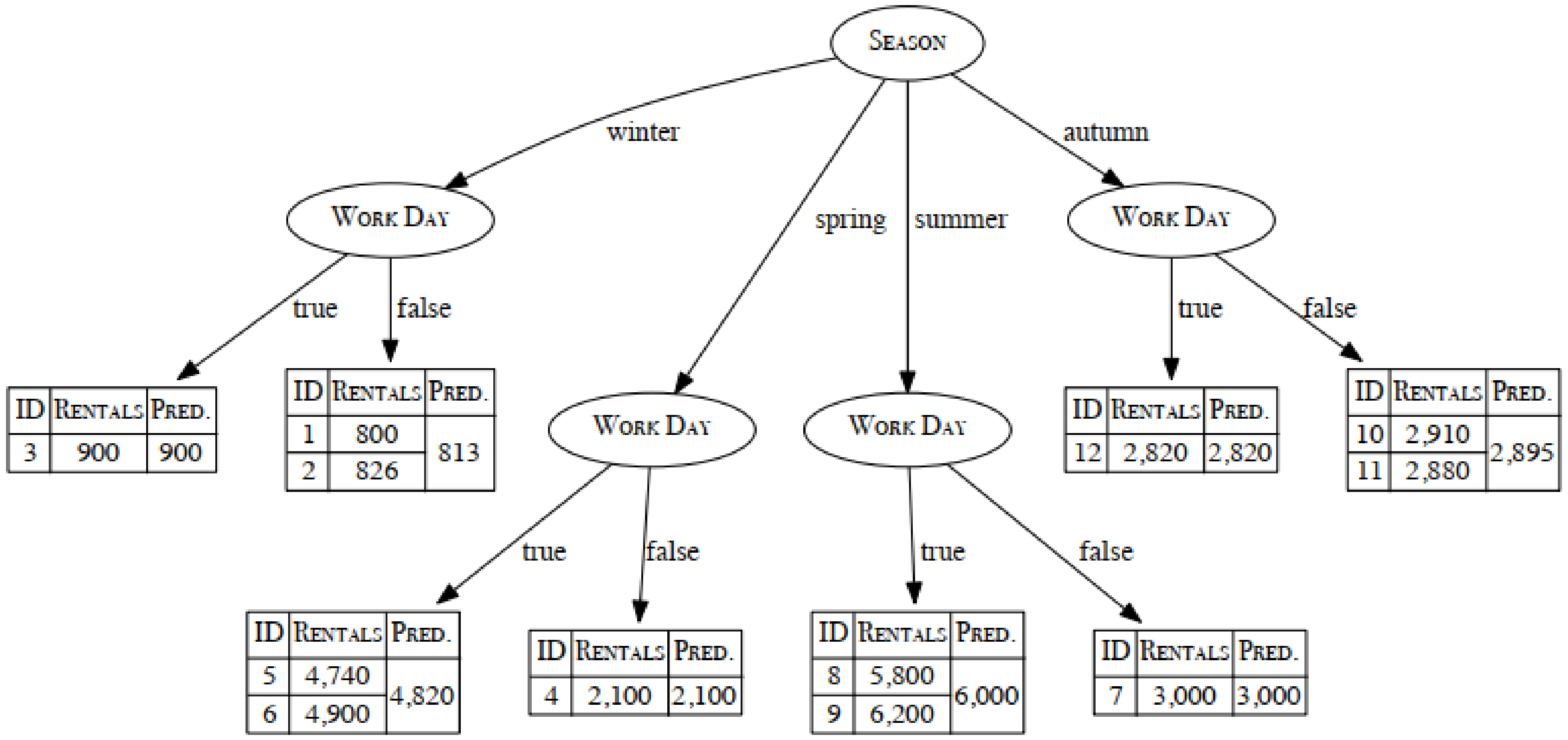
(a) and (b) show two decision trees that are consistent with the instances in the spam dataset. (c) shows the path taken through the tree shown in (a) to make a prediction for the query instance: Suspicious Words = *'true'*, Unknown Sender = *'true'*, Contains Images = *'true'*.

Regression: bike rentals per day



ID	Season	Work Day	Rentals
1	winter	false	800
2	winter	false	826
3	winter	true	900
4	spring	false	2 100
5	spring	true	4 740
6	spring	true	4 900
7	summer	false	3 000
8	summer	true	5 800
9	summer	true	6 200
10	autumn	false	2 910
11	autumn	false	2 880
12	autumn	true	2 820

Regression tree



The final decision tree induced from the dataset. This tree lists the instances that ended up at each leaf node and the prediction (PRED.) made by each leaf node.

Contents

Binary decision trees

- ❑ Apache Spark only builds binary decision trees
  - Each node can only have two branches

- ❑ Binary partitions at each node are done recursively

- ❑ Each partition is chosen greedily by selecting the best split from a set of possible splits

Best split

- ❑ The best split maximizes the information gain at a tree node

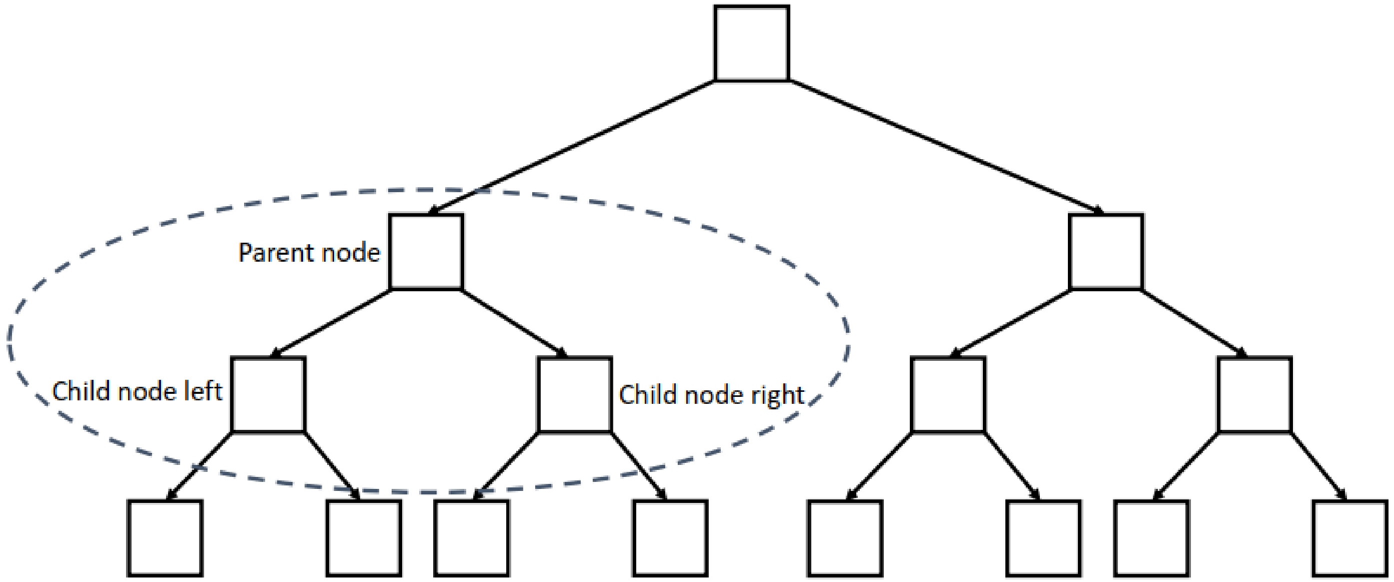
- ❑ The split chosen at each tree node is chosen from the set,

$$\arg\max_{s} \; IG\,(D, s)$$

Here, $\boldsymbol{IG(D, s)}$ is the information gain when split $\boldsymbol{s}$ is applied to dataset $\boldsymbol{D}$

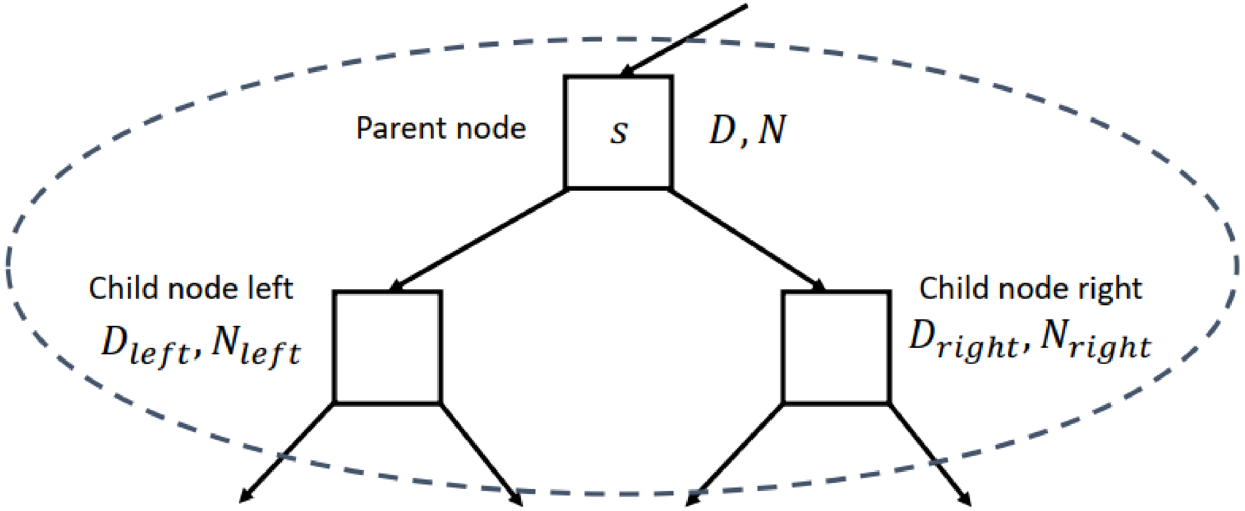
Information gain

- The <u>information gain</u> is the difference between the parent node impurity and the weighted sum of the two child node impurities



Information gain

- Assuming, that a split $\boldsymbol{s}$ partitions the dataset $\boldsymbol{D}$ of size $\boldsymbol{N}$ into two datasets $\boldsymbol{D}_{\mathbf{left}}$ and $\boldsymbol{D}_{\mathbf{right}}$ of size $\boldsymbol{N}_{\mathbf{left}}$ and $\boldsymbol{N}_{\mathbf{right}}$



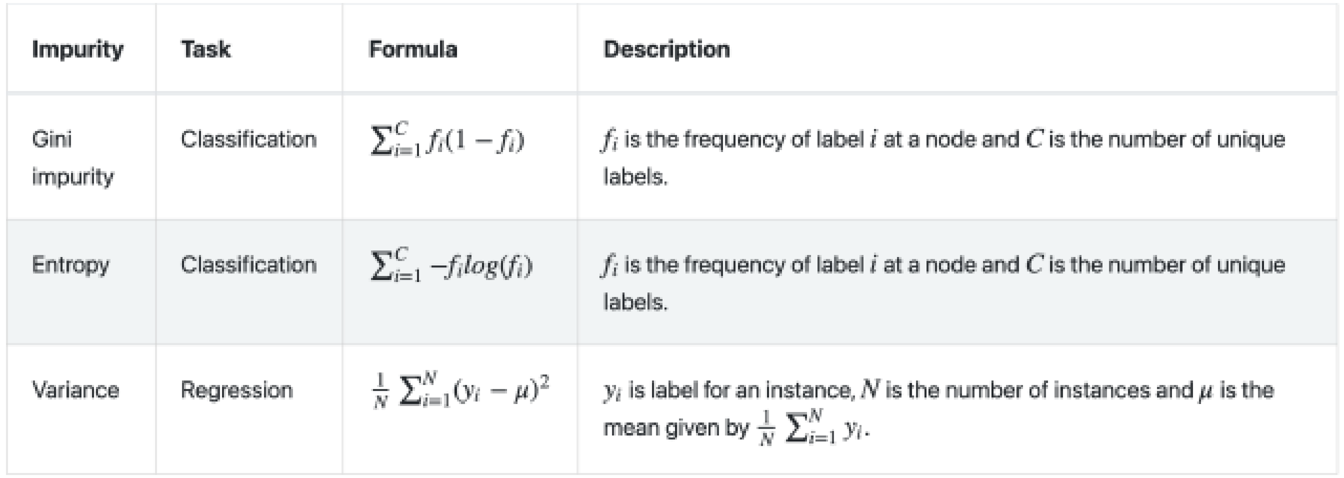
The information gain is computed as,

$$IG(D, s) = \text{Impurity}(D) - \left(\frac{N_{\text{left}}}{N}\, Impurity\,(D_{\text{left}}) + \frac{N_{\text{right}}}{N}\,\text{Impurity}\,(D_{\text{right}})\right)$$

Node impurity

- Recall, node impurity is a measure of how homogeneous are the labels at a node

- The table below shows the impurity measures currently implemented in Spark



Impurity	Task	Formula	Description
Gini impurity	Classification	$\sum_{i=1}^{C} f_i(1-f_i)$	f_i is the frequency of label i at a node and C is the number of unique labels.
Entropy	Classification	$\sum_{i=1}^{C} -f_i log(f_i)$	f_i is the frequency of label i at a node and C is the number of unique labels.
Variance	Regression	$\frac{1}{N}\sum_{i=1}^{N}(y_i-\mu)^2$	y_i is label for an instance, N is the number of instances and μ is the mean given by $\frac{1}{N}\sum_{i=1}^{N} y_i$.

