The caret package

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```
options(width=100)
if(!require("knitr")) install.packages("knitr")
library("knitr")
#getOption("width")
knitr::opts_chunk$set(comment=NA,echo = TRUE, cache=TRUE)
```

Introduction to `caret`

```
if(!require("caret")) install.packages("caret")
if(!require("mlbench")) install.packages("mlbench")
library("caret")
```

The `caret` package, short for classification and regression training, was built with several goals in mind:

- Create a unified interface for modelling and prediction (interfaces to more than 200 models),
- Develop a set of semi-automated, reasonable approaches for optimizing the values of the tuning parameters for many of these models and
- Increase computational efficiency using parallel processing.

That is `caret` has been developed to facilitate building, evaluating and comparing predictive models and as such it is an interesting alternative to using multiple different packages for distinct tasks, which, not only requires more time to learn how to use each of them, but especially makes it much harder to compare them.

Learning to use `caret`

There are multiple resources to learn `caret`that go from simple tutorials like this one or similars to courses, papers and a book by Max Kuhn, the creator or the package.

Guiding example

- The `caret` package can be used to perform a study from beginning to end.
- For this, it implements a set of general functions that can roughly be associated with the distinct steps of an analytical pipeline.
- We follow an example based on the `sonar data` from the `mlbench` package to illustrate the multiple functionalities of the package .

The goal is to predict two classes:

- M for metal cylinder
- R for rock

Data loading

```
library("mlbench")
data(Sonar)
names(Sonar)
```

```
 [1] "V1"     "V2"     "V3"     "V4"     "V5"     "V6"     "V7"     "V8"     "V9"     "V10"    "V11"    "V
[13] "V13"    "V14"    "V15"    "V16"    "V17"    "V18"    "V19"    "V20"    "V21"    "V22"    "V23"    "V
[25] "V25"    "V26"    "V27"    "V28"    "V29"    "V30"    "V31"    "V32"    "V33"    "V34"    "V35"    "V
[37] "V37"    "V38"    "V39"    "V40"    "V41"    "V42"    "V43"    "V44"    "V45"    "V46"    "V47"    "V
[49] "V49"    "V50"    "V51"    "V52"    "V53"    "V54"    "V55"    "V56"    "V57"    "V58"    "V59"    "V
[61] "Class"
```

The `sonar`package has 208 data points collected on 60 predictors (energy within a particular frequency band).

Train/test splitting

We will most of the time want to split the data into two groups: a training set and a test set.

This may be done with the `createDataPartition` function:

```
set.seed(1234) # Control of data generation
inTrain <- createDataPartition(y=Sonar$Class, p=.75, list=FALSE)
str(inTrain)
```

```
 int [1:157, 1] 2 3 4 6 7 8 9 11 14 15 ...
 - attr(*, "dimnames")=List of 2
  ..$ : NULL
  ..$ : chr "Resample1"
```

```
training <- Sonar[inTrain,]
testing <- Sonar[-inTrain,]
nrow(training)
```

```
[1] 157
```

Others similar functions are: `createFolds` and `createResample`,

Preprocessing and training

Usually, before prediction, data may have to be cleaned and pre-processed.

Caret allows to integrate it with the training step using the `train` function.

This function has multiple parameter such as:

- method: Can choose from more than 200 models
- preprocess: all type of filtering and transformations

```
CART1Model <- train (Class ~ .,
                     data=training,
                     method="rpart1SE",
                     preProc=c("center","scale"))
CART1Model
```

```
CART

157 samples
 60 predictor
  2 classes: 'M', 'R'

Pre-processing: centered (60), scaled (60)
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 157, 157, 157, 157, 157, 157, ...
Resampling results:

  Accuracy   Kappa
  0.6752493  0.350363
```

Refining specifications

Many specifications can be passed using the `trainControl` instruction.

```r
ctrl <- trainControl(method = "repeatedcv", repeats=3)
CART1Model3x10cv <- train (Class ~ .,
                          data=training,
                          method="rpart1SE",
                          trControl=ctrl,
                          preProc=c("center","scale"))

CART1Model3x10cv
```

```
CART

157 samples
 60 predictor
  2 classes: 'M', 'R'

Pre-processing: centered (60), scaled (60)
Resampling: Cross-Validated (10 fold, repeated 3 times)
Summary of sample sizes: 141, 142, 142, 141, 141, 142, ...
Resampling results:

  Accuracy   Kappa
  0.7087173  0.4168066
```

We can change the method used by changing the `trainControl` parameter.

In the example below we fit a classification tree with different options:

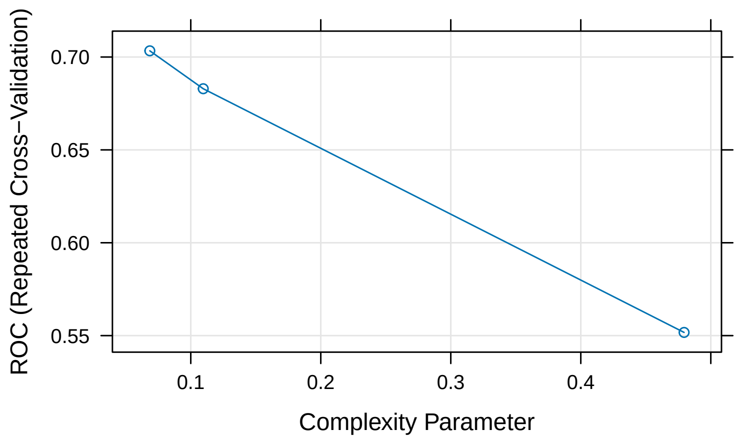
```r
ctrl <- trainControl(method = "repeatedcv", repeats=3,
                     classProbs=TRUE,
                     summaryFunction=twoClassSummary)

CART1Model3x10cv <- train (Class ~ .,
                          data=training,
                          method="rpart1SE",
                          trControl=ctrl,
                          metric="ROC",
                          preProc=c("center","scale"))

CART1Model3x10cv
```

```
CART

157 samples
 60 predictor
  2 classes: 'M', 'R'

Pre-processing: centered (60), scaled (60)
Resampling: Cross-Validated (10 fold, repeated 3 times)
Summary of sample sizes: 141, 141, 142, 141, 141, 142, ...
Resampling results:

  ROC        Sens   Spec
  0.7757068  0.775  0.6869048
```

```
CART2Fit3x10cv <- train (Class ~ .,
                       data=training,
                       method="rpart",
                       trControl=ctrl,
                       metric="ROC",
                       preProc=c("center","scale"))
CART2Fit3x10cv
```

```
CART

157 samples
 60 predictor
  2 classes: 'M', 'R'

Pre-processing: centered (60), scaled (60)
Resampling: Cross-Validated (10 fold, repeated 3 times)
Summary of sample sizes: 142, 142, 142, 142, 142, 140, ...
Resampling results across tuning parameters:

  cp          ROC        Sens       Spec
  0.06849315  0.7033441  0.6851852  0.6779762
  0.10958904  0.6829282  0.7523148  0.5922619
  0.47945205  0.5517196  0.8629630  0.2404762

ROC was used to select the optimal model using the largest value.
The final value used for the model was cp = 0.06849315.
```

```r
plot(CART2Fit3x10cv)
```

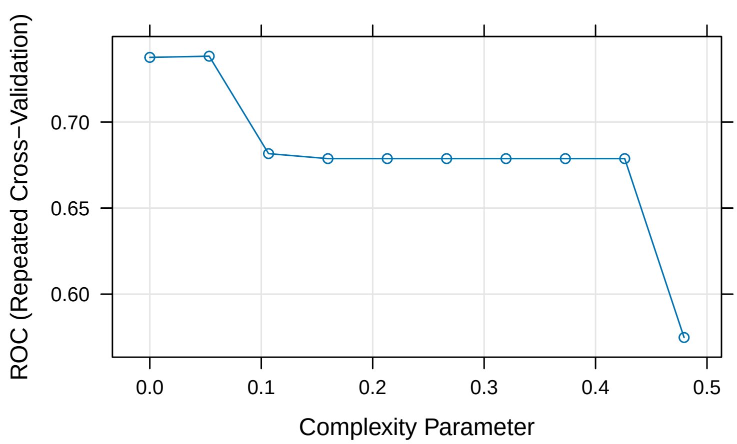



```r
CART2Fit3x10cv <- train (Class ~ .,
                         data=training,
                         method="rpart",
                         trControl=ctrl,
                         metric="ROC",
                         tuneLength=10,
                         preProc=c("center","scale"))
CART2Fit3x10cv
```

```
CART

157 samples
 60 predictor
  2 classes: 'M', 'R'

Pre-processing: centered (60), scaled (60)
Resampling: Cross-Validated (10 fold, repeated 3 times)
Summary of sample sizes: 141, 142, 140, 141, 141, 142, ...
Resampling results across tuning parameters:

  cp          ROC        Sens       Spec
  0.00000000  0.7375744  0.7305556  0.6220238
```

