Hands-on Machine Learning with R - Module 2

Hands-on webinar

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hands-on-machine-learning-R-module-2 | January 14 & 21, 2021

Prologue

Introduction

Course

https://github.com/katrienantonio/hands-on-machine-learning-R-module-2

The course repo on GitHub, where you can find the data sets, lecture sheets, R scripts and R markdown files.

Us

- ✓ katrien.antonio@kuleuven.be & roel.henckaerts@kuleuven.be
- (Katrien) Professor in insurance data science
- (Roel) PhD student in insurance data science

Checklist

☑ Do you have a fairly recent version of R?

```
version$version.string
## [1] "R version 4.0.3 (2020-10-10)"
```

☑ Do you have a fairly recent version of RStudio?

```
RStudio.Version()$version
## Requires an interactive session but should return something like "[1] '1.3.1093'"
```

☑ Have you installed the R packages listed in the software requirements?

or

☑ Have you created an account on RStudio Cloud (to avoid any local installation issues)?

Why this course?

The goals of this module

- develop foundations of working with regression and decision trees
- step from simple trees to ensembles of trees, with **bagging** and **boosting**
- focus on the use of these ML methods for the analysis of frequency + severity data
- discuss and construct some useful interpretation tools, e.g. variable importance plots, partial dependence plots.

Module 2's Outline

Prologue

Decision tree

- what is tree-based machine learning?
- tree basics: structure, terminology, growing process
- using {rpart}
- pruning via cross-validation
- examples on regression and classification
- modelling claim frequency and severity data with trees

• Interpretation tools

- feature importance
- partial dependence plot
- the {vip} and {pdp} packages

Bagging

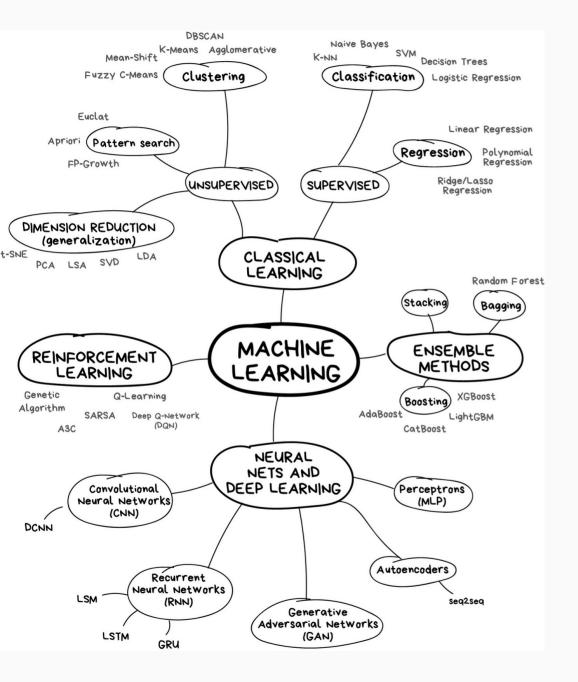
- from a single tree to Bootstrap Aggregating
- out-of-bag error

Random forest

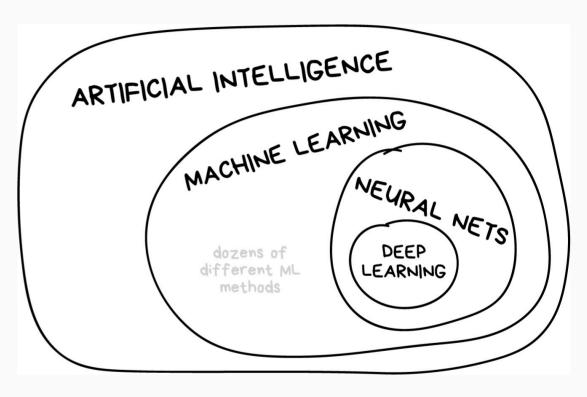
- from bagging to random forests
- tuning

Gradient boosting

- (stochastic) gradient boosting with trees
- training process and tuning parameters
- using {gbm}
- modelling claim frequencies and severities
- using {xgboost}



Some roadmaps to explore the ML landscape...



Source: Machine Learning for Everyone In simple words. With real-world examples. Yes, again.

Background reading



Henckaerts et al. (2020) paper on Boosting insights in insurance tariff plans with tree-based machine learning methods

- full algorithmic details of regression trees, bagging, random forests and gradient boosting machines
- with focus on claim frequency and severity modelling
- including interpretation tools (VIP, PDP, ICE, H-statistic)
- model comparison (GLMs, GAMs, trees, RFs, GBMs)
- managerial tools (e.g. loss ratio, discrimination power).

The paper comes with two notebooks, see examples tree-based paper and severity modelling.

The paper comes with an R package for fitting random forests on insurance data, see distRforest.

What is tree-based machine learning?

Machine learning (ML) according to Wikipedia:

"Machine learning algorithms build a **mathematical model** based on sample data, known as training data, in order to make predictions or decisions without being explicitly programmed to perform the task."

This definition goes all the way back to Arthur Samuel, who coined the term "machine learning" in 1959.

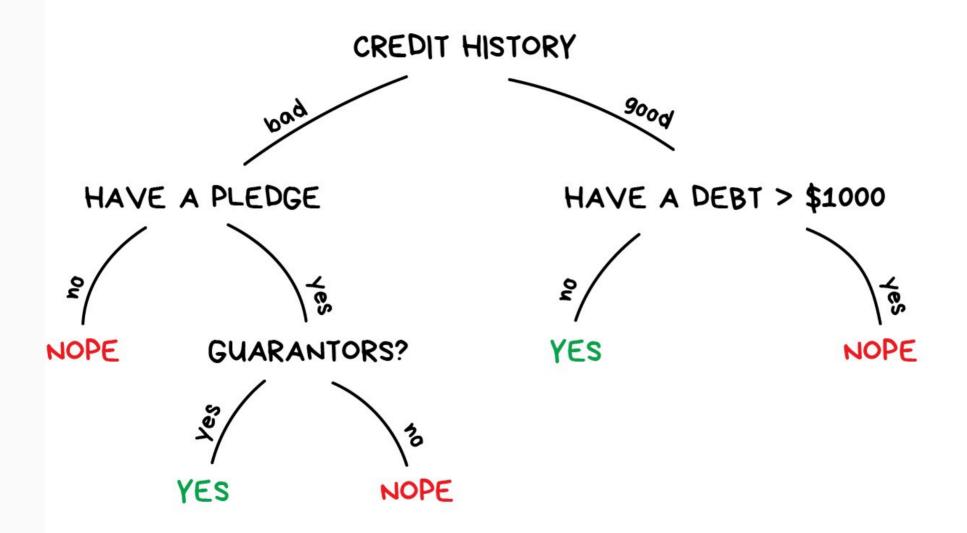
Tree-based ML makes use of a tree as building block for the mathematical model.



So, a natural question to start from is: what is a **tree**?

Tree basics

GIVE A LOAN?



Tree structure and terminology

The top of the tree contains all available training observations: the **root node**.

We partition the data into homogeneous non-overlapping subgroups: the nodes

We create subgroups via simple yes-no questions.

A tree then predicts the output in a **leaf node** as follows:

- average of the response for regression
- majority voting for classification

Tree structure and terminology

The top of the tree contains all available training observations: the root node.

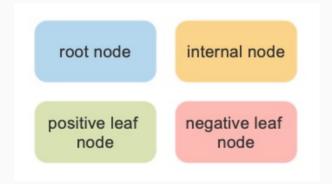
We partition the data into homogeneous non-overlapping subgroups: the nodes.

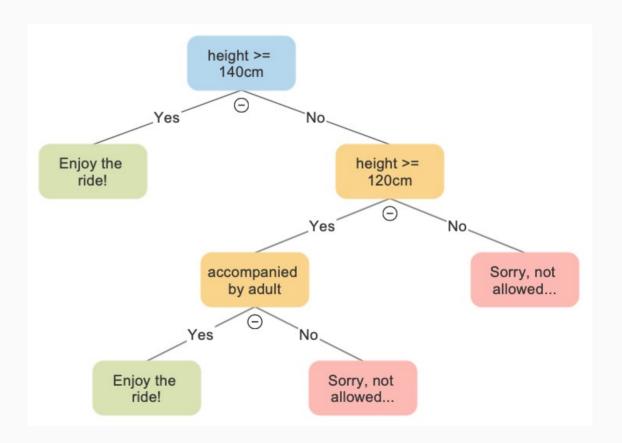
We create subgroups via simple yes-no questions.

A tree then predicts the output in a **leaf node** as follows:

- average of the response for regression
- majority voting for classification.

Different types of nodes:





Tree growing process

A golden standard is the Classification And Regression Tree algorithm: CART (Breiman et al., 1984).

CART uses binary recursive partitioning to split the data in subgroups.

In each node, we search for the best feature to partition the data into two regions: R_1 and R_2 (hence, **binary**).

Take-away ✓ - what is best?

Minimize the **overall loss** between observed responses and leaf node prediction

- overall loss = loss in region R₁ + loss in region R₂
- for regression: mean squared or absolute error, deviance,...
- for classification: cross-entropy, Gini index,...

After splitting the data, this process is repeated for region R_1 and R_2 separately (hence, **recursive**).

Repeat until stopping criterion is satisfied, e.g., maximum depth of a tree or minimum loss improvement.

Using {rpart}

- formula: a formula as response ~ feature1 + feature2 + ...
- N

no need to include the interactions!

- data: the observation data containing the response and features
- method: a string specifying which loss function to use
 - "anova" for regression (SSE as loss)
 - "class" for classification (Gini as loss)
 - "poisson" for Poisson regression (Poisson deviance as loss, see more later)
- cp: complexity parameter specifying the proportion by which the overall error should improve for a split to be attempted
- maxdepth: the maximum depth of the tree
- minsplit: minimum number of observations in a node for a split to be attempted
- minbucket: minimum number of observations in a leaf node.