*frequency refers to probability

Contents

How are the split candidates chosen?

- We saw that Spark only implements binary decision trees

- This means splits are always of the kind:

```
if feature $i \leq$ threshold then
    Move to the left/right branch
else
    Move to the right/left branch
end if
```

- Computation of `threshold` values depend on whether the features are continuous or categorical

Handling continuous features

- When working with small datasets, we can either:
  - Directly use the values of the feature as the thresholds
  - Sort the values of the feature and compute the corresponding thresholds from the sorted values

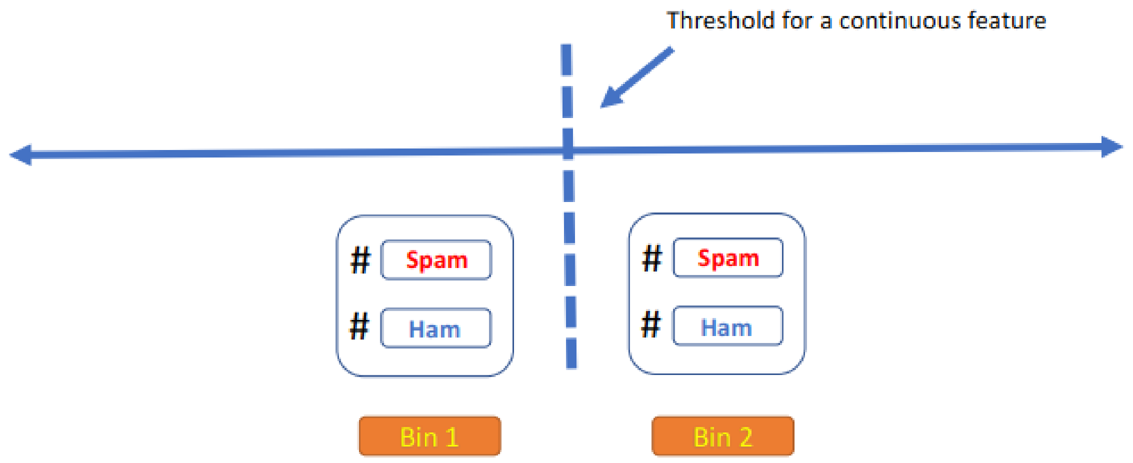
- However, these alternatives are not possible for use for large distributed datasets
  - It is not feasible to use the values of the feature as the thresholds
  - Sorting is an option, but it is expensive

Handling continuous features

- ❑ Spark's implementation computes an approximate set of split candidates by performing a quantile calculation over a sample fraction of the data

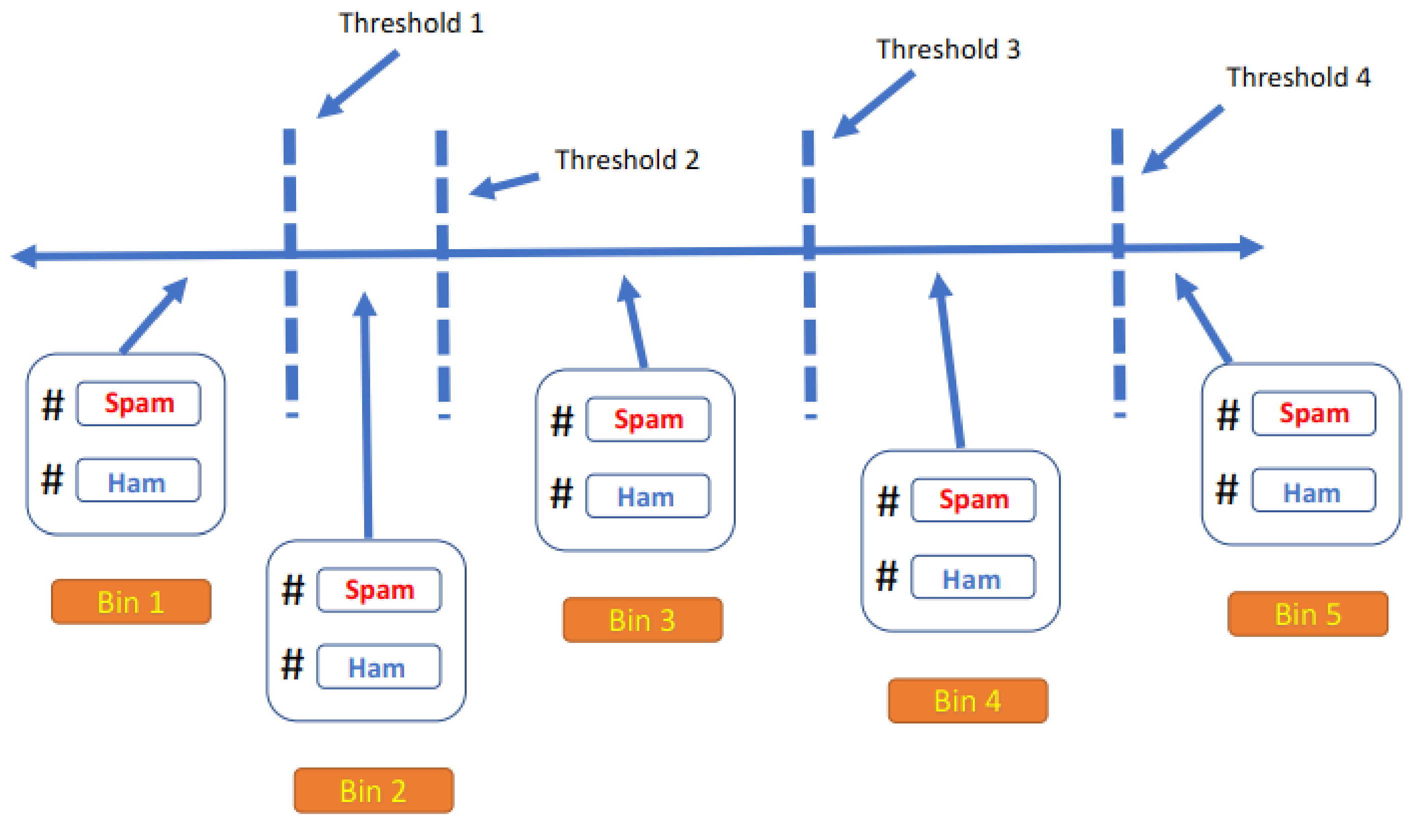
- ❑ The ordered splits create "bins" and the maximum number of such bins can be specified using the `maxBins` parameter

Bins for continuous features



Bins in continuous features

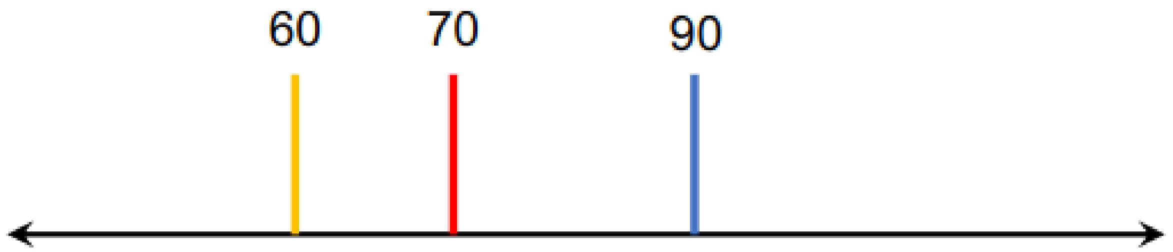
Bins for continuous features



Bins in continuous features

Why bins? Naïve approach

ID	Frequency of word “free”	Class
908	95	Spam
345	90	Spam
657	60	Ham
501	70	Ham



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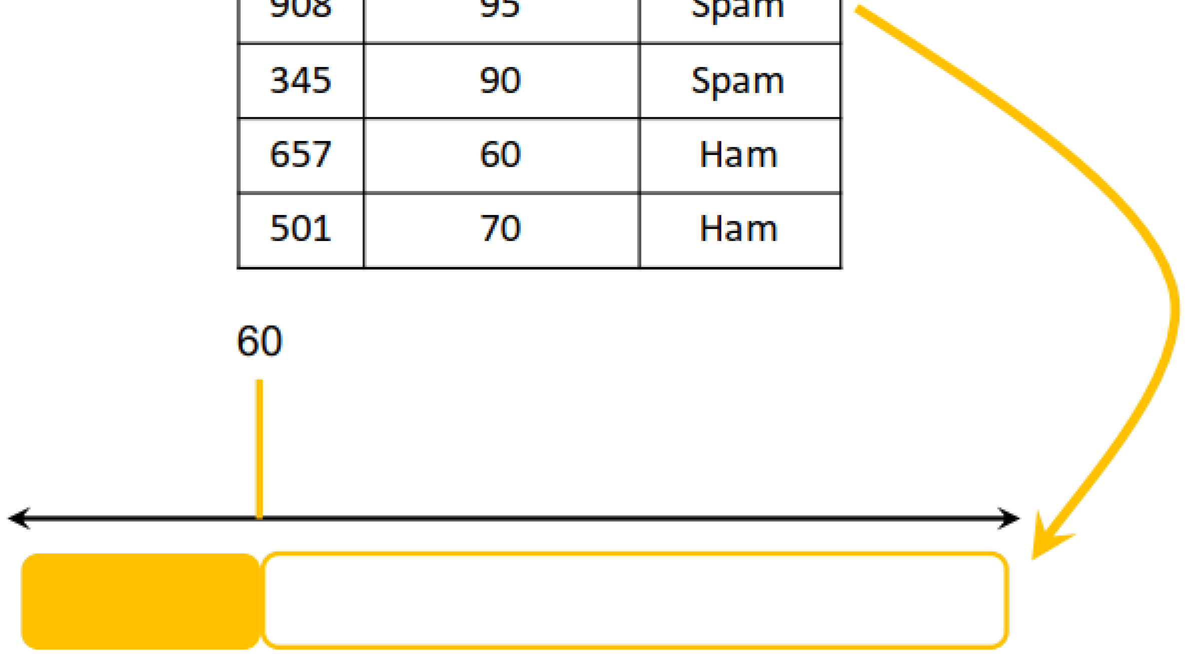

