CARET_Lab

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2023-11-27

Package loading

```
library(caret)

## Warning: package 'caret' was built under R version 4.3.2

## Loading required package: ggplot2

## Loading required package: lattice

Load Data

# attach the iris dataset to the environment
data(iris)
# rename the dataset
dataset <- iris</pre>
```

Task1: Create a Validation/Training Dataset You need to split the loaded dataset into two, 80% of which we will use to train our models and 20% that we will hold back as a validation dataset. Hint: use create-DataPartition function

```
# Create the training and test datasets
set.seed(100)

# Step 1: Get row numbers for the training data
trainRowNumbers <- createDataPartition(dataset$Species, p=0.8, list=FALSE)

# Step 2: Create the training dataset
trainData <- dataset[trainRowNumbers,]

# Step 3: Create the test dataset
testData <- dataset[-trainRowNumbers,]</pre>
```

Task2: Summarize Dataset Use skimr library to summarize the dataset

```
library(skimr)
```

```
## Warning: package 'skimr' was built under R version 4.3.2
```

```
## Warning: 'skim_to_wide' is deprecated.
## Use 'skim()' instead.
## See help("Deprecated")
```

Table 1: Data summary

Name	Piped data
Number of rows	120
Number of columns	5
Column type frequency:	
factor	1
numeric	4
Group variables	None

Variable type: factor

skimmed

skim_variable	n_missing	complete_rate	ordered	n_unique	top_counts
Species	0	1	FALSE	3	set: 40, ver: 40, vir: 40

Variable type: numeric

skim_variable	n_missing	complete_rate	mean	sd	p0	p25	p50	p75	p100	hist
Sepal.Length	0	1	5.86	0.82	4.3	5.1	5.8	6.4	7.7	
Sepal.Width	0	1	3.07	0.43	2.2	2.8	3.0	3.4	4.4	
Petal.Length	0	1	3.77	1.78	1.0	1.6	4.4	5.1	6.9	
Petal.Width	0	1	1.20	0.77	0.1	0.3	1.3	1.8	2.5	

Task3: split input and output It is the time to seperate the input attributes and the output attributes. call the inputs attributes x and the output attribute (or class) y.

```
# Store X and Y for later use.
x = trainData[, 1:4]
y = trainData[, 5]
```

Task4: Train Control for Validation Test

We will use 10-fold crossvalidation to estimate accuracy.

```
# Run algorithms using 10-fold cross validation
control <- trainControl(method="cv", number=10)
metric <- "Accuracy"</pre>
```

Task5: Model Training Train 5 different algorithms using 'train' function:

• Linear Discriminant Analysis (LDA)

Set the seed for reproducibility

• k-Nearest Neighbors (kNN).

set.seed(100)

```
# Train the model using LDA
model_LDA = train(Species ~ ., data=trainData, method = 'lda', trControl = control, metric = metric)
model_LDA
## Linear Discriminant Analysis
## 120 samples
##
    4 predictor
    3 classes: 'setosa', 'versicolor', 'virginica'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 108, 108, 108, 108, 108, 108, ...
## Resampling results:
##
##
     Accuracy Kappa
##
     0.975
               0.9625
  • Classification and Regression Trees (CART).
# Set the seed for reproducibility
set.seed(100)
# Train the model using CART
model_CART = train(Species ~ ., data=trainData, method = 'rpart', trControl = control, metric = metric
model_CART
## CART
##
## 120 samples
##
     4 predictor
     3 classes: 'setosa', 'versicolor', 'virginica'
##
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 108, 108, 108, 108, 108, 108, ...
## Resampling results across tuning parameters:
##
##
     ср
           Accuracy
                      Kappa
    0.00 0.9250000 0.8875
##
##
    0.45 0.7666667 0.6500
    0.50 0.3333333 0.0000
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was cp = 0.
```

```
# Set the seed for reproducibility
set.seed(100)
# Train the model using kNN
model_KNN = train(Species ~ ., data=trainData, method = 'knn', trControl = control, metric = metric)
model_KNN
## k-Nearest Neighbors
##
## 120 samples
     4 predictor
##
    3 classes: 'setosa', 'versicolor', 'virginica'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 108, 108, 108, 108, 108, 108, ...
## Resampling results across tuning parameters:
##
##
    k Accuracy
                   Kappa
##
    5 0.9750000 0.9625
    7 0.9833333 0.9750
##
    9 0.9750000 0.9625
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was k = 7.
  • Support Vector Machines (SVM) with a linear kernel.
# Set the seed for reproducibility
set.seed(100)
# Train the model using SVM
model_SVM = train(Species ~ ., data=trainData, method = 'svmRadial', trControl = control, metric = met.
model_SVM
## Support Vector Machines with Radial Basis Function Kernel
##
## 120 samples
##
     4 predictor
##
     3 classes: 'setosa', 'versicolor', 'virginica'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 108, 108, 108, 108, 108, 108, ...
## Resampling results across tuning parameters:
##
##
    С
           Accuracy
                      Kappa
    0.25 0.9416667 0.9125
##
##
    0.50 0.9416667 0.9125
##
     1.00 0.9416667 0.9125
```

