Quantessentials

R advice – predictive modelling with caret

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The success of machine learning and some of its practical issues

Machine learning algorithms have been very successful in applications across many fields, including finance. We have used various machine learning techniques to try and predict dividend cuts (random forest) or quarterly EPS (partial least squares, among others). Regardless of the algorithm used, the modeller always faces the same practical issues when building predictive models: from handling missing values (data pre-processing) to fine-tuning model hyper-parameters, while at the same time ensuring that the model does not overfit.

caret: the go-to package for predictive modelling in R

The *caret* package simplifies and automates supervised learning by addressing some of these practical problems. In addition, it provides consistent interface for the most powerful machine learning models in R. In this report we demonstrate some of *caret*'s most useful features and show how it can be used to train predictive models that generalise well.

Predictive modelling in R

It is common practice nowadays to generate and collect vast amounts of data to answer research questions and predict future outcomes. Alongside the rise of data, the availability of free model building software, such as Weka and increasing number of packages in R or Python, has contributed to the popularity of machine learning in many industries, including finance. In this note we are not going to introduce any of these algorithms in detail, but rather demonstrate a way of approaching predictive modelling in R.

Overwhelming number of machine learning packages

On CRAN alone, there are 96 packages related to Machine learning[1], which is both good and bad news. Thanks to the wide variety of libraries you can be almost sure that someone else has already (reasonably) implemented the algorithm you need: from simple decision trees (e.g. *rpart*) to deep belief networks (e.g. *deepnet*). The problem with this variety is that every package has its own interface: slightly different syntax (e.g. formulas vs design matrices); tools may not work well together (e.g. data pre-processing vs model training).

The *caret* package (which stands for "**C**lassification **A**nd **RE**gression **T**raining") simplifies and automates supervised learning in R by providing consistent interface for the most powerful machine learning models. It implements tools for:

- Data pre-processing and data splitting
- Model evaluation and tuning using resampling
- Variable importance estimation and feature selection

Data and models

Throughout this note we use the toy dataset from previous Quantessentials, containing 40 large-cap companies and several quantitative factors (see Appendix). We demonstrate the main features of the package by fitting a random forest model, which was discussed in detail in a previous note, and a boosted tree model to illustrate custom tuning of multiple hyper-parameters.

The golden rule: Do not overfit

The main goal of predictive modelling is to build models that perform well on **new data**. It is, however, still common practice to evaluate and select models based on performance metrics calculated with the same data that was used to train the model, i.e. in-sample. This usually leads to over-optimistic estimates of model performance and essentially guarantees overfitting. A very simple example is given in Figure 1: impute missing values with the median, fit a linear model using forward return as a target variable and everything else as predictors and calculate the Root Mean Squared Error (RMSE) – the most common error metric for regression problems.

[1] According to CRAN Task View as of June 2017
https://cran.r-project.org/web/views/MachineLearning.html

Figure 1: In-sample RMSE

```
## To reproduce the examples - please refer to the appendix for the data
library(dplyr)
# Median-impute missing values
data_imputed <- data %>%
  mutate_if(is.numeric, funs(ifelse(is.na(.), median(., na.rm = TRUE), .)))
lm_fit1 <- lm(FwdReturn ~ ., data = data_imputed)
# In-sample RMSE
sqrt(mean((predict(lm_fit1) - data_imputed$FwdReturn) ^ 2))

## [1] 1.975833
```

Source: UBS Quant.

