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Classification and regression

This page covers algorithms for Classification and Regression. It also includes sections discussing specific classes of algorithms, such as linear methods, trees, and ensembles.

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Classification

Logistic regression

Logistic regression is a popular method to predict a categorical response. It is a special case of Generalized Linear models that predicts the probability of the outcomes. In spark.ml logistic regression can be used to predict a binary outcome by using binomial logistic regression, or it can be used to predict a multiclass outcome by using multinomial logistic regression. Use the family parameter to select between these two algorithms, or leave it unset and Spark will infer the correct variant.

Multinomial logistic regression can be used for binary classification by setting the family param to "multinomial". It will produce two sets of coefficients and two intercepts.

When fitting LogisticRegressionModel without intercept on dataset with constant nonzero column, Spark MLlib outputs zero coefficients for constant nonzero columns. This behavior is the same as R glmnet but different from LIBSVM.

Binomial logistic regression

For more background and more details about the implementation of binomial logistic regression, refer to the documentation of logistic regression in spark.mllib.

Examples

The following example shows how to train binomial and multinomial logistic regression models for binary classification with elastic net regularization. elasticNetParam corresponds to α and regParam corresponds to λ .

Scala Java Python R

More details on parameters can be found in the Scala API documentation.

```
import org.apache.spark.ml.classification.LogisticRegression

// Load training data
val training = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")

val lr = new LogisticRegression()
    .setMaxIter(10)
    .setRegParam(0.3)
    .setElasticNetParam(0.8)

// Fit the model
val lrModel = lr.fit(training)
```

```
// Print the coefficients and intercept for logistic regression
println(s"Coefficients: ${\text{lrModel.coefficients}} \text{ Intercept: ${\text{lrModel.intercept}}")}

// We can also use the multinomial family for binary classification
val mlr = new LogisticRegression()
    .setMaxIter(10)
    .setRegParam(0.3)
    .setElasticNetParam(0.8)
    .setFamily("multinomial")

val mlrModel = mlr.fit(training)

// Print the coefficients and intercepts for logistic regression with multinomial family
println(s"Multinomial coefficients: ${\text{mlrModel.coefficientMatrix}}")
println(s"Multinomial intercepts: ${\text{mlrModel.interceptVector}}")
```

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/LogisticRegressionWithElasticNetExample.scala" in the Spark repo. The spark.ml implementation of logistic regression also supports extracting a summary of the model over the training set. Note that the predictions and metrics which are stored as DataFrame in LogisticRegressionSummary are annotated @transient and hence only available on the driver.

Scala Java Python

LogisticRegressionTrainingSummary provides a summary for a LogisticRegressionModel. In the case of binary classification, certain additional metrics are available, e.g. ROC curve. The binary summary can be accessed via the binarySummary method. See BinaryLogisticRegressionTrainingSummary.

Continuing the earlier example:

```
import org.apache.spark.ml.classification.LogisticRegression

// Extract the summary from the returned LogisticRegressionModel instance trained in the earlier

// example

val trainingSummary = lrModel.binarySummary

// Obtain the objective per iteration.

val objectiveHistory = trainingSummary.objectiveHistory
println("objectiveHistory:")

objectiveHistory.foreach(loss => println(loss))

// Obtain the receiver-operating characteristic as a dataframe and areaUnderROC.
val roc = trainingSummary.roc
roc.show()
println(s"areaUnderROC: ${trainingSummary.areaUnderROC}{}")
```

```
// Set the model threshold to maximize F-Measure
val fMeasure = trainingSummary.fMeasureByThreshold
val maxFMeasure = fMeasure.select(max("F-Measure")).head().getDouble(0)
val bestThreshold = fMeasure.where($"F-Measure" === maxFMeasure)
    .select("threshold").head().getDouble(0)
lrModel.setThreshold(bestThreshold)
```

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/LogisticRegressionSummaryExample.scala" in the Spark repo.

Multinomial logistic regression

Multiclass classification is supported via multinomial logistic (softmax) regression. In multinomial logistic regression, the algorithm produces K sets of coefficients, or a matrix of dimension $K \times J$ where K is the number of outcome classes and J is the number of features. If the algorithm is fit with an intercept term then a length K vector of intercepts is available.

Multinomial coefficients are available as coefficientMatrix and intercepts are available as interceptvector.

coefficients and intercept methods on a logistic regression model trained with multinomial family are not supported. Use coefficientMatrix and interceptvector instead.

The conditional probabilities of the outcome classes $k \in {1, 2, \dots, K}$ are modeled using the softmax function.

$$P(Y=k|\mathbf{X},oldsymbol{eta}_k,eta_{0k}) = rac{e^{oldsymbol{eta}_k\cdot\mathbf{X}+eta_{0k}}}{\sum_{k'=0}^{K-1}e^{oldsymbol{eta}_{k'}\cdot\mathbf{X}+eta_{0k'}}}$$

We minimize the weighted negative log-likelihood, using a multinomial response model, with elastic-net penalty to control for overfitting.

$$\min_{eta,eta_0} - \left[\sum_{i=1}^L w_i \cdot \log P(Y=y_i|\mathbf{x}_i)
ight] + \lambda \left[rac{1}{2} (1-lpha) \left| \left|oldsymbol{eta}
ight|
ight|_2^2 + lpha \left| \left|oldsymbol{eta}
ight|
ight|_1
ight]$$

For a detailed derivation please see here.

Examples

The following example shows how to train a multiclass logistic regression model with elastic net regularization, as well as extract the multiclass training summary for evaluating the model.

