UBS

Global Research

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# Machine learning

## *Trees and more trees*

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# Table of Contents

# Introduction

- This presentation focuses on classification problems.
- We will consider decision trees and two machine learning algorithms based on them: random forests and adaBoost.
- The 2014 paper, "Do we need hundreds of classifiers to solve real world classification problems?" (2014), Fernandez-Delgado et al, Journal of Machine Learning, compares the effectiveness of 179 different machine learning approaches on 121 different data sets and rank the classifiers.
- Random forests and adaBoost perform extremely well:

| Classifier | Average Accuracy | Rank (out of 179) |
|---|---|---|
| Random Forest | 81.9% | 5 / 179 |
| AdaBoost | 79.1% | 20 / 179 |
| Decision Tree | 73.5% | 108 / 179 |

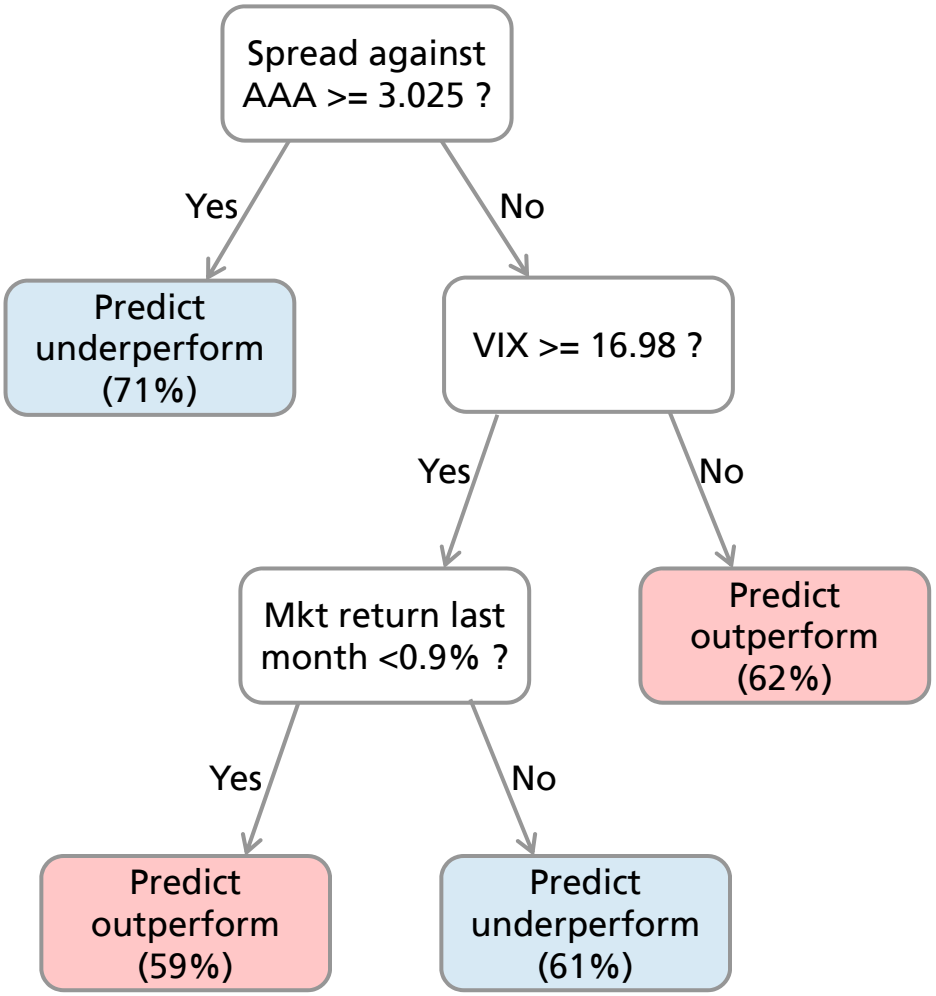
Source: "Do we need hundreds of classifiers to solve real world classification problems?" (2014), Fernandez-Delgado et al, Journal of Machine Learning, Extract from Tables 2 & 3 ,

Section 1

# Decision Trees

# How to use a tree

- The output looks like a flow chart.
- To make a prediction for today, you work your way down the tree until you reach a "leaf".
- The leaf gives you a forecast class and an attached probability e.g. underperform with a probability of 71%.




Example of a classification tree

Source: UBS Quants

# Pros and cons of decision trees

**Pros**

- Completely transparent
- Easy to interpret and communicate
- Robust to outliers / non-normal inputs and works with categorical and continuous data inputs
- Does not rely on linear relationships

**Cons**

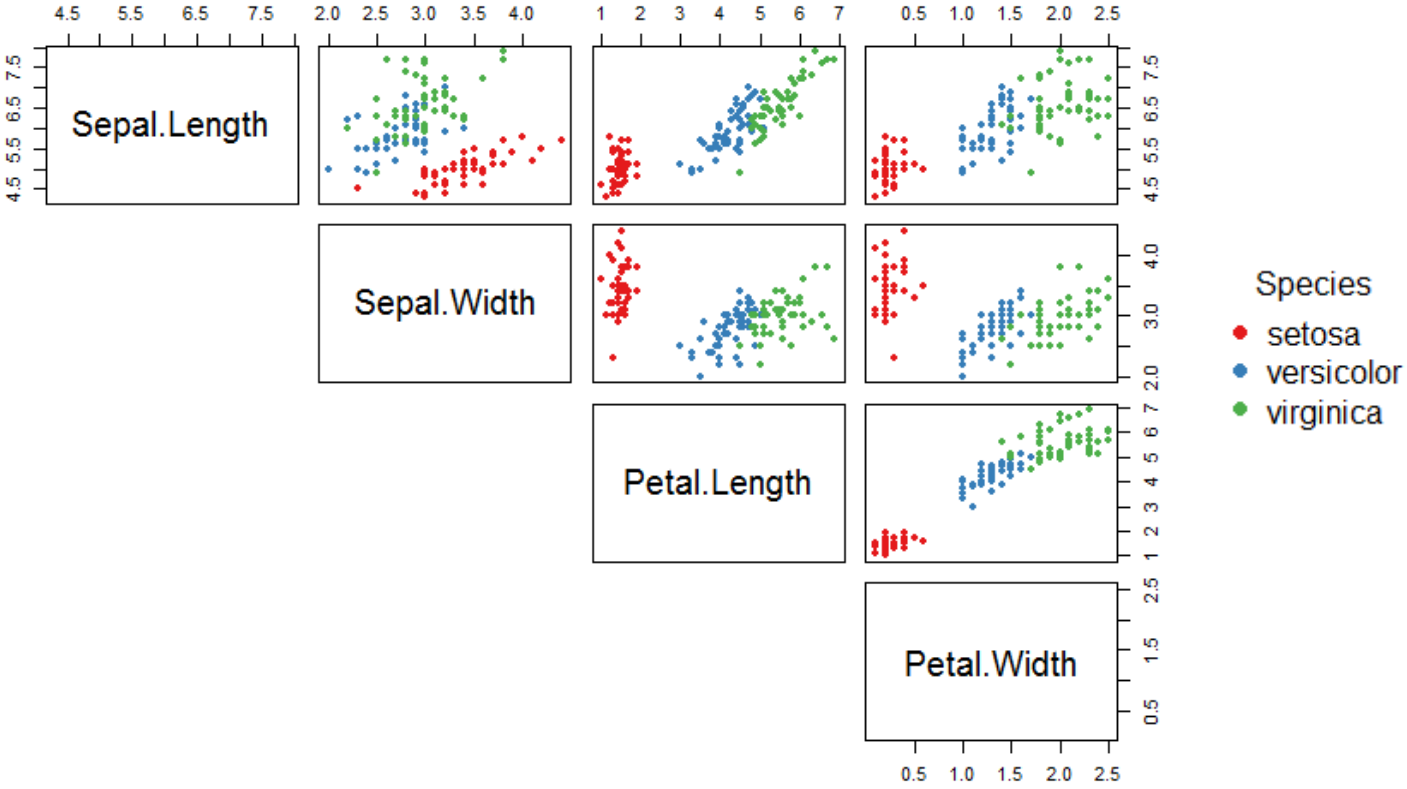
- Decision trees are often unstable i.e. the tree can change completely with the addition of an extra data-point
- Doesn't cope well with severe class imbalances
- Doesn't forecast well for inputs outside the range of its training set
- Sometimes over-fit

# Our example data

- Iris is a data-set about irises. We have data about sepal and petal lengths and widths, and we want to create a model to classify the species of iris.