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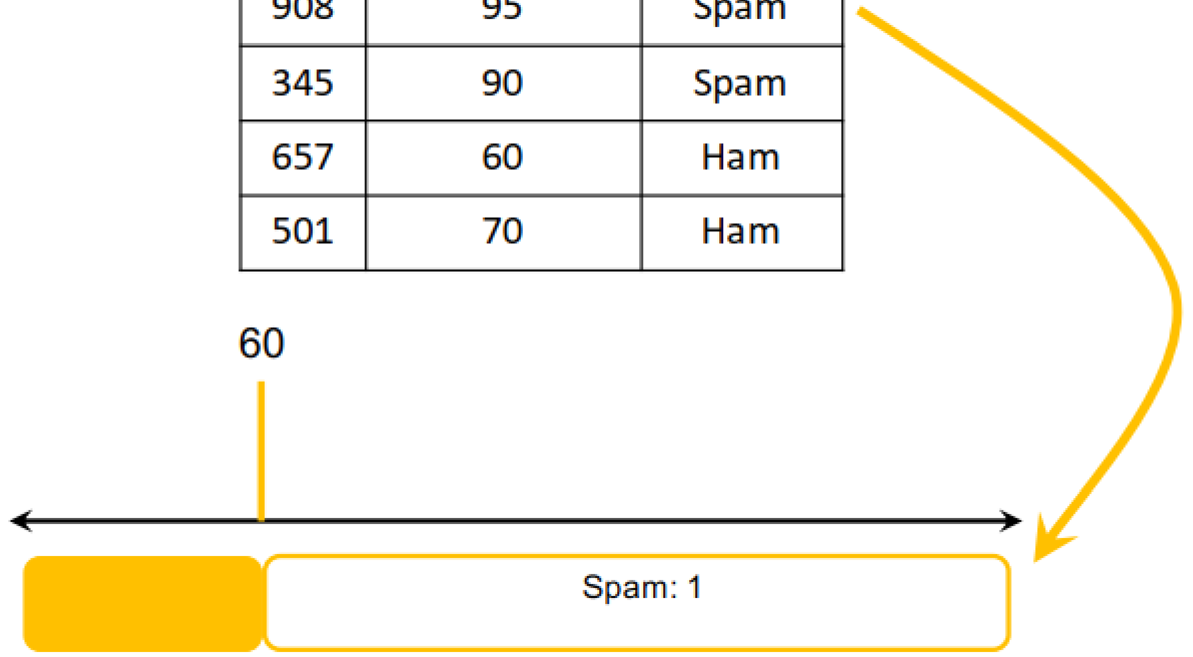

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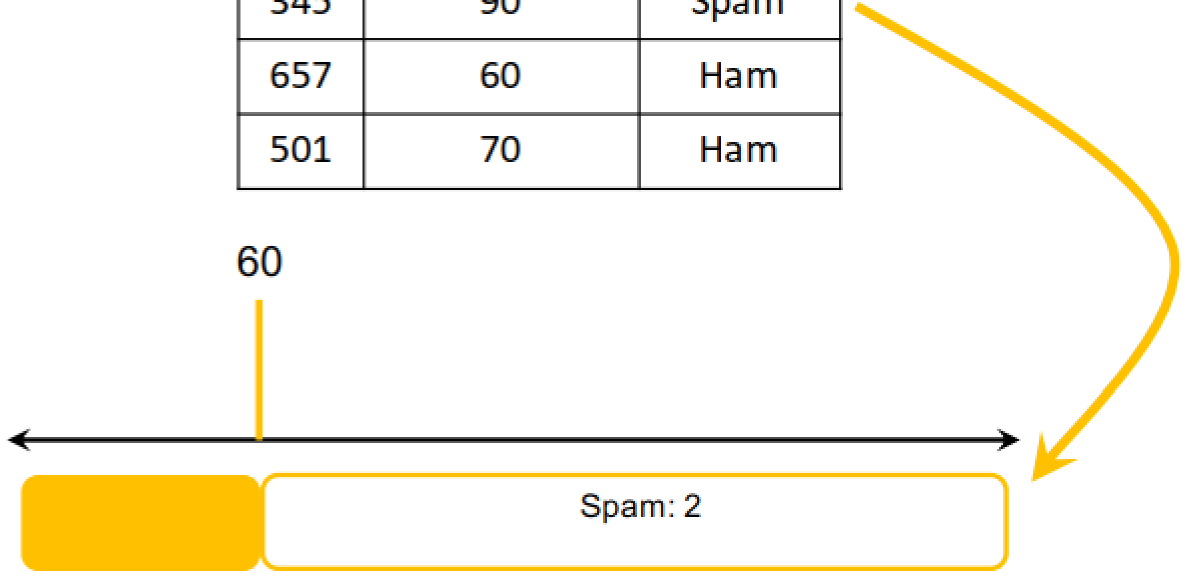

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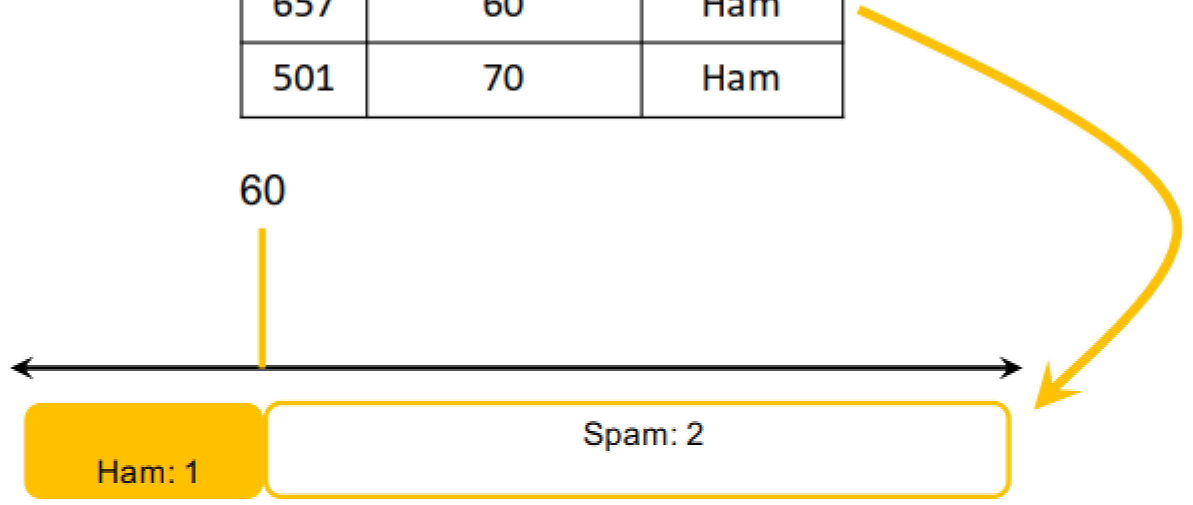

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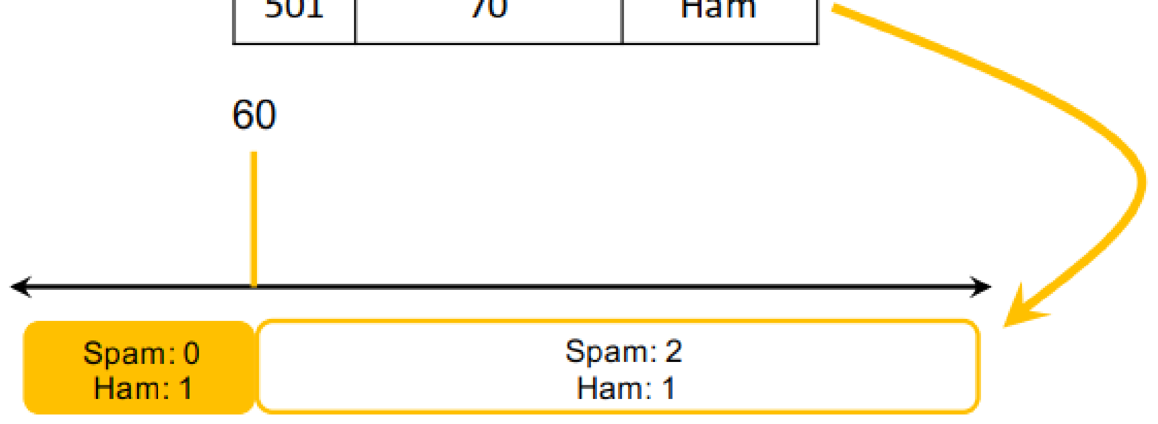

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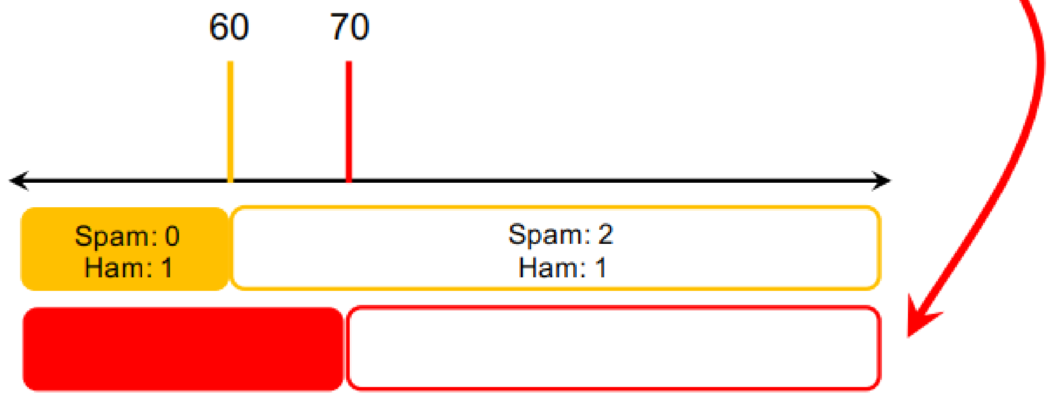

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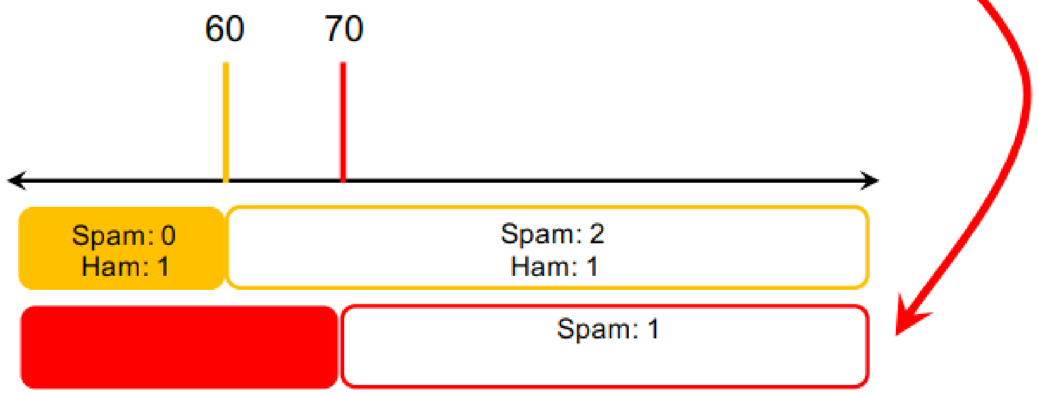

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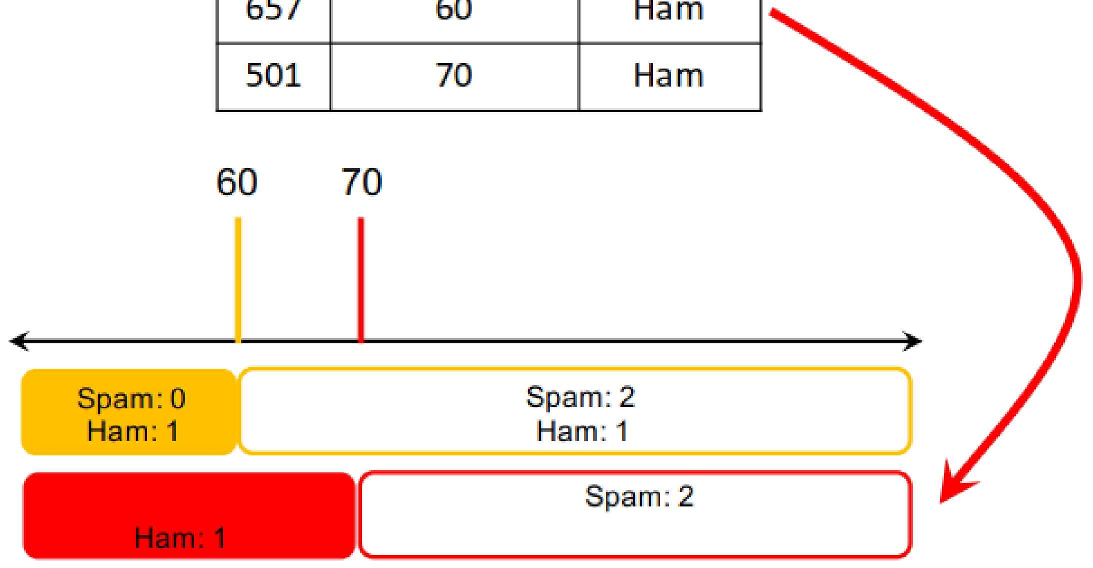