Scala Java Python R

import org.apache.spark.ml.classification.LogisticRegression
// Load training data

```
val training = spark
  .read
  .format("libsvm")
  .load("data/mllib/sample_multiclass_classification_data.txt")
val lr = new LogisticRegression()
  .setMaxIter(10)
  .setRegParam(0.3)
  .setElasticNetParam(0.8)
// Fit the model
val lrModel = lr.fit(training)
// Print the coefficients and intercept for multinomial logistic regression
println(s"Coefficients: \n${IrModel.coefficientMatrix}")
println(s"Intercepts: \n${IrModel.interceptVector}")
val trainingSummary = lrModel.summary
// Obtain the objective per iteration
val objectiveHistory = trainingSummary.objectiveHistory
println("objectiveHistory:")
objectiveHistory.foreach(println)
// for multiclass, we can inspect metrics on a per-label basis
println("False positive rate by label:")
trainingSummary.falsePositiveRateByLabel.zipWithIndex.foreach { case (rate, label) =>
 println(s"label $label: $rate")
}
println("True positive rate by label:")
trainingSummary.truePositiveRateByLabel.zipWithIndex.foreach { case (rate, label) =>
 println(s"label $1abe1: $rate")
}
println("Precision by label:")
trainingSummary.precisionByLabel.zipWithIndex.foreach { case (prec, label) =>
 println(s"label $1abe1: $prec")
}
println("Recall by label:")
trainingSummary.recallByLabel.zipWithIndex.foreach { case (rec, label) =>
 println(s"label $1abe1: $rec")
}
println("F-measure by label:")
trainingSummary.fMeasureByLabel.zipWithIndex.foreach { case (f, label) =>
 println(s"label $1abe1: $f")
```

```
val accuracy = trainingSummary.accuracy
val falsePositiveRate = trainingSummary.weightedFalsePositiveRate
val truePositiveRate = trainingSummary.weightedTruePositiveRate
val fMeasure = trainingSummary.weightedFMeasure
val precision = trainingSummary.weightedPrecision
val recall = trainingSummary.weightedRecall
println(s"Accuracy: $accuracy\nFPR: $falsePositiveRate\nTPR: $truePositiveRate\n" +
s"F-measure: $fMeasure\nPrecision: $precision\nRecall: $recall")
```

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/MulticlassLogisticRegressionWithElasticNetExample.scala" in the Spark repo.

Decision tree classifier

Decision trees are a popular family of classification and regression methods. More information about the spark.ml implementation can be found further in the section on decision trees.

Examples

The following examples load a dataset in LibSVM format, split it into training and test sets, train on the first dataset, and then evaluate on the held-out test set. We use two feature transformers to prepare the data; these help index categories for the label and categorical features, adding metadata to the DataFrame which the Decision Tree algorithm can recognize.

Scala Java Python R

More details on parameters can be found in the Scala API documentation.

```
import org.apache.spark.ml.Pipeline
import org.apache.spark.ml.classification.DecisionTreeClassificationModel
import org.apache.spark.ml.classification.DecisionTreeClassifier
import org.apache.spark.ml.evaluation.MulticlassClassificationEvaluator
import org.apache.spark.ml.feature.{IndexToString, StringIndexer, VectorIndexer}

// Load the data stored in LIBSVM format as a DataFrame.
val data = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")

// Index labels, adding metadata to the label column.
// Fit on whole dataset to include all labels in index.
val labelIndexer = new StringIndexer()
.setInputCol("label")
.setOutputCol("indexedLabel")
.fit(data)
// Automatically identify categorical features, and index them.
val featureIndexer = new VectorIndexer()
```

```
.setInputCol("features")
  .setOutputCol("indexedFeatures")
  .setMaxCategories(4) // features with > 4 distinct values are treated as continuous.
  .fit(data)
// Split the data into training and test sets (30% held out for testing).
val Array(trainingData, testData) = data.randomSplit(Array(0.7, 0.3))
// Train a DecisionTree model.
val dt = new DecisionTreeClassifier()
  .setLabelCol("indexedLabel")
  .setFeaturesCol("indexedFeatures")
// Convert indexed labels back to original labels.
val labelConverter = new IndexToString()
  .setInputCol("prediction")
  .setOutputCol("predictedLabel")
  .setLabels(labelIndexer.labels)
// Chain indexers and tree in a Pipeline.
val pipeline = new Pipeline()
  .setStages(Array(labelIndexer, featureIndexer, dt, labelConverter))
// Train model. This also runs the indexers.
val model = pipeline.fit(trainingData)
// Make predictions.
val predictions = model.transform(testData)
// Select example rows to display.
predictions.select("predictedLabel", "label", "features").show(5)
// Select (prediction, true label) and compute test error.
val evaluator = new MulticlassClassificationEvaluator()
  .setLabelCol("indexedLabel")
  .setPredictionCol("prediction")
  .setMetricName("accuracy")
val accuracy = evaluator.evaluate(predictions)
println(s"Test Error = \{(1.0 - accuracy)\}")
val treeModel = model.stages(2).asInstanceOf[DecisionTreeClassificationModel]
println(s"Learned classification tree model:\n ${\footnote{treeModel.toDebugString}}")
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/DecisionTreeClassificationExample.scala" in the Spark repo.

Random forest classifier

Random forests are a popular family of classification and regression methods. More information about the spark.ml implementation can be found further in the section on random forests.

Examples

The following examples load a dataset in LibSVM format, split it into training and test sets, train on the first dataset, and then evaluate on the held-out test set. We use two feature transformers to prepare the data; these help index categories for the label and categorical features, adding metadata to the DataFrame which the tree-based algorithms can recognize.

» Scala

Java Python

R

```
import org.apache.spark.ml.Pipeline
import org.apache.spark.ml.classification.{RandomForestClassificationModel, RandomFore
stClassifier}
import org.apache.spark.ml.evaluation.MulticlassClassificationEvaluator
import org.apache.spark.ml.feature.{IndexToString, StringIndexer, VectorIndexer}
// Load and parse the data file, converting it to a DataFrame.
val data = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")
// Index labels, adding metadata to the label column.
// Fit on whole dataset to include all labels in index.
val labelIndexer = new StringIndexer()
  .setInputCol("label")
  .setOutputCol("indexedLabel")
  .fit(data)
// Automatically identify categorical features, and index them.
// Set maxCategories so features with > 4 distinct values are treated as continuous.
val featureIndexer = new VectorIndexer()
  .setInputCol("features")
  .setOutputCol("indexedFeatures")
  .setMaxCategories(4)
  .fit(data)
// Split the data into training and test sets (30% held out for testing).
val Array(trainingData, testData) = data.randomSplit(Array(0.7, 0.3))
// Train a RandomForest model.
val rf = new RandomForestClassifier()
  .setLabelCol("indexedLabel")
  .setFeaturesCol("indexedFeatures")
  .setNumTrees(10)
// Convert indexed labels back to original labels.
val labelConverter = new IndexToString()
```