| Sepal.Length | Sepal.Width | Petal.Length | Petal.Width | Species |
|---|---|---|---|---|
| 5.9 | 3.0 | 5.1 | 1.8 | viriginica |
| 5.6 | 2.9 | 3.6 | 1.3 | versicolor |
| 5.0 | 3.6 | 1.4 | 0.2 | setosa |
| 5.1 | 3.7 | 1.5 | 0.4 | setosa |
| etc | | | | |

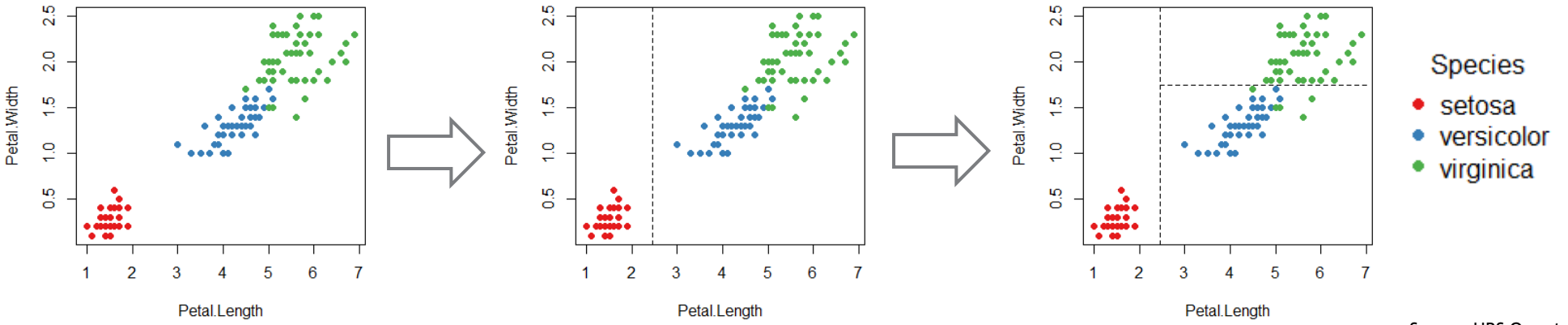
Source: UBS Quants




Source: UBS Quants

# How do we grow a tree?

- We start with all of our data.
- If your data-set is finite then for each feature there are a finite number of possible thresholds, so we can test every possible combination of feature and threshold and choose the one which divides the data "most cleanly" into two homogenous sub-groups.
- Then we repeat the process with each of those two sub-groups separately and so on recursively.




Source: UBS Quants

# How do we choose the feature and threshold at each node?(1)

- Start by defining the impurity of the data with the Gini coefficient:

$$Impurity = 1 - \sum_{i=1}^{\#\ of\ classes} {p_i}^2$$

where pi is the proportion of the data from class i. In this example, we have three classes for each of the three species of iris.

  - This will be zero if all the group is from a single class and bigger if the data is more mixed.
  - The worst case scenario is if the group has equal numbers of points from each class.

- If we cut the data into two sub-groups then the overall impurity is a weighted sum of the impurity in each sub-group:

$Overall\ impurity =$ % of data in 1st subgroup x impurity in 1st subgroup +
% of data in 2nd subgroup x impurity in 2nd subgroup

- We want to choose the cut which minimises the overall impurity i.e. creates two sub-groups which are almost exclusively a single class.

# How do we choose the feature and threshold at each node?(2)

- As an example, here is a table showing the breakdown of iris species where the sepal length is longer or shorter than 5 cm:

| | Species of iris | | | |
|---|---|---|---|---|
| | Setosa | Versicolor | Virginica | Total |
| Overall | 50 | 50 | 50 | 150 |
| Sepal.Length ≤ 5 | 28 | 3 | 1 | 32 |
| Sepal.Length > 5 | 22 | 47 | 49 | 118 |

Source: UBS Quants

$$Overall\ impurity\ before\ cut = 1 - (\frac{50}{150})^2 - (\frac{50}{150})^2 - (\frac{50}{150})^2 = \mathbf{0.66}$$

$$Impurity\ in\ short\ sepal\ subgroup = 1 - (\frac{28}{32})^2 - (\frac{3}{32})^2 - (\frac{1}{32})^2 = \mathbf{0.22}$$

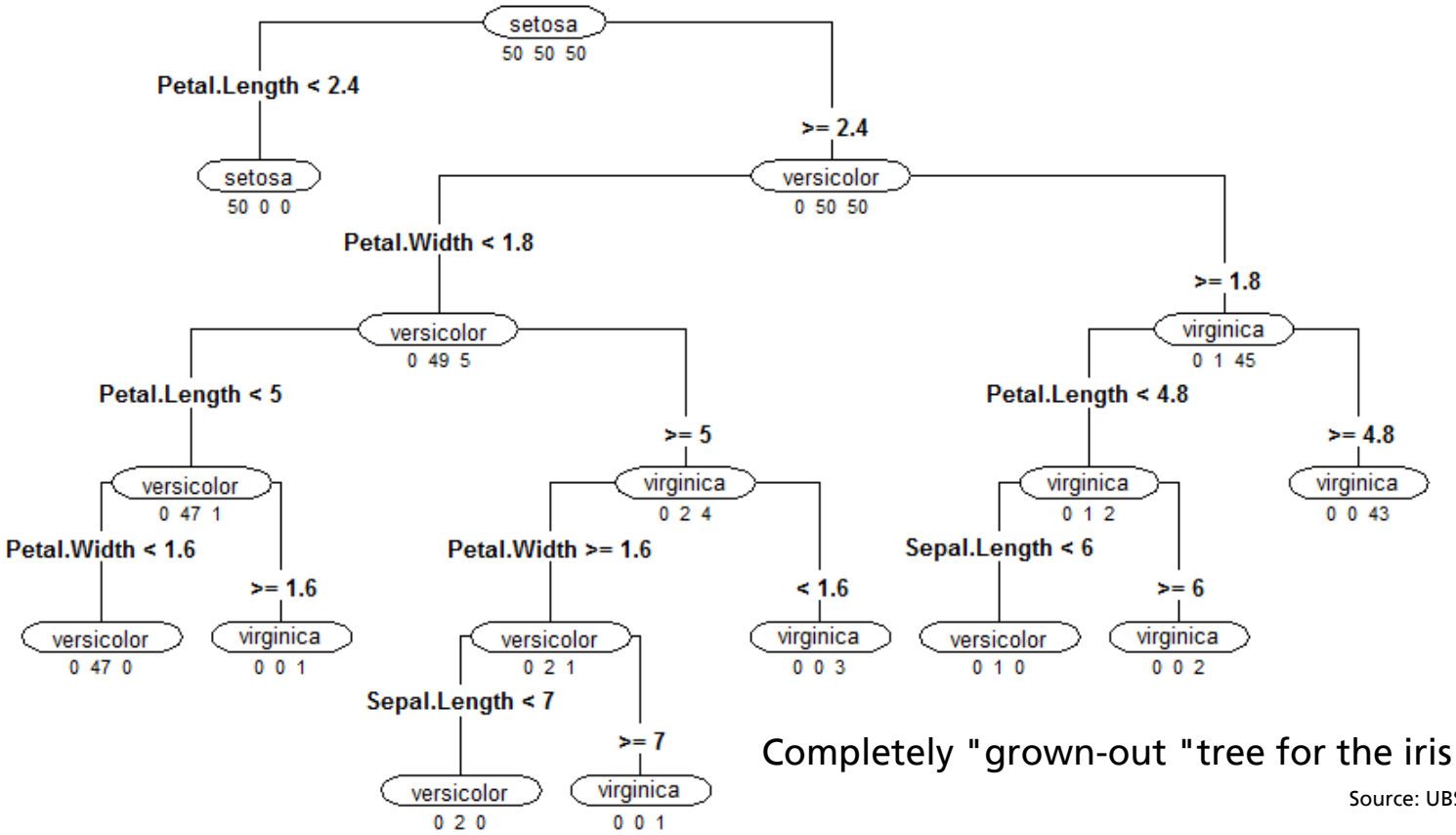
$$Impurity\ in\ long\ sepal\ subgroup = 1 - \left(\frac{22}{118}\right)^2 - \left(\frac{47}{118}\right)^2 - (\frac{49}{118})^2 = \mathbf{0.63}$$

$$Overall\ impurity\ after\ cut = \frac{32}{150} \times 0.22 + \frac{118}{150} \times 0.63 = \mathbf{0.55}$$

Lower impurity after the cut

# Over-fitting: The problem

- The rules we have seen so far will make the tree grow until every node is completely homogenous.
- This will typically lead to a big, complicated tree which over-fits the data.