Main rule in Machine Learning: Do not overfit

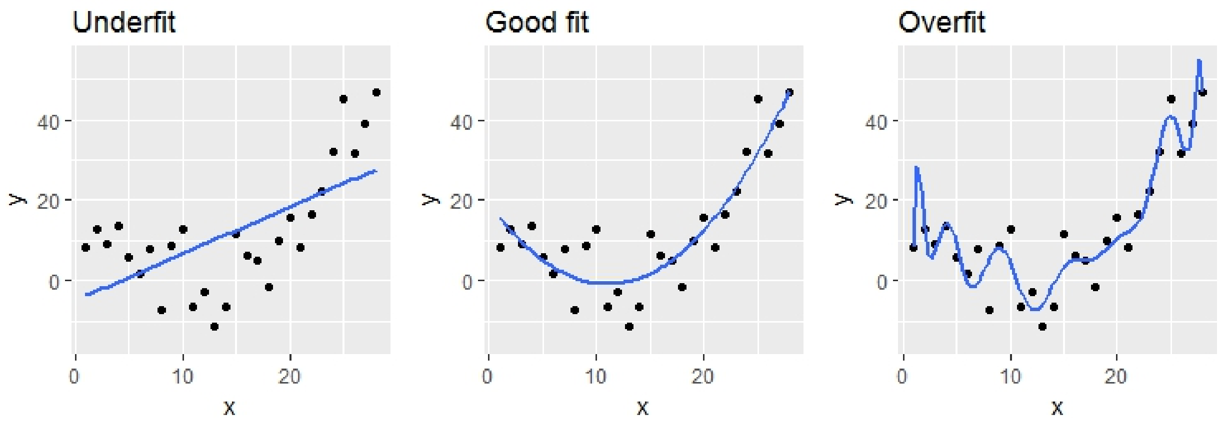
How well will this model perform on new data? The simplest way to check this is to split the data into training and test sets, use the former to fit the regression and the latter to make predictions and calculate out-of-sample RMSE as shown in Figure 2. As expected, the out-of-sample accuracy of this model is significantly worse.

Figure 2: Out-of-sample RMSE, single train-test split

```
# Use the first 30 data points to fit the model and the rest to test
training <- data_imputed[1:30, ]
test <- data_imputed[-(1:30), ]
lm_fit2 <- lm(FwdReturn ~ ., data = training)
preds <- predict(lm_fit2, newdata = test)
# Out-of-sample RMSE
sqrt(mean((preds - test$FwdReturn) ^ 2))

## [1] 4.110101
```

Source: UBS Quant.

Figure 3: Overfitting vs Underfitting



Source: UBS Quant. The figure illustrates the problem of underfitting and overfitting. The linear model in the leftmost plot is insufficient to describe the relationship in the data and will produce high in-sample and high out-of-sample RMSE. The polynomial model in the rightmost plot learns the noise in the data as opposed to the signal (i.e. overfits), which will result in small in-sample but high out-of-sample errors. The quadratic model (the true relationship) in the middle describes the data most appropriately and therefore would generalise best on new data.

Model training *a-la*-caret

To get a more precise estimate of the true out-of-sample error and therefore be able to choose models that generalise well, there are a few modifications to the simple methodology above that need to be made:

(1) Pre-process the data after splitting it (in the case above missing values should have been imputed after defining the training set)

(2) Use multiple train-test splits and take the average OOS RMSE to reduce the influence of outliers

(3) Tune the model (if it has hyper-parameters)

In the rest of the note we fit a random forest model, focusing on each of the steps outlined above. The main function in *caret* for training models is `caret::train`, whose basic syntax is demonstrated in Figure 4, which also shows the ease with which one can specify hundreds of different models by simply changing the `method` argument[2]. Prediction is also straightforward as the package implements the standard base-R interface.

Figure 4: Model fitting with caret

```
library(caret)
set.seed(20170629)
# To fit a linear model, specify method = "lm"
lm_fit <- train(
  FwdReturn ~ .,
  data = data_imputed,
  method = "lm"
)
lm_fit
# Change the method argument to "rf" to fit a random forest
rf_fit <- train(
  FwdReturn ~ .,
  data = data_imputed,
  method = "rf"
)
rf_fit
# Predictions are made with the standard interface
predict(rf_fit)
```

Source: UBS Quant.

Pre-processing

One of the most common data pre-processing tasks when it comes to machine learning is missing values imputation. One way to handle these is to throw away all the rows containing missing data. Despite being the most straightforward, this method is often a bad idea as it may lead to biases in the data, over-confident models and in some extreme scenarios leave us with little or no data to work with.

The *caret* package implements 3 types of missing values imputation: *median impute*, which is the quickest and works well when data is missing at random, *K*-

[2] See http://topepo.github.io/caret/available-models.html for a full list of available models.

nearest neighbours (KNN), which is slower but works better if data is not missing at random, and *bagged trees* - an accurate method, but with much higher computational cost.