```
.setInputCol("prediction")
       .setOutputCol("predictedLabel")
       .setLabels(labelIndexer.labels)
     // Chain indexers and forest in a Pipeline.
     val pipeline = new Pipeline()
       .setStages(Array(labelIndexer, featureIndexer, rf, labelConverter))
     // Train model. This also runs the indexers.
    val model = pipeline.fit(trainingData)
>>
     // Make predictions.
     val predictions = model.transform(testData)
     // Select example rows to display.
     predictions.select("predictedLabel", "label", "features").show(5)
     // Select (prediction, true label) and compute test error.
     val evaluator = new MulticlassClassificationEvaluator()
       .setLabelCol("indexedLabel")
       .setPredictionCol("prediction")
       .setMetricName("accuracy")
     val accuracy = evaluator.evaluate(predictions)
     println(s"Test Error = \{(1.0 - accuracy)\}")
     val rfModel = model.stages(2).asInstanceOf[RandomForestClassificationModel]
     println(s"Learned classification forest model:\n ${rfModel.toDebugString}")
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/RandomForestClassifierExample.scala" in the Spark repo.

Gradient-boosted tree classifier

Gradient-boosted trees (GBTs) are a popular classification and regression method using ensembles of decision trees. More information about the spark.ml implementation can be found further in the section on GBTs.

Examples

The following examples load a dataset in LibSVM format, split it into training and test sets, train on the first dataset, and then evaluate on the held-out test set. We use two feature transformers to prepare the data; these help index categories for the label and categorical features, adding metadata to the DataFrame which the tree-based algorithms can recognize.

Scala Java Python R

```
import org.apache.spark.ml.Pipeline
import org.apache.spark.ml.classification.{GBTClassificationModel, GBTClassifier}
import org.apache.spark.ml.evaluation.MulticlassClassificationEvaluator
import org.apache.spark.ml.feature.{IndexToString, StringIndexer, VectorIndexer}
// Load and parse the data file, converting it to a DataFrame.
val data = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")
// Index labels, adding metadata to the label column.
// Fit on whole dataset to include all labels in index.
val labelIndexer = new StringIndexer()
  .setInputCol("label")
  .setOutputCol("indexedLabel")
  .fit(data)
// Automatically identify categorical features, and index them.
// Set maxCategories so features with > 4 distinct values are treated as continuous.
val featureIndexer = new VectorIndexer()
  .setInputCol("features")
  .setOutputCol("indexedFeatures")
  .setMaxCategories(4)
  .fit(data)
// Split the data into training and test sets (30% held out for testing).
val Array(trainingData, testData) = data.randomSplit(Array(0.7, 0.3))
// Train a GBT model.
val gbt = new GBTClassifier()
  .setLabelCol("indexedLabel")
  .setFeaturesCol("indexedFeatures")
  .setMaxIter(10)
  .setFeatureSubsetStrategy("auto")
// Convert indexed labels back to original labels.
val labelConverter = new IndexToString()
  .setInputCol("prediction")
  .setOutputCol("predictedLabel")
  .setLabels(labelIndexer.labels)
// Chain indexers and GBT in a Pipeline.
val pipeline = new Pipeline()
  .setStages(Array(labelIndexer, featureIndexer, gbt, labelConverter))
// Train model. This also runs the indexers.
val model = pipeline.fit(trainingData)
// Make predictions.
val predictions = model.transform(testData)
```

```
// Select example rows to display.
predictions.select("predictedLabel", "label", "features").show(5)

// Select (prediction, true label) and compute test error.

val evaluator = new MulticlassClassificationEvaluator()
    .setLabelCol("indexedLabel")
    .setPredictionCol("prediction")
    .setMetricName("accuracy")

val accuracy = evaluator.evaluate(predictions)
println(s"Test Error = ${1.0 - accuracy}")

val gbtModel = model.stages(2).asInstanceOf[GBTClassificationModel]
println(s"Learned classification GBT model:\n ${gbtModel.toDebugString}")
```

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/GradientBoostedTreeClassifierExample.scala" in the Spark repo.

Multilayer perceptron classifier

Multilayer perceptron classifier (MLPC) is a classifier based on the feedforward artificial neural network. MLPC consists of multiple layers of nodes. Each layer is fully connected to the next layer in the network. Nodes in the input layer represent the input data. All other nodes map inputs to outputs by a linear combination of the inputs with the node's weights ${\bf w}$ and bias ${\bf b}$ and applying an activation function. This can be written in matrix form for MLPC with K+1 layers as follows:

$$\mathbf{y}(\mathbf{x}) = \mathbf{f}_{\mathrm{K}}(\dots \mathbf{f}_{2}(\mathbf{w}_{2}^{T}\mathbf{f}_{1}(\mathbf{w}_{1}^{T}\mathbf{x} + b_{1}) + b_{2})\dots + b_{K})$$

Nodes in intermediate layers use sigmoid (logistic) function:

$$\mathrm{f}(z_i) = \frac{1}{1+e^{-z_i}}$$

Nodes in the output layer use softmax function:

$$\mathrm{f}(z_i) = rac{e^{z_i}}{\sum_{k=1}^N e^{z_k}}$$

The number of nodes N in the output layer corresponds to the number of classes.

MLPC employs backpropagation for learning the model. We use the logistic loss function for optimization and L-BFGS as an optimization routine.