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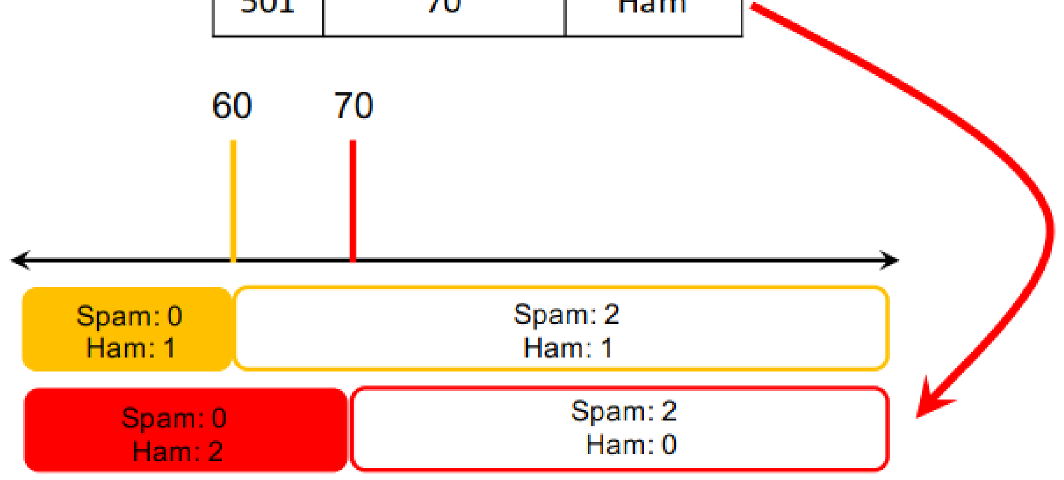

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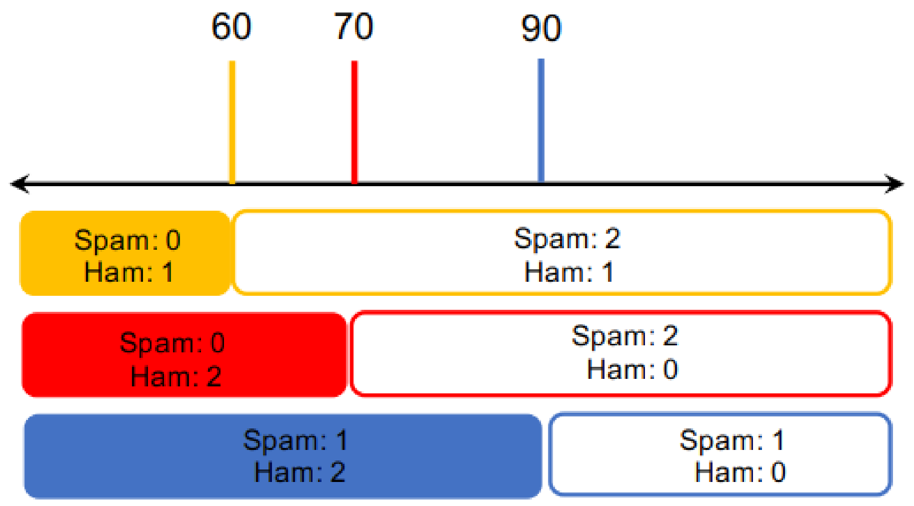

Why bins? Binary search

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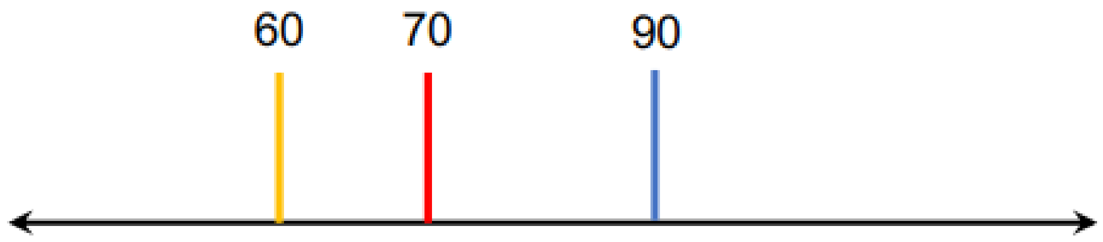

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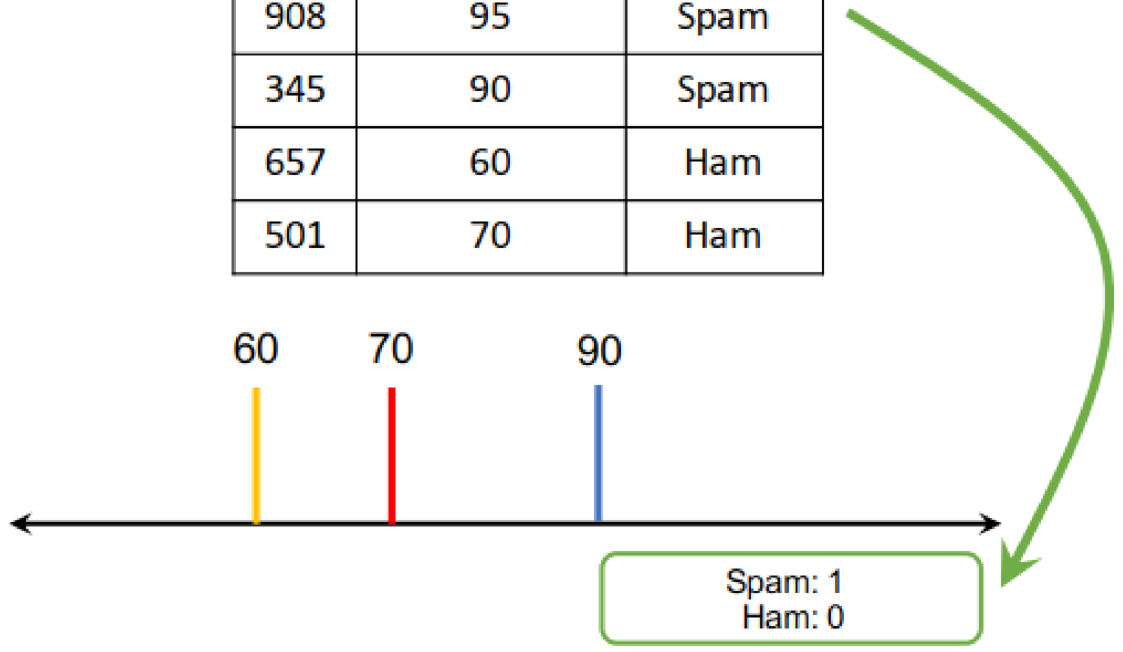

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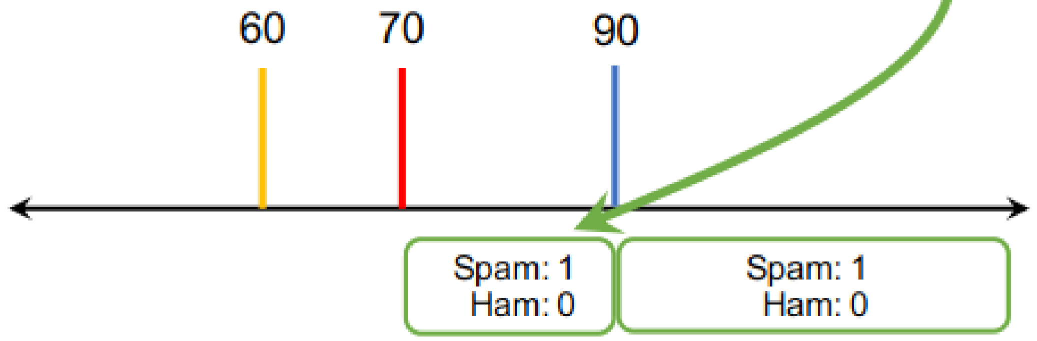

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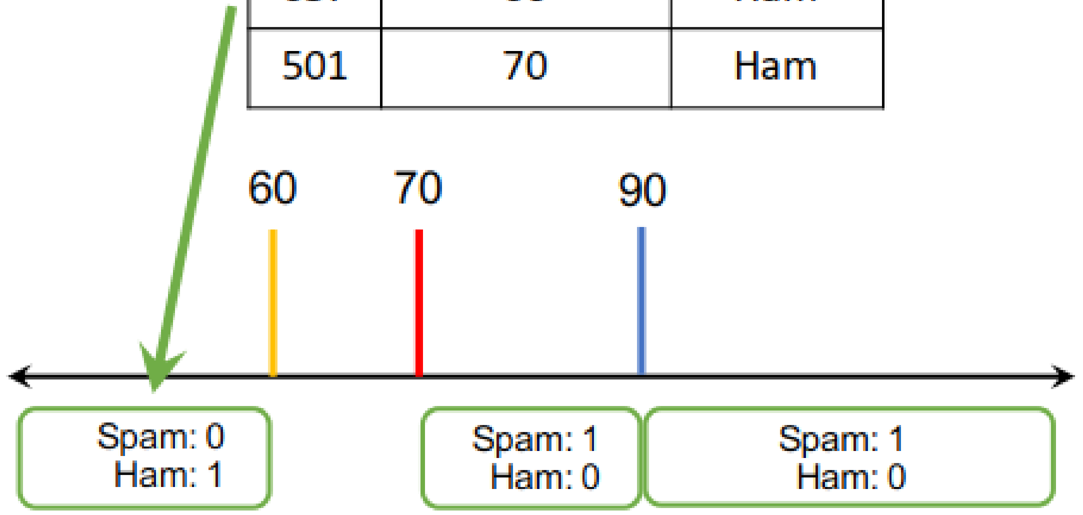

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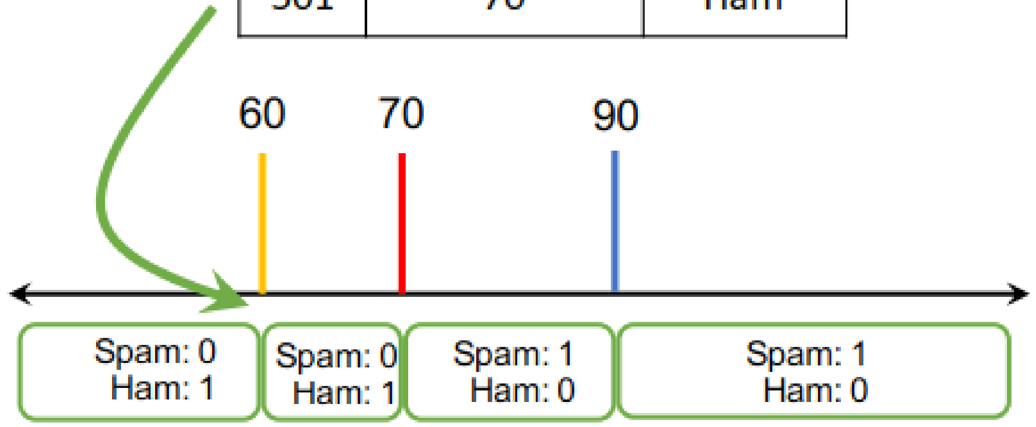

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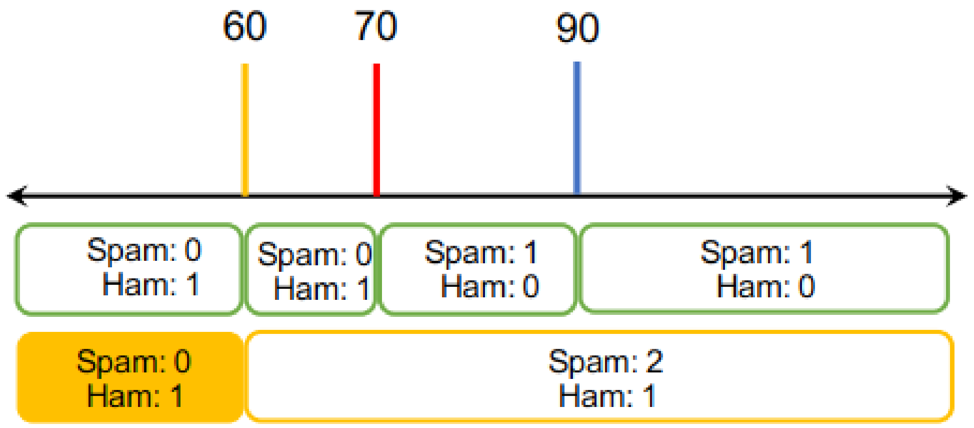

