Big data: architectures and data analytics

Spark MLlib - Part 3

Regression problem

Regression problem

- Predict the value of a continuous attribute (the target attribute)
- Regression is a logical extension of classification:
 - Harder from a mathematical perspective since there are infinite number of possible output values
 - Aim at optimizing metrics of error between predicted and true values (no accuracy rate)

Regression applications

- Use cases can be
 - Predicting usage of bike-sharing in an area and in a day
 - Predicting throughput of an internet connection
 - Predicting movie box-office takings
 - Predicting company revenue

- ...

- Spark MLlib provides also a set of regression algorithms
 - E.g., Linear regression
- A regression algorithm is used to predict the target continuous attribute by applying a model on the predictive attributes
- The model is trained on a set of training data
 - i.e., a set of data for which the value of the target attribute is know

- The regression algorithms available in Spark work only on numerical data
 - They work similarly to classification algorithms, but they predict continuous numerical values (the target attribute is a continuous numerical attribute)
- The input data must be transformed in a DataFrame having the following attributes:
 - label: double
 - The continuous numerical value to be predicted
 - features: Vector of doubles
 - Predictive features

- Many regression algorithms are available in Mllib
 - Linear regression
 - Decision tree regression
 - Random forest regression
 - Survival regression
 - Isotonic regression

- ...

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- ...

These algos are shown in the slides

Regression algorithms: scalability

Model	Number of features	Training size
Linear regression	> millions	No limit
Decision tree regression	> 1 000	No limit
Random forest regression	> 10 000	No limit
	•••	•••

Regression and parameter setting

- The tuning approach that we used for the classification problem can also be used to optimize the regression problem
 - CrossValidation
 - TrainValidationSplit
- The only difference is given by the used evaluator
 - In this case the difference between the actual value and the predicted one must be computed

Regression and performance evaluation

- As for classification, in order to test the goodness of algorithms there is an evaluator
- The evaluator is RegressionEvaluator from pyspark.ml.evaluation
- The instantiated estimator has the method evaluate() that is applied to a dataframe
- It compares the prediction with the true value
- Output: the double value of the performance

Regression and Performance evaluation

- Parameters of RegressionEvaluator:
 - MetricName: string for metric name in evaluation. Supports:
 - "rmse" (default): root mean squared error
 - "mse": mean squared error
 - "r2": R2 metric
 - "mae": mean absolute error
 - labelCol: input column with the true double target
 - predictionCol: input column with the predicted double value

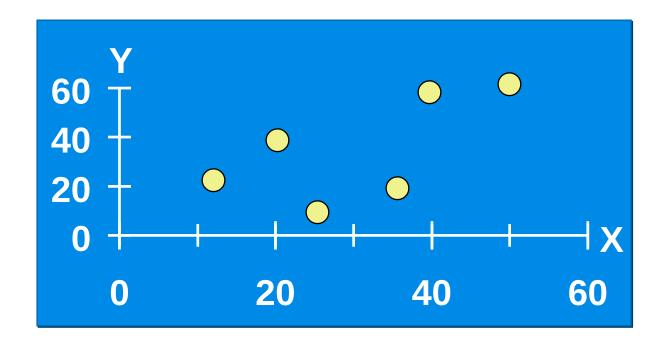
Linear regression

Linear regression

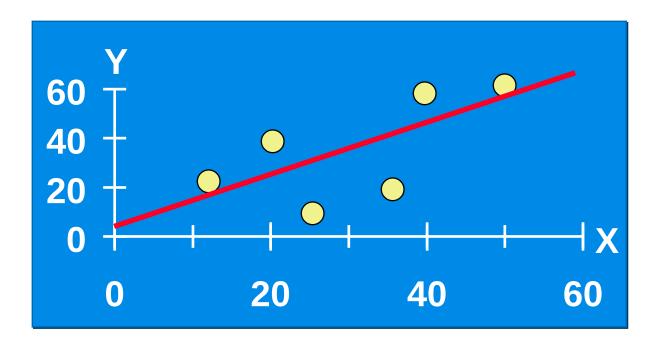
- Linear regression is a popular, effective and efficient regression algorithm
- It assumes a linear combination of your input features – sum of each feature multiplied by a weight
- The input features can be preprocessed (e.g, you can apply a non-linear function of them)
- Produce Gaussian error in the output

1-D example: suppose X is the feature and Y the target value

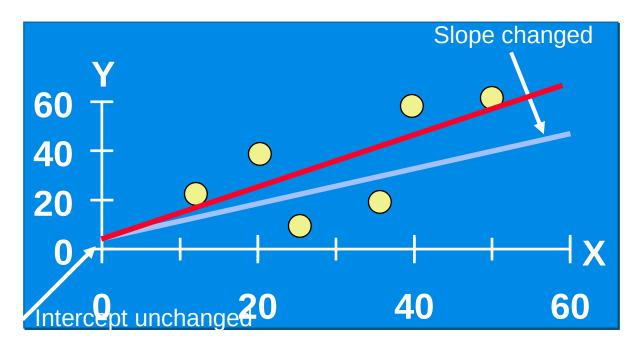
$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$



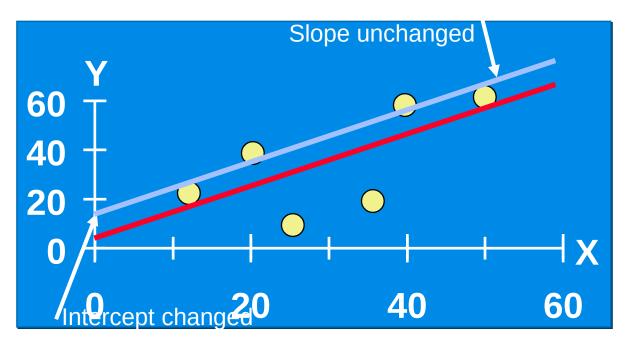
$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$



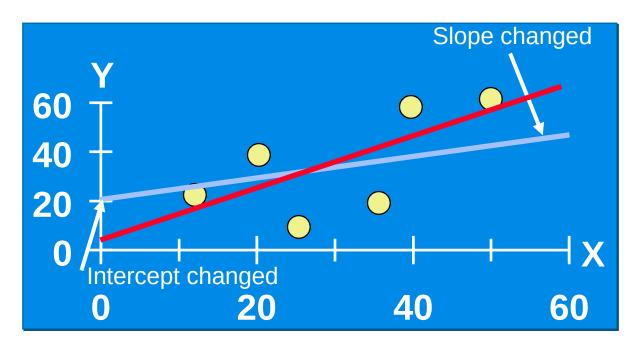
$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$