Examples

Scala Java Python R

```
import org.apache.spark.ml.classification.MultilayerPerceptronClassifier
import org.apache.spark.ml.evaluation.MulticlassClassificationEvaluator
```

```
// Load the data stored in LIBSVM format as a DataFrame.
val data = spark.read.format("libsvm")
  .load("data/mllib/sample_multiclass_classification_data.txt")
// Split the data into train and test
val splits = data.randomSplit(Array(0.6, 0.4), seed = 1234L)
val train = splits(0)
val test = splits(1)
// specify layers for the neural network:
// input layer of size 4 (features), two intermediate of size 5 and 4
// and output of size 3 (classes)
val layers = Array[Int](4, 5, 4, 3)
// create the trainer and set its parameters
val trainer = new MultilayerPerceptronClassifier()
  .setLayers(layers)
  .setBlockSize(128)
  .setSeed(1234L)
  .setMaxIter(100)
// train the model
val model = trainer.fit(train)
// compute accuracy on the test set
val result = model.transform(test)
val predictionAndLabels = result.select("prediction", "label")
val evaluator = new MulticlassClassificationEvaluator()
  .setMetricName("accuracy")
println(s"Test set accuracy = ${evaluator.evaluate(predictionAndLabels)}")
```

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/MultilayerPerceptronClassifierExample.scala" in the Spark repo.

Linear Support Vector Machine

A support vector machine constructs a hyperplane or set of hyperplanes in a high- or infinite-dimensional space, which can be used for classification, regression, or other tasks. Intuitively, a good separation is achieved by the hyperplane that has the largest distance to the nearest training-data points of any class (so-called functional margin), since in general the larger the margin the lower the generalization error of the classifier. LinearSVC in Spark ML supports binary classification with linear SVM. Internally, it optimizes the Hinge Loss using OWLQN optimizer.

Examples

Scala Java Python R

Refer to the Scala API docs for more details.

```
import org.apache.spark.ml.classification.LinearSVC

// Load training data
val training = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")

val lsvc = new LinearSVC()
    .setMaxIter(10)
    .setRegParam(0.1)

// Fit the model
val lsvcModel = lsvc.fit(training)

// Print the coefficients and intercept for linear svc
println(s"Coefficients: ${\lsvcModel.coefficients} \text{ Intercept: ${\lsvcModel.intercept}}")
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/LinearSVCExample.scala" in the Spark repo.

One-vs-Rest classifier (a.k.a. One-vs-All)

OneVsRest is an example of a machine learning reduction for performing multiclass classification given a base classifier that can perform binary classification efficiently. It is also known as "One-vs-All."

onevsRest is implemented as an Estimator. For the base classifier it takes instances of Classifier and creates a binary classification problem for each of the k classes. The classifier for class i is trained to predict whether the label is i or not, distinguishing class i from all other classes.

Predictions are done by evaluating each binary classifier and the index of the most confident classifier is output as label.

Examples

The example below demonstrates how to load the Iris dataset, parse it as a DataFrame and perform multiclass classification using onevsrest. The test error is calculated to measure the algorithm accuracy.

Scala Java Python

```
import org.apache.spark.ml.classification.{LogisticRegression, OneVsRest}
import org.apache.spark.ml.evaluation.MulticlassClassificationEvaluator

// load data file.
val inputData = spark.read.format("libsvm")
    .load("data/mllib/sample_multiclass_classification_data.txt")
```

```
// generate the train/test split.
val Array(train, test) = inputData.randomSplit(Array(0.8, 0.2))
// instantiate the base classifier
val classifier = new LogisticRegression()
  .setMaxIter(10)
  .setTol(1E-6)
  .setFitIntercept(true)
// instantiate the One Vs Rest Classifier.
val ovr = new OneVsRest().setClassifier(classifier)
// train the multiclass model.
val ovrModel = ovr.fit(train)
// score the model on test data.
val predictions = ovrModel.transform(test)
// obtain evaluator.
val evaluator = new MulticlassClassificationEvaluator()
  .setMetricName("accuracy")
// compute the classification error on test data.
val accuracy = evaluator.evaluate(predictions)
println(s"Test Error = ${1 - accuracy}")
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/OneVsRestExample.scala" in the Spark repo.

Naive Bayes

Naive Bayes classifiers are a family of simple probabilistic classifiers based on applying Bayes' theorem with strong (naive) independence assumptions between the features. The spark.ml implementation currently supports both multinomial naive Bayes and Bernoulli naive Bayes. More information can be found in the section on Naive Bayes in MLlib.

Examples

Scala Java Python R

```
import org.apache.spark.ml.classification.NaiveBayes
import org.apache.spark.ml.evaluation.MulticlassClassificationEvaluator

// Load the data stored in LIBSVM format as a DataFrame.
val data = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")
```

```
// Split the data into training and test sets (30% held out for testing)
    val Array(trainingData, testData) = data.randomSplit(Array(0.7, 0.3), seed = 1234L)
     // Train a NaiveBayes model.
    val model = new NaiveBayes()
       .fit(trainingData)
    // Select example rows to display.
    val predictions = model.transform(testData)
>>
    predictions.show()
    // Select (prediction, true label) and compute test error
    val evaluator = new MulticlassClassificationEvaluator()
       .setLabelCol("label")
       .setPredictionCol("prediction")
       .setMetricName("accuracy")
    val accuracy = evaluator.evaluate(predictions)
    println(s"Test set accuracy = $accuracy")
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/NaiveBayesExample.scala" in the Spark repo.

Regression

Linear regression

The interface for working with linear regression models and model summaries is similar to the logistic regression case.

When fitting LinearRegressionModel without intercept on dataset with constant nonzero column by "I-bfgs" solver, Spark MLlib outputs zero coefficients for constant nonzero columns. This behavior is the same as R glmnet but different from LIBSVM.

Examples

The following example demonstrates training an elastic net regularized linear regression model and extracting model summary statistics.

Scala Java Python

More details on parameters can be found in the Scala API documentation.