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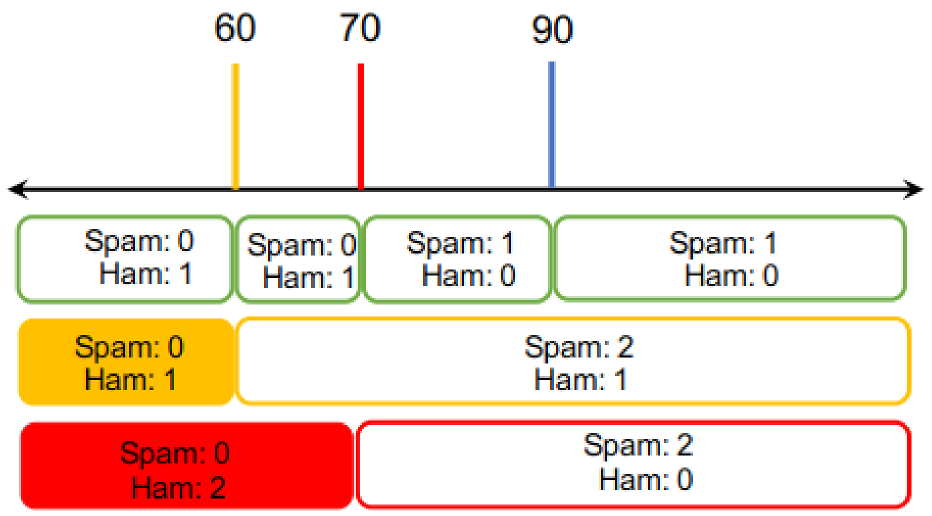

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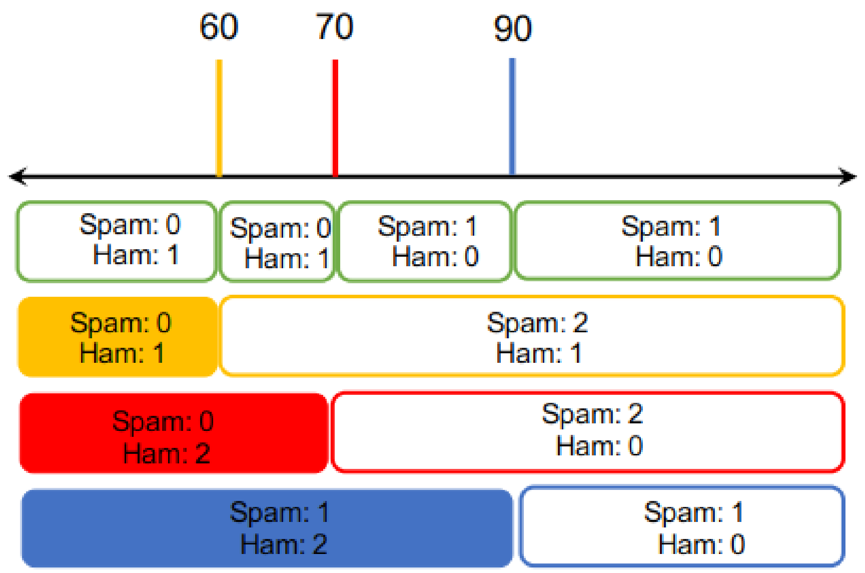


What is the difference?

- Assume there are *m* thresholds

- In the naïve approach, for each observation, we need to perform *m* operations

- When using binning, it is possible to use binary search for each observation to fill out the bins

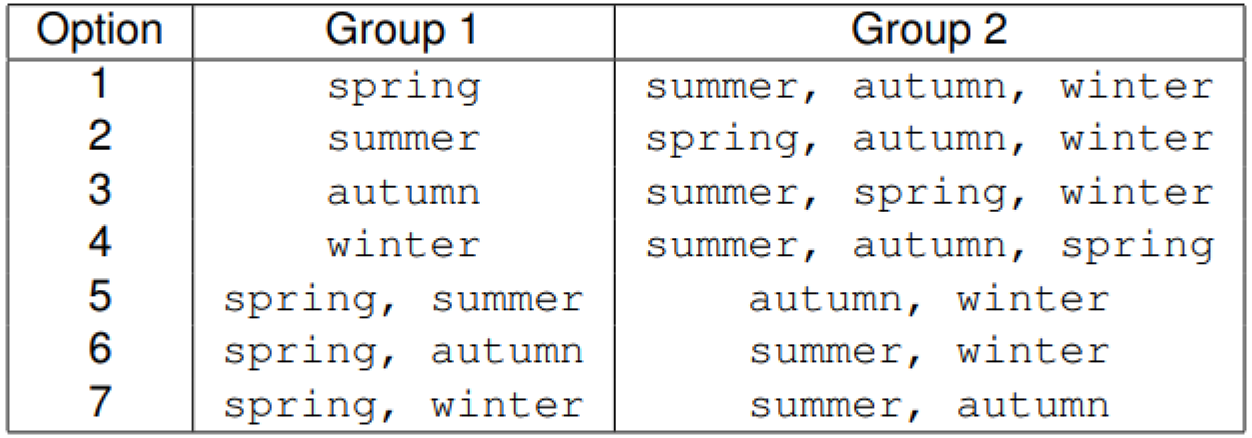
- Binary search takes $\log(m)$ operations

Categorical features

- ❑ Say we have a categorical feature that can take *M* unordered values
- ❑ We need to make a binary partition based on this categorical feature
- ❑ It can be shown there are $2^{M-1} - 1$ possible partitions of the *M* values into two groups

Categorical features

- As an example, consider the feature `weather` that takes values `[spring, summer, autumn, winter]`
- We would then have $2^{M-1} - 1 = 2^{4-1} - 1 = 7$ possible partitions of two groups



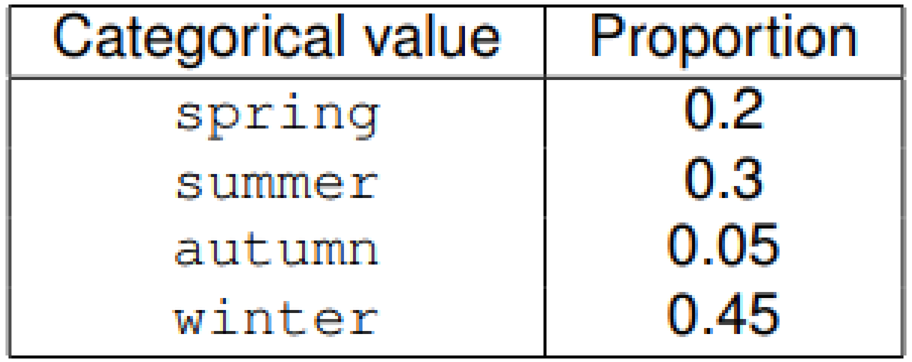
Option	Group 1	Group 2
1	`spring`	`summer, autumn, winter`
2	`summer`	`spring, autumn, winter`
3	`autumn`	`summer, spring, winter`
4	`winter`	`summer, autumn, spring`
5	`spring, summer`	`autumn, winter`
6	`spring, autumn`	`summer, winter`
7	`spring, winter`	`summer, autumn`

- For large *M*, computation becomes prohibitive
- There are heuristics to optimally reduce the number of partitions

Categorical features: binary classification

- For binary classification, the number of partitions can be reduced to $M - 1$ by order the categorical feature values by proportion falling in the outcome class 1

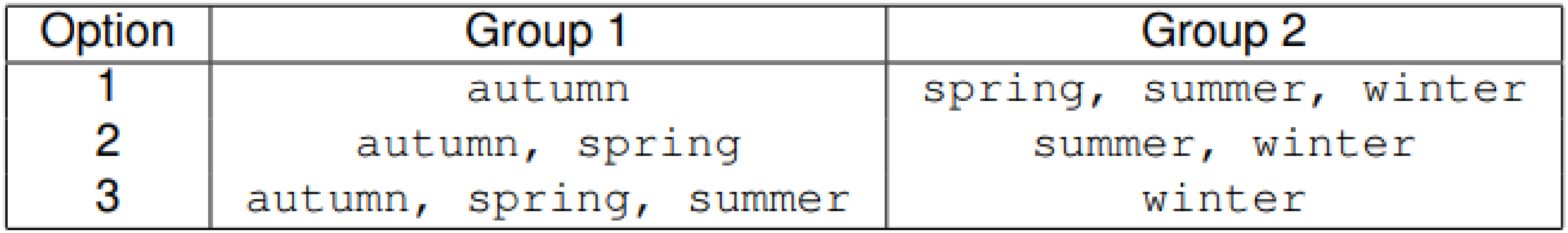
- For instance, lets consider the `weather` example and consider that the proportions contributed by the categorical values for outcome class 1 are as follows



Categorical value	Proportion
`spring`	0.2
`summer`	0.3
`autumn`	0.05
`winter`	0.45

Categorical features: binary classification

- By ordering the categorical values, we get
  - `[autumn, spring, summer, winter]`
  - Number of partitions = $M - 1 = 3$



Option	Group 1	Group 2
1	`autumn`	`spring, summer, winter`
2	`autumn, spring`	`summer, winter`
3	`autumn, spring, summer`	`winter`

- Essentially, we are transforming an unordered feature into an ordered feature

Categorical features: regression

- One can show this gives the optimal split, in terms of cross-entropy or Gini index, among all possible $2^{M-1} - 1$ splits
- This result also holds for a regression problem when using the square error loss
- In this case, the categories are ordered by increasing mean of the outcome
- More details can be found in book *The Elements of Statistical Learning*, 2nd edition, section 9.2.4

Categorical features: multi-class classification

- In Spark, for multiclass classification, all $2^{M-1} - 1$ possible split are used whenever possible

- When $2^{M-1} - 1$ is greater than the `maxBins` parameter, Spark uses a heuristic method similar to the method used for binary classification and regression

- The M categorical feature values are ordered by impurity and the resulting $M - 1$ split candidates are considered

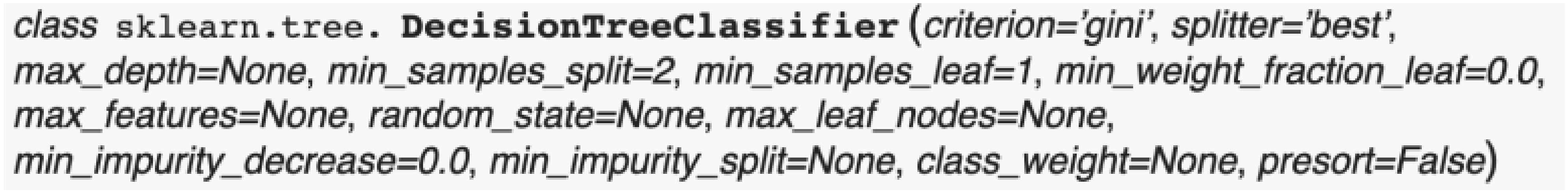
Contents

APIs for decision trees

- Class for Classification: `DecisionTreeClassifier`
- Class for Regression: `DecisionTreeRegressor`

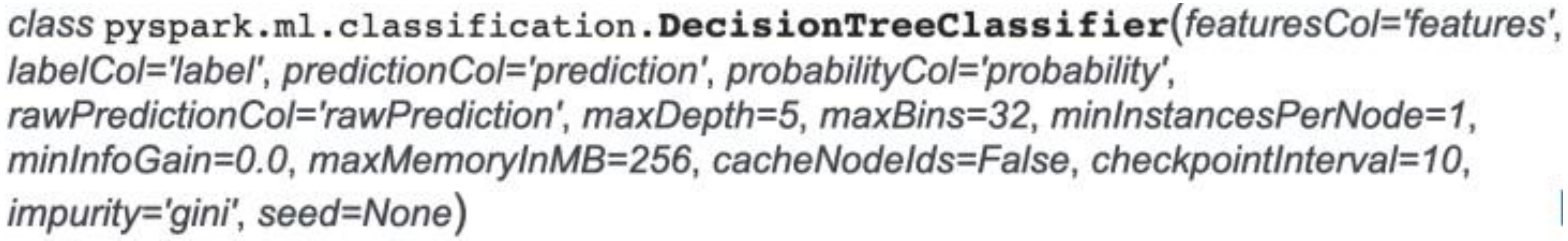
The `DecisionTreeClassifier` class

- In scikit-learn



```
class sklearn.tree. DecisionTreeClassifier(criterion='gini', splitter='best',
max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0,
max_features=None, random_state=None, max_leaf_nodes=None,
min_impurity_decrease=0.0, min_impurity_split=None, class_weight=None, presort=False)
```