$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$



$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$



Linear regression: Least Squares

'Best Fit' means difference between actual Y values and predicted Y values are a minimum.

$$\sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} \hat{\varepsilon}_i^2$$

Least squares minimizes the sum of the squared differences (errors)

Linear regression: Least Squares

LS minimizes
$$\sum_{i=1}^{n} \hat{\varepsilon}_{i}^{2} = \hat{\varepsilon}_{1}^{2} + \hat{\varepsilon}_{2}^{2} + \hat{\varepsilon}_{3}^{2} + \hat{\varepsilon}_{4}^{2}$$

$$Y_{2} = \hat{\beta}_{0} + \hat{\beta}_{1}X_{2} + \hat{\varepsilon}_{2}$$

$$\hat{Y}_{i} = \hat{\beta}_{0} + \hat{\beta}_{1}X_{i}$$

Linear regression: interpretation of coefficients

1) Slope (β_1)

- Estimated Y changes by β_1 for each unit increase in X
 - -If $\beta_1 = 2$, then Y increase by 2 for each 1 unit increase in X

2) Y-Intercept (β_0)

- Value of Y when X = 0-If $\beta_0 = 4$, then Y is 4 when X is 0

Linear regression

- Strong points
 - Very fast to train
 - Simple and interpretable model
 - Hard to overfit
- Weak points
 - Linear assumption often does not hold
 - Even if it holds, the errors (the noise)
 might not be gaussian

Linear regression in MLlib

- How to instantiate a linear regression algorithm in Spark an apply it on unlabeled data using MLlib
- The input dataset is a structured dataset with a fixed number of attributes
 - One attribute is the target attribute (the label)
 - The others are predictive attributes that are used to predict the value of the target attribute

Linear regression in MLlib

- Use the LinearRegression estimator from pyspark.ml.regression on a DataFrame
- Explicitly specify input columns featuresCol (vector) and labelCol (double)
- Output column:
 - predictionCol with the predicted double value

Linear regression in MLlib

- (Some) parameters:
 - maxIter: maximum number of iterations to fit the data (>0)
 - **fitIntercept**: whether to fit an intercept term ("True" or "False")
 - **loss:** "squaredError" or "huber", i.e., the function to minimize

•

Linear regression in Mllib: model characteristics and performance

- Model characteristics
 - IrModel.coefficients return a python list of the coefficients of the linear regressor
 - IrModel.intercept return the double value of the intercept
- We can get detailed information about the regressor we trained. The summary method of the transformer returns a summary object with many fields
- For examples:
 - Residuals of each training data (summary.residuals is a dataframe)
 - Root mean square error of residuals (summary.rootMeanSquaredError is a double)

Consider the following example file about bike sharing usage

+	+	+
weekDay distan	ceCenter re	ntals
+	+	+
Monday	1.5	358
Saturday	1.0	272
Saturday	0.5	390
Monday	3.0	120
Saturday	0.3	439
Monday	0.9	509
Saturday	1.9	102
Saturday	2.7	43
Monday	0.6	597
+	+	-

- It contains 10 records
- Each record has two predictive attributes and the target attribute
 - "rentals" is the target attribute
 - The other attributes are predictive attributes
 - They represent the day of the week and the distance of the station from the center in km.

Preprocessing the data

```
from pyspark.ml.feature import StringIndexer
from pyspark.ml.feature import OneHotEncoderEstimator
from pyspark.ml.feature import VectorAssembler
# Load training data
rentalsDF=spark.read.csv('rentals.txt',header=True,inferSchema=True)
indexer = StringIndexer(inputCol="weekDay",
 outputCol="weekDayIndex", handleInvalid="keep")
indexerModel = indexer.fit(rentalsDF)
indexedDF=indexerModel.transform(rentalsDF)
va=VectorAssembler(inputCols=["weekDayIndex","distanceCenter"],
 outputCol="features")
assembledDF=va.transform(indexedDF)
```

Input DataFrame

+ weekDay distan	ceCenter re	+ ntals
++ Monday Saturday Saturday Monday Saturday Monday Saturday	1.5 1.0 0.5 3.0 0.3 0.9 1.9 2.7	358 272 390 120 439 509 102
Monday 	0.6	597 +

Preprocessed DataFrame

++		+		-
weekDay	distanceCenter	rentals	weekDayIndex	features
++		+	+	+ -
Monday	1.5	358	1.0	[1.0,1.5]
Saturday	1.0	272	0.0	[0.0,1.0]
Saturday	0.5	390	0.0	[0.0,0.5]
Monday	3.0	120	1.0	[1.0,3.0]
Saturday	0.3	439	0.0	[0.0,0.3]
Monday	0.9	509	1.0	[1.0,0.9]
Saturday	1.9	102	0.0	[0.0,1.9]
Saturday	2.7	43	0.0	[0.0,2.7]
Monday	0.6	597	1.0	[1.0,0.6]
++		+		++

Input DataFrame

+----+

As we saw in the preprocessing part, scaling the attribute "distanceCenter" and encoding the "weekDay" to many binary features might produce better results

Saturuay	1.9	102
Saturday	2.7	43
Monday	0.6	597
+		+

Preprocessed DataFrame

+		+		+
weekDay	distanceCenter	rentals	weekDayIndex	features
+	+ -	+		++
Monday	1.5	358	1.0	[1.0,1.5]
Saturday	1.0	272	0.0	[0.0,1.0]
Saturday	0.5	390	0.0	[0.0,0.5]
Monday	3.0	120	1.0	[1.0,3.0]
Saturday	0.3	439	0.0	[0.0,0.3]
Monday	0.9	509	1.0	[1.0,0.9]
Saturday	1.9	102	0.0	[0.0,1.9]
Saturday	2.7	43	0.0	[0.0,2.7]
Monday	0.6	597	1.0	[1.0,0.6]
+	+	+		++

Training the linear regressor

```
from pyspark.ml.regression import LinearRegression

Ir = LinearRegression(labelCol="rentals",featuresCol="features",maxIter=10)

# Fit the model
IrModel = Ir.fit(assembledDF)

# Create the predictions
predictionDF=IrModel.transform(assembledDF)
```