Completely "grown-out "tree for the iris data

Source: UBS Quants

# Over-fitting: Overview of how R solves this

- Rpart has two stages to prevent over-fitting:

1. It does not allow the tree to grow out completely
2. It returns some statistics to show what a "sensible size" is.

# Over-fitting: Don't let the tree grow all the way out

Step 1

- To stop the tree from growing out completely, Rpart has some rules. The defaults cause the tree to stop when:
  - The node is very small (defaults to 20)
  - The best available split leads to a very small leaf (defaults to minsplit/3)
  - The best available split does not improve the fit by a certain amount (defaults to 0.01).
- You can change these defaults using the control variable in the rpart function, but it isn't typically necessary.
- This *can* still lead to an over-fitted tree, but it is much less likely.

# Over-fitting: Using the rpart output to choose the complexity of your tree (1)

## Step 2

- R will usually return an appropriately fitted tree, but the choice of how complex it should be is often more of an art than a science, so you may want a different tree to the default.
- The rpart function returns some statistics to help us:

```
myTree$cptable
```

```
      CP nsplit rel error xerror  xstd
1  0.500      0      1.00   1.21 0.0484
2  0.440      1      0.50   0.67 0.0609
3  0.020      2      0.06   0.10 0.0306
4  0.010      3      0.04   0.10 0.0306
5  0.005      6      0.01   0.07 0.0258
6 -1.000      8      0.00   0.07 0.0258
```

**Complexity parameter**

Lower values indicate a more complex tree.

**Relative error**

# of misclassified / # of misclassified in tree without any splits

**Cross validated relative error**

# of misclassified estimated from cross-validation / # of misclassified in tree without any splits

**Cross validated standard error**

Source: UBS Quants

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# Over-fitting: Using the rpart output to choose the complexity of your tree (2)

| | CP | nsplit | rel error | xerror | xstd |
|---|---|---|---|---|---|
| 1 | 0.500 | 0 | 1.00 | 1.21 | 0.0484 |
| 2 | 0.440 | 1 | 0.50 | 0.67 | 0.0609 |
| 3 | 0.020 | 2 | 0.06 | 0.10 | 0.0306 |
| 4 | 0.010 | 3 | 0.04 | 0.10 | 0.0306 |
| **5** | **0.005** | **6** | **0.01** | **0.07** | **0.0258** |
| 6 | -1.000 | 8 | 0.00 | 0.07 | 0.0258 |

Source: UBS Quants

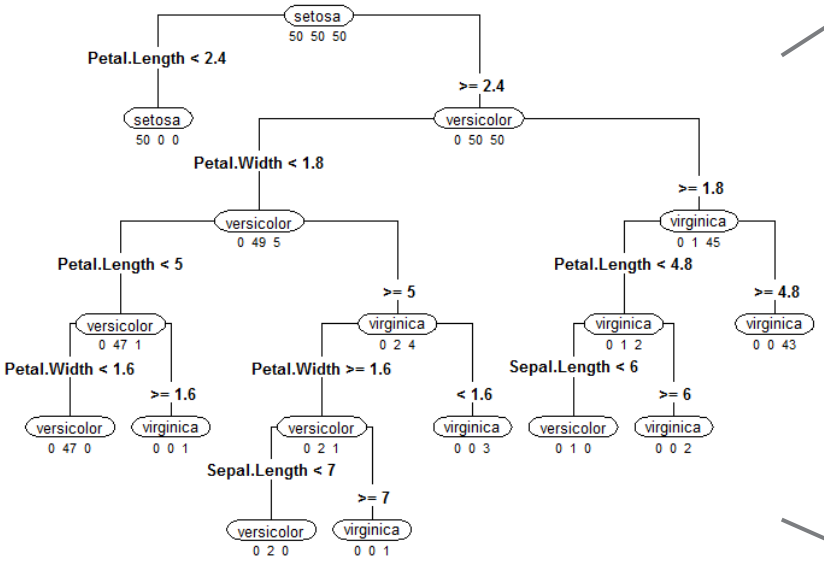
- We could choose the tree with the smallest cross-validated relative error i.e. the tree with six splits here.
- An alternative, more conservative approach is to take the smallest tree within one standard error of the smallest cross-validated relative error i.e. the smallest tree with:

$$\text{xerror} < 0.07 + 0.0258 = 0.0958$$

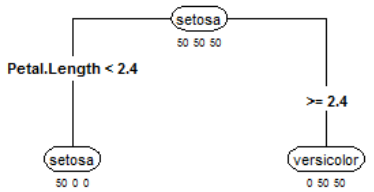
- … which would give us the tree with two splits
- Then we prune the tree to this size by specifying the cp parameter.

```
newTree = prune(myTree, cp=0.02)
```

# Over-fitting: Using the rpart output to choose the complexity of your tree (3)

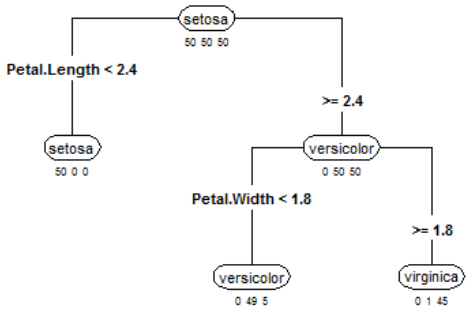



Prune at cp = 0.44



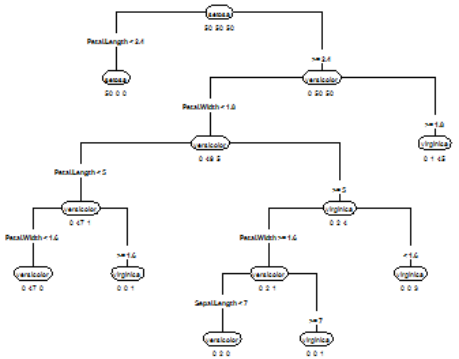

Too simple

Prune at cp = 0.02




**Just right**

Prune at cp = 0.005



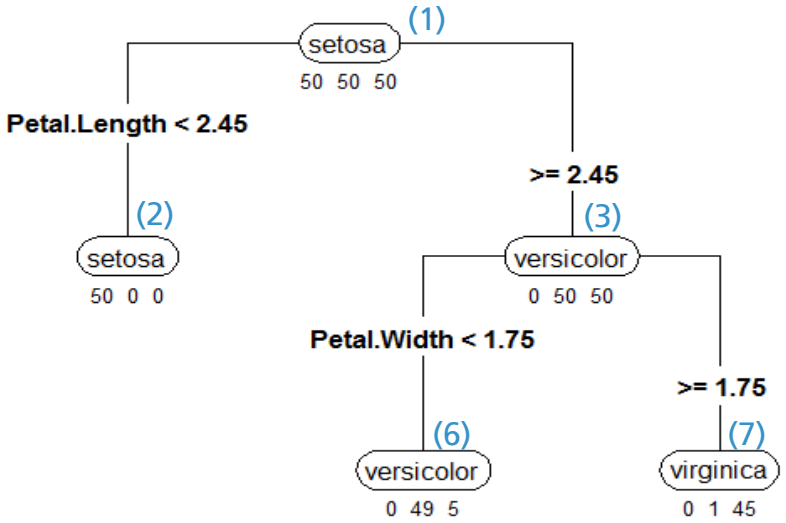
Too complex

Source: UBS Quants

# Trees in R: Create a decision tree

- Here is the R code to create a classification decision tree and the main output:

```
library(rpart)
myTree = rpart(Species ~., data=iris)
```




Source: UBS Quants

```
1) root 150 100 setosa (0.33 0.33 0.33)
  2) Petal.Length< 2.45 50   0 setosa (1.00 0.00 0.00) *
  3) Petal.Length>=2.45 100  50 versicolor (0.00 0.50 0.50)
    6) Petal.Width< 1.75 54   5 versicolor (0.00 0.91 0.09) *
    7) Petal.Width>=1.75 46   1 virginica (0.00 0.02 0.98) *
```

Node

Split

# of the data-points which go through that node

# of the data-points which are *incorrectly* predicted

Predicted classification

Breakdown of actual classifications at that node

Is this a leaf?