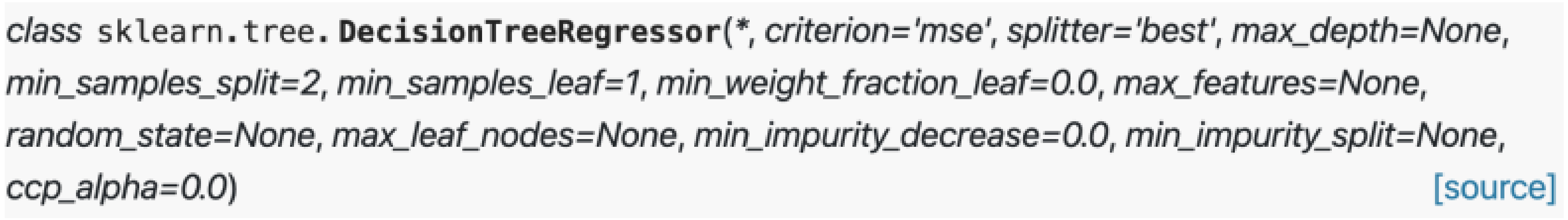
- In PySpark



```
class pyspark.ml.classification.DecisionTreeClassifier(featuresCol='features',
labelCol='label', predictionCol='prediction', probabilityCol='probability',
rawPredictionCol='rawPrediction', maxDepth=5, maxBins=32, minInstancesPerNode=1,
minInfoGain=0.0, maxMemoryInMB=256, cacheNodeIds=False, checkpointInterval=10,
impurity='gini', seed=None)
```

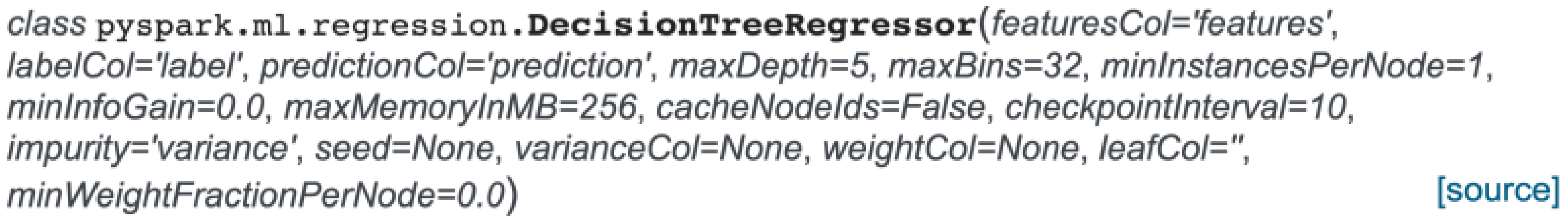
The DecisionTreeRegressor class

- In scikit-learn



```
class sklearn.tree.DecisionTreeRegressor(*, criterion='mse', splitter='best', max_depth=None,
min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None,
random_state=None, max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None,
ccp_alpha=0.0)                                                                         [source]
```

- In PySpark



```
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labelCol='label', predictionCol='prediction', maxDepth=5, maxBins=32, minInstancesPerNode=1,
minInfoGain=0.0, maxMemoryInMB=256, cacheNodeIds=False, checkpointInterval=10,
impurity='variance', seed=None, varianceCol=None, weightCol=None, leafCol='',
minWeightFractionPerNode=0.0)                                                          [source]
```

Parameters to adjust

- `maxDepth`: Maximum depth of a tree

- `maxBins`: Maximum number of bins for discretizing continuous features. It must be ≥ 2 and $\geq$ number of categories for any categorical feature

- `impurity`: Criterion used for information gain calculation.
  - Supported options:
    - `entropy` or `gini` for classification
    - `variance` for regression

- Several other parameters will be explored in the lab session

Contents

PLANET: horizontal partitioning

- PLANET is the standard algorithm to train a decision in a distributed dataset or horizontal partitioning

- Let $X \in \mathbb{R}^{n \times p}$ be the input matrix

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix}$$

  - Here, $\mathrm{x_k} \in \mathbb{R}^{\mathrm{p} \times 1}$, meaning there are *p* features

- Horizontal partitioning refers to the fact that each worker will receive a subset of the n instances or row vectors

Setup

- Assume there are B potential thresholds for each of the p features that were considered
- Let us define S as the set of cardinality $p \times B$ that contains all the split candidates
- Assume there are k workers. Each worker j computes c sufficient statistics over a subset of the original data, $\boldsymbol{X}_j$
- What are these sufficient statistics?
  - For classification: label counts (e.g. $c = 4$ for binary classification, i.e., 2 per branch)
  - For regression: count, sum, and sum^2 (so, $c = 6$, i.e., 3 per branch)
- Details can be found in the paper, **Yggdrasil: An Optimized System for Training Depp Decision Trees at Scale**

Setup

- Each worker *j* then computes the sufficient statistics $g_j(s)$ over $\mathbf{X}_j$ for each $s \in S$

- For a parent node I in the tree, the optimal split s* is found by solving

$$s^* = \arg\max_{s \in S} f(\sum_{j=1}^{k} g_j(s))$$

  - Where, $f\colon \mathbb{R}^c \rightarrow \mathbb{R}$ computes the information gains

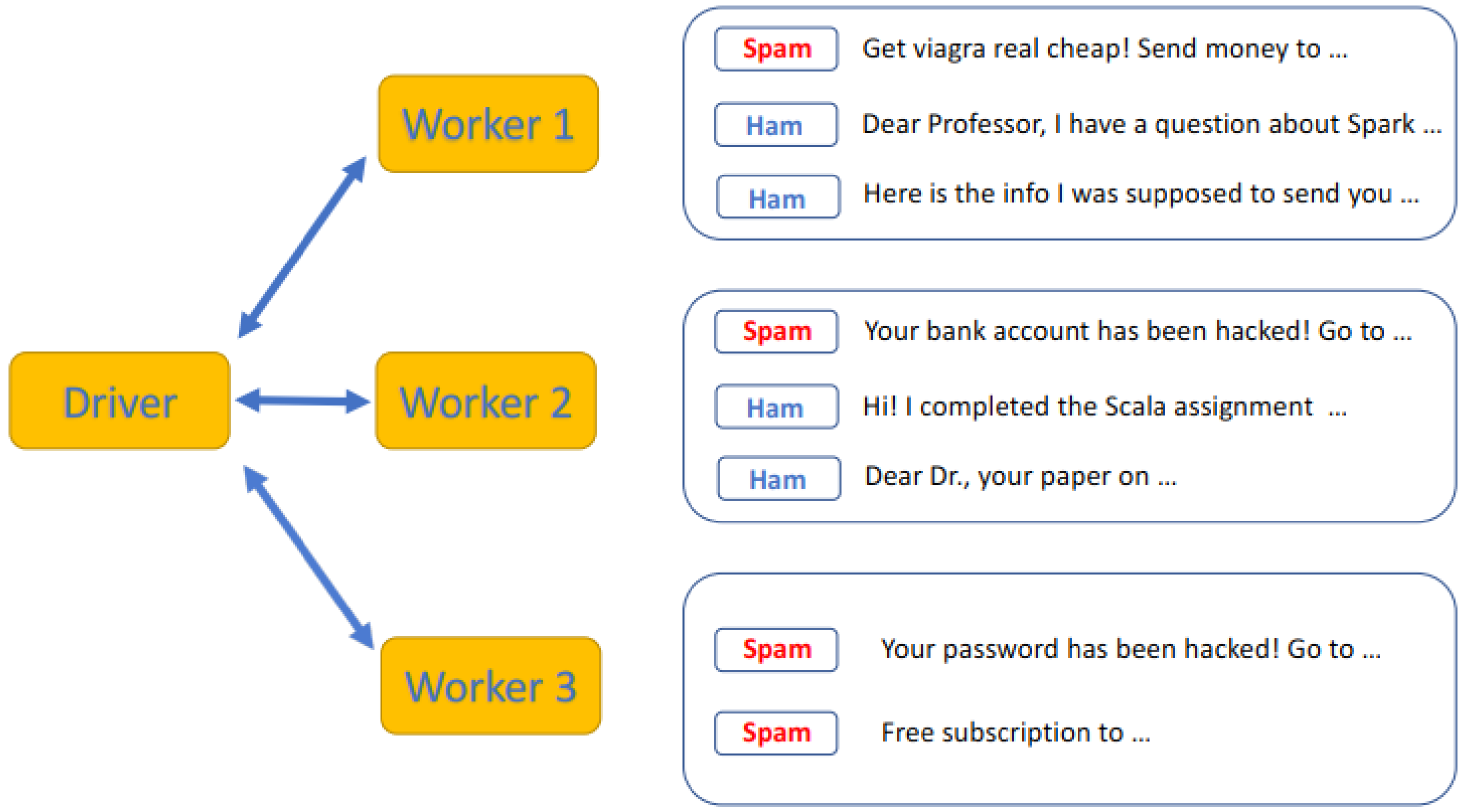
Algorithm to compute s^* in a distributed fashion

- We start by assuming the depth of the tree is fixed to *D*

- At iteration *t*,
  - the algorithm computes the optimal splits for all the nodes on the level *t* of the tree
  - there is a single round trip of communication between the master and the workers

- Each tree node *i* is split as follows
  1. The *j*-th worker locally computes sufficient statistics $g_j(s)$ for all $s \in S$
  2. Each worker communicates all statistics $g_j(s)$ to the master (*Bp* in total)
  3. The master computes the best split s^*
  4. The master broadcasts s^* to the workers, who update their local states to keep track of which instances are assigned to which child nodes

