MONASH University

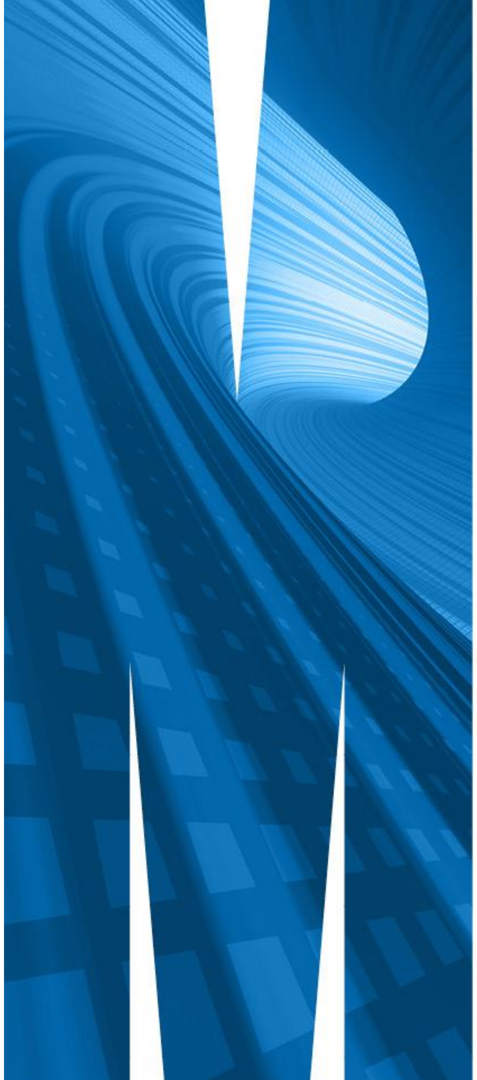
Week 7

FIT5202 Big Data Processing

K-Means Clustering

Model Selection

Updated by CM Ting – 11 April 2025



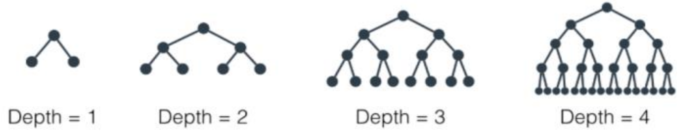
Week 7 Agenda

- **Part - A**
- Week 6 Review
- K-means Clustering
  - Shilouette Score
- Tutorial Instructions
  - Use case : Identify if 3 hackers were involved

- **Part - B**
- Model Selection
  - Hyperparameter Tuning
  - Cross Validation
    - K-fold Cross Validation
  - TrainValidationSplit
- Model Persistance
  - Saving and Loading a Model

Model Selection (a.k.a Hyperparameter Tuning)

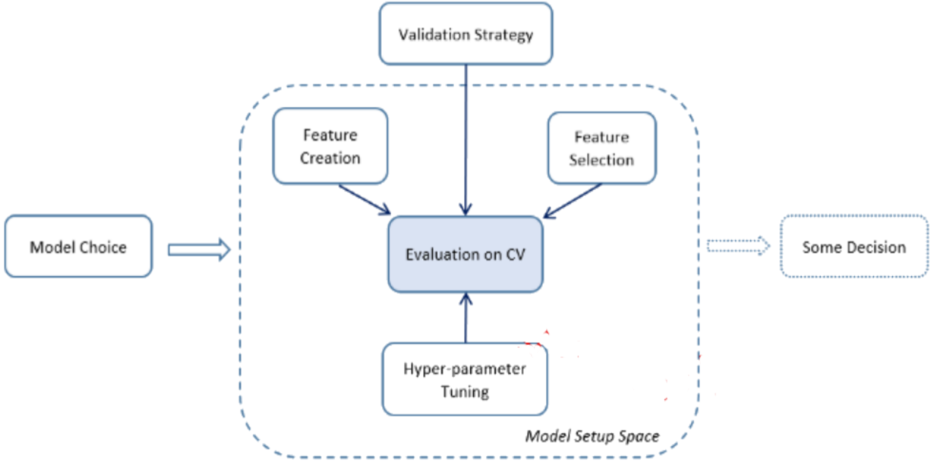
All models are wrong; some are useful (George E.P. Box)