Tuning parameter 'sigma' was held constant at a value of 0.9021222

```
## Accuracy was used to select the optimal model using the largest value. ## The final values used for the model were sigma = 0.9021222 and C = 0.25.
```

• Random Forest (RF)

Accuracy

##

LDA

CART

KNN

```
# Set the seed for reproducibility
set.seed(100)
# Random Forest (RF)
model_RF = train(Species ~ ., data=trainData, method = 'rf', trControl = control, metric = metric)
model_RF
## Random Forest
##
## 120 samples
    4 predictor
##
     3 classes: 'setosa', 'versicolor', 'virginica'
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 108, 108, 108, 108, 108, 108, ...
## Resampling results across tuning parameters:
##
##
     mtry Accuracy
                      Kappa
##
           0.9666667 0.9500
##
           0.9666667 0.9500
     3
           0.9583333 0.9375
##
     4
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was mtry = 2.
```

Task6: Select the Best Model We now have 5 models and accuracy estimations for each. We need to compare the models to each other and select the most accurate. Use resamples function to complete this task

```
#Compare all 5 using resample
models_compare <- resamples(list(LDA = model_LDA, CART = model_CART, KNN = model_KNN, SVMLinear = model
summary(models_compare)

##
## Call:
## summary.resamples(object = models_compare)
##
## Models: LDA, CART, KNN, SVMLinear, RF
## Number of resamples: 10
##</pre>
```

Mean 3rd Qu. Max. NA's

1

1

1

1

0

0

Median

1st Qu.

0.9166667 0.9375000 1.0000000 0.9750000

0.8333333 0.8541667 0.9166667 0.9250000

0.9166667 1.0000000 1.0000000 0.9833333

Min.

```
## SVMLinear 0.8333333 0.9166667 0.9583333 0.9416667
## R.F
             0.9166667 0.9166667 1.0000000 0.9666667
##
## Kappa
##
              Min. 1st Qu. Median
                                     Mean 3rd Qu. Max. NA's
             0.875 0.90625 1.0000 0.9625
## LDA
                                                1
## CART
             0.750 0.78125 0.8750 0.8875
             0.875 1.00000 1.0000 0.9750
## KNN
                                                1
                                                      1
                                                           0
## SVMLinear 0.750 0.87500 0.9375 0.9125
                                                1
                                                      1
                                                           0
## RF
             0.875 0.87500 1.0000 0.9500
                                                           0
                                                1
```

What was the most accurate model? The most accurate models were the KNN model with accuracy 98.3% and LDA model with accuracy 97.5%

Task7: Make Prediction (Confusion Matrix) Now we want to get an idea of the accuracy of the best model on our validation set. Use 'predict' and confusionMatrix functions to complete this task.

LDA Confusion Matrix & Prediction

```
predicted <- predict(model_LDA, testData)
confusionMatrix(reference = testData$Species, data = predicted)</pre>
```

```
## Confusion Matrix and Statistics
##
##
               Reference
## Prediction
                setosa versicolor virginica
##
     setosa
                     10
                      0
                                 9
                                            0
##
     versicolor
     virginica
                      0
                                 1
                                           10
##
## Overall Statistics
##
##
                  Accuracy: 0.9667
                     95% CI : (0.8278, 0.9992)
##
       No Information Rate: 0.3333
##
##
       P-Value [Acc > NIR] : 2.963e-13
##
##
                      Kappa: 0.95
##
   Mcnemar's Test P-Value : NA
##
##
## Statistics by Class:
##
##
                         Class: setosa Class: versicolor Class: virginica
                                                   0.9000
## Sensitivity
                                1.0000
                                                                     1.0000
## Specificity
                                1.0000
                                                   1.0000
                                                                     0.9500
## Pos Pred Value
                                1.0000
                                                   1.0000
                                                                     0.9091
## Neg Pred Value
                                1.0000
                                                   0.9524
                                                                     1.0000
## Prevalence
                                0.3333
                                                   0.3333
                                                                     0.3333
## Detection Rate
                                0.3333
                                                   0.3000
                                                                     0.3333
## Detection Prevalence
                                0.3333
                                                   0.3000
                                                                     0.3667
## Balanced Accuracy
                                1.0000
                                                   0.9500
                                                                     0.9750
```