```
import org.apache.spark.ml.regression.LinearRegression

// Load training data
val training = spark.read.format("libsvm")
```

```
.load("data/mllib/sample_linear_regression_data.txt")
val lr = new LinearRegression()
  .setMaxIter(10)
  .setRegParam(0.3)
  .setElasticNetParam(0.8)
// Fit the model
val lrModel = lr.fit(training)
// Print the coefficients and intercept for linear regression
println(s"Coefficients: ${\text{IrModel.coefficients}} Intercept: ${\text{IrModel.intercept}}")
// Summarize the model over the training set and print out some metrics
val trainingSummary = lrModel.summary
println(s"numIterations: ${trainingSummary.totalIterations}")
println(s"objectiveHistory: [${trainingSummary.objectiveHistory.mkString(",")}]")
trainingSummary.residuals.show()
println(s"RMSE: ${trainingSummary.rootMeanSquaredError}")
println(s"r2: ${trainingSummary.r2}")
```

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/LinearRegressionWithElasticNetExample.scala" in the Spark repo.

Generalized linear regression

Contrasted with linear regression where the output is assumed to follow a Gaussian distribution, generalized linear models (GLMs) are specifications of linear models where the response variable Y_i follows some distribution from the exponential family of distributions. Spark's GeneralizedLinearRegression interface allows for flexible specification of GLMs which can be used for various types of prediction problems including linear regression, Poisson regression, logistic regression, and others. Currently in <code>spark.ml</code>, only a subset of the exponential family distributions are supported and they are listed below.

NOTE: Spark currently only supports up to 4096 features through its GeneralizedLinearRegression interface, and will throw an exception if this constraint is exceeded. See the advanced section for more details. Still, for linear and logistic regression, models with an increased number of features can be trained using the LinearRegression and LogisticRegression estimators.

GLMs require exponential family distributions that can be written in their "canonical" or "natural" form, aka natural exponential family distributions. The form of a natural exponential family distribution is given as:

$$f_Y(y| heta, au) = h(y, au) \exp\left(rac{ heta\cdot y - A(heta)}{d(au)}
ight)$$

where θ is the parameter of interest and τ is a dispersion parameter. In a GLM the response variable Y_i is assumed to be drawn from a natural exponential family distribution:

$$Y_i \sim f\left(\cdot | heta_i, au
ight)$$

where the parameter of interest $heta_i$ is related to the expected value of the response variable μ_i by

$$\mu_i = A'(\theta_i)$$

Here, $A'(\theta_i)$ is defined by the form of the distribution selected. GLMs also allow specification of a link function, which defines the relationship between the expected value of the response variable μ_i and the so called *linear predictor* η_i :

$$g(\mu_i) = \eta_i = \overrightarrow{x_i}^T \cdot ec{eta}$$

Often, the link function is chosen such that $A'=g^{-1}$, which yields a simplified relationship between the parameter of interest θ and the linear predictor η . In this case, the link function $g(\mu)$ is said to be the "canonical" link function.

$$\theta_i=A'^{-1}(\mu_i)=g(g^{-1}(\eta_i))=\eta_i$$

A GLM finds the regression coefficients $\vec{\beta}$ which maximize the likelihood function.

$$\max_{ec{eta}} \mathcal{L}(ec{ heta} | ec{y}, X) = \prod_{i=1}^N h(y_i, au) \exp\left(rac{y_i heta_i - A(heta_i)}{d(au)}
ight)$$

where the parameter of interest θ_i is related to the regression coefficients $\vec{\beta}$ by

$$heta_i = A'^{-1}(g^{-1}(\overrightarrow{x_i} \cdot \overrightarrow{eta}))$$

Spark's generalized linear regression interface also provides summary statistics for diagnosing the fit of GLM models, including residuals, p-values, deviances, the Akaike information criterion, and others.

See here for a more comprehensive review of GLMs and their applications.

Available families

Family	Response Type	Supported Links	
Gaussian	Continuous	Identity*, Log, Inverse	
Binomial	Binary	Logit*, Probit, CLogLog	
Poisson	Count	Log*, Identity, Sqrt	
Gamma	Continuous	Inverse*, Idenity, Log	
Tweedie	Zero-inflated continuous	Power link function	
rweedle	Zero-inilated continuous	Power link function	

^{*} Canonical Link

Examples

The following example demonstrates training a GLM with a Gaussian response and identity link function and extracting model summary statistics.

Scala Java Python R

Refer to the Scala API docs for more details.

```
import org.apache.spark.ml.regression.GeneralizedLinearRegression
// Load training data
val dataset = spark.read.format("libsvm")
  .load("data/mllib/sample_linear_regression_data.txt")
val glr = new GeneralizedLinearRegression()
  .setFamily("gaussian")
  .setLink("identity")
  .setMaxIter(10)
  .setRegParam(0.3)
// Fit the model
val model = glr.fit(dataset)
// Print the coefficients and intercept for generalized linear regression model
println(s"Coefficients: ${model.coefficients}")
println(s"Intercept: ${model.intercept}")
// Summarize the model over the training set and print out some metrics
val summary = model.summary
println(s"Coefficient Standard Errors: ${summary.coefficientStandardErrors.mkString(",")}
")
println(s"T Values: ${summary.tValues.mkString(",")}")
println(s"P Values: ${summary.pValues.mkString(",")}")
println(s"Dispersion: ${summary.dispersion}")
println(s"Null Deviance: ${summary.nullDeviance}")
println(s"Residual Degree Of Freedom Null: ${summary.residualDegreeOfFreedomNull}}")
println(s"Deviance: ${summary.deviance}")
println(s"Residual Degree Of Freedom: ${\summary.residualDegreeOfFreedom}")
println(s"AIC: ${summary.aic}")
println("Deviance Residuals: ")
summary.residuals().show()
```

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/GeneralizedLinearRegressionExample.scala" in the Spark repo.

Decision tree regression

Decision trees are a popular family of classification and regression methods. More information about the spark.ml implementation can be found further in the section on decision trees.

Examples

The following examples load a dataset in LibSVM format, split it into training and test sets, train on the first dataset, and then evaluate on the held-out test set. We use a feature transformer to index categorical features, adding metadata to the DataFrame which the Decision Tree algorithm can recognize.

Scala Java Python R

More details on parameters can be found in the Scala API documentation.