Toy example of a regression tree

Simulated data

```
library(tidyverse)
set.seed(54321) # reproducibility
dfr \(
\times \text{tibble}(::tibble(
    x = seq(0, 2 * pi, length.out = 500),
    m = 2 * sin(x),
    y = m + rnorm(length(x), sd = 1)
    )
}
```

```
## 1 0.00000000 0.00000000 -0.1789007

## 2 0.01259155 0.02518244 -0.9028617

## 3 0.02518311 0.05036089 -0.7336728

## 4 0.03777466 0.07553136 -1.5750691

## 5 0.05036621 0.10068985 -0.3073767

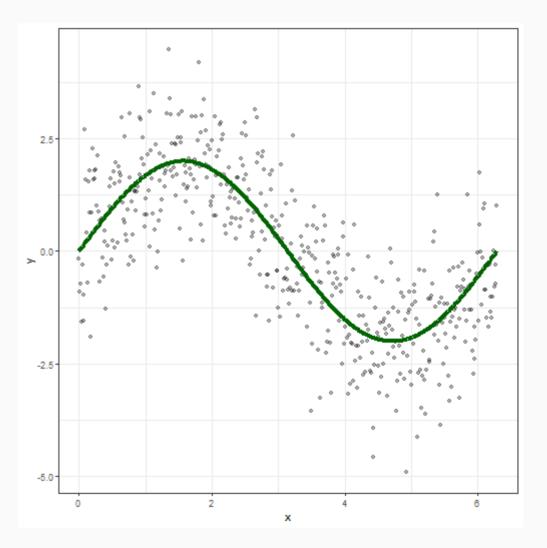
## 6 0.06295777 0.12583237 -0.9696970

## 7 0.07554932 0.15095495 -1.5412872

## 8 0.08814088 0.17605359 2.6920994

## 9 0.10073243 0.20112432 1.5964765

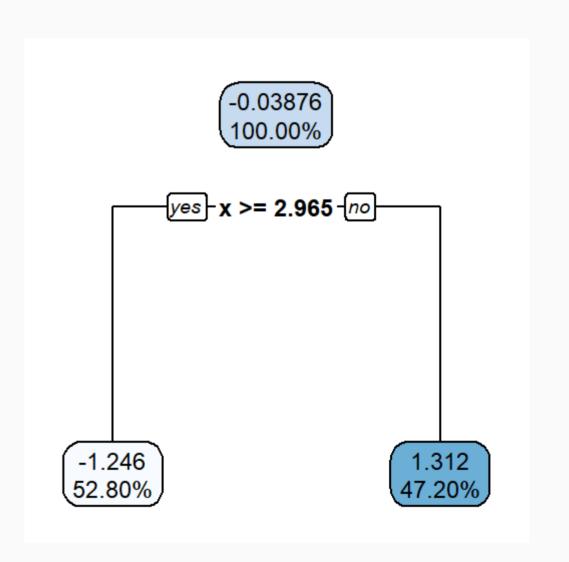
## 10 0.11332398 0.22616316 0.4061405
```



Decision stump - a tree with only one split

```
library(rpart)
fit \leftarrow rpart(formula = y \sim x,
             data = dfr,
             method = 'anova',
             control = rpart.control(
               maxdepth = 1
print(fit)
\#\# n = 500
##
## node), split, n, deviance, yval
    * denotes terminal node
   1) root 500 1498.4570 -0.03876172
    2) x ≥ 2.965311 264 384.3336 -1.24604800 *
   3) x< 2.965311 236 298.8888 1.31176200 *
```

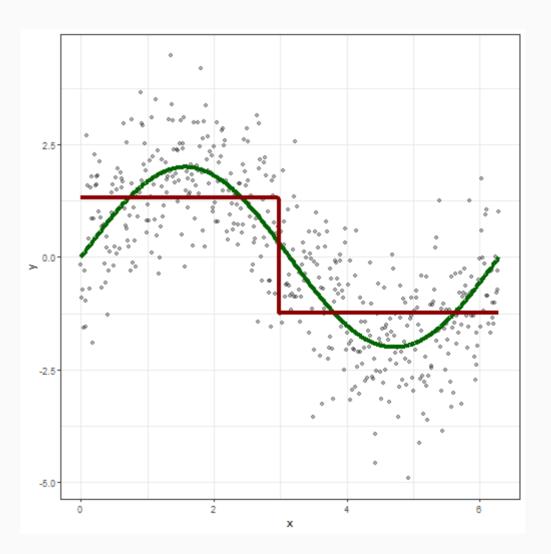
```
library(rpart.plot) # for nice plots
rpart.plot(fit, digits = 4, cex = 2)
```



Decision stump - a tree with only one split

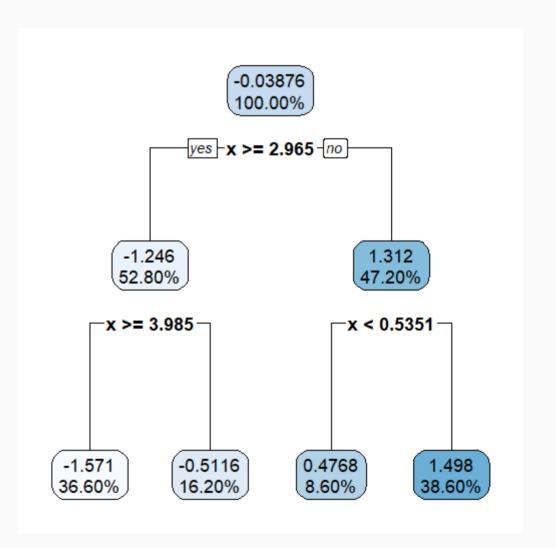
```
fit \leftarrow rpart(formula = y \sim x,
             data = dfr,
             method = 'anova',
             control = rpart.control(
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print(fit)
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     2) x ≥ 2.965311 264 384.3336 -1.24604800 *
    3) x< 2.965311 236 298.8888 1.31176200 *
```

```
# Get predictions via the predict function
pred ← predict(fit, dfr)
```



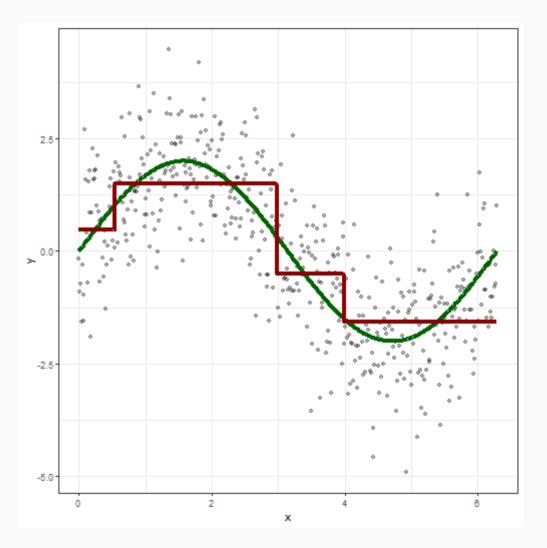
Adding splits

```
fit \leftarrow rpart(formula = y \sim x,
             data = dfr.
             method = 'anova',
             control = rpart.control(
               maxdepth = 2
print(fit)
\#\# n = 500
## node), split, n, deviance, yval
        * denotes terminal node
   1) root 500 1498.45700 -0.03876172
    2) x \ge 2.965311 264 384.33360 -1.24604800
     4) x ≥ 3.985227 183 228.44490 -1.57111200 *
      5) x < 3.985227 81 92.86428 -0.51164310 *
     3) x< 2.965311 236 298.88880 1.31176200
     6) x< 0.535141 43 55.23637 0.47680020 *
      7) x \ge 0.535141 193 206.99550 1.49779000 *
```



Adding splits (cont.)

```
fit \leftarrow rpart(formula = y \sim x,
             data = dfr.
             method = 'anova',
             control = rpart.control(
               maxdepth = 2
print(fit)
\#\# n = 500
  node), split, n, deviance, yval
         * denotes terminal node
   1) root 500 1498.45700 -0.03876172
     2) x \ge 2.965311 264 384.33360 -1.24604800
      4) x ≥ 3.985227 183 228.44490 -1.57111200 *
      5) x < 3.985227 81 92.86428 -0.51164310 *
     3) x< 2.965311 236 298.88880 1.31176200
     6) x< 0.535141 43 55.23637 0.47680020 *
      7) x \ge 0.535141 193 206.99550 1.49779000 *
```





Your turn

Let's get familiar with the structure of a decision tree.

Q: choose one of the trees from the previously discussed examples and pick a leaf node, but keep it simple for now.

- 1. Replicate the **predictions** for that leaf node, based on the split(s) and the training data.
- 2. Replicate the **deviance** measure for that leaf node, based on the split(s), the training data and your predictions from Q1.

Hint: the deviance used in an anova {rpart} tree is the **Sum of Squared Errors (SSE)**:

$$ext{SSE} = \sum_{i=1}^n (y_i - \hat{f}\left(x_i
ight))^2,$$

Take for example the tree with depth two:

```
print(fit)
## n= 500
##

## node), split, n, deviance, yval
## * denotes terminal node
##

## 1) root 500 1498.45700 -0.03876172
## 2) x ≥ 2.965311 264 384.33360 -1.24604800
## 4) x ≥ 3.985227 183 228.44490 -1.57111200 *
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## 3) x < 2.965311 236 298.88880 1.31176200
## 3) x < 2.965314 43 55.23637 0.47680020 *
## 7) x ≥ 0.535141 193 206.99550 1.49779000 *</pre>
```

Let's predict the values for leaf node 6.

Q.1: calculate the prediction

```
# Subset observations in node 6
obs ← dfr %>% dplyr::filter(x < 0.535141)

# Predict
pred ← obs$y %>% mean
pred
## [1] 0.4768002
```

Q.2: calculate the deviance

```
# Deviance
dev ← (obs$y - pred)^2 %>% sum
dev
## [1] 55.23637
```

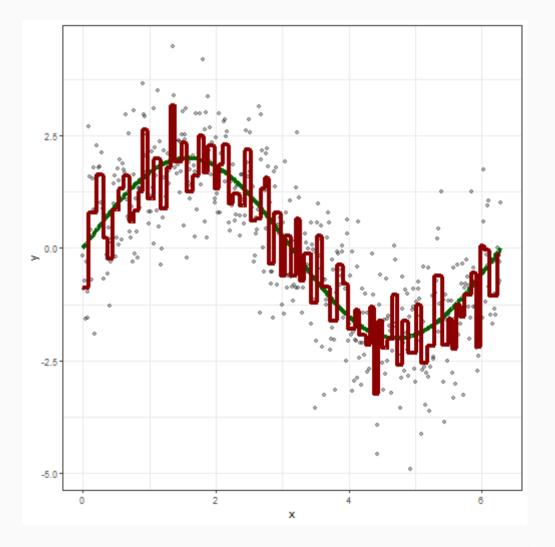
A very deep tree

```
fit \leftarrow rpart(formula = y \sim x,
              data = dfr,
              method = 'anova',
              control = rpart.control(
                maxdepth = 20,
                minsplit = 10,
                minbucket = 5,
                CD = 0
```

Take-away - understanding the cp

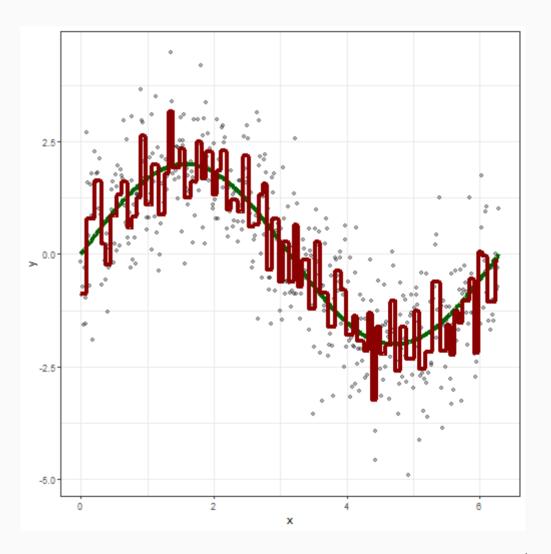
parameter:

- unitless in {rpart} (different from original CART)
- cp = 1 returns a **root node**, without splits
- cp = 0 returns the **deepest tree possible**, allowed by the other stopping criteria.