In addition to missing values imputation, caret implements other common pre-processing operations, including variable transformation (centering, scaling, PCA), removing highly correlated predictors or such with (near) zero variance. Some of these are demonstrated in Figure 5.

Note that *caret* does not provide support for feature engineering (constructing new variables from existing) or other general data manipulation tasks (filtering observations); see our notes on [data.table]() or [dplyr]() for such operations.

Figure 5: Data pre-processing

```r
set.seed(20170630)
rf_fit1 <- train(
  FwdReturn ~ .,
  data = data,
  preProcess = "medianImpute",
  na.action = na.pass,  #!! Set na.action to pass
  method = "rf"
)
rf_fit1
```

```
## Random Forest
##
## 24 samples
## 14 predictors
## Pre-processing: median imputation (20)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 40, 40, 40, 40, 40, 40, ...
## Resampling results across tuning parameters:
##
##   mtry  RMSE      Rsquared
##    2    3.526280  0.4923369
##   11    3.547843  0.4648829
##   20    3.638426  0.4322584
##
## RMSE was used to select the optimal model using  the smallest value.
## The final value used for the model was mtry = 2.
```

```r
# You can also pass multiple arguments to preProcess. E.g.:
# 1. remove columns with zero or near-zero variance ("nzv")
# 2. median impute missing values
# 3. center and 4. scale all variables
rf_fit2 <- train(
  FwdReturn ~ .,
  data = data,
  preProcess = c("nzv", "medianImpute", "center", "scale"),
  na.action = na.pass,  #!! Set na.action to pass
  method = "rf"
)
```

Source: UBS Quant. There is an order in which operations should be applied (e.g. centering comes before scaling), but you don't need to worry about it – caret will execute them in the correct order.

Resampling

The default resampling scheme used to calculate out-of-sample performance metrics is bootstrap validations (with 25 replications). Another common option is (repeated) K-fold cross validation (CV), which we show how to implement Figure 6. In practice the two yield similar results.

Figure 6: Defining repeated cross-validation resampling scheme

```
# Define the resampling scheme using the trainControl function
my_cv_control <- trainControl(
  method = "repeatedcv",
  number = 5,          # number of folds
  repeats = 10,        # number of repeats
  verboseIter = TRUE   #
)
rf_fit3 <- train(
  FwdReturn ~ .,
  data = data,
  preProcess = "medianImpute",
  na.action = na.pass,
  method = "rf",
  trControl = my_cv_control # pass the trainControl object to trControl
)
```

Source: UBS Quant. The resampling scheme is controlled by the `trControl` argument in `train`.

Time series resampling requires more care

Clearly, neither the bootstrap nor CV can be applied to time series, as they will break the temporal structure in the data. To deal with this problem *caret* implements a "time-slice" resampling scheme that allows you to specify initial training period, forecasting horizon and whether the model is to be fitted on a rolling or expanding window basis .

As an example, suppose we have monthly data and wish to fit a model on a rolling window basis using 5 years of training data (60 observations), aiming to predict next month's value, i.e. the forecast horizon is 1 month. The appropriate train-control object to use in such an experiment is defined in Figure 7.

Figure 7: Time series validation

```
my_time_control <- trainControl (
  method = "timeslice",
  initialWindow = 60,  # use the first 60 data points to train
  horizon = 1,         # forecast one ahead
  fixedWindow = TRUE   # use rolling window (the default)
)
```

Source: UBS Quant. The train-control object should be passed to the `trControl` argument in `train.`

Model tuning

Most machine learning models have *hyper-parameters*, which unlike regular parameters, cannot be inferred from the data, yet they impact how well the model performs. In most cases there are no "optimal" values or meaningful defaults hence hyper-parameters require *tuning*.