```
import org.apache.spark.ml.Pipeline
import org.apache.spark.ml.evaluation.RegressionEvaluator
import org.apache.spark.ml.feature.VectorIndexer
import org.apache.spark.ml.regression.DecisionTreeRegressionModel
import org.apache.spark.ml.regression.DecisionTreeRegressor
// Load the data stored in LIBSVM format as a DataFrame.
val data = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")
// Automatically identify categorical features, and index them.
// Here, we treat features with > 4 distinct values as continuous.
val featureIndexer = new VectorIndexer()
  .setInputCol("features")
  .setOutputCol("indexedFeatures")
  .setMaxCategories(4)
  .fit(data)
// Split the data into training and test sets (30% held out for testing).
val Array(trainingData, testData) = data.randomSplit(Array(0.7, 0.3))
// Train a DecisionTree model.
val dt = new DecisionTreeRegressor()
  .setLabelCol("label")
  .setFeaturesCol("indexedFeatures")
// Chain indexer and tree in a Pipeline.
val pipeline = new Pipeline()
  .setStages(Array(featureIndexer, dt))
// Train model. This also runs the indexer.
val model = pipeline.fit(trainingData)
// Make predictions.
val predictions = model.transform(testData)
```

```
// Select example rows to display.
predictions.select("prediction", "label", "features").show(5)

// Select (prediction, true label) and compute test error.

val evaluator = new RegressionEvaluator()
    .setLabelCol("label")
    .setPredictionCol("prediction")
    .setMetricName("rmse")

val rmse = evaluator.evaluate(predictions)
println(s"Root Mean Squared Error (RMSE) on test data = $rmse")

val treeModel = model.stages(1).asInstanceOf[DecisionTreeRegressionModel]
println(s"Learned regression tree model:\n ${treeModel.toDebugString}}")
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/DecisionTreeRegressionExample.scala" in the Spark repo.

Random forest regression

Random forests are a popular family of classification and regression methods. More information about the spark.ml implementation can be found further in the section on random forests.

Examples

The following examples load a dataset in LibSVM format, split it into training and test sets, train on the first dataset, and then evaluate on the held-out test set. We use a feature transformer to index categorical features, adding metadata to the DataFrame which the tree-based algorithms can recognize.

Scala Java Python R

```
import org.apache.spark.ml.Pipeline
import org.apache.spark.ml.evaluation.RegressionEvaluator
import org.apache.spark.ml.feature.VectorIndexer
import org.apache.spark.ml.regression.{RandomForestRegressionModel, RandomForestRegres
sor}

// Load and parse the data file, converting it to a DataFrame.
val data = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")

// Automatically identify categorical features, and index them.
// Set maxCategories so features with > 4 distinct values are treated as continuous.
val featureIndexer = new VectorIndexer()
.setInputCol("features")
.setOutputCol("indexedFeatures")
.setMaxCategories(4)
.fit(data)
```

```
// Split the data into training and test sets (30% held out for testing).
val Array(trainingData, testData) = data.randomSplit(Array(0.7, 0.3))
// Train a RandomForest model.
val rf = new RandomForestRegressor()
  .setLabelCol("label")
  .setFeaturesCol("indexedFeatures")
// Chain indexer and forest in a Pipeline.
val pipeline = new Pipeline()
  .setStages(Array(featureIndexer, rf))
// Train model. This also runs the indexer.
val model = pipeline.fit(trainingData)
// Make predictions.
val predictions = model.transform(testData)
// Select example rows to display.
predictions.select("prediction", "label", "features").show(5)
// Select (prediction, true label) and compute test error.
val evaluator = new RegressionEvaluator()
  .setLabelCol("label")
  .setPredictionCol("prediction")
  .setMetricName("rmse")
val rmse = evaluator.evaluate(predictions)
println(s"Root Mean Squared Error (RMSE) on test data = $rmse")
val rfModel = model.stages(1).asInstanceOf[RandomForestRegressionModel]
println(s"Learned regression forest model:\n ${rfModel.toDebugString}")
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/RandomForestRegressorExample.scala" in the Spark repo.

Gradient-boosted tree regression

Gradient-boosted trees (GBTs) are a popular regression method using ensembles of decision trees. More information about the spark.ml implementation can be found further in the section on GBTs.

Examples

Note: For this example dataset, GBTRegressor actually only needs 1 iteration, but that will not be true in general.

Scala Java Python R