A very deep tree (cont.)

What is your opinion on the tree shown on the right?



Pruning via cross-validation in {rpart}

How deep should a tree be?

The bias-variance trade off:

- a **shallow** tree will underfit:
 - bias **1** and variance
- a **deep** tree will overfit:
 - bias **v** and variance
- find right balance between bias and variance!

Typical approach to get the right fit:

- fit an overly complex deep tree
- prune the tree to find the optimal subtree.

How to prune?

How deep should a tree be?

The bias-variance trade off:

- a **shallow** tree will underfit:
 - bias **1** and variance
- a deep tree will overfit:
 - bias **4** and variance **4**
- find right balance between bias and variance!

Typical approach to get the right fit:

- fit an overly complex deep tree
- prune the tree to find the optimal subtree.

How to prune?

Look for the smallest subtree that minimizes a **penalized** loss function:

$$\min\{f_{\mathrm{loss}} + \alpha \cdot |T|\}$$

- ullet loss function $f_{
 m loss}$
- ullet complexity parameter lpha
- ullet number of leaf nodes |T|.

A shallow tree results when lpha is large and a deep tree when lpha is small.

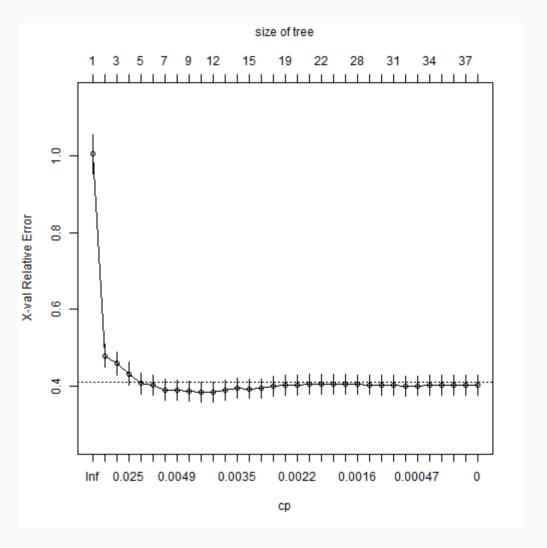
Perform **cross-validation** on the complexity parameter:

- cp is the complexity parameter in {rpart}
- ullet cp is lpha divided by $f_{
 m loss}$ evaluated in root node.

Cfr. tuning of the regularization paramater in lasso from {glmnet} in **Module 1**.

Pruning via cross-validation

```
# Plot the cross-validation results
plotcp(fit)
```



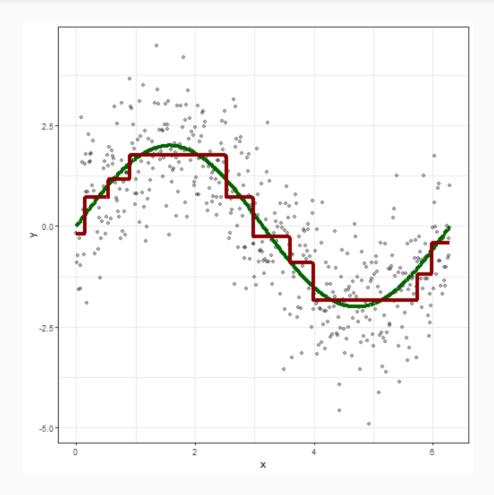
Pruning via cross-validation

```
set.seed(87654) # reproducibility
fit \leftarrow rpart(formula = y \sim x,
              data = dfr.
             method = 'anova',
              control = rpart.control(
               maxdepth = 10.
               minsplit = 20,
               minbucket = 10,
                cp = 0,
                xval = 5
# Get xval results via 'cptable' attribute
cpt ← fit$cptable
```

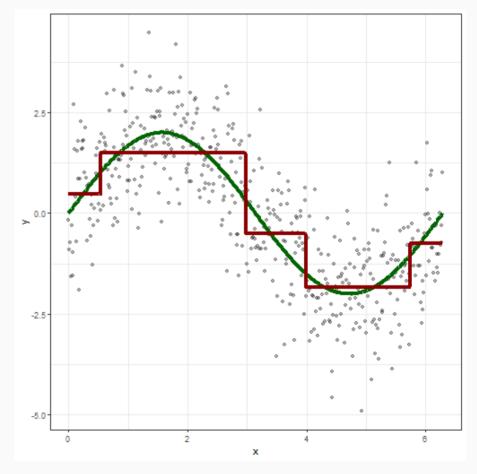
```
CP nsplit rel error
                                   xerror
                                                xstd
     0.54404922
                         1.000000 1.004726 0.0514072
     0.04205955
                         0.455951 0.479691 0.0306899
     0.02638545
                         0.413891 0.459565 0.0303987
     0.02446313
                         0.387506 0.432619 0.0288631
     0.01686947
                         0.363043 0.407090 0.0271596
     0.00556730
                         0.346173 0.402555 0.0269263
     0.00537029
                         0.340606 0.390939 0.0263032
     0.00455035
                         0.335236 0.389550 0.0259170
     0.00438010
                         0.330685 0.387857 0.0262972
  10 0.00437052
                         0.326305 0.384689 0.0262569
  11 0.00417651
                         0.317564 0.384689 0.0262569
## 12 0.00413572
                         0.313388 0.389304 0.0264134
  13 0.00288842
                         0.309252 0.394634 0.0263896
  14 0.00248513
                         0.306363 0.393097 0.0255738
## 15 0.00230656
                         0.301393 0.394084 0.0254549
  16 0.00227479
                         0.299087 0.401089 0.0260820
## 17 0.00222192
                         0.296812 0.403132 0.0258395
  18 0.00218218
                         0.294590 0.403132 0.0258395
                         0.292408 0.405123 0.0258289
  19 0.00189012
## 20 0.00177060
                         0.290518 0.405770 0.0258239
```

Minimal CV error or 1 SE rule

fit_1 ← prune(fit, cp = cpt[min_xerr, 'CP'])



fit_2 ← prune(fit, cp = cpt[se_rule, 'CP'])





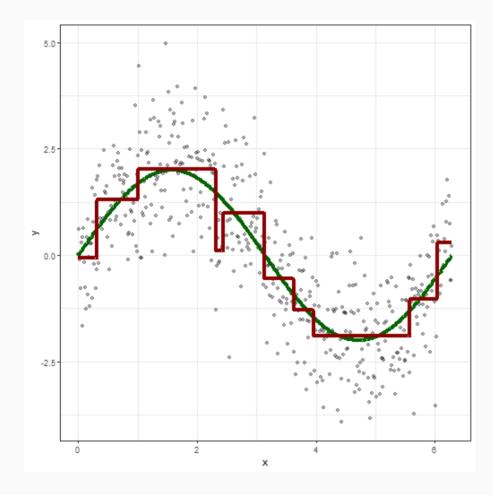
Your turn

- **Q**: Trees are often associated with **high variance**, meaning that the resulting model can be very sensitive to the input data. Let's explore this statement!
 - 1. Generate a second data set dfr2 with a different seed.
 - 2. Fit an optimal tree to this data following the pruning strategy.
 - 3. Can you spot substantial differences with the trees from before?

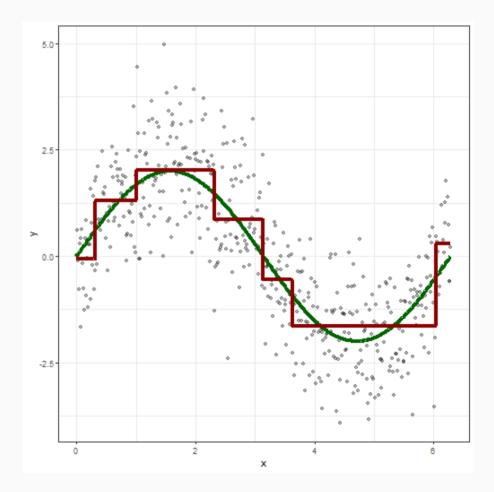
Q.1: a brand new data set

```
# Generate the data
set.seed(83625493)
dfr2 ← tibble(
    x = seq(0, 2 * pi, length.out = 500),
    m = 2 * sin(x),
    y = m + rnorm(length(x), sd = 1)
    )
```

Q.2a: optimal tree with min CV error



Q.2b: optimal tree with one SE rule

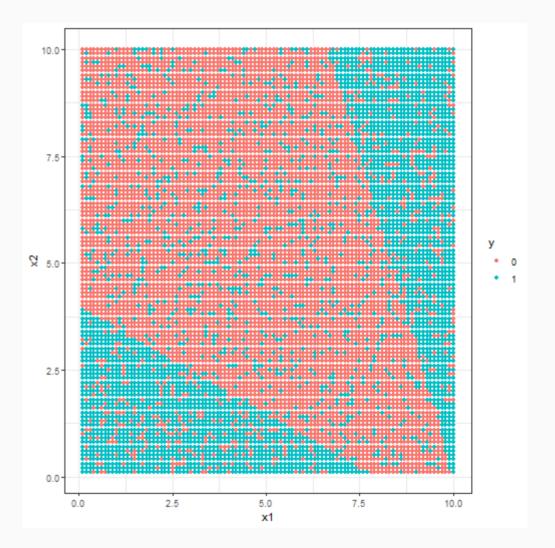


Q.3: trees look rather different compared to those from before, even though they try to approximate the same function.