Preprocessed dataframe

+	+	+	+
weekDay dista	anceCenter re	entals wee	ekDayIndex features
+	+	+	+
Monday	1.5	358	1.0 [1.0,1.5]
Saturday	1.0	272	0.0 [0.0,1.0]
Saturday	0.5	390	0.0 [0.0,0.5]
Monday	3.0	120	1.0 [1.0,3.0]
Saturday	0.3	439	0.0 [0.0,0.3]
Monday	0.9	509	1.0 [1.0,0.9]
Saturday	1.9	102	0.0 [0.0,1.9]
Saturday	2.7	43	0.0 [0.0,2.7]
Monday	0.6	597	1.0 [1.0,0.6]
+	-	· · ·	+

Output dataframe with regression

4	+					++
ļ	weekDay	distanceCenter	rentals	weekDayIndex	features	prediction
1	Monday Saturday Saturday Monday Saturday Monday Saturday Saturday Saturday	1.0 0.5 3.0 0.3 0.9 1.9 2.7	272 390 120 439 509 102 43	0.0 0.0 1.0 0.0 1.0 0.0 0.0	[0.0,1.0] [0.0,0.5] [1.0,3.0] [0.0,0.3] [1.0,0.9] [0.0,1.9] [0.0,2.7]	395.82984014193653 299.82396947108407 389.98082944364353 125.3592602242581 426.04357343266736 504.01807210900796 137.541621520477 -6.709354435618195 558.1121880925436
4	+			+		++

Information about the created regressor

```
# Print the coefficients and intercept for linear regression print("Coefficients: %s" % str(lrModel.coefficients)) print("Intercept: %s" % str(lrModel.intercept))
```

```
# Summarize the model over the training set and print out some
metrics
trainingSummary = IrModel.summary
print("RMSE: %f" % trainingSummary.rootMeanSquaredError)
trainingSummary.residuals.show()
```

Output dataframe with regression

++-	+	+	+		++
weekDay d	istanceCenter	rentals	weekDayIndex	features	prediction
++-	+	+	+		++
Monday	1.5	358	1.0	[1.0,1.5]	395.82984014193653
Saturday	1.0	272	0.0	[0.0,1.0]	299.82396947108407
Saturday	0.5	390	0.0	[0.0,0.5]	389.98082944364353
Monday	3.0	120	1.0	[1.0,3.0]	125.3592602242581
Saturday	0.3	439	0.0	[0.0,0.3]	426.04357343266736
Monday	0.9	509	1.0	[1.0,0.9]	504.01807210900796
Saturday	1.9	102	0.0	[0.0,1.9]	137.541621520477
Saturday	2.7	43	0.0	[0.0,2.7]	-6.709354435618195
Monday	0.6	597	1.0	[1.0,0.6]	558.1121880925436
++-	+	+	·	- 	++

Regressor information

Coefficients: [186.162730643412, -180.31371994511898]

Intercept: 480.13768941620305

RMSE: 29.198876

++
residuals
++
-37.82984014193653
-27.82396947108407
0.019170556356471025
-5.359260224258094
12.956426567332642
4.98192789099204
-35.54162152047701
49.709354435618195
38.88781190745635

Test DataFrame

+	+-	+
weekDay distan	ceCenter r	entals
+		+
Monday	0.1	641.0
Saturday	2.1	129.0
Saturday	1.5	199.0
Monday	2.0	231.0
Sunday	0.5	393.0
+		+

Preprocess test

```
# Load test data
rentalsTestDF=spark.read.csv('rentalsTest.txt',header=True,inferSchem
a=True)
```

indexedTestDF=indexerModel.transform(rentalsTestDF)

assembledTestDF=va.transform(indexedTestDF)

Test DataFrame

+	+ -	+
weekDay distar	nceCenter r	entals
+	+ -	+
Monday	0.1	641.0
Saturday	2.1	129.0
Saturday	1.5	199.0
Monday	2.0	231.0
Sunday	0.5	393.0
+	+ -	+

Test DataFrame preprocessed

Test DataFrame

"Sunday" does not produce an error since in the StringIndexer we selected to keep linvalid values. They are stored in another category (i.e., 2.0)

```
-----+
 weekDay|distanceCenter|rentals|weekDayIndex| features|
  Monday I
                        641.0
                                      1.0|[1.0,0.1]
|Saturday|
                   2.1
                        129.01
                                      0.0|[0.0,2.1]
Saturdayl
                   1.5l
                                      0.0|[0.0,1.5]|
                        199.0l
  Mondayl
                        231.01
                                      1.0|[1.0,2.0]|
                                      2.0|[2.0,0.5]
  Sunday
                   0.51
                        393.01
```

Apply model to test data

```
from pyspark.ml.evaluation import RegressionEvaluator
predictionTestDF=IrModel.transform(assembledTestDF)
```

```
# compute test error
evaluator = RegressionEvaluator(
    labelCol="rentals", predictionCol="prediction", metricName="rmse")
rmse = evaluator.evaluate(predictionTestDF)
print("Root Mean Squared Error (RMSE) on test data = %g" % rmse)
```

Test DataFrame

++ weekDay	distanceCenter	rentals
Monday Saturday Saturday Monday Sunday	2.1 1.5	129.0 199.0 231.0

Output test DataFrame with predictions

++		+	+		++
weekDay	distanceCenter	rentals	weekDayIndex	features	prediction
++		+	·+		++
Monday	0.1	641.0	1.0	[1.0,0.1]	648.2690480651031
Saturday	2.1	129.0	0.0	[0.0, 2.1]	101.47887753145318
Saturday	1.5	199.0	0.0	[0.0,1.5]	209.66710949852455
Monday	2.0	231.0	1.0	[1.0, 2.0]	305.67298016937707
Sunday	0.5	393.0	2.0	[2.0,0.5]	762.3062907304675
++		+	+		++

Root Mean Squared Error (RMSE) on test data = 169.049

- Decision trees applied to regression work similarly to the ones for classification
- In regression, the trees output a single number per leaf node instead of a label
- A tree can predict a non linear function

- Use the DecisionTreeRegressor estimator from pyspark.ml.regression on a DataFrame
- Explicitly specify input columns featuresCol (vector) and labelCol (double)
- Output column:
 - predictionCol with the predicted double value

- Parameters are the same as for the classification
- Only difference is:
 - impurity: it represents the metric for wheter or not the model should split a particular leaf node with a particular value. The only currently supported metric is "variance"

- Consider the same previous example about predicting bike sharing usage
- Let's start already from the preprocessed dataframe