CART Confusion Matrix & Prediction

```
predicted <- predict(model_CART, testData)</pre>
confusionMatrix(reference = testData$Species, data = predicted)
## Confusion Matrix and Statistics
##
##
               Reference
## Prediction
                setosa versicolor virginica
##
     setosa
                     10
                                 0
                     0
                                 9
                                           3
##
     versicolor
                     0
                                           7
##
                                 1
     virginica
##
## Overall Statistics
##
##
                  Accuracy : 0.8667
                    95% CI: (0.6928, 0.9624)
##
       No Information Rate: 0.3333
##
       P-Value [Acc > NIR] : 2.296e-09
##
##
##
                     Kappa : 0.8
##
##
   Mcnemar's Test P-Value : NA
## Statistics by Class:
##
##
                         Class: setosa Class: versicolor Class: virginica
## Sensitivity
                                1.0000
                                                   0.9000
                                                                     0.7000
                                                   0.8500
                                                                     0.9500
                                1.0000
## Specificity
## Pos Pred Value
                                1.0000
                                                   0.7500
                                                                     0.8750
## Neg Pred Value
                                1.0000
                                                   0.9444
                                                                     0.8636
## Prevalence
                                0.3333
                                                   0.3333
                                                                     0.3333
## Detection Rate
                                                   0.3000
                                                                    0.2333
                                0.3333
## Detection Prevalence
                                0.3333
                                                   0.4000
                                                                    0.2667
                                                                     0.8250
## Balanced Accuracy
                                1.0000
                                                   0.8750
KNN Confusion Matrix & Prediction
predicted <- predict(model_KNN, testData)</pre>
confusionMatrix(reference = testData$Species, data = predicted)
## Confusion Matrix and Statistics
##
##
               Reference
## Prediction
                setosa versicolor virginica
##
     setosa
                     10
                                 0
##
     versicolor
                     0
                                 9
                                           2
                                           8
                     0
                                 1
##
     virginica
##
## Overall Statistics
##
##
                  Accuracy: 0.9
##
                    95% CI : (0.7347, 0.9789)
##
       No Information Rate: 0.3333
```

```
P-Value [Acc > NIR] : 1.665e-10
##
##
                     Kappa : 0.85
##
##
##
   Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##
                         Class: setosa Class: versicolor Class: virginica
## Sensitivity
                                1.0000
                                                   0.9000
                                                                     0.8000
## Specificity
                                1.0000
                                                   0.9000
                                                                     0.9500
## Pos Pred Value
                                1.0000
                                                                     0.8889
                                                   0.8182
## Neg Pred Value
                                1.0000
                                                   0.9474
                                                                     0.9048
## Prevalence
                                0.3333
                                                                     0.3333
                                                   0.3333
## Detection Rate
                                0.3333
                                                   0.3000
                                                                     0.2667
## Detection Prevalence
                                0.3333
                                                   0.3667
                                                                     0.3000
## Balanced Accuracy
                                1.0000
                                                   0.9000
                                                                     0.8750
SVM Confusion Matrix & Prediction
predicted <- predict(model_SVM, testData)</pre>
confusionMatrix(reference = testData$Species, data = predicted)
## Confusion Matrix and Statistics
##
               Reference
##
## Prediction
               setosa versicolor virginica
                    10
                                 0
     setosa
##
     versicolor
                     0
                                 9
                                            1
##
     virginica
                     0
                                 1
                                            9
##
## Overall Statistics
##
##
                  Accuracy: 0.9333
##
                    95% CI: (0.7793, 0.9918)
##
       No Information Rate: 0.3333
       P-Value [Acc > NIR] : 8.747e-12
##
##
##
                      Kappa : 0.9
##
##
    Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##
                         Class: setosa Class: versicolor Class: virginica
                                1.0000
                                                   0.9000
                                                                     0.9000
## Sensitivity
## Specificity
                                1.0000
                                                   0.9500
                                                                     0.9500
## Pos Pred Value
                                1.0000
                                                   0.9000
                                                                     0.9000
## Neg Pred Value
                                1.0000
                                                   0.9500
                                                                     0.9500
## Prevalence
                                0.3333
                                                   0.3333
                                                                     0.3333
## Detection Rate
                                0.3333
                                                   0.3000
                                                                     0.3000
## Detection Prevalence
                                0.3333
                                                   0.3333
                                                                     0.3333
```

0.9250

1.0000

Balanced Accuracy

0.9250

```
predicted <- predict(model_RF, testData)
confusionMatrix(reference = testData$Species, data = predicted)</pre>
```

```
## Confusion Matrix and Statistics
##
##
               Reference
## Prediction
               setosa versicolor virginica
##
     setosa
                    10
                                0
##
     versicolor
                     0
                                9
                                           1
     virginica
                     0
                                1
                                           9
##
##
## Overall Statistics
##
##
                  Accuracy : 0.9333
                    95% CI : (0.7793, 0.9918)
##
       No Information Rate : 0.3333
##
       P-Value [Acc > NIR] : 8.747e-12
##
##
##
                     Kappa : 0.9
##
##
   Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##
                        Class: setosa Class: versicolor Class: virginica
## Sensitivity
                               1.0000
                                                  0.9000
                                                                   0.9000
## Specificity
                               1.0000
                                                  0.9500
                                                                   0.9500
## Pos Pred Value
                               1.0000
                                                  0.9000
                                                                   0.9000
## Neg Pred Value
                               1.0000
                                                  0.9500
                                                                   0.9500
## Prevalence
                               0.3333
                                                  0.3333
                                                                   0.3333
## Detection Rate
                               0.3333
                                                  0.3000
                                                                   0.3000
## Detection Prevalence
                               0.3333
                                                  0.3333
                                                                   0.3333
## Balanced Accuracy
                               1.0000
                                                  0.9250
                                                                   0.9250
```