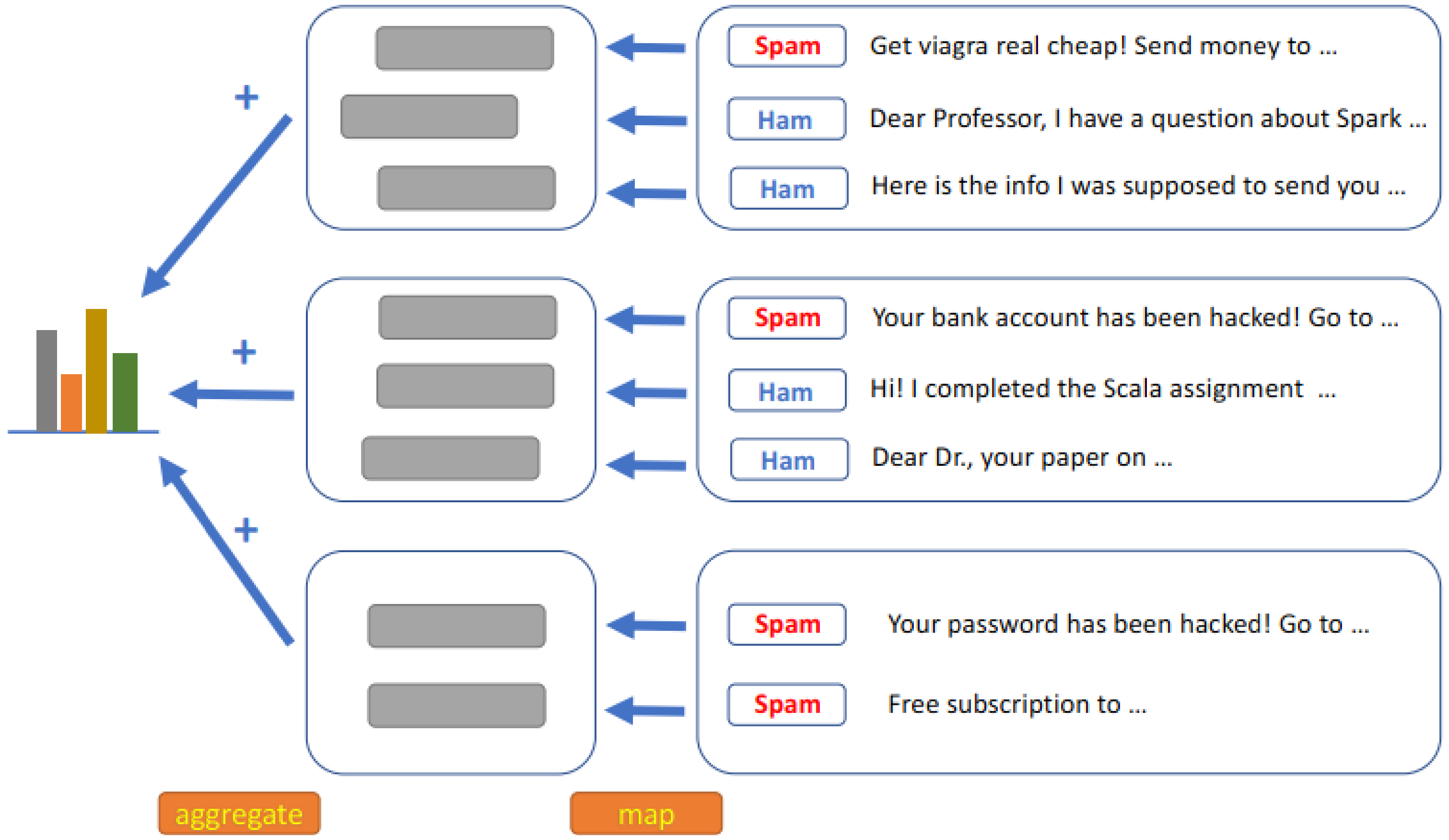
The distributed dataset



Driver
Worker 1
Worker 2
Worker 3
Spam
Get viagra real cheap! Send money to …
Ham
Dear Professor, I have a question about Spark …
Ham
Here is the info I was supposed to send you …
Spam
Your bank account has been hacked! Go to …
Ham
Hi! I completed the Scala assignment …
Ham
Dear Dr., your paper on …
Spam
Your password has been hacked! Go to …
Spam
Free subscription to …

A distributed dataset

The distributed dataset



Spam
Get viagra real cheap! Send money to ...
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Dear Professor, I have a question about Spark ...
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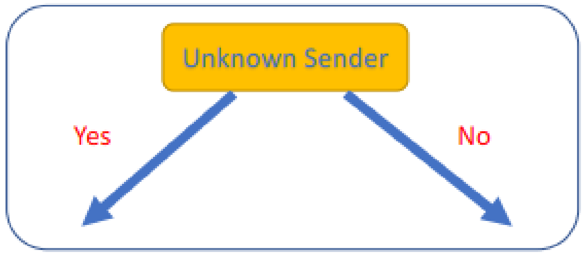
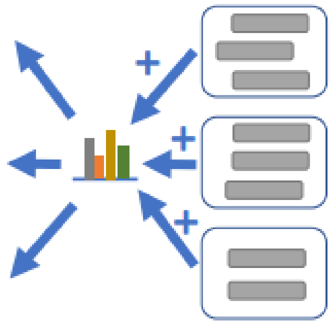
Ham
Dear Dr., your paper on ...
Spam
Your password has been hacked! Go to ...
Spam
Free subscription to ...
+
+
+
aggregate
map

A distributed dataset

Building a decision tree

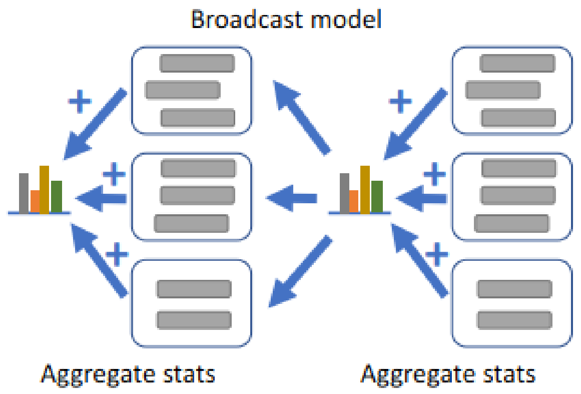


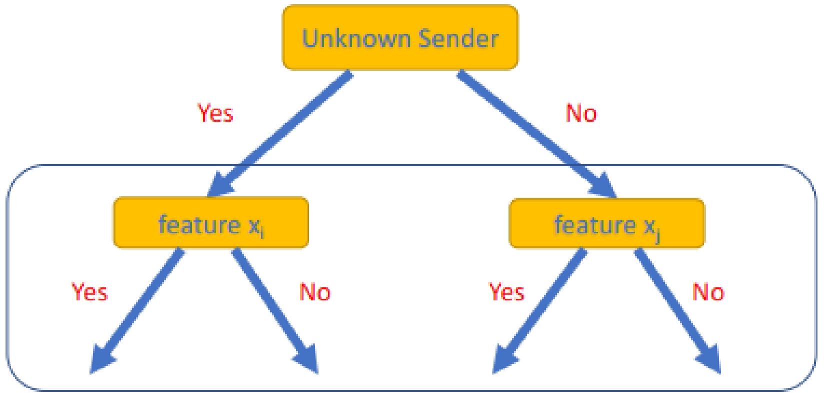


Aggregate stats

Building the tree in Spark

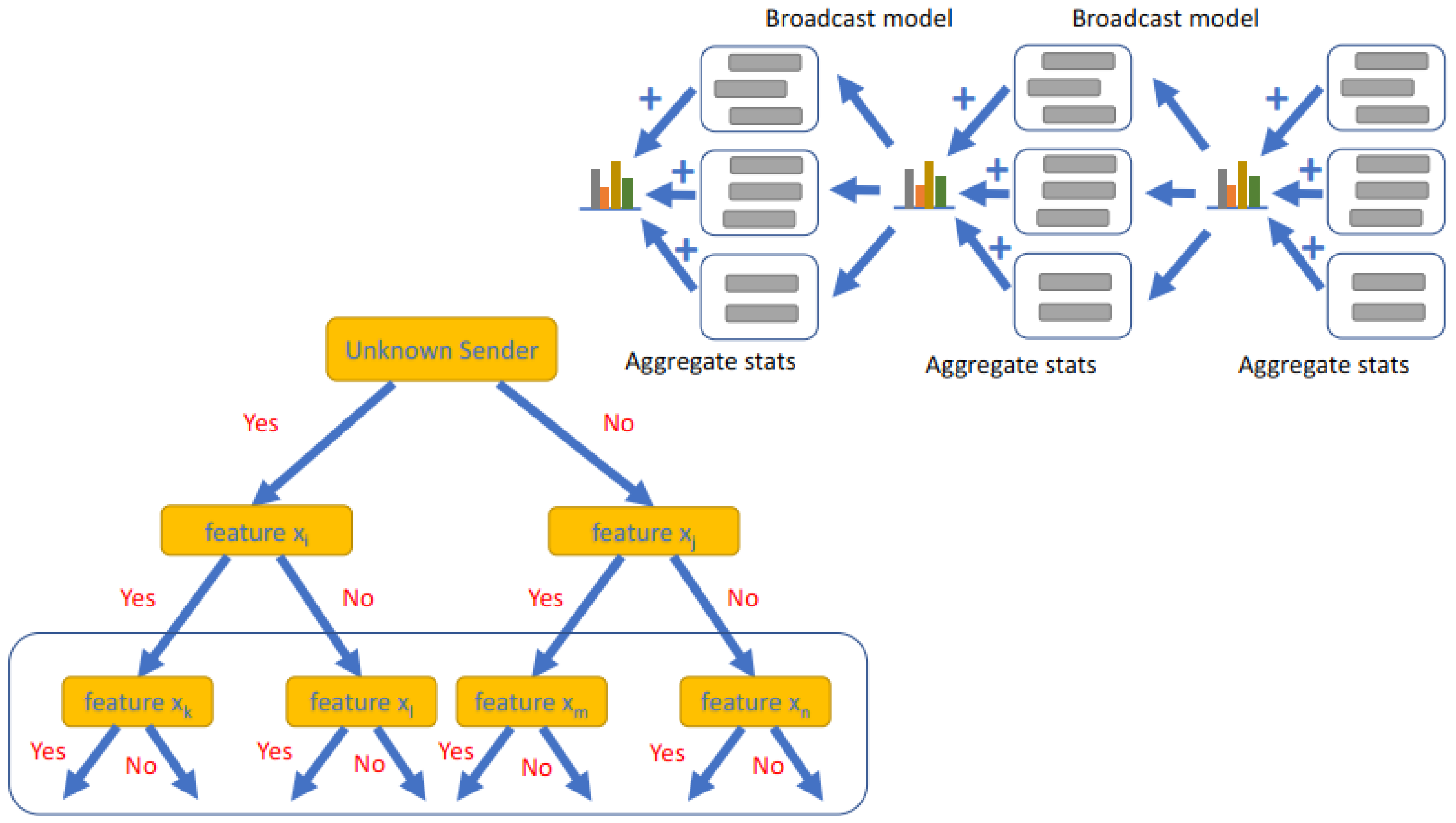
Building a decision tree





Building the tree in Spark

Building a decision tree



Building the tree in Spark

Computational and communication complexity

- Computation is linear in *n*, *p* and *D*, so it’s easy to parallelize
- The issue is the communication overhead
- For each tree node, step 2 in the algorithm before, require communicating *kBp* tuples of size *c*
- With 2^D total nodes, the total communication is $\boldsymbol{2^D kBpc}$ floating point values
- Communication is then exponential in tree depth *D* and linear in thresholds *B*

Contents

Bagging and boosting

- Rather than creating a single model, they generate a set of models and then make predictions by aggregating the outputs of these models

- A prediction model that is composed of a set of models is called a model ensemble

- In order for this approach to work, the models that are in the ensemble must be different from each other

- There are two standard approaches to creating ensembles:
  - Bagging
  - Boosting

Bagging: Definition

- In **bagging** (or **bootstrap aggregating**) each model in the ensemble is trained on a random sample of the dataset known as **bootstrap samples**

- Each random sample is the same size as the dataset and **sampling with replacement** is used

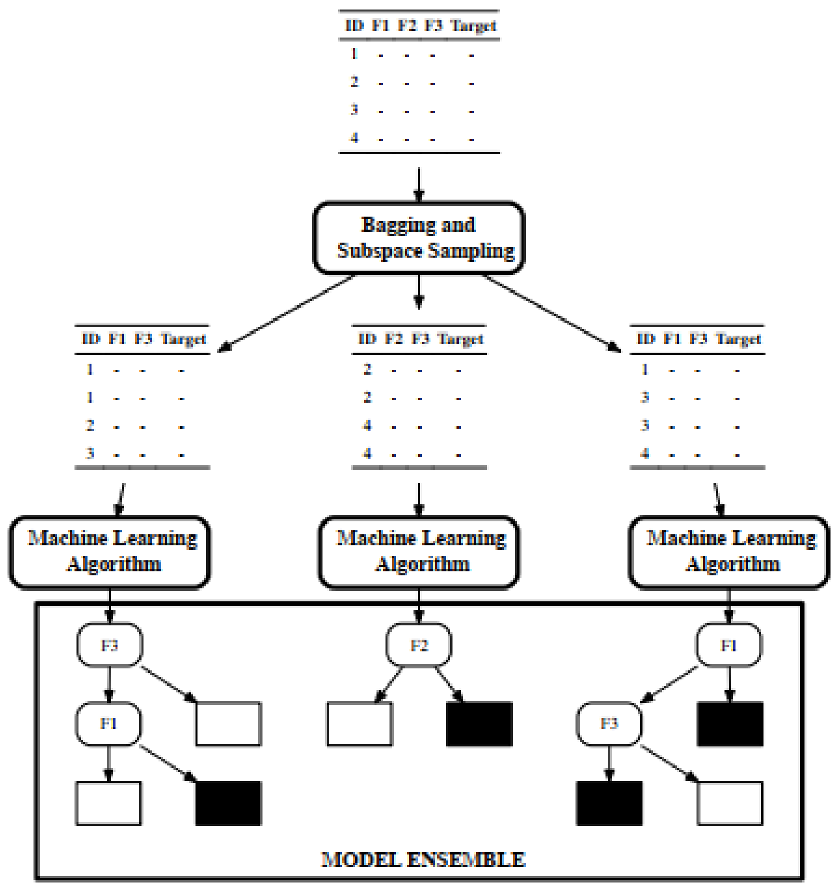
- Hence, every bootstrap sample will be missing some of the instance from the dataset. Consequently,
  - Each bootstrap sample will be different
  - Therefore, models trained on different bootstrap samples will also be different

Bagging: Random forest

- When bagging is used with decision trees, each boostrap sample only uses a randomly selected subset of the descriptive features in the dataset
  - This is known as **subspace sampling**

- The combination of bagging, subspace sampling and decision trees is known as a **random forest** model

Example of using bagging


ID F1 F2 F3 Target
Bagging and Subspace Sampling
ID F1 F3 Target
ID F2 F3 Target
ID F1 F3 Target
Machine Learning Algorithm
Machine Learning Algorithm
Machine Learning Algorithm
F3
F1
F2
F1
F3
MODEL ENSEMBLE

The process of creating a model ensemble using bagging and subspace sampling.