Toy example of a classification tree

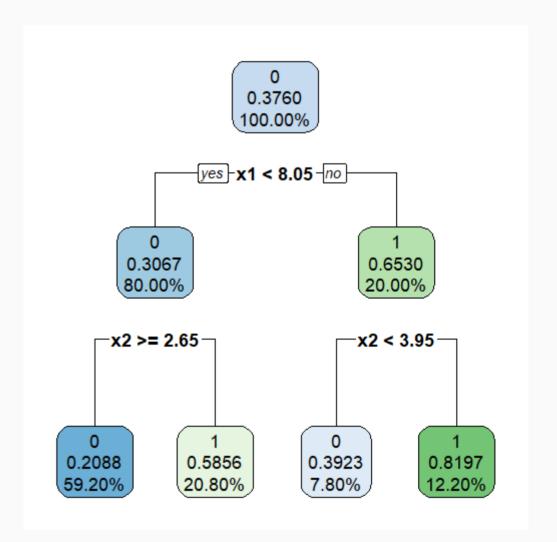
Simulated data

```
set.seed(54321) # reproducibility
dfc ← tibble::tibble(
 x1 = rep(seq(0.1,10,by = 0.1), times = 100),
 x2 = rep(seq(0.1,10,by = 0.1), each = 100),
 y = as.factor(
   pmin(1,
         pmax(0,
             round(
     1*(x1+2*x2<8) + 1*(3*x1+x2>30) +
       rnorm(10000, sd = 0.5))
```



Fitting a simple tree

```
fit \leftarrow rpart(formula = y \sim x1 + x2,
             data = dfc,
             method = 'class',
             control = rpart.control(
               maxdepth = 2
print(fit)
\#\# n= 10000
## node), split, n, loss, yval, (yprob)
         * denotes terminal node
   1) root 10000 3760 0 (0.6240000 0.3760000)
    2) x1< 8.05 8000 2454 0 (0.6932500 0.3067500)
      4) x2 ≥ 2.65 5920 1236 0 (0.7912162 0.2087838) *
       5) x2< 2.65 2080 862 1 (0.4144231 0.5855769) *
     3) x1 \ge 8.05 \ 2000 \ 694 \ 1 \ (0.3470000 \ 0.6530000)
      6) x2< 3.95 780 306 0 (0.6076923 0.3923077) *
      7) x2 \ge 3.95 1220 220 1 (0.1803279 0.8196721) *
```



Fitting a simple tree (cont.)

```
fit \leftarrow rpart(formula = y \sim x1 + x2,
             data = dfc,
             method = 'class',
             control = rpart.control(
               maxdepth = 2
print(fit)
\#\# n= 10000
## node), split, n, loss, yval, (yprob)
         * denotes terminal node
   1) root 10000 3760 0 (0.6240000 0.3760000)
     2) x1< 8.05 8000 2454 0 (0.6932500 0.3067500)
      4) x2 \ge 2.65 5920 1236 0 (0.7912162 0.2087838) *
       5) x2< 2.65 2080 862 1 (0.4144231 0.5855769) *
     3) x1 \ge 8.05 \ 2000 \ 694 \ 1 \ (0.3470000 \ 0.6530000)
      6) x2< 3.95 780 306 0 (0.6076923 0.3923077) *
      7) x2 \ge 3.95 1220 220 1 (0.1803279 0.8196721) *
```

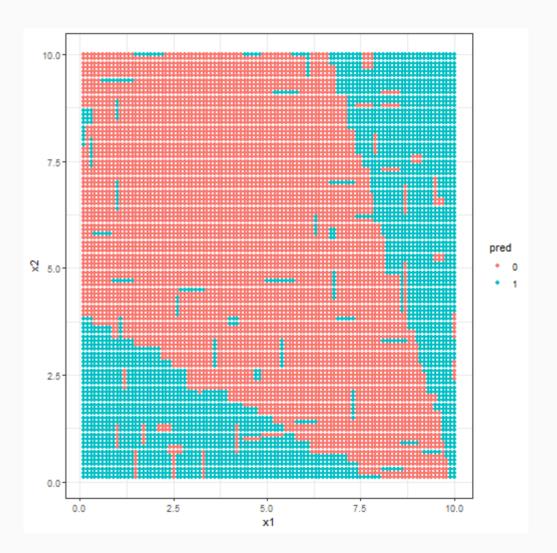


What about an overly complex tree?



What about an overly complex tree?

Clearly **overfitting**!





Your turn

Let's find a satisfying fit for this classification example.

Q: perform cross-validation on cp to find the optimal pruned subtree.

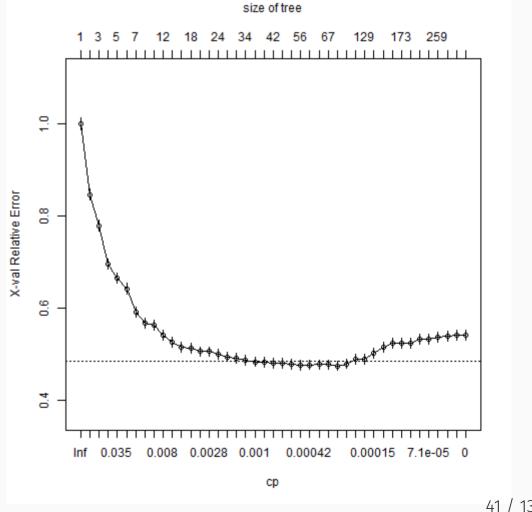
- 1. Set xval = 5 in rpart.control() (do not forget to set a **seed** beforehand).
- 2. Graphically inspect the xval results via plotcp().
- 3. Extract the xval results via \$cptable.
- 4. Apply the min xerror and/or the one SE rule to find the **optimal** cp.
- 5. Show the resulting classifier graphically.

Q.1: fit a complex tree and perform cross-validation

```
set.seed(87654) # reproducibility
fit \leftarrow rpart(formula = y \sim x1 + x2,
             data = dfc,
             method = 'class',
             control = rpart.control(
               maxdepth = 20,
               minsplit = 10,
               minbucket = 5,
               cp = 0,
               xval = 5
```

Q.2: inspect the xval results graphically

plotcp(fit)



Q.3: extract the xval results in a table

```
# Get xval results via 'cptable' attribute
cpt ← fit$cptable
```

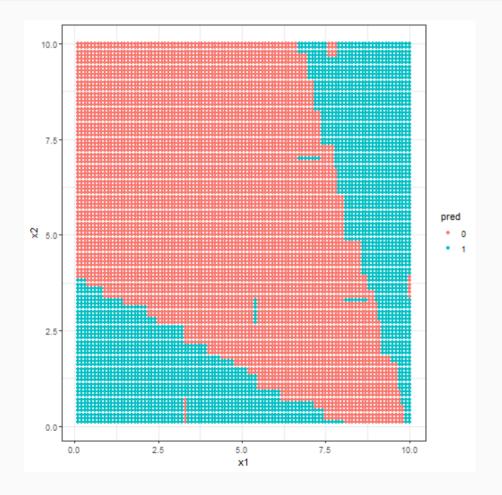
Q.4: optimal cp via min CV error or one SE rule

```
unname(min_xerr)
## [1] 29
```

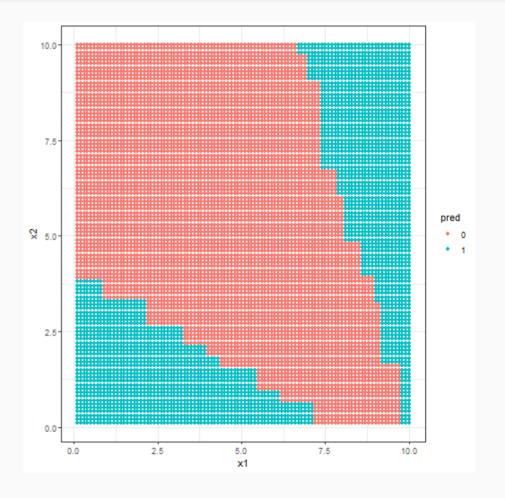
```
se_rule
## [1] 20
```

```
print(cpt[16:35,], digits = 6)
               CP nsplit rel error
                                                 xstd
                                     xerror
## 16 0.001861702
                          0.471543 0.500000 0.0103913
## 17 0.001595745
                          0.467819 0.494149 0.0103443
## 18 0.001329787
                          0.466223 0.490957 0.0103184
  19 0.001063830
                          0.456915 0.487234 0.0102880
                          0.455851 0.483245 0.0102552
  20 0.000930851
## 21 0.000797872
                          0.453989 0.482713 0.0102508
  22 0.000709220
                          0.450000 0.480319 0.0102310
## 23 0.000664894
                          0.447872 0.480319 0.0102310
## 24 0.000531915
                          0.443883 0.478457 0.0102155
  25 0.000443262
                          0.441223 0.476330 0.0101978
## 26 0.000398936
                          0.439894 0.476596 0.0102000
  27 0.000354610
                          0.439096 0.477660 0.0102089
## 28 0.000332447
                          0.436968 0.477660 0.0102089
  29 0.000265957
                          0.434309 0.474734 0.0101844
## 30 0.000199468
                          0.426330 0.478989 0.0102200
## 31 0.000177305
                          0.424468 0.488830 0.0103011
  32 0.000166223
                          0.421543 0.488830 0.0103011
## 33 0.000132979
                          0.419681 0.502128 0.0104082
## 34 0.000113982
                          0.417819 0.515160 0.0105105
## 35 0.000106383
                          0.416223 0.523936 0.0105780
```

Q.5a: optimal subtree via min CV error



Q.5b: optimal subtree via one SE rule



Claim frequency and severity modeling with {rpart}

Claim frequency prediction on the MTPL data

Recall the MTPL data set introduced in Module 1.

The Poisson GLM is a classic approach for modelling claim frequency data.

How to deal with claim counts in a decision tree?

Use the **Poisson deviance** as **loss function**:

$$D^{ ext{Poi}} = 2 \cdot \sum_{i=1}^{n} oldsymbol{y}_i \cdot \ln rac{oldsymbol{y}_i}{\exp _i \cdot \hat{f}\left(oldsymbol{x}_i
ight)} - \{oldsymbol{y}_i - \exp _i \cdot \hat{f}\left(oldsymbol{x}_i
ight)\},$$

with **expo** the exposure measure.