```
import org.apache.spark.ml.Pipeline
import org.apache.spark.ml.evaluation.RegressionEvaluator
import org.apache.spark.ml.feature.VectorIndexer
import org.apache.spark.ml.regression.{GBTRegressionModel, GBTRegressor}
// Load and parse the data file, converting it to a DataFrame.
val data = spark.read.format("libsvm").load("data/mllib/sample_libsvm_data.txt")
// Automatically identify categorical features, and index them.
// Set maxCategories so features with > 4 distinct values are treated as continuous.
val featureIndexer = new VectorIndexer()
  .setInputCol("features")
  .setOutputCol("indexedFeatures")
  .setMaxCategories(4)
  .fit(data)
// Split the data into training and test sets (30% held out for testing).
val Array(trainingData, testData) = data.randomSplit(Array(0.7, 0.3))
// Train a GBT model.
val gbt = new GBTRegressor()
  .setLabelCol("label")
  .setFeaturesCol("indexedFeatures")
  .setMaxIter(10)
// Chain indexer and GBT in a Pipeline.
val pipeline = new Pipeline()
  .setStages(Array(featureIndexer, gbt))
// Train model. This also runs the indexer.
val model = pipeline.fit(trainingData)
// Make predictions.
val predictions = model.transform(testData)
// Select example rows to display.
predictions.select("prediction", "label", "features").show(5)
// Select (prediction, true label) and compute test error.
val evaluator = new RegressionEvaluator()
  .setLabelCol("label")
  .setPredictionCol("prediction")
  .setMetricName("rmse")
val rmse = evaluator.evaluate(predictions)
println(s"Root Mean Squared Error (RMSE) on test data = $rmse")
```

val gbtModel = model.stages(1).asInstanceOf[GBTRegressionModel]
println(s"Learned regression GBT model:\n \${gbtModel.toDebugString}")

Find full example code at

"examples/src/main/scala/org/apache/spark/examples/ml/GradientBoostedTreeRegressorExample.scala" in the Spark repo.

Survival regression

In spark.ml, we implement the Accelerated failure time (AFT) model which is a parametric survival regression model for censored data. It describes a model for the log of survival time, so it's often called a log-linear model for survival analysis. Different from a Proportional hazards model designed for the same purpose, the AFT model is easier to parallelize because each instance contributes to the objective function independently.

Given the values of the covariates x^i , for random lifetime t_i of subjects i = 1, ..., n, with possible right-censoring, the likelihood function under the AFT model is given as:

$$L(eta,\sigma) = \prod_{i=1}^n [rac{1}{\sigma} f_0(rac{\log t_i - x^{'}eta}{\sigma})]^{\delta_i} S_0(rac{\log t_i - x^{'}eta}{\sigma})^{1-\delta_i}$$

Where δ_i is the indicator of the event has occurred i.e. uncensored or not. Using $\epsilon_i = \frac{\log t_i - x^i \beta}{\sigma}$, the log-likelihood function assumes the form:

$$\iota(eta,\sigma) = \sum_{i=1}^n [-\delta_i \log \sigma + \delta_i \log f_0(\epsilon_i) + (1-\delta_i) \log S_0(\epsilon_i)]$$

Where $S_0(\epsilon_i)$ is the baseline survivor function, and $f_0(\epsilon_i)$ is the corresponding density function.

The most commonly used AFT model is based on the Weibull distribution of the survival time. The Weibull distribution for lifetime corresponds to the extreme value distribution for the log of the lifetime, and the $S_0(\epsilon)$ function is:

$$S_0(\epsilon_i) = \exp(-e^{\epsilon_i})$$

the $f_0(\epsilon_i)$ function is:

$$f_0(\epsilon_i) = e^{\epsilon_i} \exp(-e^{\epsilon_i})$$

The log-likelihood function for AFT model with a Weibull distribution of lifetime is:

$$\iota(eta,\sigma) = -\sum_{i=1}^n [\delta_i \log \sigma - \delta_i \epsilon_i + e^{\epsilon_i}]$$

Due to minimizing the negative log-likelihood equivalent to maximum a posteriori probability, the loss function we use to optimize is $-\iota(\beta, \sigma)$. The gradient functions for β and $\log \sigma$ respectively are:

$$rac{\partial (-\iota)}{\partial eta} = \sum_{1=1}^n [\delta_i - e^{\epsilon_i}] rac{x_i}{\sigma}$$

$$rac{\partial (-\iota)}{\partial (\log \sigma)} = \sum_{i=1}^n [\delta_i + (\delta_i - e^{\epsilon_i})\epsilon_i]$$

The AFT model can be formulated as a convex optimization problem, i.e. the task of finding a minimizer of a convex function $-\iota(\beta,\sigma)$ that depends on the coefficients vector β and the log of scale parameter $\log \sigma$. The optimization algorithm underlying the implementation is L-BFGS. The implementation matches the result from R's survival function survreg

When fitting AFTSurvivalRegressionModel without intercept on dataset with constant nonzero column, Spark MLlib outputs zero coefficients for constant nonzero columns. This behavior is different from R survival::survreg.

Examples



Refer to the Scala API docs for more details.

```
import org.apache.spark.ml.linalg.Vectors
import org.apache.spark.ml.regression.AFTSurvivalRegression
val training = spark.createDataFrame(Seq(
  (1.218, 1.0, Vectors.dense(1.560, -0.605)),
  (2.949, 0.0, Vectors.dense(0.346, 2.158)),
  (3.627, 0.0, Vectors.dense(1.380, 0.231)),
  (0.273, 1.0, Vectors.dense(0.520, 1.151)),
  (4.199, 0.0, Vectors.dense(0.795, -0.226))
)).toDF("label", "censor", "features")
val quantileProbabilities = Array(0.3, 0.6)
val aft = new AFTSurvivalRegression()
  .setQuantileProbabilities(quantileProbabilities)
  .setQuantilesCol("quantiles")
val model = aft.fit(training)
// Print the coefficients, intercept and scale parameter for AFT survival regression
println(s"Coefficients: ${model.coefficients}")
println(s"Intercept: ${model.intercept}")
println(s"Scale: ${model.scale}")
model.transform(training).show(false)
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/AFTSurvivalRegressionExample.scala" in the Spark repo.

Isotonic regression

Isotonic regression belongs to the family of regression algorithms. Formally isotonic regression is a problem where given a finite set of real numbers $Y=y_1,y_2,\ldots,y_n$ representing observed responses and $X=x_1,x_2,\ldots,x_n$ the unknown response values to be fitted finding a function that minimises

$$f(x) = \sum_{i=1}^{n} w_i (y_i - x_i)^2 \tag{1}$$

with respect to complete order subject to $x_1 \le x_2 \le ... \le x_n$ where w_i are positive weights. The resulting function is called isotonic regression and it is unique. It can be viewed as least squares problem under order restriction. Essentially isotonic regression is a monotonic function best fitting the original data points.

We implement a pool adjacent violators algorithm which uses an approach to parallelizing isotonic regression. The training input is a DataFrame which contains three columns label, features and weight.

Additionally IsotonicRegression algorithm has one optional parameter called isotonic defaulting to true. This argument specifies if the isotonic regression is isotonic (monotonically increasing) or antitonic (monotonically decreasing).

Training returns an IsotonicRegressionModel that can be used to predict labels for both known and unknown features. The result of isotonic regression is treated as piecewise linear function. The rules for prediction therefore are:

- If the prediction input exactly matches a training feature then associated prediction is returned. In case there are multiple predictions with the same feature then one of them is returned. Which one is undefined (same as java.util.Arrays.binarySearch).
- If the prediction input is lower or higher than all training features then prediction with lowest or highest feature is returned respectively. In case there are multiple predictions with the same feature then the lowest or highest is returned respectively.
- If the prediction input falls between two training features then prediction is treated as piecewise linear
 function and interpolated value is calculated from the predictions of the two closest features. In case
 there are multiple values with the same feature then the same rules as in previous point are used.