Boosting: How does it work?

- ❑ Boosting works by iteratively creating models and adding them to the ensemble
- ❑ The iteration stops when a predefined number of models have been added
- ❑ When we use **boosting** each new model added to the ensemble is biased to pay more attention to instance that previous models miss-classified
- ❑ This is done by incrementally adapting the dataset used to train the models. To do this, we use a **weighted dataset**

Boosting: Weighted Dataset

- Each instance has an associated weight, $\mathrm{w}_i \geq 0$
- Initially set to $\frac{1}{n}$ where n is the number of instances in the dataset
- After each model is added to the ensemble, it is tested on the **training data**
  - Weights of the instances that the model accurately predicts are **decreased**
  - Weights of the instances that the model predicts incorrectly are **increased**
- These weights are used as a distribution over which the dataset is sampled to create a **replicated training set**
  - Replication of an instance is proportional to its weight

Algorithm

- During each **training iteration**, the algorithm does the following:
  1. Induces a model and calculates the total error, ϵ, by summing the weights of the training instances for which the predictions made by the model were incorrect
  2. Increases the weights for the instances that were misclassified by using the formula:
  $$\mathbf{w}[i] \leftarrow \mathbf{w}[i] \times \left(\frac{1}{2 \times \epsilon}\right)$$
  3. Decreases the weights for the instances correctly classified:
  $$\mathbf{w}[i] \leftarrow \mathbf{w}[i] \times \left(\frac{1}{2 \times (1 - \epsilon)}\right)$$
  4. Calculates a confidence factor, α, for the model such that α increases as ϵ decreases
  $$\alpha = \frac{1}{2} \times \log_e\left(\frac{1 - \epsilon}{\epsilon}\right)$$

Predictions

- Once the set of models have been created, the ensemble makes **predictions** using a weighted aggregate of the predictions made by the individual models

- The weights used in this aggregation are simply the confidence factors associated with each model

Contents

Bagging and Boosting in PySpark

- ❑ Random forests can be implement in PySpark

- ❑ The boosting model implemented in PySpark is the Gradient-Boosted Trees (GBTs)

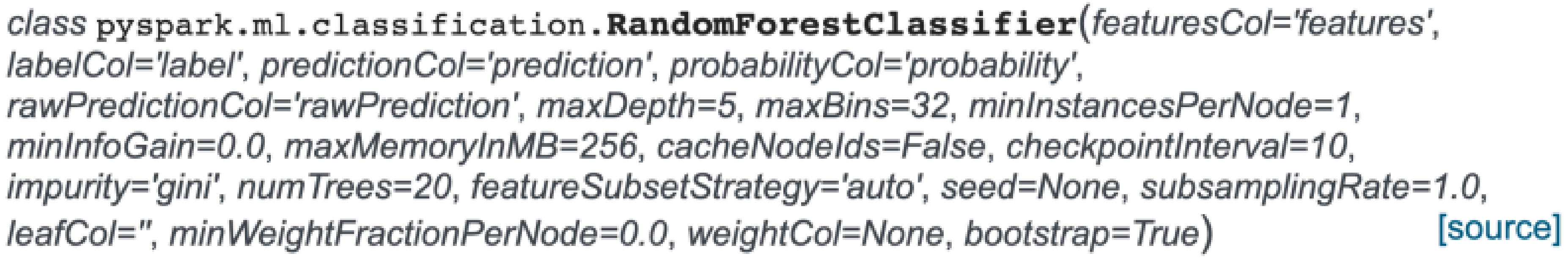
Random forests

- `spark.ml` supports random forests for binary and multiclass classification and for regression, suing both continuous and categorical features

- `spark.ml` implements random forests using the existing decision tree implementation

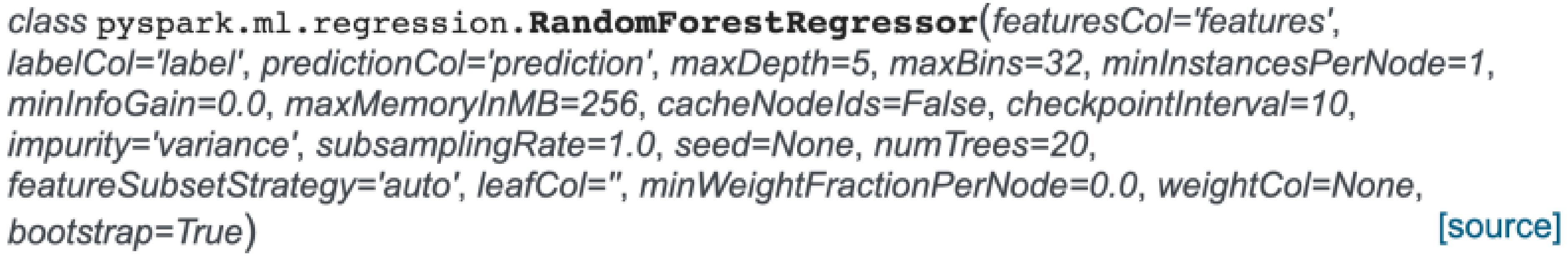
Random forest API

- `RandomForestClassifier` **class in PySpark**



class **pyspark.ml.classification.RandomForestClassifier**(*featuresCol='features', labelCol='label', predictionCol='prediction', probabilityCol='probability', rawPredictionCol='rawPrediction', maxDepth=5, maxBins=32, minInstancesPerNode=1, minInfoGain=0.0, maxMemoryInMB=256, cacheNodeIds=False, checkpointInterval=10, impurity='gini', numTrees=20, featureSubsetStrategy='auto', seed=None, subsamplingRate=1.0, leafCol='', minWeightFractionPerNode=0.0, weightCol=None, bootstrap=True*) [source]

- `RandomForestRegressor` **class in PySpark**



class **pyspark.ml.regression.RandomForestRegressor**(*featuresCol='features', labelCol='label', predictionCol='prediction', maxDepth=5, maxBins=32, minInstancesPerNode=1, minInfoGain=0.0, maxMemoryInMB=256, cacheNodeIds=False, checkpointInterval=10, impurity='variance', subsamplingRate=1.0, seed=None, numTrees=20, featureSubsetStrategy='auto', leafCol='', minWeightFractionPerNode=0.0, weightCol=None, bootstrap=True*) [source]

Important parameter to adjust

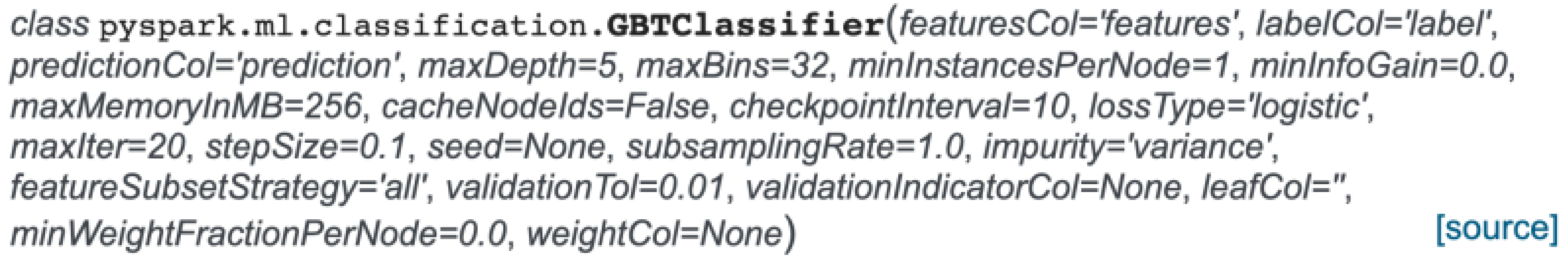
- `numTrees`: Number of trees in the forest
- `maxDepth`: Maximum depth of each tree in the forest
- Several other parameters will be explored in the lab session

Gradient-boosted trees

- `spark.ml` supports GBTs for binary classification and for regression, using both continuous and categorical features
- `spark.ml` implements GBTs using the existing decision tree implementation
- GBTs do not yet support multiclass classification

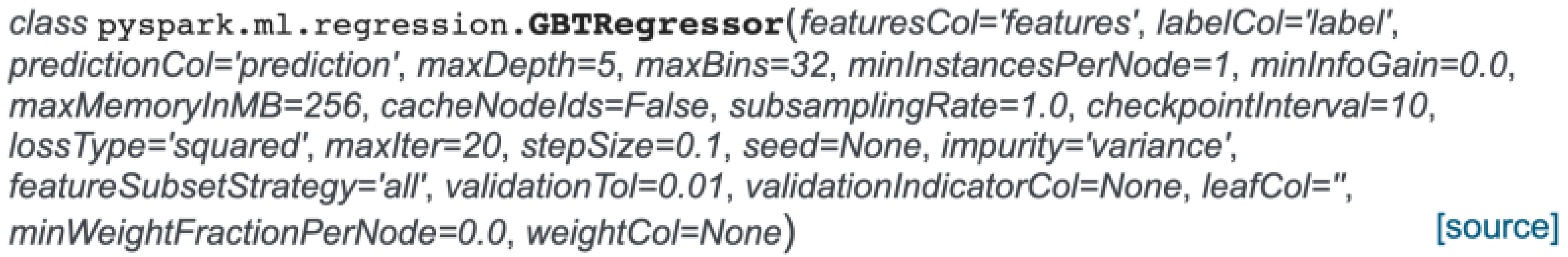
Gradient-boosted trees API

- `GBTClassifier` class in PySpark



class **pyspark.ml.classification.GBTClassifier**(*featuresCol='features', labelCol='label', predictionCol='prediction', maxDepth=5, maxBins=32, minInstancesPerNode=1, minInfoGain=0.0, maxMemoryInMB=256, cacheNodeIds=False, checkpointInterval=10, lossType='logistic', maxIter=20, stepSize=0.1, seed=None, subsamplingRate=1.0, impurity='variance', featureSubsetStrategy='all', validationTol=0.01, validationIndicatorCol=None, leafCol='', minWeightFractionPerNode=0.0, weightCol=None*) [source]

- `GBTRegressor` class in PySpark



class **pyspark.ml.regression.GBTRegressor**(*featuresCol='features', labelCol='label', predictionCol='prediction', maxDepth=5, maxBins=32, minInstancesPerNode=1, minInfoGain=0.0, maxMemoryInMB=256, cacheNodeIds=False, subsamplingRate=1.0, checkpointInterval=10, lossType='squared', maxIter=20, stepSize=0.1, seed=None, impurity='variance', featureSubsetStrategy='all', validationTol=0.01, validationIndicatorCol=None, leafCol='', minWeightFractionPerNode=0.0, weightCol=None*) [source]

Parameters to adjust

- ❑ The parameters to adjust are similar to the ones used for random forests

- ❑ Some of these will be reviewed in the lab session

Contents

References

- ❑ Lecture slides were adapted from [Dr Mauricio Alvarez], who contributed to this module from 2017 to 2022

Contents

References

- Book: Fundamentals of Machine Learning for Predictive Analytics by Kelleher, Mac Namee and D’Arcy, 2015

- Website: Spark API documentation

- YouTube videos:
  - *Scalable Decision Trees in Spark MLlib* by Manish Amde (contributor to the MLlib implementation of Decision Trees in Spark)
  - *Decision Trees on Spark* by Joseph Bradley (Databricks)

- Paper: *PLANET: Massively Parallel Learning of Tree Ensembles with MapReduce* by B. Panda et al. (Google)