- **HyperParameter Tuning**
- Finding the best model or parameters (e.g. maxDepth of DT, number of clusters in k-means clustering)
- Tuning can be done for individual Estimators or the entire Pipeline

Model selection for MLlib has the following tools:

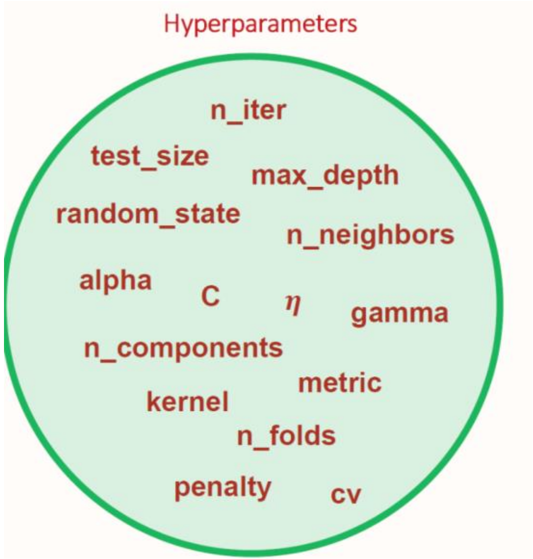
1. CrossValidator
2. TrainValidationSplit



https://spark.apache.org/docs/latest/ml-tuning.html
https://medium.com/pythoneers/hyperparameter-tuning-in-data-science-ad1a03d830b9

Hyperparameter Tuning

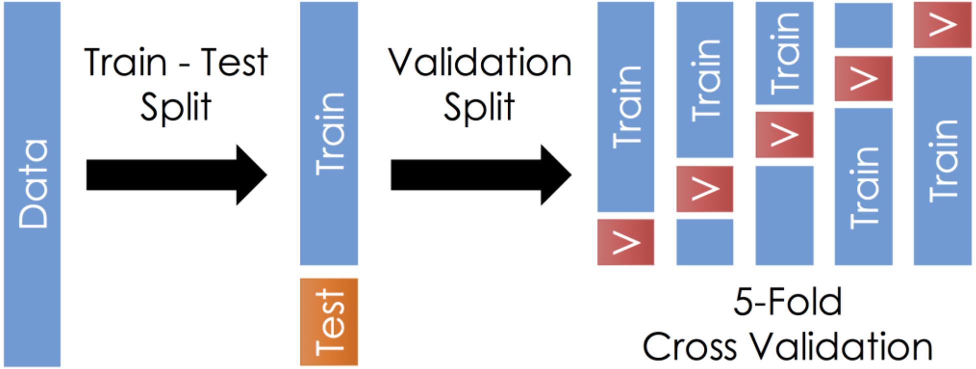
- Hyper-parameters are not model parameters : they cannot be trained from the data
- Hyperparameter tuning : choosing a set of optimal hyperparameters for a learning algorithm
- model.extractParamMap() to get the list of hyperparameters for the model



https://www.analyticsvidhya.com/blog/2024/06/parameters-and-hyperparameters/

Cross Validation (K-Fold)

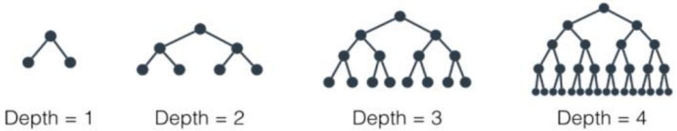
- Splitting dataset into a set of folds, which are used as separate training and test datasets.



Model Selection:

❑ Evaluate performance over a range of model hyper-parameters on validation set,

❑ Choose the model which give highest performance

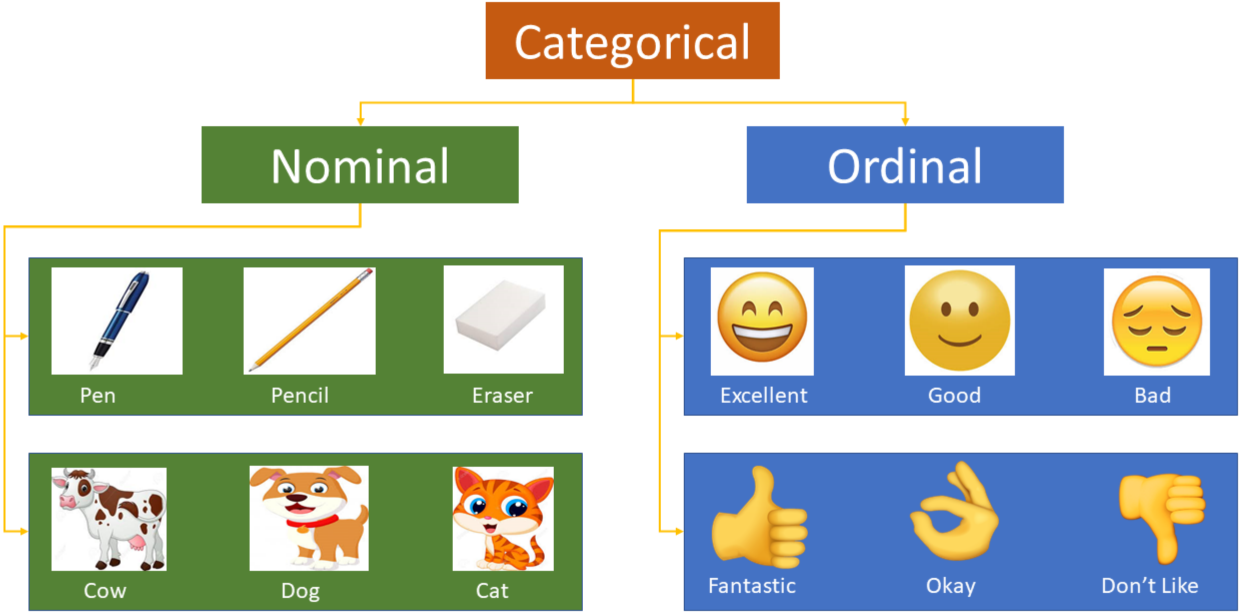


Why not just tune hyperparamters on the test set?

http://www.ds100.org/sp17/assets/notebooks/linear_regression/Cross_Validation_and_the_Bias_Variance_Tradeoff.html

Categorical features

Categorical variables represent types of data which may be divided into groups.



No ordering

The variables have natural, ordered categories

DT Hyperparameter: maxBins

Continuous features

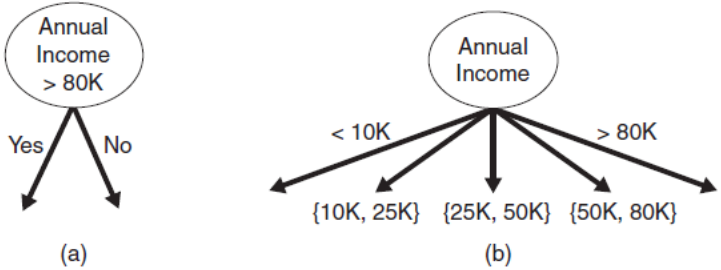


Figure 4.11. Test condition for continuous attributes.

- ❑ The test condition can be expressed as a comparison test ($A < v$) and ($A > v$) with binary outcome, or a range of outcomes $v_i < A < v_{i+1}$ for i=1,…, *k*
- ❑ For binary tree, algorithm will consider all split position *v* (splitting point / threshold)

Example

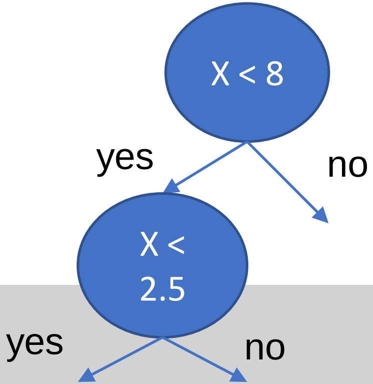
Consider variable *X* with instances [1,3,4,6,2,5,18,10,-3,-5]

We can sort data, and cluster data into **bins** to choose splitting point (e.g., -1,2.5,4.5, and 8)

[-5,-3,1,2,3,4,5,6,10,18]

[-5,-3],[1,2],[3,4],[5,6],[10,18]

Maximum number of bins can be specified using maxBins.