```
  0.05327245  0.7382523  0.7453704  0.6130952
  0.10654490  0.6816468  0.7773148  0.5696429
  0.15981735  0.6787368  0.8092593  0.5482143
  0.21308980  0.6787368  0.8092593  0.5482143
  0.26636225  0.6787368  0.8092593  0.5482143
  0.31963470  0.6787368  0.8092593  0.5482143
  0.37290715  0.6787368  0.8092593  0.5482143
  0.42617960  0.6787368  0.8092593  0.5482143
  0.47945205  0.5748016  0.8680556  0.2815476

ROC was used to select the optimal model using the largest value.
The final value used for the model was cp = 0.05327245.
```

```r
plot(CART2Fit3x10cv)
```



Predict & confusionMatrix functions

To predict new samples can be used predict function.

- type = prob : to compute class probabilities
- type = raw : to predict the class

The `confusionMatrix` function will compute the confusion matrix and associated statistics for the model fit.

```
CART2Probs <- predict(CART2Fit3x10cv, newdata = testing, type = "prob")
CART2Classes <- predict(CART2Fit3x10cv, newdata = testing, type = "raw")
confusionMatrix(data=CART2Classes,testing$Class)
```

```
Confusion Matrix and Statistics

          Reference
Prediction  M  R
         M 21  5
         R  6 19

               Accuracy : 0.7843
                 95% CI : (0.6468, 0.8871)
    No Information Rate : 0.5294
    P-Value [Acc > NIR] : 0.0001502

                  Kappa : 0.5681

 Mcnemar's Test P-Value : 1.0000000

            Sensitivity : 0.7778
            Specificity : 0.7917
         Pos Pred Value : 0.8077
         Neg Pred Value : 0.7600
             Prevalence : 0.5294
         Detection Rate : 0.4118
   Detection Prevalence : 0.5098
      Balanced Accuracy : 0.7847

       'Positive' Class : M
```

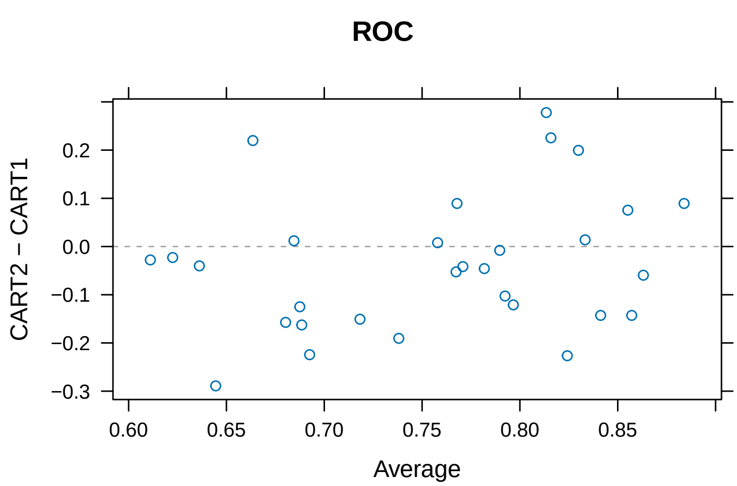
Model comparison

The `resamples`function enable smodel comparison

```
resamps=resamples(list(CART2=CART2Fit3x10cv,
                       CART1=CART1Model3x10cv))
summary(resamps)
```

```
Call:
summary.resamples(object = resamps)

Models: CART2, CART1
Number of resamples: 30

ROC
           Min.   1st Qu.    Median      Mean   3rd Qu.     Max. NA's
CART2 0.5000000 0.6294643 0.7455357 0.7382523 0.8058036 0.952381    0
CART1 0.5535714 0.7249504 0.7926587 0.7757068 0.8315972 0.937500    0

Sens
           Min.   1st Qu.    Median      Mean 3rd Qu. Max. NA's
CART2 0.4444444 0.6250000 0.7500000 0.7453704   0.875    1    0
CART1 0.4444444 0.6666667 0.7777778 0.7750000   0.875    1    0

Spec
       Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
CART2 0.250 0.5714286 0.6250000 0.6130952 0.7142857 0.8750000    0
CART1 0.375 0.5714286 0.7142857 0.6869048 0.8571429 0.8571429    0
```

```
xyplot(resamps,what="BlandAltman")
```



```r
diffs<-diff(resamps)
summary(diffs)
```

```
Call:
summary.diff.resamples(object = diffs)

p-value adjustment: bonferroni
Upper diagonal: estimates of the difference
Lower diagonal: p-value for H0: difference = 0