+	+	++	+	
weekDay	distanceCenter	rentals	weekDayIndex	features
+	t	++	+	+
Monday	1.5	358	1.0	[1.0,1.5]
Saturday	1.0	272	0.0	[0.0,1.0]
Saturday	0.5	390	0.0	[0.0,0.5]
Monday	3.0	120	1.0	[1.0,3.0]
Saturday	0.3	439	0.0	[0.0,0.3]
Monday	0.9	509	1.0	[1.0,0.9]
Saturday	1.9	102	0.0	[0.0,1.9]
Saturday	2.7	43	0.0	[0.0,2.7]
Monday	0.6	597	1.0	[1.0,0.6]
+	+	++	+	+

Training the decision tree

```
from pyspark.ml.regression import DecisionTreeRegressor
from pyspark.ml.evaluation import RegressionEvaluator
# Train a DecisionTree model.
dt = DecisionTreeRegressor(labelCol="rentals",featuresCol="features",maxDepth=4)
# Fit the model
dtModel = dt.fit(assembledDF)
# Predict output
predictionDF=dtModel.transform(assembledDF)
# Compute training error
evaluator = RegressionEvaluator(
  labelCol="rentals", predictionCol="prediction", metricName="rmse")
rmse = evaluator.evaluate(predictionDF)
print("Root Mean Squared Error (RMSE) on training data = %g" % rmse)
```

Preprocessed dataframe

+	+	+	+
weekDay dist	anceCenter re	entals we	ekDayIndex features
+	+	+	+
Monday	1.5	358	1.0 [1.0,1.5]
Saturday	1.0	272	0.0 [0.0,1.0]
Saturday	0.5	390	0.0 [0.0,0.5]
Monday	3.0	120	1.0 [1.0,3.0]
Saturday	0.3	439	0.0 [0.0,0.3]
Monday	0.9	509	1.0 [1.0,0.9]
Saturday	1.9	102	0.0 [0.0,1.9]
Saturday	2.7	43	0.0 [[0.0, 2.7]]
Monday	0.6	597	1.0 [1.0,0.6]
+	+	+	+

Output dataframe with regression

+	+	+	LPayInday faaturas pro	
weekbay uista +	ecenter re	+	kDayIndex features pre	
Monday	1.5	358	1.0 [1.0,1.5]	358.0
Saturday	1.0	272	0.0 [0.0,1.0]	272.0
Saturday	0.5	390	0.0 [0.0,0.5]	390.0
Monday	3.0	120	1.0 [1.0,3.0]	120.0
Saturday	0.3	439	0.0 [0.0,0.3]	439.0
Monday	0.9	509	1.0 [1.0,0.9]	509.0
Saturday	1.9	102	0.0 [0.0,1.9]	102.0
Saturday	2.7	43	0.0 [0.0,2.7]	43.0
Monday	0.6	597	1.0 [1.0,0.6]	597.0
+		+	+	

Root Mean Squared Error (RMSE) on training data = 0

Preprocessed dataframe

```
weekDay|distanceCenter|rentals|weekDayIndex| features|
                                            1.0|[1.0,1.5]|
  Monday|
                     1.5
                              3581
|Saturday|
                      1.0
                              272
                                            0.0|[0.0,1.0]|
                     0.5|
                                            0.0|[0.0,0.5]|
|Saturday|
                              3901
                                            1.0|[1.0,3.0]|
  Monday|
                      3.0
                              120|
|Saturday|
                      0.3|
                              439|
                                            0.0|[0.0,0.3]|
                                            1.0|[1.0,0.9]|
                      0.91
                              509 l
  Monday|
```

The model is perfect with respect to training data

+-----

Output dataframe with regression

```
weekDay|distanceCenter|rentals|weekDayIndex| features|prediction
                                            1 0 | [1.0, 1.5] |
  Monday|
                     1.5
                              358
                                                                358.0
|Saturday|
                     1.0
                              272
                                            0.0|[0.0,1.0]|
                                                                272.0
                                            0.0|[0.0,0.5]|
|Saturday|
                     0.5
                              390 l
                                                                390.0
  Mondayl
                     3.01
                              120
                                            1.0|[1.0,3.0]|
                                                                120.0
|Saturday|
                     0.31
                              439
                                            0.0|[0.0,0.3]|
                                                                439.0
  Mondayl
                     0.91
                              509
                                            1.0 [1.0,0.9]
                                                                509.0
|Saturday|
                     1.9
                              102
                                            0.0 \ [0.0, 1.9]
                                                                102.0
                                            0.0|[0.0,2.7]|
|Saturday|
                     2.7
                              43|
                                                                43.0
                                            1.0|1.0,0.6]|
  Mondayl
                     0.6
                              597
                                                                597.0
```

Root Mean Squared Error (RMSE) on training data = 0

Test DataFrame

++	- +
weekDay distanceCenter rental	s
Monday 0.1 641. Saturday 2.1 129. Saturday 1.5 199. Monday 2.0 231. Sunday 0.5 393.	0 0 0

Apply model to test data

```
from pyspark.ml.evaluation import RegressionEvaluator predictionTestDF=lrModel.transform(assembledTestDF)
```

```
# compute test error
evaluator = RegressionEvaluator(
    labelCol="rentals", predictionCol="prediction", metricName="rmse")
rmse = evaluator.evaluate(predictionTestDF)
```

print("Root Mean Squared Error (RMSE) on test data = %g" % rmse)

Test DataFrame

+	+-	+
weekDay distan	ceCenter r	entals
+	+-	+
Monday	0.1	641.0
Saturday	2.1	129.0
Saturday	1.5	199.0
Monday	2.0	231.0
Sunday	0.5	393.0
+	+-	+

Output test DataFrame with predictions

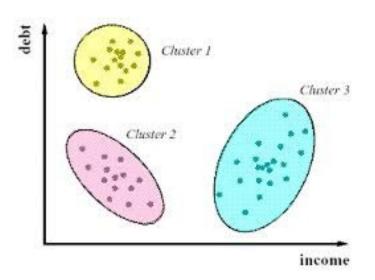
```
weekDay|distanceCenter|rentals|weekDayIndex| features|prediction|
                                   1.0|[1.0,0.1]|
0.0|[0.0.2.1]|
              0.1| 641.0|
2.1| 129.0|
  Mondayl
                                                         597.01
                                       0.0|[0.0,2.1]|
|Saturday|
                                                         102.0
|Saturday| 1.5| 199.0|
                                       0.0|[0.0,1.5]|
                                                         272.0
                  2.0| 231.0|
                                       1.0|[1.0,2.0]|
  Monday|
                                                         120.0
              0.5| 393.0|
                                       2.0|[2.0,0.5]|
  Sunday|
                                                         597.0
```