Examples

Scala Java Python R

Refer to the IsotonicRegression Scala docs for details on the API.

```
import org.apache.spark.ml.regression.IsotonicRegression

// Loads data.
val dataset = spark.read.format("libsvm")
    .load("data/mllib/sample_isotonic_regression_libsvm_data.txt")

// Trains an isotonic regression model.
val ir = new IsotonicRegression()
val model = ir.fit(dataset)

println(s"Boundaries in increasing order: ${\text{model.boundaries}}\n")
println(s"Predictions associated with the boundaries: ${\text{model.predictions}}\n")

// Makes predictions.
model.transform(dataset).show()
```

Find full example code at "examples/src/main/scala/org/apache/spark/examples/ml/IsotonicRegressionExample.scala" in the Spark repo.

Linear methods

We implement popular linear methods such as logistic regression and linear least squares with L_1 or L_2 regularization. Refer to the linear methods guide for the RDD-based API for details about implementation and tuning; this information is still relevant.

We also include a DataFrame API for Elastic net, a hybrid of L_1 and L_2 regularization proposed in Zou et al, Regularization and variable selection via the elastic net. Mathematically, it is defined as a convex combination of the L_1 and the L_2 regularization terms:

$$lpha\left(\lambda\|\mathbf{w}\|_{1}
ight)+\left(1-lpha
ight)\left(rac{\lambda}{2}\|\mathbf{w}\|_{2}^{2}
ight), lpha\in[0,1], \lambda\geq0$$

By setting α properly, elastic net contains both L_1 and L_2 regularization as special cases. For example, if a linear regression model is trained with the elastic net parameter α set to 1, it is equivalent to a Lasso model. On the other hand, if α is set to 0, the trained model reduces to a ridge regression model. We implement Pipelines API for both linear regression and logistic regression with elastic net regularization.

Decision trees

Decision trees and their ensembles are popular methods for the machine learning tasks of classification and regression. Decision trees are widely used since they are easy to interpret, handle categorical features, extend to the multiclass classification setting, do not require feature scaling, and are able to capture non-linearities and feature interactions. Tree ensemble algorithms such as random forests and boosting are among the top performers for classification and regression tasks.

The spark.ml implementation supports decision trees for binary and multiclass classification and for regression, using both continuous and categorical features. The implementation partitions data by rows, allowing distributed training with millions or even billions of instances.

Users can find more information about the decision tree algorithm in the MLlib Decision Tree guide. The main differences between this API and the original MLlib Decision Tree API are:

- support for ML Pipelines
- separation of Decision Trees for classification vs. regression
- · use of DataFrame metadata to distinguish continuous and categorical features

The Pipelines API for Decision Trees offers a bit more functionality than the original API. In particular, for classification, users can get the predicted probability of each class (a.k.a. class conditional probabilities); for regression, users can get the biased sample variance of prediction.

Ensembles of trees (Random Forests and Gradient-Boosted Trees) are described below in the Tree ensembles section.

Inputs and Outputs

We list the input and output (prediction) column types here. All output columns are optional; to exclude an output column, set its corresponding Param to an empty string.

Input Columns

Param name	Type(s)	Default	Description
labelCol	Double	"label"	Label to predict
featuresCol	Vector	"features"	Feature vector

Output Columns

Param name	Type(s)	Default	Description	Notes
predictionCol	Double	"prediction"	Predicted label	
rawPredictionCol	Vector	"rawPrediction"	Vector of length # classes, with the counts of training instance labels at the tree node which makes the prediction	Classification only
probabilityCol	Vector	"probability"	Vector of length # classes equal to rawPrediction normalized to a multinomial distribution	Classification only
varianceCol	Double		The biased sample variance of prediction	Regression only

Tree Ensembles

The DataFrame API supports two major tree ensemble algorithms: Random Forests and Gradient-Boosted Trees (GBTs). Both use spark.ml decision trees as their base models.

Users can find more information about ensemble algorithms in the MLlib Ensemble guide. In this section, we demonstrate the DataFrame API for ensembles.

The main differences between this API and the original MLlib ensembles API are:

- support for DataFrames and ML Pipelines
- · separation of classification vs. regression
- · use of DataFrame metadata to distinguish continuous and categorical features
- more functionality for random forests: estimates of feature importance, as well as the predicted probability of each class (a.k.a. class conditional probabilities) for classification.

Random Forests

Random forests are ensembles of decision trees. Random forests combine many decision trees in order to reduce the risk of overfitting. The spark.ml implementation supports random forests for binary and multiclass classification and for regression, using both continuous and categorical features.

For more information on the algorithm itself, please see the spark.mllib documentation on random forests.

Inputs and Outputs

We list the input and output (prediction) column types here. All output columns are optional; to exclude an output column, set its corresponding Param to an empty string.

Input Columns

Param name	Type(s)	Default	Description
labelCol	Double	"label"	Label to predict
featuresCol	Vector	"features"	Feature vector

Output Columns (Predictions)

Param name	Type(s)	Default	Description	Notes
predictionCol	Double	"prediction"	Predicted label	
rawPredictionCol	Vector	"rawPrediction"	Vector of length # classes, with the counts of training instance labels at the tree node which makes the prediction	Classification only
probabilityCol	Vector	"probability"	Vector of length # classes equal to rawPrediction normalized to a multinomial distribution	Classification only

Gradient-Boosted Trees (GBTs)

Gradient-Boosted Trees (GBTs) are ensembles of decision trees. GBTs iteratively train decision trees in order to minimize a loss function. The spark.ml implementation supports GBTs for binary classification and for regression, using both continuous and categorical features.

For more information on the algorithm itself, please see the spark.mllib documentation on GBTs.

Inputs and Outputs

We list the input and output (prediction) column types here. All output columns are optional; to exclude an output column, set its corresponding Param to an empty string.

Input Columns

Param name	Type(s)	Default	Description
labelCol	Double	"label"	Label to predict
featuresCol	Vector	"features"	Feature vector

Note that GBTClassifier currently only supports binary labels.

Output Columns (Predictions)

 Param name
 Type(s)
 Default
 Description
 Notes

 predictionCol
 Double
 "prediction"
 Predicted label

In the future, GBTClassifier will also output columns for rawPrediction and probability, just as RandomForestClassifier does.

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