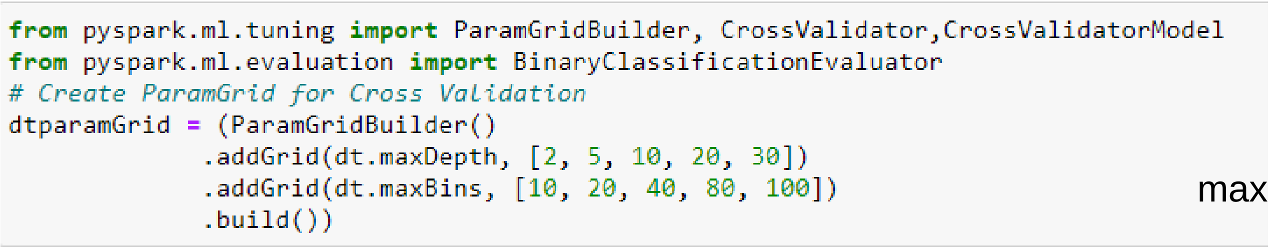


If maxBins is large, more splitting points to consider in building the tree.

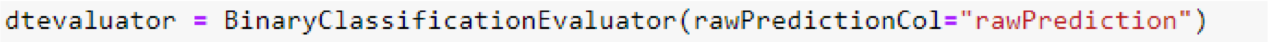
https://spark.apache.org/docs/1.1.0/mllib-decision-tree.html
https://www-users.cs.umn.edu/~kumar001/dmbook/ch4.pdf

Cross Validation (Decision Tree)

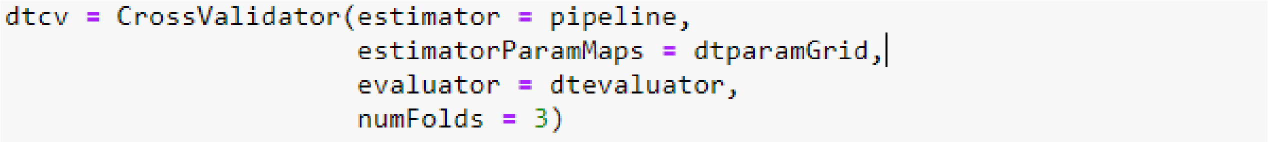
Grid-based
Hyperparameter tuning



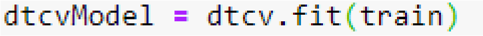
```
from pyspark.ml.tuning import ParamGridBuilder, CrossValidator,CrossValidatorModel
from pyspark.ml.evaluation import BinaryClassificationEvaluator
# Create ParamGrid for Cross Validation
dtparamGrid = (ParamGridBuilder()
             .addGrid(dt.maxDepth, [2, 5, 10, 20, 30])
             .addGrid(dt.maxBins, [10, 20, 40, 80, 100])
             .build())
```



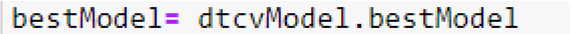
```
dtevaluator = BinaryClassificationEvaluator(rawPredictionCol="rawPrediction")
```



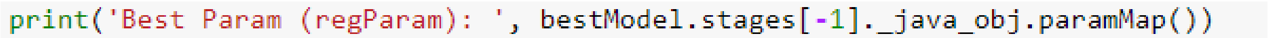
```
dtcv = CrossValidator(estimator = pipeline,
                      estimatorParamMaps = dtparamGrid,
                      evaluator = dtevaluator,
                      numFolds = 3)
```



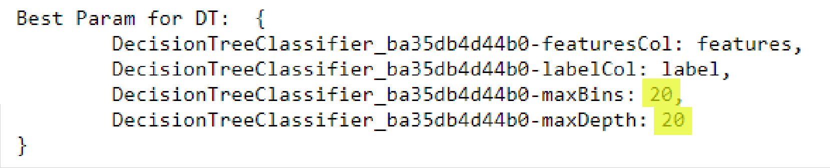
```
dtcvModel = dtcv.fit(train)
```



```
bestModel= dtcvModel.bestModel
```



```
print('Best Param (regParam): ', bestModel.stages[-1]._java_obj.paramMap())
```



```
Best Param for DT:  {
	DecisionTreeClassifier_ba35db4d44b0-featuresCol: features,
	DecisionTreeClassifier_ba35db4d44b0-labelCol: label,
	DecisionTreeClassifier_ba35db4d44b0-maxBins: 20,
	DecisionTreeClassifier_ba35db4d44b0-maxDepth: 20
}
```