Here we go:

Fitting a simple tree to the MTPL data

```
print(fit)
```

Take-away → Poisson tree in {rpart}:

- Poisson deviance via method = 'poisson'
- response as two-column matrix: cbind(expo,y).

```
## n= 163231
## node), split, n, deviance, yval
         * denotes terminal node
##
   1) root 163231 89944.320 0.13933520
      2) bm< 6.5 127672 63455.290 0.11784050
       4) bm< 1.5 88621 41252.130 0.10550490
          8) ageph ≥ 55.5 33646 14281.360 0.08899811 *
          9) ageph< 55.5 54975 26835.800 0.11598320 *
        5) bm ≥ 1.5 39051 21872.010 0.14641040
##
         10) ageph ≥ 57.5 8463 4324.098 0.11963920 *
         11) ageph< 57.5 30588 17496.720 0.15408620 *
     3) bm ≥ 6.5 35559 24843.720 0.22188630
        6) bm< 10.5 22657 15022.440 0.19808030
         12) ageph ≥ 26.5 17196 10950.970 0.18565170 *
         13) ageph< 26.5 5461 4025.443 0.23668440 *
##
        7) bm ≥ 10.5 12902 9678.292 0.26753260
         14) agec< 6.5 4472 3181.981 0.23435030 *
         15) agec ≥ 6.5 8430 6471.783 0.28640140 *
##
```

Fitting a simple tree to the MTPL data

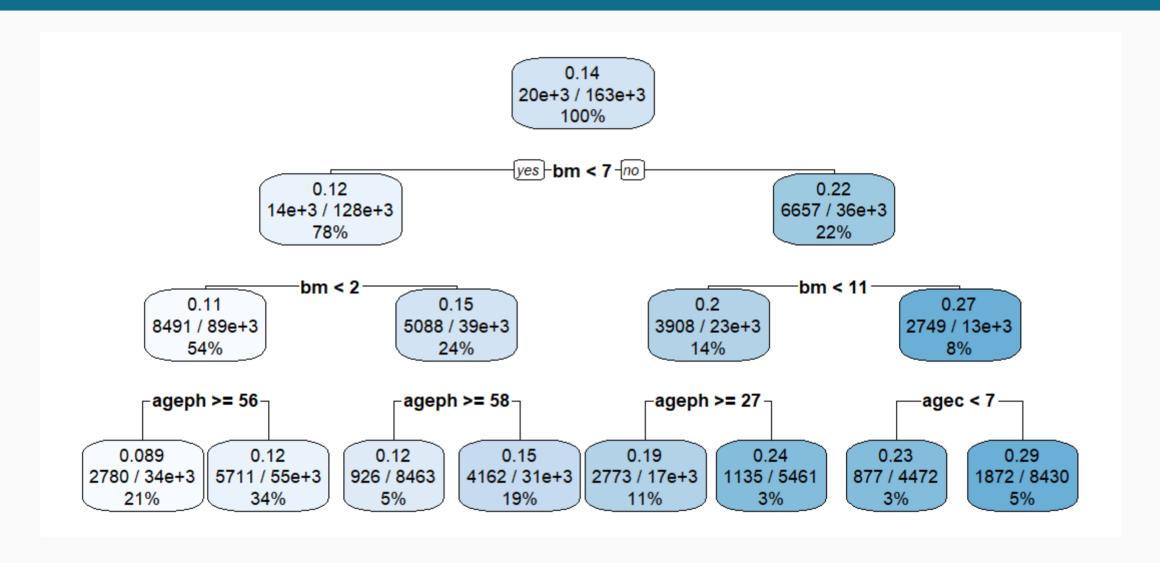
```
print(fit)
```

Easier way to **understand** this tree?

Try rpart.plot from the package {rpart.plot}

```
## n= 163231
##
## node), split, n, deviance, yval
         * denotes terminal node
##
    1) root 163231 89944.320 0.13933520
      2) bm< 6.5 127672 63455.290 0.11784050
##
       4) bm< 1.5 88621 41252.130 0.10550490
          8) ageph ≥ 55.5 33646 14281.360 0.08899811 *
          9) ageph< 55.5 54975 26835.800 0.11598320 *
        5) bm ≥ 1.5 39051 21872.010 0.14641040
##
         10) ageph ≥ 57.5 8463 4324.098 0.11963920 *
         11) ageph< 57.5 30588 17496.720 0.15408620 *
     3) bm ≥ 6.5 35559 24843.720 0.22188630
##
        6) bm< 10.5 22657 15022.440 0.19808030
##
         12) ageph ≥ 26.5 17196 10950.970 0.18565170 *
         13) ageph< 26.5 5461 4025.443 0.23668440 *
        7) bm ≥ 10.5 12902 9678.292 0.26753260
##
         14) agec< 6.5 4472 3181.981 0.23435030 *
##
        15) agec ≥ 6.5 8430 6471.783 0.28640140 *
##
```

Fitting a simple tree to the MTPL data





Your turn

Verify whether the **prediction** in a leaf node is **what you would expect**.

- **Q**: take the leftmost node as an example: bm < 2 and $ageph \ge 56$.
 - 1. Subset the data accordingly.
 - 2. Calculate the expected claim frequency as sum(nclaims)/sum(expo).
 - 3. Compare with the {rpart} prediction of 0.08899811.

Q.1-Q.2: subset the data and calculate the claim frequency

```
## claim_freq
## 1 0.08898655
```

Q.3: the prediction and our DIY calculation do not match!

Is this due to a rounding error?

Or is there something spooky going on?

Unraveling the mystery of {rpart}

Conceptually: no events in a leaf node lead to division by zero in the deviance!

Solution: assume **Gamma prior** on the mean of the Poisson in the leaf nodes:

- set $\mu = \sum y_i / \sum \exp \! \mathrm{o}_i$
- ullet use coefficient of variation $k=\sigma/\mu$ as ${\sf user\ input}$
- k=0 extreme **pessimism** (all leaf nodes equal)
- $k=\infty$ extreme **optimism** (let the data speak)
- default in {rpart}: k=1.

The resulting leaf node prediction:

$$rac{lpha + \sum y_i}{eta + \sum \mathrm{expo}_i}, \quad lpha = 1/k^2, \quad eta = lpha/\mu.$$

```
## prediction
## 1 0.08899811
```

More details in Section 8.2 of the vignette on Poisson regression.

Coefficient of variation very low

```
## n= 163231
##

## node), split, n, deviance, yval
## * denotes terminal node
##

## 1) root 163231 89944.320 0.1393352
## 2) bm< 6.5 127672 63858.770 0.1393352
## 5) bm > 1.5 88621 41974.470 0.1393352 *

## 5) bm > 1.5 39051 21884.300 0.1393352 *

## 10) ageph > 57.5 8463 4346.787 0.1393352 *

## 3) bm > 6.5 35559 26085.560 0.1393353 *
```

Notice that **all** leaf nodes predict the **same value**.

Coefficient of variation very high

```
## claim_freq
## 1 0.08898655
```

```
## n= 163231
## node), split, n, deviance, yval
         * denotes terminal node
##
   1) root 163231 89944.320 0.13933520
      2) bm< 6.5 127672 63455.290 0.11783920
       4) bm< 1.5 88621 41252.130 0.10550180
          8) ageph ≥ 55.5 33646 14281.360 0.08898655 *
          9) ageph< 55.5 54975 26835.800 0.11597980 *
        5) bm ≥ 1.5 39051 21872.010 0.14641180
##
         10) ageph ≥ 57.5 8463 4324.098 0.11962090 *
         11) ageph< 57.5 30588 17496.720 0.15409010 *
     3) bm ≥ 6.5 35559 24843.720 0.22190600
        6) bm< 10.5 22657 15022.440 0.19810170
         12) ageph \geq 26.5 17196 10950.970 0.18567400 *
         13) ageph< 26.5 5461 4025.443 0.23683020 *
        7) bm ≥ 10.5 12902 9678.292 0.26762210
         14) agec< 6.5 4472 3181.980 0.23453270 *
##
        15) agec ≥ 6.5 8430 6471.783 0.28656300 *
##
```



Your turn

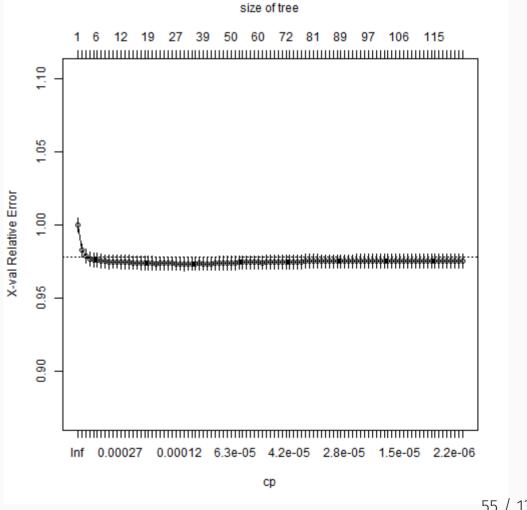
- **Q**: Follow the **pruning strategy** to develop a proper frequency tree model for the MTPL data.
 - 1. Start from an overly complex tree. Do not forget your favorite random **seed** upfront!
 - 2. Inspect the cross-validation results.
 - 3. Choose the cp value minimizing xerror for pruning.
 - 4. Visualize the pruned tree with rpart.plot.

Q.1: fit an overly complex tree

```
set.seed(9753) # reproducibilty
fit ← rpart(formula =
               cbind(expo,nclaims) ~
              ageph + agec + bm + power +
               coverage + fuel + sex + fleet + use,
             data = mtpl,
            method = 'poisson',
             control = rpart.control(
              maxdepth = 20,
              minsplit = 2000,
              minbucket = 1000,
               cp = 0,
               xval = 5
```

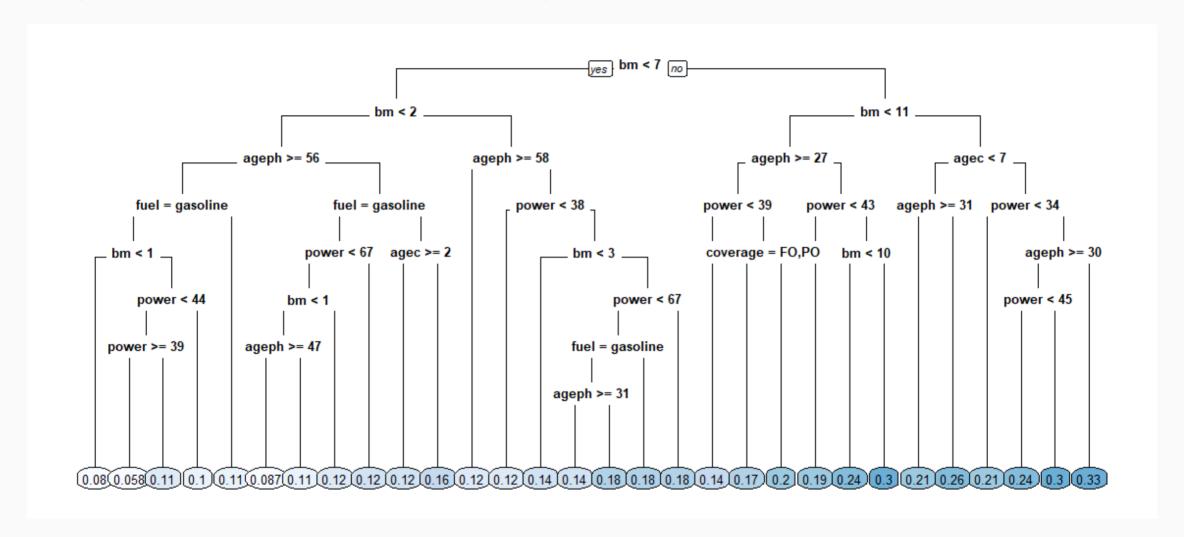
Q.2: inspect the cross-validation results

plotcp(fit)



Q.3: choose the cp value that minimizes xerror for pruning

Q.4: try to understand how the final model looks like. Can you make sense of it?



Interpretation tools

Interpreting a tree model

Interpretability depends on the size of the tree

- is easy with a **shallow** tree but hard with a **deep** tree
- luckily there are some tools to aid you.