Root Mean Squared Error (RMSE) on test data = 111.293

Unsupervised learning: clustering

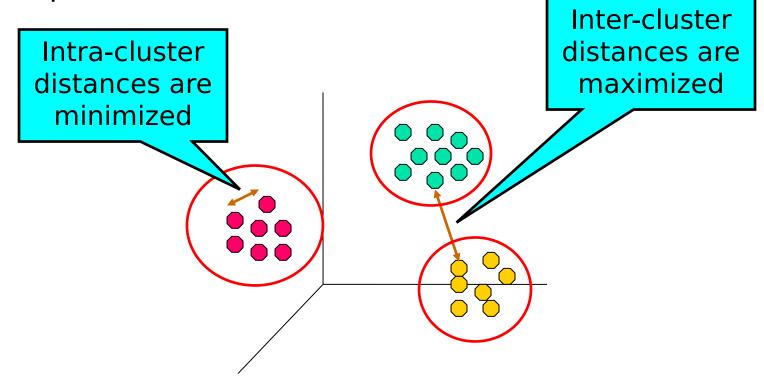
Unsupervised learning

- Learning "what normally happens"
- No output
- Clustering: Grouping similar instances
- Other applications: Summarization, Association Analysis



Clustering

Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups

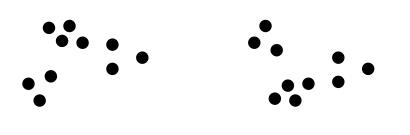


Clustering: use cases

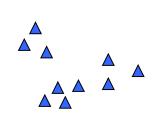
- Finding users with similar behaviour without the need to set thresholds
- Finding anomalies in data
- Topic modelling

Clustering: ambiguity

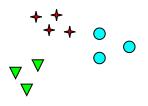
Notion of a cluster can be ambiguous



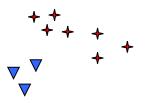
How many clusters?



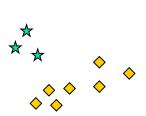
Two Clusters



Six Clusters







Clustering: weak points

- It is usually hard to define and measure success
- For big data, the problem is exacerbated
- Clustering in high dimensional space can create odd clusters
- Curse of dimensionality: as feature space expands in dimensionality, it become more sparse and not statistically significant

Clustering

"The validation of clustering structures is the most difficult and frustrating part of cluster analysis.

Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

From: Algorithms for Clustering Data, Jain and Dubes

Clustering algorithms

- Spark MLlib provides a (limited) set of clustering algorithms
 - K-means
 - Gaussian mixture models
 - Bisecting K-means
 - Latent Dirichlet Allocation
 - ...

Clustering algorithms

- Spark MLlib provides a (limited) set of clustering algorithms
 - K-means
 - Gaussian mixture models
 - Bisecting K-means
 - Latent Dirichlet Allocation
 - . . .

These algos are shown in the slides

Clustering model scalability

Model	Statistical recommendation	Computation limits	Training size
k-means	features<100	Features x clusters < 10 million	No limit
Bisecting k-means	features<100	Features x clusters < 10 million	No limit
Gaussian Mixture models	features<100	Features x clusters< 10 million	No limit
Latent Dirichlet Allocation	An interpretable number	> 1000 clusters	No limit

Clustering

- Each clustering algorithm has its own parameters
- However, all the provided algorithms identify a set of groups of objects/clusters and assign each input object to one single cluster
- All the clustering algorithms available in Spark work only with numerical data
 - Categorical values must be mapped to integer values (i.e., numerical values)

Clustering

- The input of the MLlib clustering algorithms is a DataFrame containing a feature column
 - Data type: pyspark.ml.linalg.Vectors
- The clustering algorithm clusters the input records by considering only the content of features
 - The other columns, if any, are not considered

Clustering: Example

- Example: credit score
 - A set of customer profiles
 - For each customer we have savings and income
 - We want to automatically group customer in groups based on their characteristics

+		 +
Savings	Income	User
15000		!
0	5000	Luca
20000	800	Martino
6000	1300	Mike
50000	2500	Francesca
2000	1100	Steve
700	1500	Maria
75000	0	Guido
4000	500	Roberta
7000	3000	Idilio
3000	900	Marco
6000	1200	Dena
+		+

Clustering: Example

Preprocess data for clustering

```
from pyspark.ml.feature import StandardScaler
from pyspark.ml.feature import VectorAssembler
data=spark.read.csv('credit score cluster.txt',header=True,inferSche
  ma=True)
va=VectorAssembler(inputCols=["Savings","Income"],
  outputCol="features")
assembledDF=va.transform(data)
scaler = StandardScaler(inputCol="features",
  outputCol="scaledFeatures", withStd=True, withMean=True)
scalerModel = scaler.fit(assembledDF)
scaledDF=scalerModel.transform(assembledDF)
```

Clustering: Example

Input DataFrame

+ Savings	Income	+ User
+		++
15000	1000	Paolo
0	5000	Luca
20000	800	Martino
6000	1300	Mike
50000	2500	Francesca
2000	1100	Steve
700	1500	Maria
75000	0	Guido
4000	500	Roberta
7000	3000	Idilio
3000	900	Marco
6000	1200	Dena
+		·

Preprocessed DataFrame

+	+	+	++
Savings Income	User	features	scaledFeatures
+	+	++	+
15000 1000	Paolo	[15000.0,1000.0]	[-0.0312169519277
0 5000	Luca	[0.0,5000.0]	[-0.6770849228476]
20000 800	Martino	[20000.0,800.0]	[0.18407237171215]
6000 1300	Mike	[6000.0,1300.0]	[-0.4187377344796]
50000 2500	Francesca	[50000.0,2500.0]	[1.47580831355180]
2000 1100	Steve	[2000.0,1100.0]	[-0.5909691933916]
700 1500	Maria	[700.0,1500.0]	[-0.6469444175380]
75000 0	Guido	[75000.0,0.0]	[2.55225493175152]
4000 500	Roberta	[4000.0,500.0]	[-0.5048534639356]
7000 3000	Idilio	[7000.0,3000.0]	[-0.3756798697517]
3000 900	Marco	[3000.0,900.0]	[-0.5479113286636]
6000 1200	Dena	[6000.0,1200.0]	[-0.4187377344796]
+	+	+	++

Clustering performance: silhouette

- Silhouette measures consistency within clusters of data.
- The silhouette value is a measure of how similar an object is to its own cluster (cohesion) compared to other clusters (separation).
- It ranges from −1 to +1, where a high value indicates that the object is well matched to its own cluster and poorly matched to neighboring clusters.
- If most objects have a high value, then the clustering configuration is appropriate.
- The silhouette can be calculated with any distance metric