maxDepth

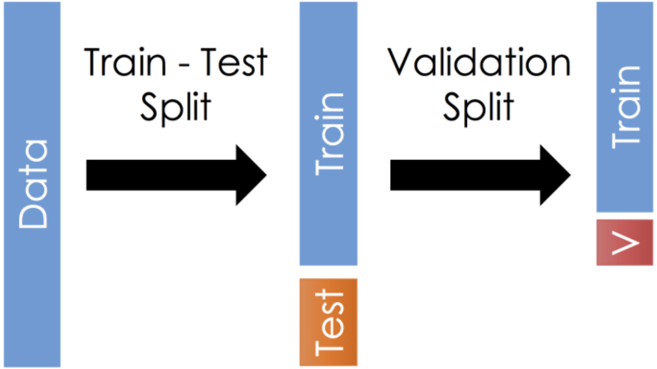
maxBins

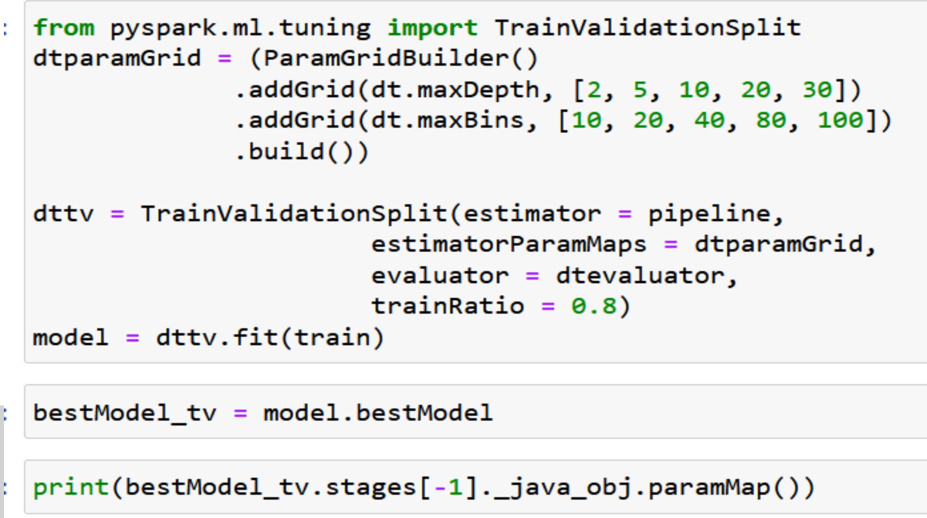
	2	5	10	20	30
10					
20					
40					
80					
100					

- ○ Evaluate performance for each pair of hyperparameters on validation set
- ○ Choose the best set of hyperparameters

TrainValidationSplit

- Creates a single dataset pair
- Only evaluates each combination of parameter once as opposed to k-times in case of CrossValidator
- Less expensive but not reliable if the training dataset is not large enough





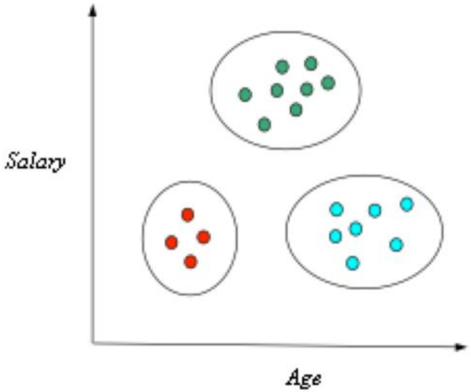
```
from pyspark.ml.tuning import TrainValidationSplit
dtparamGrid = (ParamGridBuilder()
             .addGrid(dt.maxDepth, [2, 5, 10, 20, 30])
             .addGrid(dt.maxBins, [10, 20, 40, 80, 100])
             .build())

dttv = TrainValidationSplit(estimator = pipeline,
                      estimatorParamMaps = dtparamGrid,
                      evaluator = dtevaluator,
                      trainRatio = 0.8)
model = dttv.fit(train)
```

```
bestModel_tv = model.bestModel
```

```
print(bestModel_tv.stages[-1]._java_obj.paramMap())
```