Feature importance

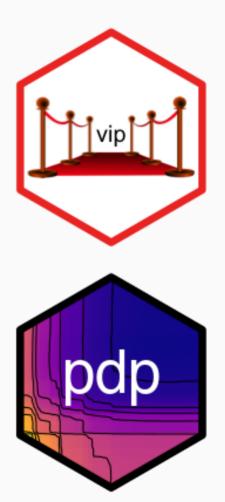
- identify the most **important** features
- implemented in the package {vip}.

Partial dependence plot

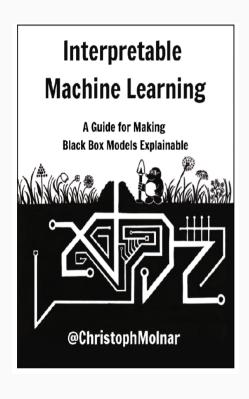
- measure the marginal effect of a feature
- implemented in the package {pdp}.

Excellent source on interpretable machine learning:

Interpretable Machine Learning book by Christophe Molnar.



Feature importance and partial dependence



With feature importance:

- ullet sum improvements in loss function over all splits on a variable x_ℓ
- important variables appear high and often in a tree.

With partial dependence:

univariate

$$ar{f}_{\ell}(x_{\ell}) = rac{1}{n} \sum_{i=1}^n f_{ ext{tree}}(x_{\ell}, oldsymbol{x}_{-\ell}^i).$$

bivariate

$$ar{f}_{k,\ell}(x_k,x_\ell) = rac{1}{n} \sum_{i=1}^n f_{ ext{tree}}(x_k,x_\ell,oldsymbol{x}_{-k,\ell}^i)$$

• marginal effects, interactions can stay hidden!

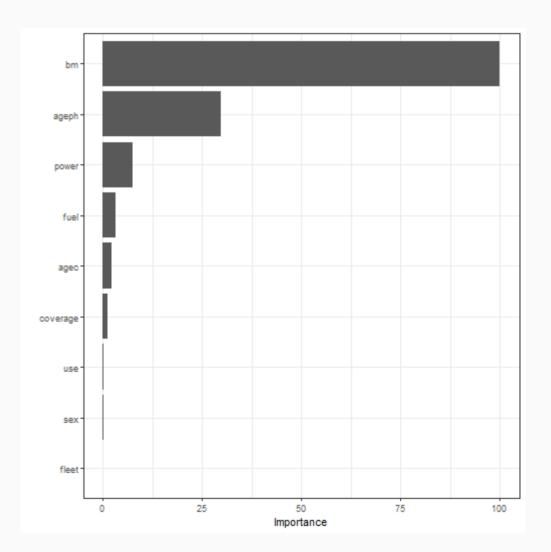
Feature importance



```
library(vip)
# Function vi gives you the data
var_imp ← vip::vi(fit_srt)
```

```
Variable
               Importance
          bm 2186.5664729
             651.1768792
       ageph
       power
              164.2502735
       fuel
              70.5542003
              45.8086193
        agec
## 6 coverage
              24.9202279
              2.2088357
         use
              0.7547625
      sex
## 9
     fleet
             0.2642045
```

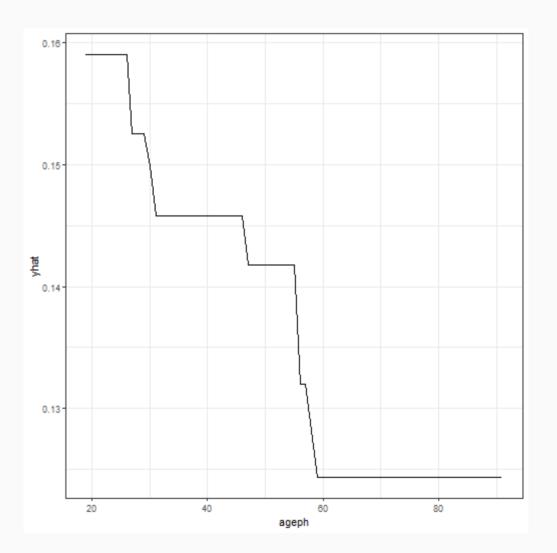
```
# Function vip makes the plot
vip::vip(fit_srt, scale = TRUE)
```



Partial dependence plot

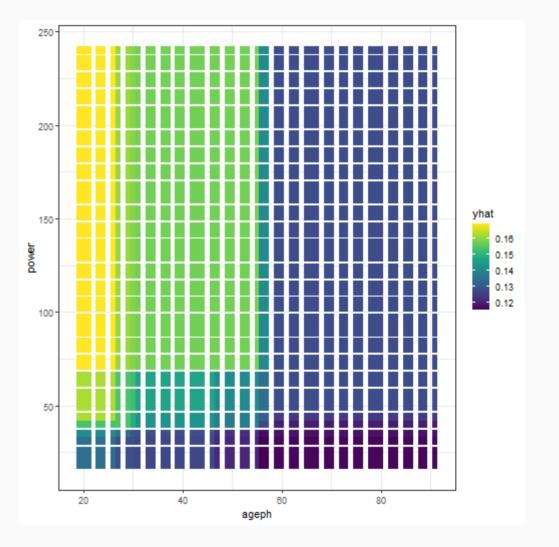


```
library(pdp)
# Need to define this helper function for Poisson
pred.fun ← function(object, newdata){
   mean(predict(object, newdata))
}
# Sample 5000 observations to speed up pdp generation
set.seed(48927)
pdp_ids ← mtpl %>% nrow %>% sample(size = 5000)
```



Partial dependence plot in two dimensions



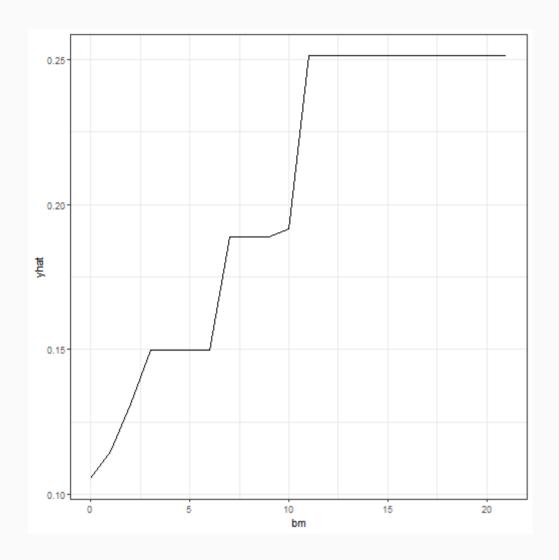




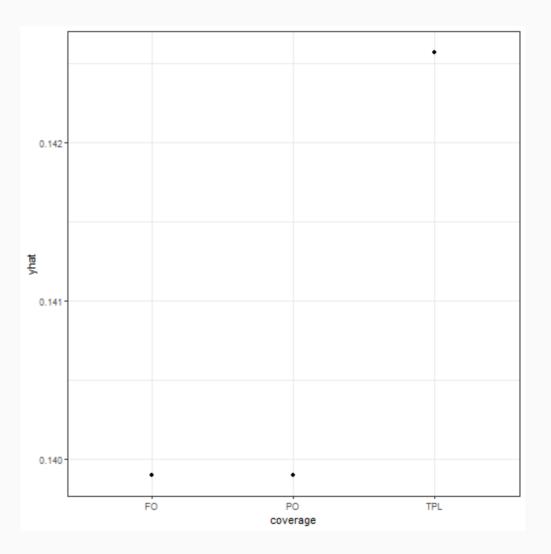
Use partial dependence plots for **other features** to gain **understanding** of your model.

Your turn

Level in the bonus-malus scale



Type of coverage



That's a wrap on single trees!

Advantages ©

- Shallow tree is easy to **explain** graphically.
- Closely mirror the human decision-making process.
- Handle all types of features without pre-processing.
- Fast and very scalable to big data.
- Automatic variable selection.
- Surrogate splits can handle **missing** data.

That's a wrap on single trees!

Advantages ©

- Shallow tree is easy to **explain** graphically.
- Closely mirror the human decision-making process.
- Handle all types of features without pre-processing.
- Fast and very scalable to big data.
- Automatic variable selection.
- Surrogate splits can handle **missing** data.

Disadvantages 😊

- Tree uses **step** functions to approximate the effect.
- Greedy heuristic approach chooses **locally** optimal split (i.e., based on all previous splits).
- Data becomes **smaller** and smaller down the tree.
- All this results in **high variance** for a tree model...
- ... which harms **predictive performance**.

From a single tree to ensembles of trees

Ensembles of trees

Remember: prediction error = bias + variance.

Good predictive performance requires low bias AND low variance.

Two popular **ensemble** algorithms (that can be applied to any type of model, not just trees) are:

Bagging (Breiman, 1996)

- low bias via detailed individual models
- (think: deep trees)
- low **variance** via averaging of those models
- (think: in parallel)

Boosting (Friedman, 2001)

- low variance via simple individual models
- (think: stumps)
- low **bias** by incrementing the model sequentially
- (think: sequentially).

Random forest (Breiman, 2001) is then a modification on bagging for trees to further improve the variance reduction.

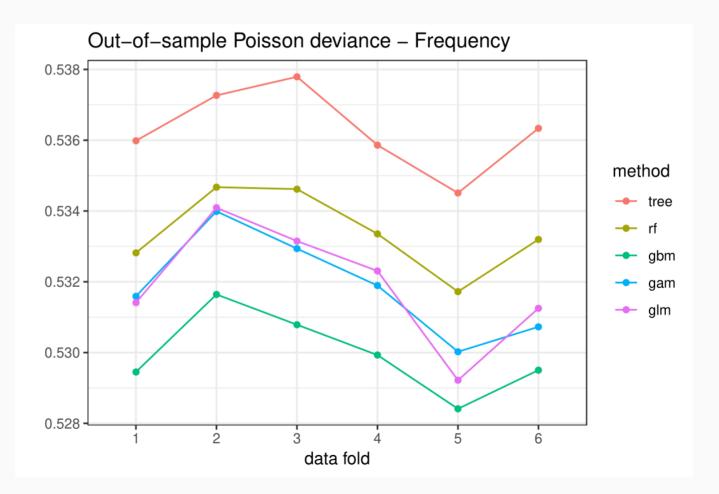
Model comparison on claim frequency data

Detailed discussion in our North American Actuarial Journal (2020) paper.

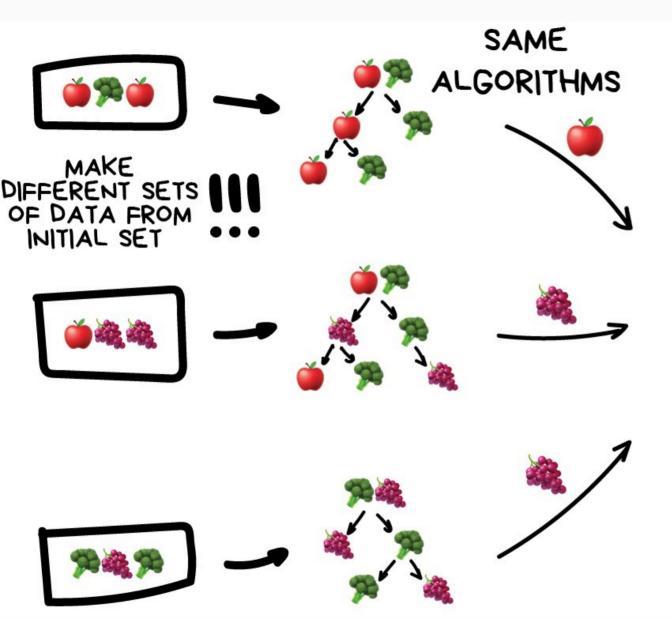
Analyzing frequency as well as severity data.