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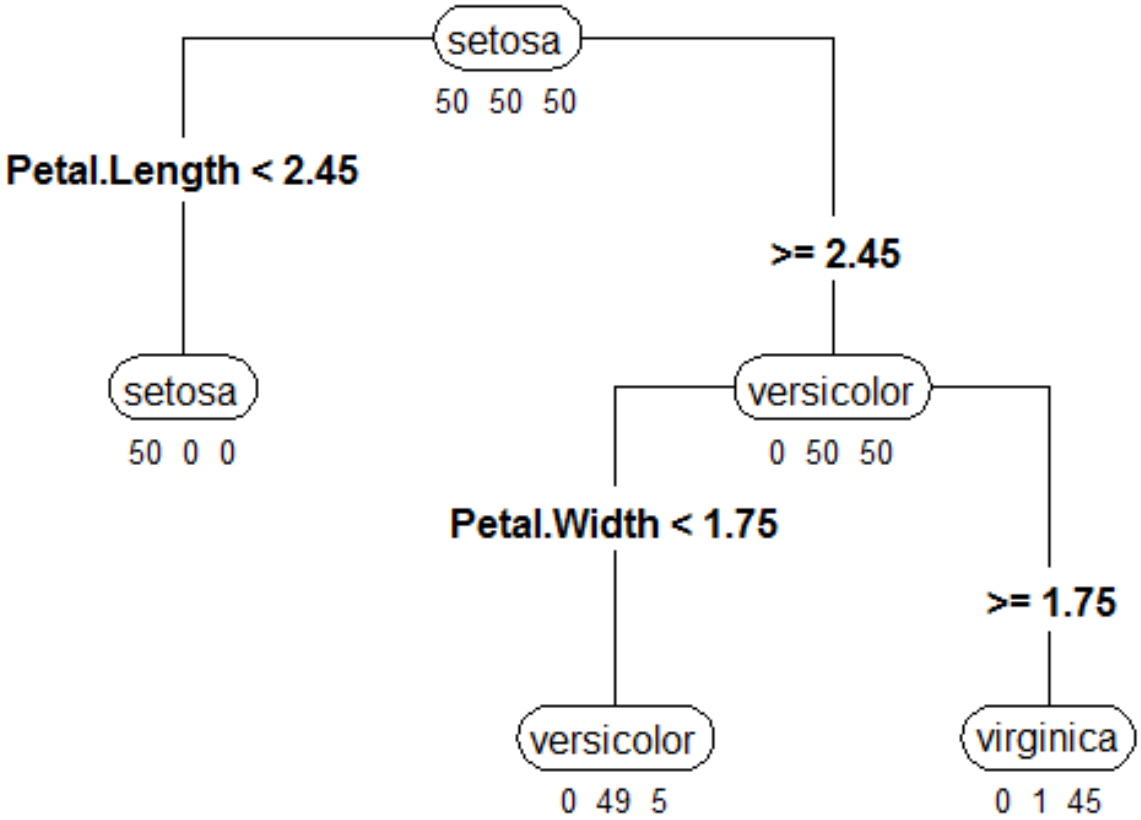
# Trees in R: Plot the tree

Simple plot

```
plot(myTree)
text(myTree)
```

Pretty plot

```
library(rpart.plot)
prp(myTree, type=4, extra=1, varlen=0, under=T, branch=1)
```




Source: UBS Quants

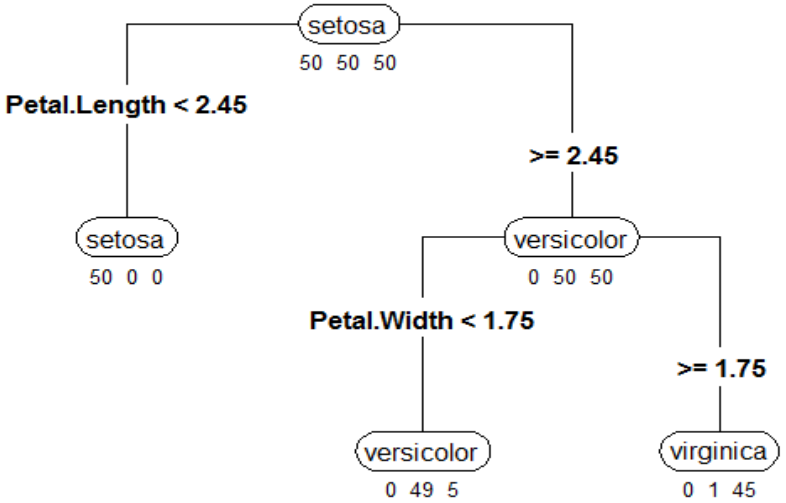
# Trees in R: Use the output

- To use your tree for predicting, put your out of sample data into the same format as your training data and use the prediction function:

```
x = data.frame(Sepal.Length=5, Sepal.Width=3.8, Petal.Length=2.5, Petal.Width=2.5)
predict(myTree, x)
```

```
  setosa versicolor virginica
1      0      0.022     0.978
```

- You get the vector of probabilities for each classification from the node of the tree that that data-point falls into.




Source: UBS Quants

Section 2

# Machine Learning Theory

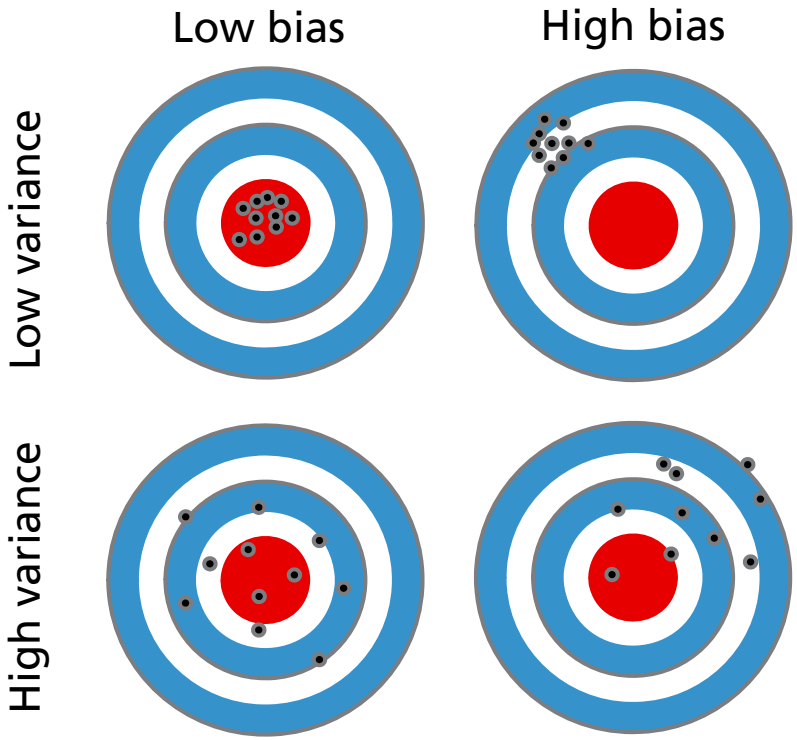
# Bias vs Variance (1)

- The **bias** is the difference between the expected prediction of the model and the correct value we are trying to predict.

  e.g. if you predict election outcomes from a survey of homeowners, the model will have high bias.

- The **variance** is how much the predictions for a given point vary between different realisations of the model.

  e.g. if you predict election outcomes from a survey of 20 people the model will have high variance.




Source: UBS Quants

# Bias vs Variance (2)

- There is typically a trade-off between bias and variance as you increase the model's complexity.

  e.g. suppose you fit a polynomial relationship between x and y with 100 data-points. As you increase the degree of the polynomial, you will decrease the bias, but increase the variance.

- If you over-fit a model you can expect to see low bias, but high variance.
- If you under-fit a model you can expect to see high bias but low variance.

- The total error on a model can be expressed as the sum of the variance and the bias$^2$, so finding the best model amounts to finding the sweet spot between variance and bias.
- Analysts often obsess over reducing bias, but variance is an equally important a source of error.

# Ensemble learning (1)

- Ensemble learning means combining a large number of simple models (often called "weak learners") to create an overall model. Typically we combine the simple models using the average or majority forecast from each model.
- Provided each simple model has better accuracy than random guessing and the models are diverse, then combining models should improve performance.
- Two of the most popular approaches are:

| **Bagging**<br>***B***ootstrap ***Agg***regat***ing*** | **Boosting** |
|---|---|
| Each model is created **independently**. This makes bagging parallelisable. | The models are created **iteratively**, so that a model focuses on forecasting the data instances which were misclassified by previous models. |
| Each model's forecast is treated equally. | Models' forecasts are weighted by their accuracy. |
| Works by reducing variance. So bagging is particularly useful for combining high variance, low bias models, such as over-fitted trees. | Works by reducing both variance and bias. So boosting is commonly used with high bias models e.g. 1-level trees ("stumps") |
| Example = Random forests | Example = adaBoost |

# Ensemble learning (2)

- Dietterich describes three conceptual reasons why ensembles can improve the performance of weak learners in his paper "Ensemble Methods in Machine Learning":
- Statistical

  When you have limited data, there are many different models which give similar accuracy on the training set. Using an ensemble allows you to reduce the risk of choosing the wrong model.
- Computational

  Many learning algorithms work by a local search, which can lead to them getting stuck in local optima. An ensemble approach allows you to try out multiple different start points which reduces this risk.
- Representational

  Sometimes by combining models you can produce hypotheses which are not available from individual models

  e.g. a decision tree will struggle to classify a diagonal boundary. The tree would have to be enormous to approximate it with any degree of accuracy. However, even a fairly small combination of trees can get a good approximation quickly.