Clustering performance in MLIib

- As for classification and regression, in order to test the goodness of clusters there is an evaluator
- The evaluator is ClusteringEvaluator from pyspark.ml.evaluation
- The instantiated estimator has the method evaluate() that is applied to a dataframe
- It compares the clusters with the input data
- It computes the silhouette measure

Clustering performance in MLIib

- Parameters of ClusteringEvaluator:
 - metricName: string for metric name in evaluation. Only supports "silhouette"
 - distanceMeasure: param for distance measure to be used in evaluation. Supports "squaredEuclidean" (default) and "cosine"
 - featuresCol: input column with the features
 - **predictionCol**: input column with the cluster assignment

K-means clustering algorithm

- K-means is one of the most popular clustering algorithms
- It is characterized by one important parameter
 - The number of clusters K
 - The choice of K is a complex operation
 - Often chosen by experimenting different values

- It uses proximity by Euclidean clustering
- It is able to identify only spherical shaped clusters
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid

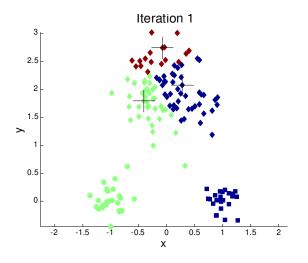
The basic algorithm is very simple:

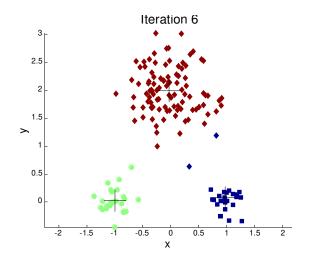
- 1: Select K points as the initial centroids.
- 2: repeat
- 3: Form K clusters by assigning all points to the closest centroid.
- 4: Recompute the centroid of each cluster.
- 5: **until** The centroids don't change

Most of the time, convergence happens in the first few iterations.

Importance of choosing initial centroids

Case 1:

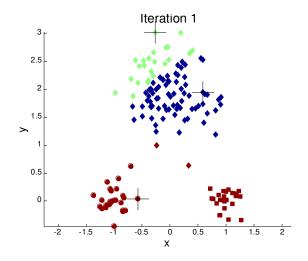


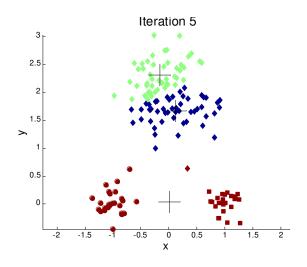


At convergence

Importance of choosing initial centroids

Case 2:





At convergence

Specific performance measure for K-means

Evaluating K-means cluster: Sum of Squared Error (SSE)

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

- x is a data point in cluster C_i and m_j is the centroid of the cluster C_i
- Given two clusters, we can choose the one with the smallest error
- One easy way to reduce SSE is to increase K, the number of clusters

K-means clustering algorithm in MLlib

- The following slides show how to apply the K-means algorithm provided by Mllib
- The input dataset is a structured dataset with a fixed number of attributes
 - All the attributes are numerical attributes

K-means in MLlib

- Use the Kmeans estimator from pyspark.ml.clustering on a DataFrame
- Explicitly specify input columns featuresCol (vector)
- Output column:
 - PredictionCol: with its predicted cluster center

K-means in MLlib

- Parameters are:
 - k: number of clusters
 - initMode: initialization of the centroids.
 Supported are "random" and "k-means||"
 - initSteps: number of steps for "k-means||" initialization mode
 - maxIter: Total number of iterations over the data before stopping
 - tol: specifies threshold for keeping optimizing centroids position

K-means: summary of results

- K-means include a summary class to evaluate our model
- It includes information about clusters created and relative size (number of data for each cluster)
- We can also compute the sum of squared error within cluster which measure how close values are from their cluster centroid (computeCost)
- Given k, k-means try to minimize the computeCost

- Example: credit score
 - Start from preprocessed dataframe

Preprocessed DataFrame

++			·+	+
Savings	Income	User	features	scaledFeatures
++			++	·+
15000	1000	Paolo	[15000.0,1000.0]	[-0.0312169519277
0	5000	Luca	[0.0,5000.0]	[-0.6770849228476]
20000	800	Martino	[20000.0,800.0]	[0.18407237171215]
6000	1300	Mike	[6000.0,1300.0]	[-0.4187377344796
50000	2500	Francesca		[1.47580831355180
2000	1100	Steve	[2000.0,1100.0]	[-0.5909691933916
700	1500	Maria	[700.0,1500.0]	[-0.6469444175380
75000	0	Guido		[2.55225493175152
4000	500	Roberta	[4000.0,500.0]	[-0.5048534639356
7000	3000	Idilio		[-0.3756798697517
3000	900	Marco		[-0.5479113286636
6000	1200	Dena	[6000.0,1200.0]	[-0.4187377344796
++		+	++	+

from pyspark.ml.clustering import KMeans

```
# Trains a k-means model.
kmeans = KMeans(k=3,featuresCol="scaledFeatures",initMode="k-means||")
model = kmeans.fit(scaledDF)

# Make predictions
predictionsDF = model.transform(scaledDF)
```

Preprocessed DataFrame

+	+	.+	++
Savings Inco	ome User	features	scaledFeatures
0 50 20000 8 6000 13 50000 25 2000 12 700 15 75000 4000 5 7000 30 3000 5	000 Luca 800 Martino 300 Mike	a [0.0,5000.0] b [20000.0,800.0] c [6000.0,1300.0] a [50000.0,2500.0] c [7000.0,1100.0] a [75000.0,00] b [75000.0,00] a [4000.0,500.0] b [7000.0,3000.0] b [3000.0,900.0]	[-0.0312169519277 [-0.6770849228476 [0.18407237171215 [-0.4187377344796 [1.47580831355180 [-0.5909691933916 [-0.6469444175380 [2.55225493175152 [-0.5048534639356 [-0.3756798697517 [-0.5479113286636 [-0.4187377344796
+	+	.+	++