ROC
      CART2  CART1
CART2        -0.03745
CART1 0.1598

Sens
      CART2  CART1
CART2        -0.02963
CART1 0.4514

Spec
      CART2   CART1
CART2         -0.07381
CART1 0.02404
```

Example: Comparison of boosting methods

We use the `caret` package and the `BreastCancer` dataset.

Adaboost

In this example, we are using the rpart algorithm as the base learner for AdaBoost. We can then use the predict function to make predictions on new data:

```
library(caret)
library(mlbench)

data(BreastCancer)

# Split the data into training and testing sets
set.seed(123)
trainIndex <- createDataPartition(BreastCancer$Class, p = 0.7, list = FALSE)
training <- BreastCancer[trainIndex, ]
testing <- BreastCancer[-trainIndex, ]

# Next, set up
# - the training control and
# - tuning parameters for the AdaBoost algorithm:

ctrl <- trainControl(method = "repeatedcv",
                     number = 10, repeats = 3,
                     classProbs = TRUE,
                     summaryFunction = twoClassSummary)

params <- data.frame(method = "AdaBoost",
                     nIter = 100,
                     interaction.depth = 1,
                     shrinkage = 0.1)

#  we are using 10-fold cross-validation with 3 repeats and the twoClassSummary function for ev
# We are also setting the number of iterations for the AdaBoost algorithm to 100, the maximum 

# Use the train function to train the AdaBoost algorithm on the training data and evaluate its

adaboost <- train(Class ~ ., data = training,
                  method = "rpart",
                  trControl = ctrl,
                  tuneGrid = params)

predictions <- predict(adaboost, newdata = testing)

# Evaluate the performance of the model
confusionMatrix(predictions, testData$diagnosis)
```

Gradient boosting

We use the `gbm` method in train() function from the caret package to build a Gradient Boosting model on the Breast Cancer dataset.

```
library(caret)
library(gbm)
data(BreastCancer)

# Convert the diagnosis column to a binary factor
BreastCancer$diagnosis <- ifelse(BreastCancer$diagnosis == "M", 1, 0)

# Split the dataset into training and testing sets
trainIndex <- createDataPartition(BreastCancer$diagnosis, p = 0.7, list = FALSE)
trainData <- BreastCancer[trainIndex, ]
testData <- BreastCancer[-trainIndex, ]

# Define the training control
ctrl <- trainControl(method = "cv", number = 10, classProbs = TRUE, summaryFunction = twoClassS

# Define the Gradient Boosting model
model <- train(diagnosis ~ ., data = trainData, method = "gbm", trControl = ctrl,
               verbose = FALSE, metric = "ROC", n.trees = 1000, interaction.depth = 3, shrinkag

# Make predictions on the testing set
predictions <- predict(model, testData)

# Evaluate the performance of the model
confusionMatrix(predictions, testData$diagnosis)
```

XGBoost

- In this example, we use the `xgbTree` method in `train()` function from the caret package to build an `XGBoost` model on the `BreastCancer` dataset.
- The hyperparameters are set to default values, except for parameters:
    - nrounds,

  - max_depth,
  - eta, lambda, and
  - alpha

- The final performance is evaluated using a confusion matrix.

```
library(caret)
library(xgboost)
data(BreastCancer)

# Convert the diagnosis column to a binary factor
BreastCancer$diagnosis <- ifelse(BreastCancer$diagnosis == "M", 1, 0)

# Split the dataset into training and testing sets
trainIndex <- createDataPartition(BreastCancer$diagnosis, p = 0.7, list = FALSE)
trainData <- BreastCancer[trainIndex, ]
testData <- BreastCancer[-trainIndex, ]

# Define the training control
ctrl <- trainControl(method = "cv", number = 10, classProbs = TRUE, summaryFunction = twoClassS

# Define the XGBoost model
model <- train(diagnosis ~ .,
               data = trainData,
               method = "xgbTree", trControl = ctrl,
               verbose = FALSE, metric = "ROC",
               nrounds = 1000, max_depth = 3,
               eta = 0.01, lambda = 1, alpha = 0)

# Make predictions on the testing set
predictions <- predict(model, testData)

# Evaluate the performance of the model
confusionMatrix(predictions, testData$diagnosis)
```

References

Official references and resources

- Caret tutorial at UseR! 2014
- The `caret` package
- JSS Paper
- Applied Predictive Modeling Blog
- Caret cheatsheet in Rstudio cheatsheet page

Other resources

- Caret Package – A Practical Guide to Machine Learning in R -Create predictive models in R with Caret
- Caret R Package for Applied Predictive Modeling