Section 3

# Random Forests

# Overview of random forests (1)

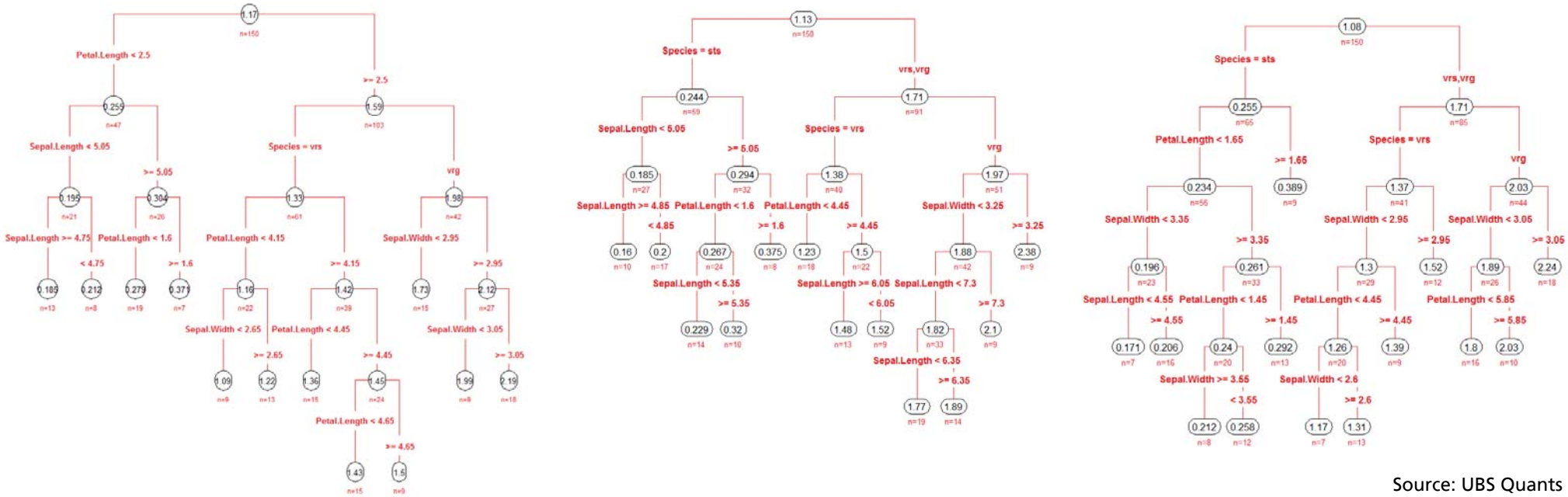
- Random forests (Breiman, 1999) is a bagging algorithm which uses decision trees.
- In brief, a random forest is a large collection of trees, with two additional sources of randomness.
- For each tree in the forest:
  1. Start with a bootstrap sample of the data.
  2. At each node, select M of the available features at random. Find the best feature and threshold to use at this node.
     - In R, the default value for M is set to √(# of variables).
  3. Continue this process with each of the two sub-groups until you have completely grown the tree out and each node is homogenous.

  Repeat until you have a large number of completely grown out trees (default in R is 500 but if there are a large number of variables in your dataset you may choose to increase that.)
- This gives us two sources of randomness; the bootstrap sample and the random selection of features at each node.

# Overview of random forests (2)

- To use the forest for prediction, you take the prediction from each of the individual trees and combine them with a majority vote.

Tree 1, Tree 2, …., Tree 500




Source: UBS Quants

# Why should a forest be better than a tree?

Intuitive argument:

- If you have multiple (somewhat independent) models with different pieces of useful information, then choosing just one of them, even if it is the best, means throwing away some of that information.
- If you instead combine models, you can keep the insights from all the models, which should produce a stronger, more robust overall model.

Bias vs Variance argument:

- In a random forest, the bias of the forest is equal to the bias of an individual (overgrown) tree, but the variance of the forest is much smaller than the variance of an individual tree, so the overall error is much lower.
- We ensure that each individual tree has low correlation to its peers by allowing them to grow all the way out, using bootstrap sampling and using random feature selection, so that the variance decreases more rapidly.

# Importance

- A random forest can also tell us which of our features is most important:
  - For each feature, we look across all the trees and find every node which uses that feature.
  - Then we compute how much each node which uses that feature decreases the Gini impurity.
  - We take the average.
- A higher value indicates the feature is very effective at distinguishing between classes and a lower value indicates the feature is less effective.
- In R, there is a function to do this automatically: `importance(myForest)`

| | MeanDecreaseGini |
|---|---|
| Sepal.Length | 9.9726 |
| Sepal.Width | 2.3978 |
| Petal.Length | 43.7739 |
| Petal.Width | 43.1792 |

Source: UBS Quants

- It can be helpful to use random forests to order a list of features to understand your data better, even if you then go on to use a different model.
- Be careful though; this statistic does not take into account the correlation between features. Two very highly correlated features will have similar importance, but there is little to be gained from including both in your model.

# Pros and cons of the random forests

## Pros

- Much more effective than an single decision tree.
- Very little pre-processing of your signals is required. Random forests can handle outliers, non-normal inputs and both categorical and continuous inputs.
- Easy to parallelise which allows for faster runtimes.
- Identifies important signals, which is helpful when you build other models.

## Cons

- Random forests are (to some extent) a black box. They are far harder to interpret and communicate than a simple decision tree.
- Can still struggle with severe class imbalances
- Random forests can struggle to generalise to new data if it lies outside the range of data it was trained on
  - e.g. if you are modelling the effect of inflation on equity returns and there is no deflationary period in your data, the model will probably not perform well at forecasting for deflationary periods.
- Random forests tend to be biased towards continuous variables or categorical variables with lots of splits.

# Random Forests: forecasting dividend cuts (1)

The problem:

- Forecast which stocks in the Russell 1000 will cut their dividend by more than 5% in the next 12 months
  - 5% requirement reduces "noise"
  - We only use ordinary dividends per share (no special dividends or stock dividends etc.)
  - We exclude firms which have had large corporate actions in the 12m before the ex-div date.

The features:

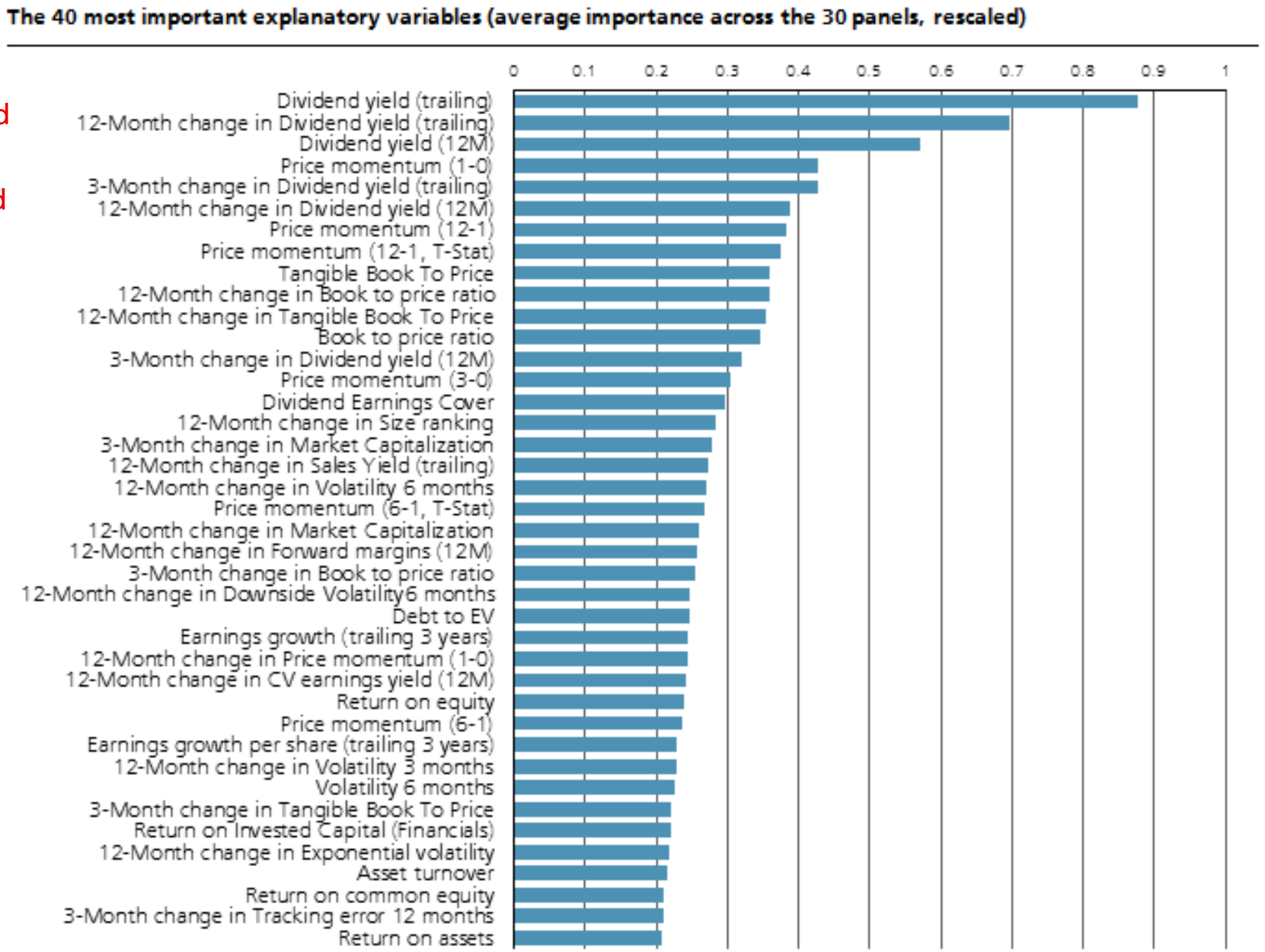
- We selected 116 factors from our daily factor database and supplemented each variable with its 3-month and 12-month changes. In total this gives us 348 explanatory variables
  - The model does not include information about the companies' dividend policies nor does it attempt to forecast changes in dividend policies
- We use 7 year rolling windows for the analysis
  - There are secular changes in dividend yields, so an expanding window is misleading
  - For long periods of time, almost no stocks cut their dividends so you need a long window.

The model:

- Random Forest with 2000 decision trees.

# Random Forests: forecasting dividend cuts (2)

1. Dividend yield
2. Changes in dividend yield
3. Price momentum
4. Book to price
5. Dividend cover
6. Debt to Enterprise Value
7. Historic earnings growth
8. Profitability
9. Volatility




Source: UBS Quantitative Research

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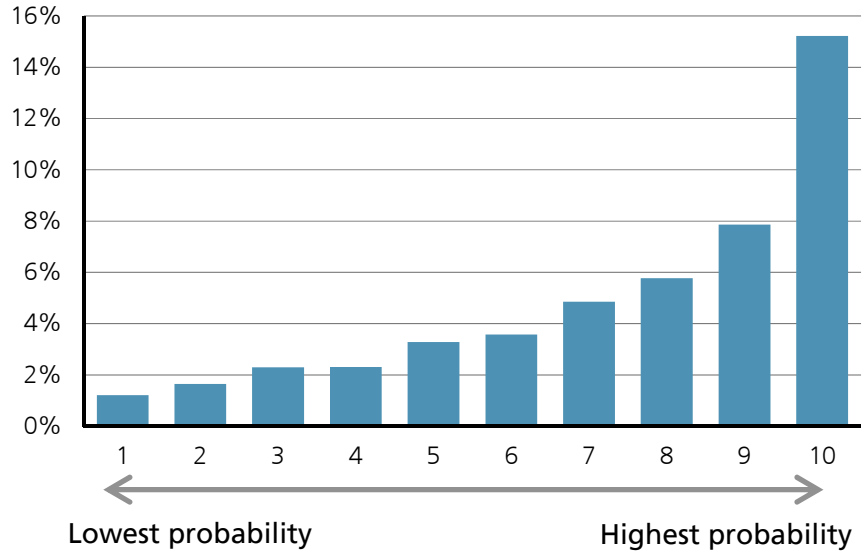
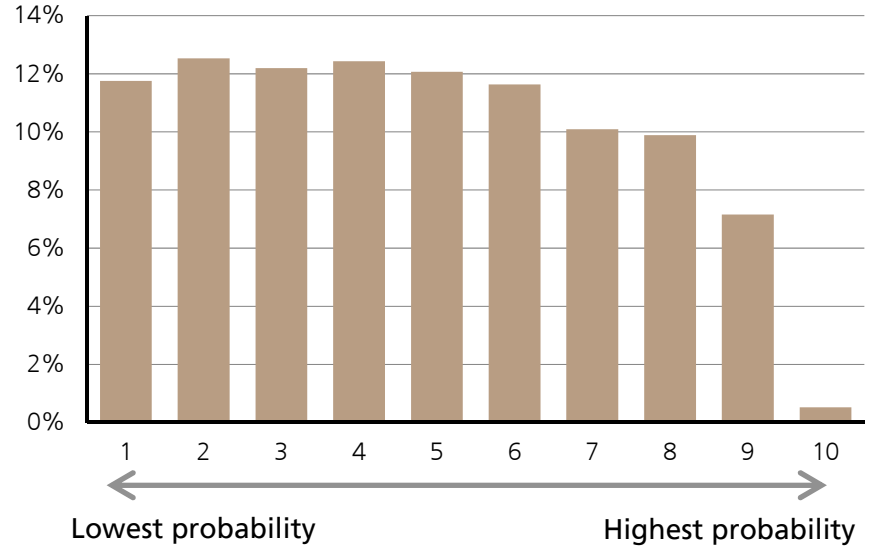
# Random Forests: forecasting dividend cuts (3)

**Proportion of dividend reduction in each decile**




Source: UBS Quantitative Research. US largest 1000 stocks.

**Average DPS growth rate in each decile**




Source: UBS Quantitative Research. Trimmed average. US largest 1000 stocks.

- More than 15% of the companies with the highest estimated likelihood of a dividend cut ended up reducing their dividends compared to just 4.8% across all the deciles.
- The companies with the highest expected probability of a dividend cut grew their dividend per share by an average of less than 2.8% over the following 12 months compared to an average growth rate of more than 10% across all the companies.

# Random forests in R: Create a forest

- Here is the R code to create a simple classification random forest and the main output:

```
library(randomForest)
myForest = randomForest(Species ~., data=iris)
```

```
Call:
 randomForest(formula = Species ~ ., data = iris)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 2

        OOB estimate of  error rate: 5.33%
Confusion matrix:
           setosa versicolor virginica class.error
setosa         50          0         0        0.00
versicolor      0         47         3        0.06
virginica       0          5        45        0.10
```

**Out-of-bag estimate of error rate**

For each entry $X_i$ in the dataset, predict that $y_i$ using only the trees which do not include $(X_i, y_i)$. Find the error.

**Confusion matrix**

This shows how the training data would be classified / misclassified by the out-of-bag estimation.