Output DataFrame with clusters

++		+			++
Savings In	come	User	features	scaledFeatures	prediction
++					++
15000	1000	Paolo	[15000.0,1000.0]	[-0.0312169519277	0
0	5000 j	Luca	[0.0,5000.0]	[-0.6770849228476	1
j 20000 j	800	Martino		[0.18407237171215	j oj
j 6000 j	1300 j	Mike	[6000.0,1300.0]	[-0.4187377344796	j oj
j 50000 j	2500 j	Francesca	[50000.0,2500.0]	[1.47580831355180	2
2000	1100 j	Steve	[2000.0,1100.0]	[-0.5909691933916	0
700	1500 j	Maria	[700.0,1500.0]	[-0.6469444175380	j 0 j
75000	0	Guido	[75000.0,0.0]	[2.55225493175152	j 2 j
4000	500	Roberta	[4000.0,500.0]	[-0.5048534639356	j 0 j
7000	3000 j	Idilio	[7000.0,3000.0]	[-0.3756798697517	j 1 j
3000	900	Marco	[3000.0,900.0]	[-0.5479113286636	j 0 j
j 6000 j	1200 j	Dena		[-0.4187377344796	j 0 j
++	i	- 		- 	++

from pyspark.ml.evaluation import ClusteringEvaluator

```
# Shows the result.
centers = model.clusterCenters()
print("Cluster Centers: ")
for center in centers:
  print(center)
print("Size of the clusters: ", model.summary.clusterSizes)
# Evaluate clustering by computing Silhouette score
evaluator = ClusteringEvaluator()
silhouette = evaluator.evaluate(predictionsDF)
print("Silhouette with squared euclidean distance = " + str(silhouette))
print("SSE: ",model.computeCost(predictionsDF))
```

Output DataFrame with clusters +-----

+	.+	+		++
Savings Incom	e User	features	scaledFeatures	prediction
+	.+	+		+
15000 100	Paolo	[15000.0,1000.0]	[-0.0312169519277	0
0 500	D Luca	[0.0,5000.0]	[-0.6770849228476	1
20000 80) Martino	[[20000.0,800.0]	[0.18407237171215	i 0 j
6000 130	O Mike		[-0.4187377344796	i 0 j
50000 250	Francesca	[50000.0,2500.0]	[1.47580831355180	2
2000 110) Steve	[[2000.0,1100.0]	[-0.5909691933916	i 0 j
700 150	o Maria	[700.0,1500.0]	[-0.6469444175380	i 0 j
75000	O Guido	[75000.0,0.0]	[2.55225493175152	2
4000 50	0 Roberta	[4000.0,500.0]	[-0.5048534639356	i 0 j
7000 300) Idilio	[[7000.0,3000.0]	[-0.3756798697517	1
j 3000 j 90	oj Marco	[3000.0,900.0]	[-0.5479113286636	i oi
6000 120	Dena Dena		[-0.4187377344796	0 j
+	+	+	+	+ -

87

Standard output

```
Cluster Centers:

[-0.37191231 -0.39159297]

[-0.5263824    1.80071098]

[ 2.01403162 -0.2343391 ]
```

Size of the clusters: [8, 2, 2]

Silhouette with squared euclidean distance = -0.09641007707651222

SSE: 4.404936191705298

Assign new data to existing clusters

```
+----+
|Savings|Income| User|
+----+
| 10000| 1860|Mariana|
| 4500| 1100| Nicola|
| 27000| 1000| Davide|
+----+
```

predictionsNewDF = model.transform(scaledNewDF)

```
# Load New data
dataNewDF=spark.read.csv('credit_score_cluster_Test.txt',header=Tr
    ue,inferSchema=True)

assembledNewDF=va.transform(dataNewDF)
scaledNewDF=scalerModel.transform(assembledNewDF)

# Make predictions
```

Assign new data to existing clusters

```
| Savings|Income| User|
| User|
| 10000| 1860|Mariana|
| 4500| 1100| Nicola|
| 27000| 1000| Davide|
```

Output dataframe with associated clusters

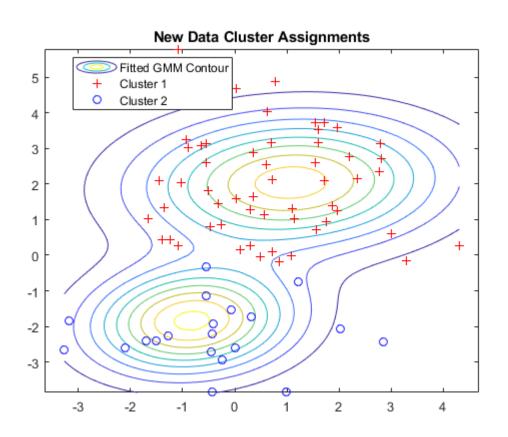
```
| Savings|Income| User| features| scaledFeatures|prediction|
| 10000| 1860|Mariana|[10000.0,1860.0]|[-0.2465062755677...| 0|
| 4500| 1100| Nicola| [4500.0,1100.0]|[-0.4833245315716...| 0|
| 27000| 1000| Davide|[27000.0,1000.0]|[0.48547742480807...|
```

Gaussian mixture model

Gaussian mixture model

- Gaussian mixture models (GMM) are another popular clustering algorithm
- It assumes each cluster produces data based upon random draws from a (multidimensional) Gaussian distribution
- Clusters should be less likely to have data at the edge
- Each Gaussian cluster has its own mean and standard deviation
- Allow for a more nuanced cluster associated with probability

Gaussian mixture model



GMM in MLlib

- Use the GaussianMixture estimator from pyspark.ml.clustering on a DataFrame
- Explicitly specify input columns featuresCol (vector)
- Output column:
 - PredictionCol: with its predicted cluster
 - ProbabilityCol: probability of each cluster

GMM in MLlib

- Parameters are:
 - k: number of clusters that you would like to end up with
 - maxIter: Total number of iterations over the data before stopping
 - **tol**: specifies threshold for keeping optimizing weights of Gaussian mixtures

GMM: summary of results

- Also GMM include a summary class to evaluate our model
- It includes information about weights of the Gaussian Mixtures and clusters created and relative size (number of data for each cluster)

- Example: credit score
 - Start from preprocessed dataframe

Preprocessed DataFrame

++			++	+
Savings	Income	User	features	scaledFeatures
++		+	++	+
15000	1000	Paolo	[15000.0,1000.0]	[-0.0312169519277
0	5000	Luca	[0.0,5000.0]	[-0.6770849228476
20000	800	Martino	[20000.0,800.0]	[0.18407237171215]
6000	1300	Mike	[6000.0,1300.0]	[-0.4187377344796]
50000	2500	Francesca	[50000.0,2500.0]	[1.47580831355180]
2000	1100	Steve	[2000.0,1100.0]	[-0.5909691933916]
700	1500	Maria	[700.0,1500.0]	[-0.6469444175380]
75000	0	Guido	[75000.0,0.0]	[2.55225493175152]
4000	500	Roberta	[4000.0,500.0]	[-0.5048534639356]
7000	3000	Idilio	[7000.0,3000.0]	[-0.3756798697517]
3000	900	Marco	[3000.0,900.0]	[-0.5479113286636]
6000	1200	Dena	[6000.0,1200.0]	[-0.4187377344796
++		+ -	·+	+

from pyspark.ml.clustering import GaussianMixture

```
# Trains a GMM model.
gmm = GaussianMixture(k=3,featuresCol="scaledFeatures")
model = gmm.fit(scaledDF)

# Make predictions
predictionsDF = model.transform(scaledDF)
predictionsDF.show(truncate=False)
```