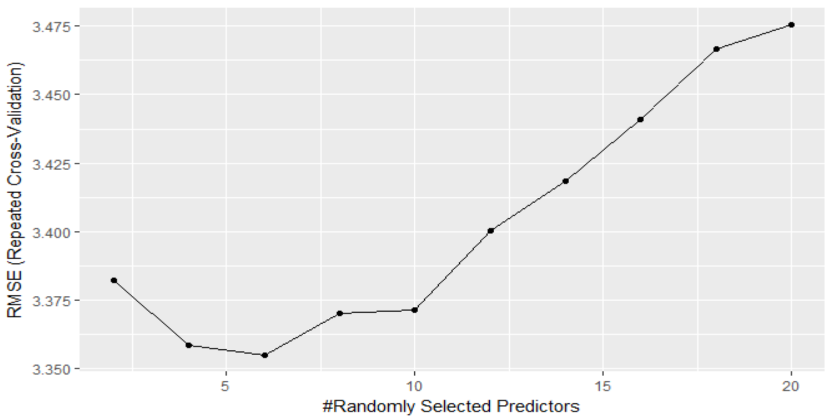
The only tuning parameter in random forest is *mtry* – the number of randomly selected variables used at each split, and its default values typically work well ($p/3$

for regression and $\sqrt{p}$ for classification, where p is number of variables). More complex machine learning algorithms, however, have no good defaults (e.g. KNN) or have several tuning parameters (e.g. boosted trees with 4) in which case calibrating the model becomes crucial.

Figure 8 shows how to implement simple tuning, where you only need to specify how many variations of the hyper-parameters to try and *caret* will decide on the exact values.

Figure 8: Simple tuning via `tuneLength`

```
set.seed(20170627)
rf_fit4 <- train(
  FwdReturn ~ .,
  data = data,
  preProcess = "medianImpute",
  na.action = na.pass,
  method = "rf",
  trControl = my_cv_control,
  tuneLength = 10
)
# Optimal mtry
rf_fit4$bestTune
## mtry
## 3 6
# Lowest RMSE
min(rf_fit4$results$RMSE)
## [1] 3.354858
ggplot(rf_fit4)
```

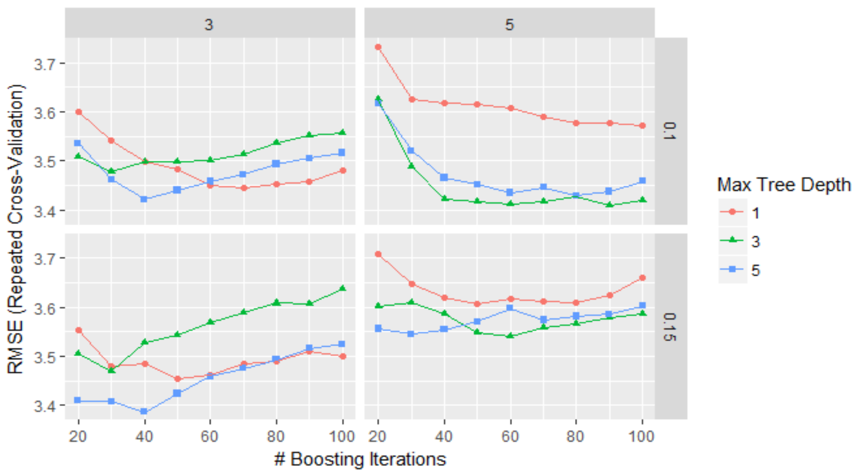


Source: UBS Quant.

Figure 9 demonstrates a custom tuning grid for boosted trees model, which requires you to explicitly specify the values of the parameters for which the model is to be fitted.

Figure 9: Custom tuning via tuneGrid

```
# Boosted trees (gbm package) have 4 tuning parameters
gbm_grid <- expand.grid(
   n.trees  = seq(20, 100, by = 10),
   interaction.depth = c(1, 3, 5),
   shrinkage = c(0.1, 0.15),
   n.minobsinnode = c(3, 5)
)
nrow(gbm_grid)
## [1] 108   # gbm will be fitted for 108 values of the parameters
set.seed(20170627)
gbm_fit <- train(
  FwdReturn ~ .,
  data = data,
  preProcess = c("nzv", "medianImpute", "center", "scale"),
  na.action = na.pass,
  method = "gbm",
  trControl = my_cv_control,
  tuneGrid =  gbm_grid,
  verbose = FALSE # gbm output is verbose, may want to supress it
)
# Optimal paramters

gbm_fit$bestTune

##    n.trees interaction.depth shrinkage n.minobsinnode
## 93      40                 5      0.15              3

# Lowest RMSE

min(gbm_fit$results$RMSE)
## [1] 3.38652

ggplot(gbm_fit)
```



Source: UBS Quant.