Source: UBS Quants

# Random forests in R: Use the output

- To use your random forest for predicting then, just as before, put your out of sample data into the same format as your training data and use the predict function:

```
x = data.frame(Sepal.Length=5, Sepal.Width=3.8, Petal.Length=2.5, Petal.Width=2.5)
predict(myForest, x, "prob")
```

```
  setosa versicolor virginica
1   0.21      0.392     0.398
```

Source: UBS Quants

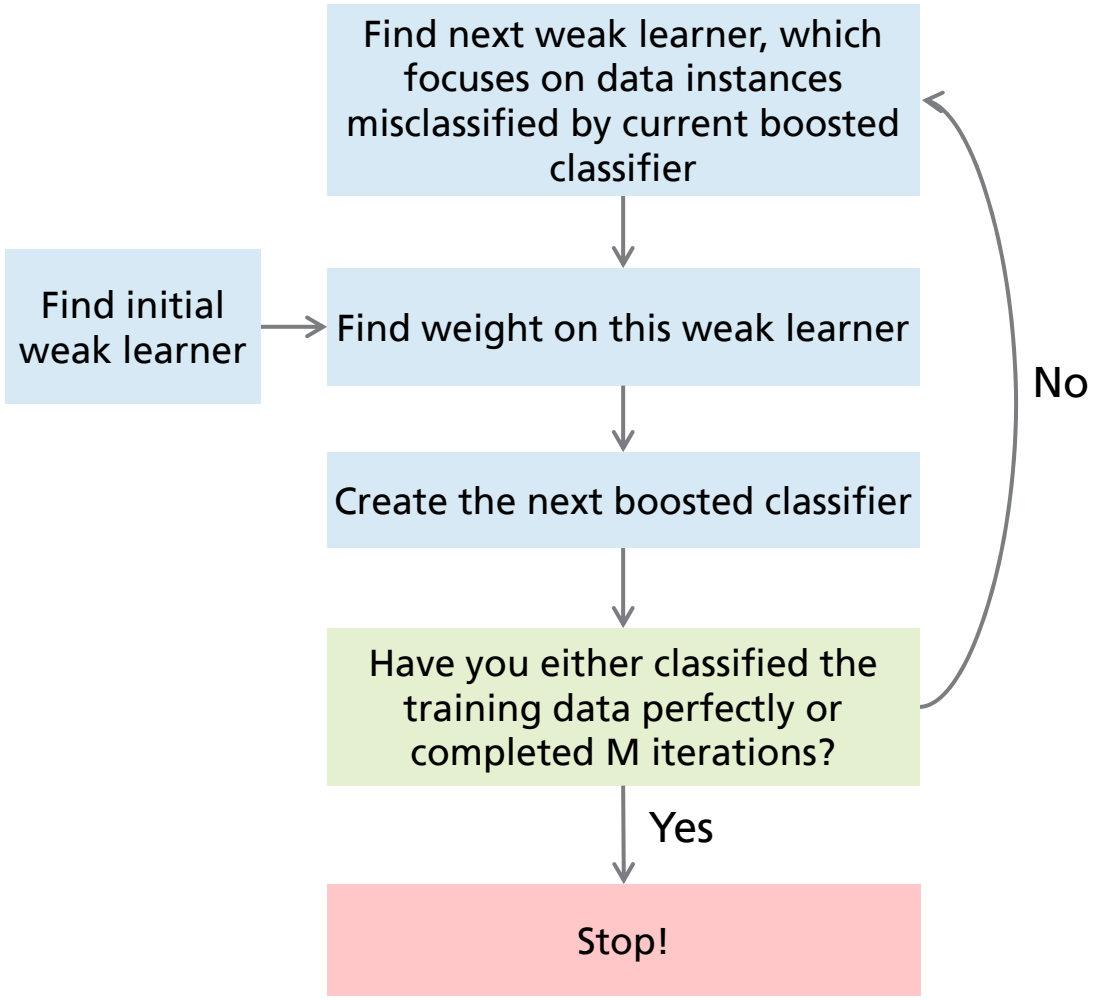
- Once again, you get the vector of probabilities for each classification.

Section 4

# AdaBoost

# AdaBoost: algorithm in words

- AdaBoost is a boosting algorithm which often (but not always) uses decision trees.
- There are many variants of AdaBoost, but we will focus on the basic, most common version.
- We *iteratively* create a series of weak classifiers (often decision trees which are constrained to have only one node) on the dataset.
- As we go, we create a boosted classifier made up of a *linear combination* of all the weak classifiers so far.
- Each new weak model is built to be expert at instances handled incorrectly by the current boosted classifier.




Source: UBS Quants

# AdaBoost: algorithm in maths

- Some definitions:
  - $w_i$ is the weight of data instance i.
  - $\kappa_m$ is the m$^{th}$ weak classifier. This is often a heavily pruned decision tree.
  - $\alpha_m$ is the weight of the m$^{th}$ weak classifier in the boosted classifier
  - $C_m$ is the m$^{th}$ boosted classifier. This is defined as a linear combination of the weak classifiers so far:

$$C_m(x_i) = \alpha_1\kappa_1(x_i) + \cdots + \alpha_m\kappa_m(x_i)$$

Start with equal weights

Initialise the weights, so that $w_i = 1$ for all i

For m in 1 to M:

Each new weak classifier focuses on data instances with bigger weights - those currently being misclassified

Find the weak classifier, $\kappa_m$, which minimises the weighted error:

$$error = \sum_{i:\, \kappa_m(x_i) \neq y_i} w_i \Big/ \sum_{i=1}^{N} w_i$$

Weak classifiers with smaller weighted errors will have a bigger impact on the boosted classifier

Define $\alpha_m = \frac{1}{2}\ln(\frac{1-error}{error})$

Define $C_m$, the m$^{th}$ boosted classifier as $C_m(x_i) = \alpha_1\kappa_1(x_i) + \cdots + \alpha_m\kappa_m(x_i)$

Give greater weight to data instances which are misclassified by the boosted classifier

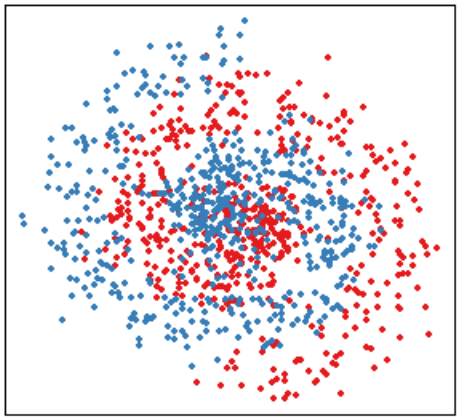
Update the weights so that $w_i = \exp(-y_i C_m(x_i))$ for all i

End

Source: UBS Quants

# AdaBoost: algorithm in pictures

Start with equal weights

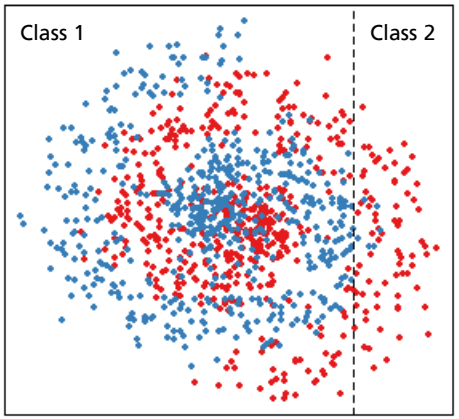


Find the first weak classifier, $\kappa_1$

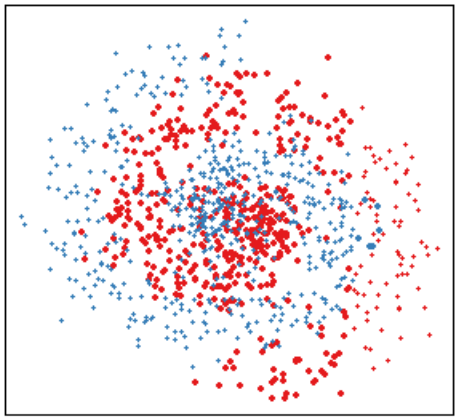
Weighted error = 43%

$\alpha_1 = 0.13$

$C_1 = 0.13\kappa_1$




Update the weights so that misclassified data instances get greater weights.



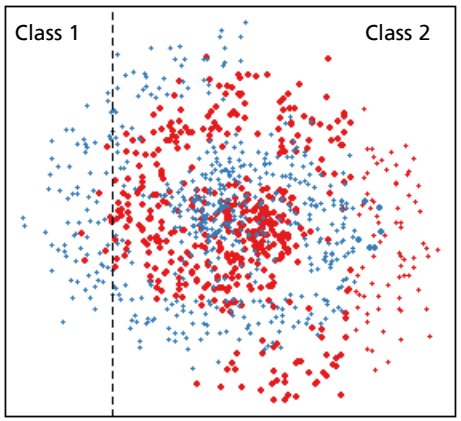
Find the second weak classifier, $\kappa_2$

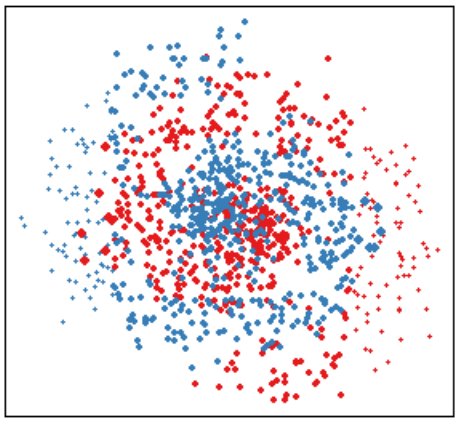
Weighted error = 39%

$\alpha_2 = 0.22$

$C_s = 0.13\kappa_1 + 0.224\kappa_2$

Update the weights so that misclassified data instances get greater weights.