Preprocessed DataFrame

++		+	+	+
Savings	Income	User +	features	scaledFeatures
15000 0 20000 6000 50000 7000 75000 4000 7000 3000	5000 800 1300	Luca Martino Mike Francesca Steve Maria Guido Roberta Idilio	[0.0,5000.0] [20000.0,800.0] [6000.0,1300.0] [50000.0,2500.0] [2000.0,1100.0] [700.0,1500.0] [75000.0,0.0] [4000.0,500.0] [7000.0,3000.0] [3000.0,900.0]	[-0.0312169519277 [-0.6770849228476 [0.18407237171215 [-0.4187377344796 [1.47580831355180 [-0.5909691933916 [-0.6469444175380 [2.55225493175152 [-0.5048534639356 [-0.3756798697517 [-0.5479113286636 [-0.4187377344796
++		+	+	+

Output DataFrame with clusters and probabilities

Savings Income User	features		prediction	 probability
0	[[0.0,5000.0] [[20000.0,800.0] [[6000.0,1300.0] [[50000.0,2500.0] [[2000.0,1100.0] [[700.0,1500.0] [[75000.0,0.0] [[4000.0,500.0] [[7000.0,3000.0] [[7000.0,3000.0]		1 0 2 1 2 2 2 0 2 1	[0.9997461383843239, 2.5339239436132E-4, 4.6922131486960353E-7]

```
print("Gaussians weights shown as a DataFrame: ")
model.gaussiansDF.show(truncate=False)
print("Size of the clusters: ", model.summary.clusterSizes)
from pyspark.ml.evaluation import ClusteringEvaluator
# Evaluate clustering by computing Silhouette score
evaluator = ClusteringEvaluator()
silhouette = evaluator.evaluate(predictionsDF)
print("Silhouette with squared euclidean distance = " +
  str(silhouette))
```

Output DataFrame with clusters

```
|Savings|Income|User
                                          IscaledFeatures
                                                                                       |prediction|probability
                         |[15000.0,1000.0]|[-0.031216951927791736,-0.4193436518555962]|0
       1000
              |Paolo
                                                                                                  |[0.9997461383843239,2.5339239436132E-4,4.6922131486960353E-7]
        15000
              Luca
                         1[0.0,5000.0]
                                          | [-0.6770849228476208, 2.5407291847721423]
                                                                                                  [7.67384821545586E-15,0.99999999999847,7.67384821545586E-15]
                         [20000.0,800.0] [0.18407237171215127,-0.5673472936869831]
                                                                                       10
                                                                                                  [0.9997781944193962,2.2180558059577122E-4,8.08697666663197E-15]
120000
        1800
               |Martino
                          [6000.0,1300.0] [[-0.41873773447968915,-0.1973381891085158]
6000
        1300
               |Mike
                                                                                      12
                                                                                                  [3.370858048561919E-5,5.087928478827556E-5,0.9999154121347261]
150000
        12500
              [Francesca|[50000.0,2500.0]][1.4758083135518092,0.6906836618798058]
                                                                                       11
                                                                                                  [7.671883651274481E-15,0.99999999999847,7.671883651274481E-15]
12000
       11100
              Steve
                         [2000.0,1100.0] [-0.5909691933916436,-0.3453418309399027]
                                                                                                  [0.09756437460176307,2.851666521106474E-6,0.9024327737317159]
1700
       11500
              IMaria
                         [700.0,1500.0] [-0.6469444175380287,-0.04933454727712887] |2
                                                                                                  [1.414987519906597E-10,8.114221331490605E-5,0.9999188576451863]
                                          |[2.5522549317515244,-1.159361861012531]
                                                                                                   [0.9987350372281458, 0.0012649627718535413, 6.71135687338088E-16]
175000
               |Guido
                         [75000.0,0.0]
                                         [-0.5048534639356663, -0.7893527564340636]
                                                                                       2
                                                                                                   [2.9326429379156076E-16,4.3649700681163853E-7,0.9999995635029929]
4000
       1500
               |Roberta
                         [4000.0,500.0]
17000
        13000
              IIdilio
                         [7000.0,3000.0] [-0.37567986975170053,1.060692766458273]
                                                                                                  [7.66296622775793E-15,0.9999999226529782,7.734701413156046E-8]
        900
                         [3000.0,900.0] [-0.547911328663655,-0.49334547277128965]
                                                                                                  [4.378058313062203E-6,1.107903359412824E-6,0.9999945140383275]
13000
               |Marco
                         [6000.0,1200.0] [-0.41873773447968915,-0.27134001002420927] 2
                                                                                                  [0.020490483344952695,2.355096422577629E-5,0.9794859656908216]
```

Standard output

Silhouette with squared euclidean distance = 0.14433979161213353

Assign new data to existing clusters

```
+----+
|Savings|Income| User|
+----+
| 10000| 1860|Mariana|
| 4500| 1100| Nicola|
| 27000| 1000| Davide|
+----+
```

Make predictions

```
# Load New data
dataNewDF=spark.read.csv('credit_score_cluster_Test.txt',header=Tr
    ue,inferSchema=True)

assembledNewDF=va.transform(dataNewDF)
scaledNewDF=scalerModel.transform(assembledNewDF)
```

predictionsNewDF = model.transform(scaledNewDF)

Assign new data to existing clusters

```
+-----+
|Savings|Income| User|
+-----+
| 10000| 1860|Mariana|
| 4500| 1100| Nicola|
| 27000| 1000| Davide|
+-----+
```

Output dataframe with associated clusters

Savings Income	User	features	scaledFeatures	prediction	 probability
10000 1860 4500 1100	Mariana [100 Nicola [45 Davide [270	000.0,1860.0] [-0 500.0,1100.0] [-0 000.0,1000.0] [0.	0.2465062755677 0.4833245315716 48547742480807	2 2 0	[9.83009952163732 [1.32063772202194 [0.99999756357385