Variable importance

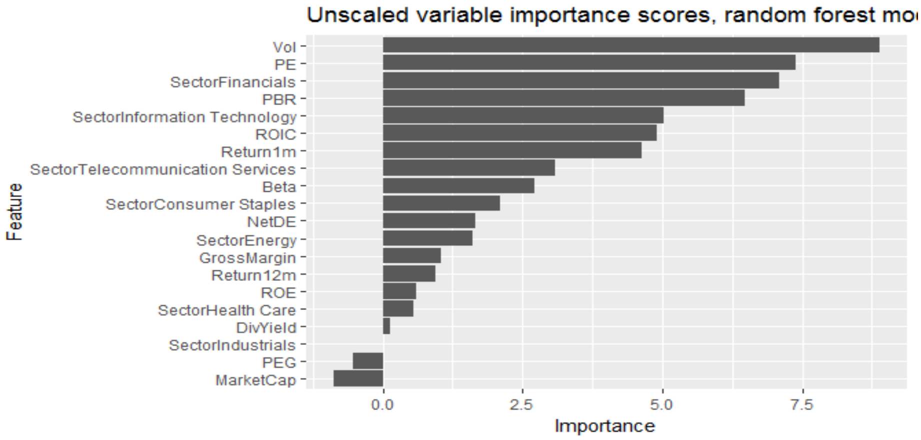
Machine learning algorithms have been very successful in applications across many fields, yet there are still significant concerns about transparency (and rightly so). Although there is a fundamental difference between explanatory modelling and predictive modelling[3], we often require causal explanation and inference from a model that is trained to be good at prediction (e.g. 10% increase in x results in 5% decrease in y). Extracting such causal information from predictive models is often very difficult due to their high non-linearities; however, ranking predictors according to some measure of strength or relevance with the response can often give us confidence that the model is doing something meaningful.

The only thing harder than training a good model is interpreting it

caret allows you to compute variable importance metrics both for models that have "built-in" measurements of predictor importance (such as linear models or random forests) and those that don't (e.g. SVMs). Figure 10 and Figure 11 show how to extract (`varImp` function) and visualise variable importance scores.

Figure 10: Variable importance, random forest model

```r
# For rf, you need to explicitly set importance = TRUE in train()
set.seed(20170628)
rf_fit <- train(
  FwdReturn ~ .,
  data = data,
  preProcess = "medianImpute",
  na.action = na.pass,
  method = "rf",
  trControl = my_cv_control,
  importance = TRUE
)
# By default, scores are scaled between 0 and 100; to get raw scores, set scale to FALSE
rf_imp <- varImp(rf_fit, scale = FALSE)
ggplot(rf_imp) +
  ggtitle("Unscaled variable importance scores, random forest model ")
```

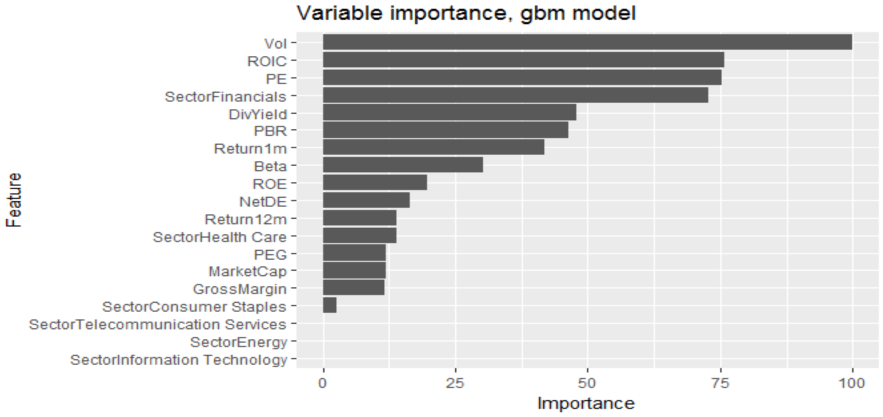


Source: UBS Quant.