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Source: UBS Quants

# Pros and cons of AdaBoost

## Pros

- Very robust to data inputs – doesn't need to be normal or continuous
- Unlikely to over-fit
- Can reduce both bias and variance

## Cons

- Very sensitive to incorrect classification of data in its training set.
- Sometimes struggles with very noisy data.
- Cannot be run in parallel.

# AdaBoost in R: Create your model

- Here is the R code to create an adaBoost model. Currently the package ada only supports classification problems with two classes.

```
library(ada)
myAdaBoost = ada(Species~., data=subset(iris, Species!='setosa'))
```

```
Call:
ada(Species ~ ., data = subset(iris, Species != "setosa"))
Loss: exponential Method: discrete   Iteration: 50


Final Confusion Matrix for Data:
            Final Prediction
True value   versicolor virginica
  versicolor         47         3
  virginica           2        48


Train Error: 0.05
Out-Of-Bag Error:  0.04  iteration= 11
```

Confusion matrix

This shows how the training data would be classified / misclassified.

Error estimates

Source: UBS Quants

Section 5

# Machine Learning Horse Race

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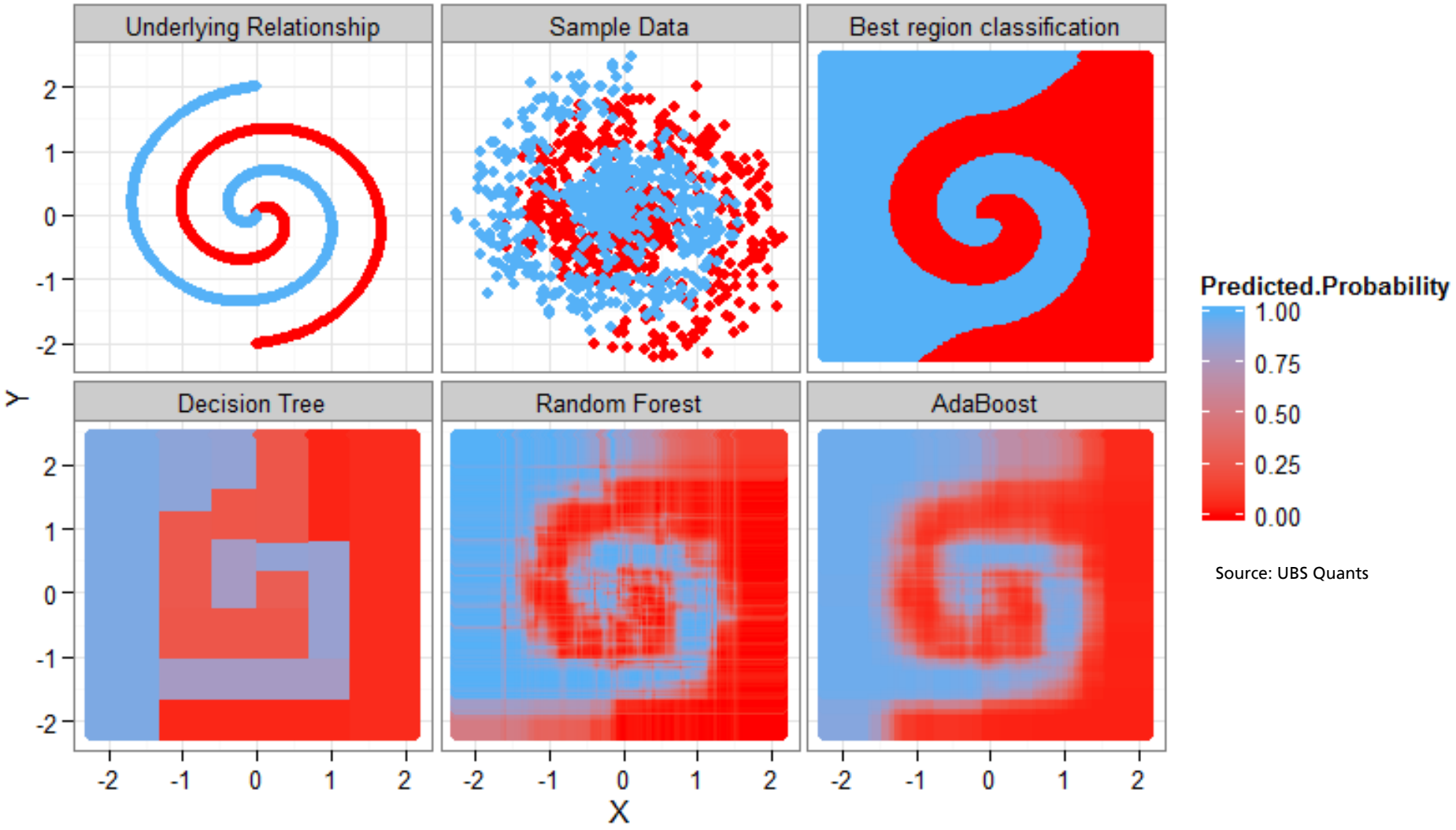
# Machine learning horse race




Source: UBS Quants

| | Decision Tree | Random forest | AdaBoost |
|---|---|---|---|
| Out of sample accuracy | 70% | 76% | 76% |
| Time taken | 0.05 secs | 0.435 secs | 0.863 secs |

Source: UBS Quants

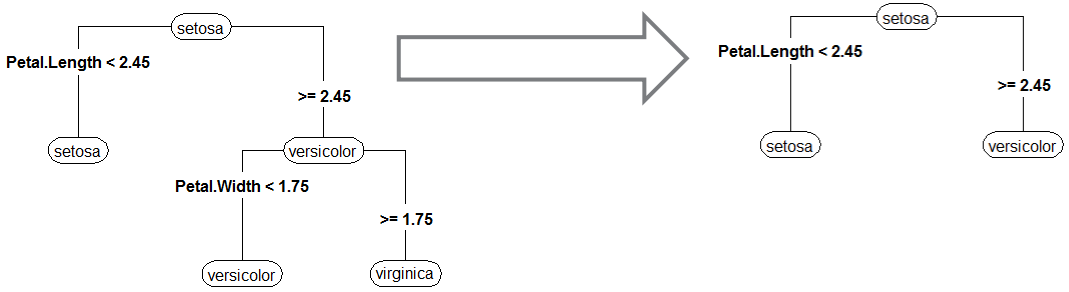
Section 6

# Appendix

# Over-fitting: Optional extra details (1)

First some definitions:

- A sub-tree of a tree T is any smaller tree you can make by pruning one or more nodes, for example:




- The big, over-grown tree which is step 1 in R's process is called $T_{max.}$
- We define: $\mathbf{R_\alpha(T)} = \%\ \text{of errors} + \alpha \times \#\ \text{of leaves}$

  And: $\mathbf{T_\alpha} = \text{subtree of } T_{Max} \text{ which minimises } R_\alpha(T_\alpha)$
- As you increase alpha, so you penalise bigger trees more, you get a series of nested sub-trees of decreasing complexity. This series is finite and one of these trees will be our optimal tree.
- $T_0$ is simply $T_{max}$, the fully grown tree, and for large enough $\alpha$, $T_\alpha$ will be the minimal tree with no splits (just the root).

# Over-fitting: Optional extra details (2)

- We use cross-validation to find the best alpha to use and hence the best sub-tree which has both a good fit and is parsimonious.

- First: Divide the data into 10 sub-sets $X_1$ … $X_{10}$.

  For i in 1 to 10

  > Our data-set is all the data except $X_i$ i.e. nine-tenths of the full data-set.
  >
  > Find $T_{max}$, the (overgrown) tree for this data-set.
  >
  > For any alpha
  >
  > > Find $T_\alpha$, the sub-tree of $T_{max}$ which minimises the error adjusted for complexity
  > >
  > > $$R_\alpha(T_\alpha) = \%\ \text{of errors} + \ \alpha \times \#\ \text{of leaves}$$
  > >
  > > Then, using the out-of-sample data $X_i$ find $R_\alpha(T_\alpha)$
  >
  > End

  End

- Then: For any alpha

  > Find the average out-of-sample value of the error adjusted for complexity, $R_\alpha(T_\alpha)$.

  End

  The "best" alpha is the one with the smallest average.

- Finally: Use all of the data, X, to find $T_{max}$ (the overgrown tree).

  Then, using the best alpha, find $T_\alpha$, the sub-tree of $T_{max}$ which minimises $R_\alpha(T_\alpha)$

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