Picture taken from Henckaerts et al. (2020).

Boosting > Random forest > Bagging > Decision tree



Introducing bagging



BAGGING ON TREES

II

RANDOM FOREST

JUST AVERAGING ALL THE RESULTS



BAGGING

Bagging

Bagging is for Bootstrap AGGregatING.

Simple idea:

- build a lot of different base learners on bootstrapped samples of the data
- combine their predictions.

Model **averaging** helps to:

- reduce variance
- avoid overfitting.

Bagging works best for base learners with:

- low bias and high variance
- for example: deep decison trees.

Bagging or Bootstrap AGGregatING

Take-aways

: working principles see {ipred} package, using {rpart} under the hood.

- build a lot of different base learners on bootstrapped samples of the data
- combine their predictions
- model averaging helps to:
 - reduce variance
 - avoid overfitting.
- bagging works best for base learners with:
 - low bias and high variance
 - for example: deep decison trees.

bagging with trees?

- do B times:
 - create .hi-pink[bootstrap sample] by drawing with replacement from the original data
 - fit a .hi-pink[deep tree] to the bootstrap sample.
- combine the predictions of these B trees
 - average prediction for regression
 - majorty vote for classification.

Bootstrap samples

```
# Set a seed for reproducibility
set.seed(45678)
# Generate the first bootstrapped sample
bsample 1 ← dfr %>% nrow %>%
 sample(replace = TRUE)
# Generate another bootstrapped sample
bsample 2 ← dfr %>% nrow %>%
 sample(replace = TRUE)
# Use the indices to sample the data
dfr b1 ← dfr %>%
 dplyr::slice(bsample_1)
dfr b2 ← dfr %>%
 dplyr::slice(bsample_2)
```

```
# Let's have a look at the sampled data
dfr_b1 %>% dplyr::arrange(x) %>% head()
dfr_b2 %>% dplyr::arrange(x) %>% head()
```

Sample 1:

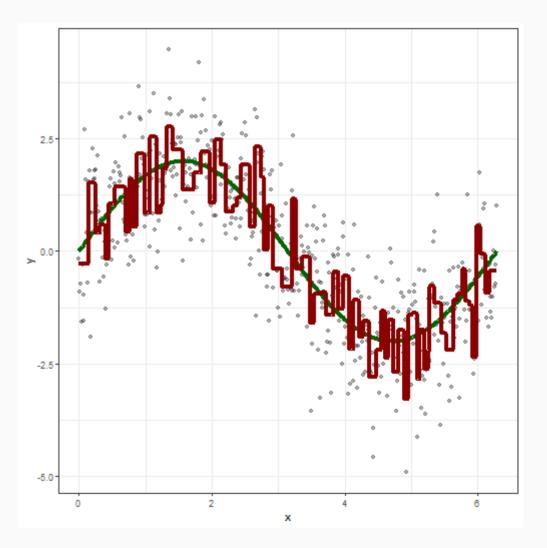
```
## x m y
## 1 0.02518311 0.05036089 -0.7336728
## 2 0.02518311 0.05036089 -0.7336728
## 3 0.03777466 0.07553136 -1.5750691
## 4 0.06295777 0.12583237 -0.9696970
## 5 0.10073243 0.20112432 1.5964765
## 6 0.11332398 0.22616316 0.4061405
```

Sample 2:

```
## x m y
## 1 0.00000000 0.00000000 -0.1789007
## 2 0.00000000 0.00000000 -0.1789007
## 3 0.00000000 0.00000000 -0.1789007
## 4 0.01259155 0.02518244 -0.9028617
## 5 0.06295777 0.12583237 -0.9696970
## 6 0.07554932 0.15095495 -1.5412872
```

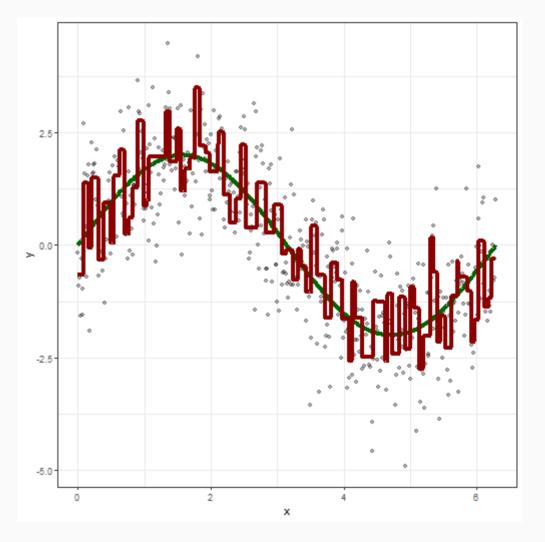
Decision tree on sample 1

On it's own, this is a **noisy prediction** with very **high** variance!



Decision tree on sample 2

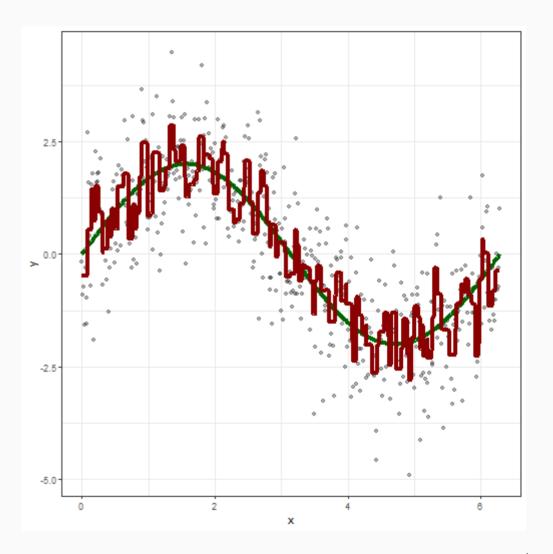
Again, very **high variance** on it's own!



Combining the predictions of both trees

Does it look like the prediction it's getting **less noisy**?

In other words: is variance reducing?





Your turn

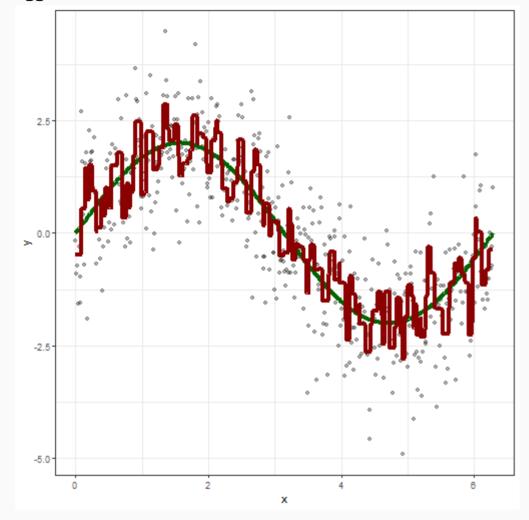
- **Q**: add a **third tree** to the **bagged ensemble** and inspect the predictions.
 - 1. Generate a **bootstrap sample** of the data (note: don't use the same seed as before because your bootstrap samples will be the same).
 - 2. Fit a **deep tree** to this bootstrap sample.
 - 3. Make predictions for this tree and average with the others.

Q.1: bootstrap sample with different seed

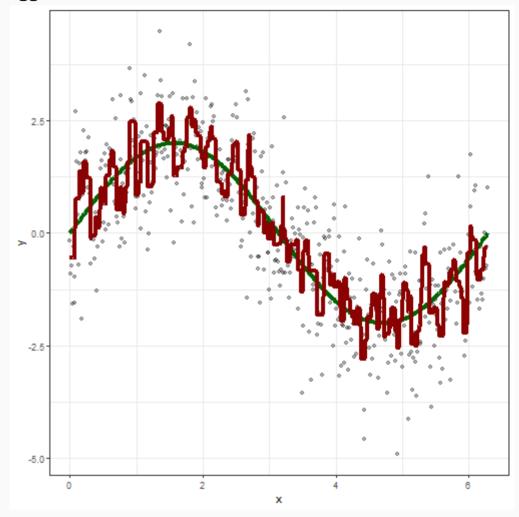
Q.2: fit a deep tree

Q.3: average the predictions

Bagged ensemble with B = 2



Bagged ensemble with B = 3



Little variance reduction might be visible, but we clearly need a lot more trees. Let's use the {ipred} package for this!

Using {ipred}

- formula: a formula as response ~ feature1 + feature2 + ...
- data: the observation data containing the response and features
- control: options to pass to rpart.control for the base learners
- nbagg: the number of bagging iterations B, i.e., the number of trees in the ensemble
- ns: number of observations to draw for the bootstrap samples (often less than N to save computational time)
- coob: a logical indicating whether an out-of-bag estimate of the error rate should be computed.

Out-of-bag (OOB) error

Bootstrap samples are constructed with replacement.

Some observations are not present in a bootstrap sample:

- they are called the **out-of-bag** observations
- use those to calculate the out-of-bag (OOB) error
- measures hold-out error like cross-validation does.

Advantage of OOB over cross-validation?

• the OOB error comes for free with bagging.

Out-of-bag (OOB) error

Bootstrap samples are constructed with replacement.

Some observations are not present in a bootstrap sample:

- they are called the **out-of-bag** observations
- use those to calculate the out-of-bag (OOB) error
- measures hold-out error like cross-validation.

Advantage of OOB over cross-validation?

• the OOB error comes for free with bagging.

But, is this a **representative** sample?

Roughly 37% of observations are OOB when N is large.