[3] See To Explain or to Predict by G. Shmueli for an excellent discussion on the topic

Figure 11: Variable importance for the gbm model

```r
gbm_imp <- varImp(gbm_fit)
ggplot(gbm_imp) +
  ggtitle("Variable importance scores, gbm model")
```



Source: UBS Quant.

Appendix

Figure 12: Data used in the report

```
data <- read.csv(row.names = 1,
text = "Ticker,Sector,MarketCap,Beta,GrossMargin,PEG,PE,PBR,DivYield,ROE,ROIC,Vol,FwdReturn,Return1m,Return12m,NetDE
AAPL UW,Information Technology,562022,1.38,38.80,2.12,11.84,4.38,2.00,39.06,27.47,21.97,2.36,11.49,-13.70,0.19
MSFT UW,Information Technology,442557,1.23,62.66,NA,19.39,5.96,2.36,12.34,8.72,22.65,2.01,13.69,27.42,-0.79
XOM UN,Energy,368876,0.82,21.54,NA,24.26,2.14,3.28,7.58,6.63,13.99,-1.18,-0.78,13.34,0.22
JNJ UN,Health Care,344596,0.75,69.43,0.20,18.06,4.74,2.40,21.89,17.51,9.79,-4.07,5.27,29.44,-0.23
AMZN UW,Consumer Discretionary,359676,1.34,33.48,0.00,91.71,24.27,0.00,9.10,4.35,27.04,1.36,6.31,43.07,0.10
GE UN,Industrials,279053,1.02,34.08,0.03,19.02,3.14,2.95,8.33,2.72,17.84,0.32,4.38,23.61,1.22
FB UW,Information Technology,355708,1.17,83.88,0.47,27.29,7.52,0.00,11.02,11.01,17.89,1.76,10.91,31.18,-0.44
NESN VX,Consumer Staples,250209,0.78,49.62,NA,22.10,3.84,2.90,13.69,11.59,13.88,0.77,5.11,10.82,0.24
T UN,Telecommunication Services,266320,0.46,38.60,NA,14.68,2.16,4.39,13.19,6.59,11.39,-5.57,2.46,30.59,0.98
JPM UN,Financials,231060,1.25,NA,0.51,10.71,1.04,2.75,9.69,4.09,24.89,5.52,8.54,-3.00,2.27
WFC UN,Financials,242176,1.07,NA,0.94,11.59,1.40,3.13,11.75,5.69,20.34,6.75,4.40,-13.69,1.82
GOOG UW,Information Technology,527988,1.21,61.78,0.40,20.29,4.27,0.00,14.24,13.93,16.61,-0.23,9.69,18.78,-0.57
PG UN,Consumer Staples,228360,0.60,50.23,NA,21.47,3.92,3.11,14.03,10.80,11.36,2.01,3.66,9.32,0.33
PFE UN,Health Care,223762,0.61,72.03,0.09,14.45,3.55,3.09,11.65,8.10,12.78,-4.86,6.48,7.43,0.32
VZ UN,Telecommunication Services,225851,0.60,47.56,2.26,13.93,12.12,4.05,128.45,14.94,12.93,-5.56,1.08,25.13,5.58
CVX UN,Energy,193144,1.23,8.07,NA,30.39,1.28,4.18,0.85,0.70,16.28,-0.83,0.16,15.52,0.22
NOVN VX,Health Care,197850,1.09,64.35,NA,16.84,2.78,3.36,9.13,7.54,18.76,-3.61,3.68,-15.70,0.32
BRK/B UN,Financials,355729,0.88,24.96,1.22,18.60,1.38,0.00,9.80,7.20,15.94,4.31,2.95,0.84,0.17
KO UN,Consumer Staples,188263,0.57,59.90,NA,22.08,7.59,3.07,27.08,13.62,13.52,-0.46,-1.20,11.11,0.99
MRK UN,Health Care,162462,0.82,62.81,0.71,15.67,3.71,3.10,10.08,6.56,16.40,7.04,5.13,5.11,0.29
ROG VX,Health Care,218243,1.04,69.34,0.02,15.97,10.05,3.27,43.70,23.02,20.07,-3.11,-0.28,-8.42,0.66
HD UN,Consumer Discretionary,170865,1.06,32.27,0.91,20.51,27.17,1.78,93.09,28.78,15.99,-2.48,8.18,22.59,2.79
INTC UW,Information Technology,164400,1.41,62.20,0.12,13.30,2.69,2.81,19.46,15.12,21.46,3.74,11.48,24.05,0.17