K-Means Clustering



Finds groups (or clusters) of data

A cluster comprises a number of “similar” objects

A member is closer to another member within the same group than to a member of a different group

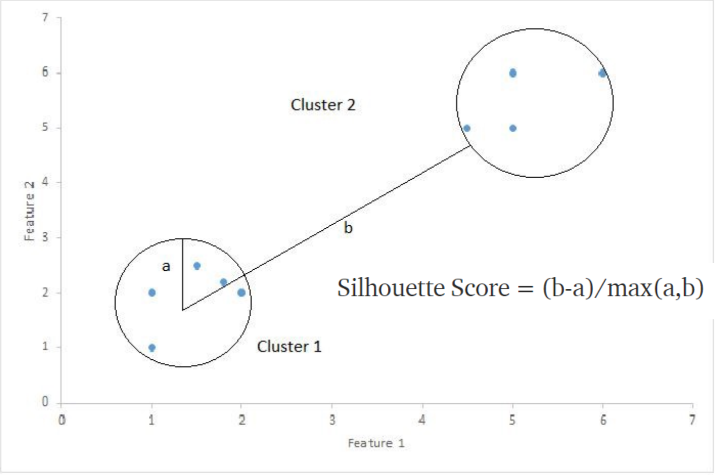
Groups have no category or label

Unsupervised learning

[Animation Demo](#) , [DEMO 2](#)

Silhouette Score [-1 1] : calculates the goodness of a clustering technique

- 1 - Clusters are well apart from each other and clearly distinguishes
- 0 - Clusters are not clearly distinguished, the distance between the clusters is not significant (overlapping cluster)
- -1 – Clusters assigned wrongly



Silhouette Score = (b-a)/max(a,b)

https://towardsdatascience.com/silhouette-coefficient-validating-clustering-techniques-e976bb81d10c

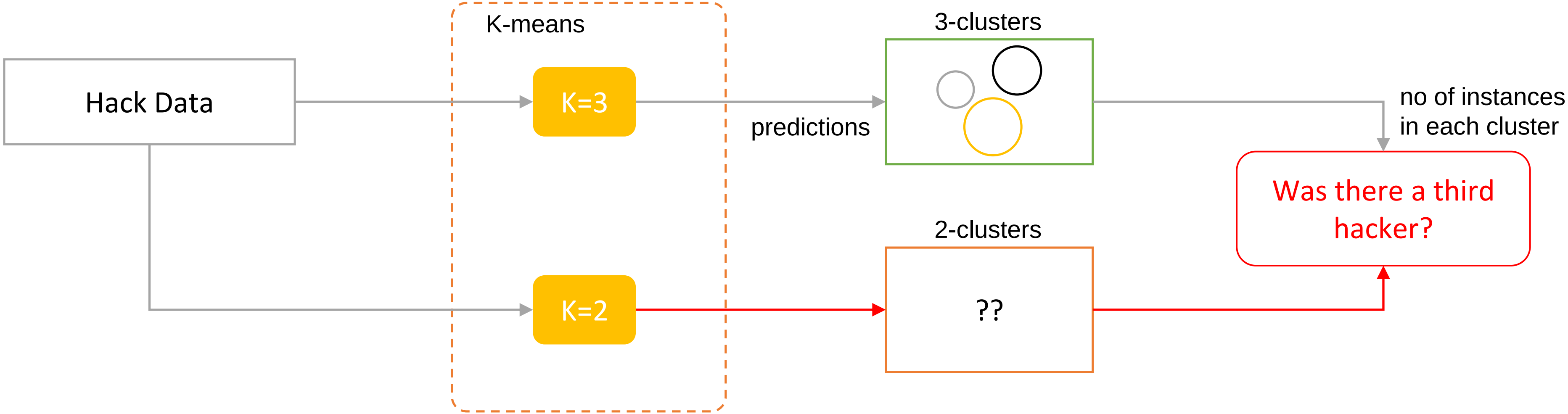
a= average intra-cluster distance

b= average inter-cluster distance

Use case : Was there a third hacker?

Assumption:
Each cluster should have the same number of records

Assumption : Hackers trade off attacks equally



Feature transformation:

(1) Vector Assembler
(2) StandardScaler (normalizing the features to have mean 0 and variance 1)

Thank You!

See you next week.