BAC UN,Financials,148041,1.46,NA,NA,10.19,0.63,1.38,6.18,3.22,33.22,11.90,15.59,-16.82,1.12
7203 JT,Consumer Discretionary,173183,0.94,20.05,5.23,10.57,1.07,3.56,13.60,8.60,33.75,5.84,17.77,-25.12,0.76
CMCSA UW,Consumer Discretionary,162195,0.69,58.39,0.99,17.97,3.10,1.52,15.72,8.27,13.67,-2.96,8.05,10.63,0.95
CSCO UW,Information Technology,153688,1.37,62.51,0.63,12.52,2.46,2.92,16.91,12.63,19.58,2.98,10.83,11.97,-0.56
V UN,Information Technology,184419,0.93,78.23,0.91,24.14,5.81,0.67,23.85,18.68,21.15,3.83,5.36,6.71,-0.17
PM UN,Consumer Staples,155536,0.72,64.38,0.03,21.19,NA,4.05,NA,50.88,16.76,-0.33,0.57,21.11,-2.11
PEP UN,Consumer Staples,156954,0.62,54.91,NA,21.84,13.99,2.58,38.27,12.83,12.88,-1.30,5.86,15.84,2.04
005930 KP,Information Technology,194464,0.99,37.45,0.54,9.58,1.28,1.36,11.65,11.54,21.70,5.26,7.80,24.56,-0.36
700 HK,Information Technology,226081,0.96,58.39,0.62,31.22,11.53,0.25,28.87,19.78,23.56,8.20,10.85,29.39,-0.83
DIS UN,Consumer Discretionary,163115,1.06,41.35,1.08,15.75,3.70,1.43,20.22,15.49,15.01,-1.55,0.57,-17.93,0.37
HSBA LN,Financials,130240,1.19,NA,NA,11.19,0.73,6.91,6.44,3.34,19.57,15.59,10.66,-7.94,0.22
IBM UN,Information Technology,153528,0.96,48.76,0.18,11.59,10.33,3.24,95.80,25.52,18.82,-0.23,10.75,4.66,2.06
C UN,Financials,127286,1.62,NA,1.22,8.83,0.61,0.46,7.16,3.81,34.88,8.97,9.40,-23.90,1.24
2330 TT,Information Technology,130621,0.97,45.46,0.80,13.34,3.49,3.48,24.33,20.89,20.60,2.03,12.42,36.80,-0.31
ORCL UN,Information Technology,169536,1.10,74.74,0.30,14.61,3.72,1.46,18.82,10.76,19.97,0.44,5.65,6.50,-0.23
MO UN,Consumer Staples,132286,0.46,62.41,0.31,21.00,48.25,3.27,205.76,35.00,11.90,-2.38,-1.18,26.19,3.29
UNH UN,Health Care,136613,0.83,NA,0.34,16.68,3.88,1.40,17.93,10.94,13.06,-4.99,2.92,19.52,0.66")
```

Source: UBS Quant. The dataset contains 40 large-cap companies and factors associated with them as of 31/Jul/2016.

Figure 13: Packages used in examples

Package	Version
caret	6.0-76
randomForest	4.6-7
gbm	2.1.1
dplyr	0.7.1

Source: UBS Quant

References

Max Kuhn, Kjell Johnson (2013) Applied Predictive Modeling. Springer Science & Business Media; http://appliedpredictivemodeling.com/

Max Kuhn (2017). Caret: Misc functions for training and plotting classification and regression models. R package version 6.0-76. https://CRAN.R-project.org/package=caret. Caret website: http://topepo.github.io/caret/index.html

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Sell	Stock price expected to fall within three months from the time the rating was assigned because of a specific catalyst or event.	<1%	<1%

Source: UBS. Rating allocations are as of 31 March 2017.
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