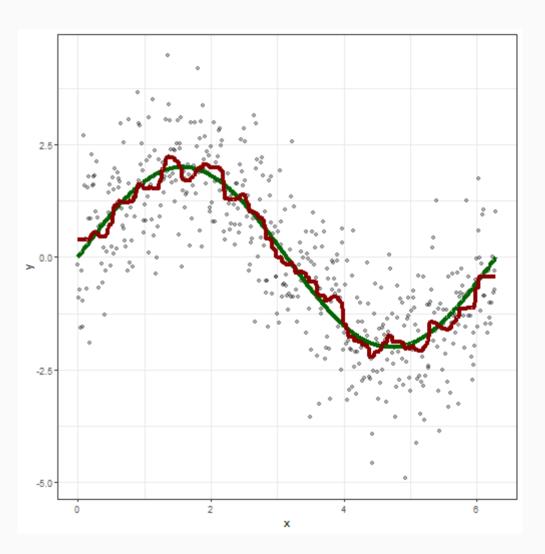
Even more when we sample $\leq N$ observations

Bagging properly

```
library(ipred)
set.seed(83946) # reproducibility
# Fit a bagged tree model
fit \leftarrow ipred::bagging(formula = y ~ x,
               data = dfr,
               nbagg = 200,
               ns = nrow(dfr),
               coob = TRUE,
               control = rpart.control(
                 maxdepth = 20,
                 minsplit = 40,
                 minbucket = 20,
                 cp = 0)
```

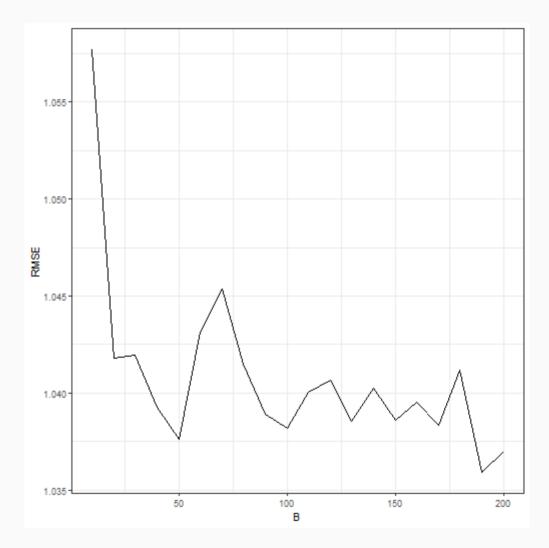
```
# Predict from this model
pred ← predict(fit, dfr)
```

With 200 trees we can see the variance reduction!



Evolution of the OOB error

```
set.seed(98765) # reproducibility
# Define a grid for B
nbags \leftarrow 10*(1:20)
oob \leftarrow rep(0, length(nbags))
# Fit a bagged tree model
for(i in 1:length(nbags)){
  fit \leftarrow ipred::bagging(formula = y ~ x,
                data = dfr,
                nbagg = nbags[i],
                ns = nrow(dfr),
                coob = TRUE,
                control = rpart.control(
                  maxdepth = 20,
                  minsplit = 40,
                  minbucket = 20,
                  cp = 0)
  oob[i] \leftarrow fit\$err
```



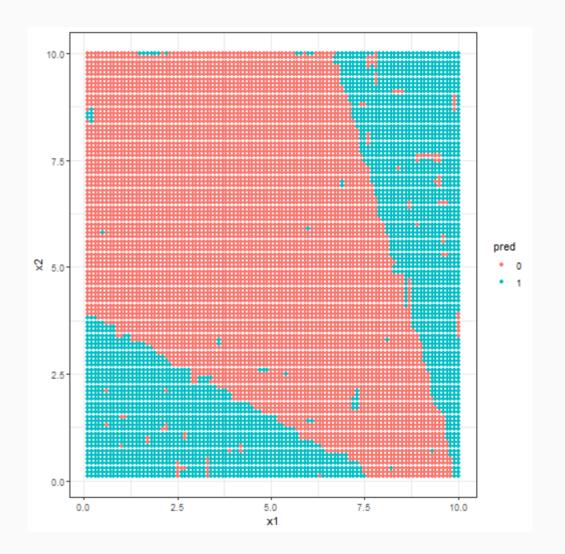


Your turn

Use {ipred} to fit a **bagged** tree ensemble for the toy **classification** problem with data dfc.

Q: experiment with the nbagg and control parameters to see their effect on the predictions.

Q: the following parameter settings seem to produce a decent fit.



From bagging to random forests

Problem of dominant features

A downside of bagging is that dominant features can cause individual trees to have a similar structure

known as tree correlation

Remember the **feature importance** results discussed earlier for the MTPL data?

- bm is a very dominant variable
- ageph was rather important
- power also, but to a lesser degree.

Problem?

- bagging gets its predictive performance from variance reduction
- however, this reduction when tree correlation
- dominant features therefore **hurt** the preditive performance of a bagged ensemble!

Random forest

Random forest is a modification on bagging to get an ensemble of de-correlated trees.

Process is very similar to bagging, with one small **trick**:

- before each split, select a **subset of features** at random as candidate features for splitting
- this essentially decorrelates the trees in the ensemble, improving predictive performance
- the number of candidates is typically considered a tuning parameter

Bagging introduces randomness in the rows of the data.

Random forest introduces randomness in the rows and columns of the data.

Many **packages** available, but a couple of popular ones:

- {randomForest}: standard for regression and classification, but not very fast
- {randomForestSRC}: fast OpenMP implementation for survival, regression and classification
- {ranger}: fast C++ implementation for survival, regression and classification.



Your turn

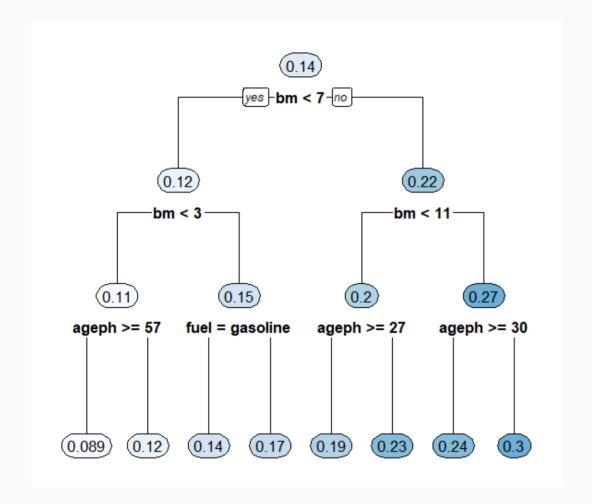
- **Q**: let's investigate the issue of dominant features.
 - 1. Take **two bootstrap samples** from the **MTPL** data.
 - 2. Fit a regression tree of **depth = 3** to each sample.
 - 3. Check the resulting tree structures.

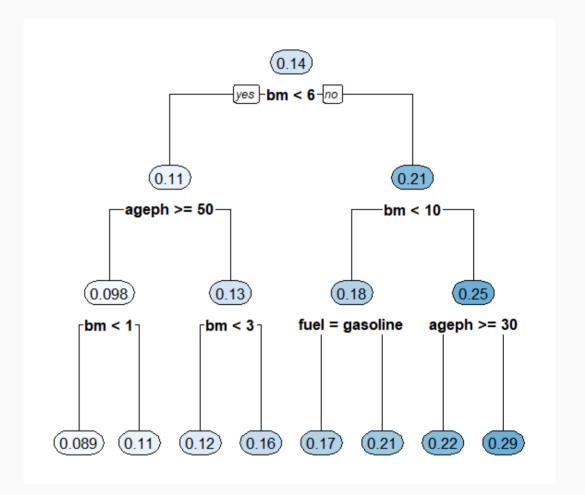
Q.1: two bootstrap samples

Q.2: Poisson regression tree for each sample

```
fit b1 ← rpart(formula =
               cbind(expo,nclaims) ~
               ageph + agec + bm + power +
               coverage + fuel + sex + fleet + use.
             data = mtpl b1,
             method = 'poisson'.
             control = rpart.control(
               maxdepth = 3,
               minsplit = 2000,
               minbucket = 1000,
               cp = 0)
fit b2 ← rpart(formula =
               cbind(expo,nclaims) ~
               ageph + agec + bm + power +
               coverage + fuel + sex + fleet + use,
             data = mtpl b2,
             method = 'poisson',
             control = rpart.control(
               maxdepth = 3,
               minsplit = 2000,
               minbucket = 1000,
               cp = 0)
```

Q.3: the resulting tree structures





Using {ranger}

```
ranger(formula, data, num.trees, mtry, min.node.size, max.depth,
    replace, sample.fraction, oob.error, num.threads, seed)
```

- formula: a formula as response ~ feature1 + feature2 + ...
- data: the observation data containing the response and features
- num.trees: the number of trees in the ensemble
- mtry: the number of candidate features for splitting
- min.node.size and max.depth: minimal leaf node size and maximal depth for the individual trees
- replace and sample.fraction: sample with/without replacement and fraction of observations to sample
- oob.error: boolean indication to calculate the OOB error
- num.threads and seed: number of threads and random seed.

Tuning strategy for random forests

Many tuning parameters in a random forest:

- number of trees
- number of candidates for splitting
- max tree depth
- minimum leaf node size
- sample fraction.

Construct a full cartesian grid via expand.grid:

```
search_grid \leftarrow expand.grid(
  num.trees = c(100,200),
  mtry = c(3,6,9),
  min.node.size = c(0.001,0.01)*nrow(mtpl),
  error = NA
)
```

```
print(search_grid)
      num.trees mtrv min.node.size error
            100
## 1
                            163.231
                                       NA
            200
                            163.231
                                       NA
            100
                            163.231
                                       NA
                            163.231
## 4
            200
                                       NA
            100
                            163.231
                                       NΑ
## 6
                            163.231
            200
                                       NA
                           1632.310
## 7
            100
                                       NA
            200
                           1632.310
                                       NA
## 9
            100
                           1632.310
                                       NA
## 10
            200
                           1632.310
                                       NA
## 11
            100
                           1632.310
                                       NΑ
## 12
            200
                           1632.310
                                       NA
```

Tuning strategy for random forests (cont.)

Perform a **grid search** and track the **OOB error**:

```
library(ranger)
for(i in seq len(nrow(search grid))) {
 # fit a random forest for the ith combination
 fit \leftarrow ranger(
    formula = nclaims ~
              ageph + agec + bm + power +
              coverage + fuel + sex + fleet + use,
   data = mtpl,
   num.trees = search_grid$num.trees[i],
   mtry = search grid$mtry[i],
   min.node.size = search grid$min.node.size[i],
   replace = TRUE,
   sample.fraction = 0.75,
   verbose = FALSE,
   seed = 54321
 # get the OOB error
 search_grid$error[i] ← fit$prediction.error
```

```
search grid %>% arrange(error)
      num.trees mtrv min.node.size
                                        error
## 1
            200
                          1632.310 0.1332844
                          1632.310 0.1333003
            100
## 3
                          1632.310 0.1333551
            200
                          1632.310 0.1333689
## 4
            200
            100
                          1632.310 0.1333754
## 6
                          1632.310 0.1333862
            100
                           163.231 0.1337361
## 7
            200
            100
                           163.231 0.1338148
## 9
            200
                           163,231 0,1341431
## 10
            100
                           163,231 0,1342326
                           163.231 0.1343189
## 11
            200
## 12
            100
                           163.231 0.1344154
```

What does the prediction error **measure** actually?

The **Mean Squared Error**, but does that make sense for us?

Random forests for actuaries

All available random forest packages (in R) only support **standard regression** based on the **Mean Squared Error**:

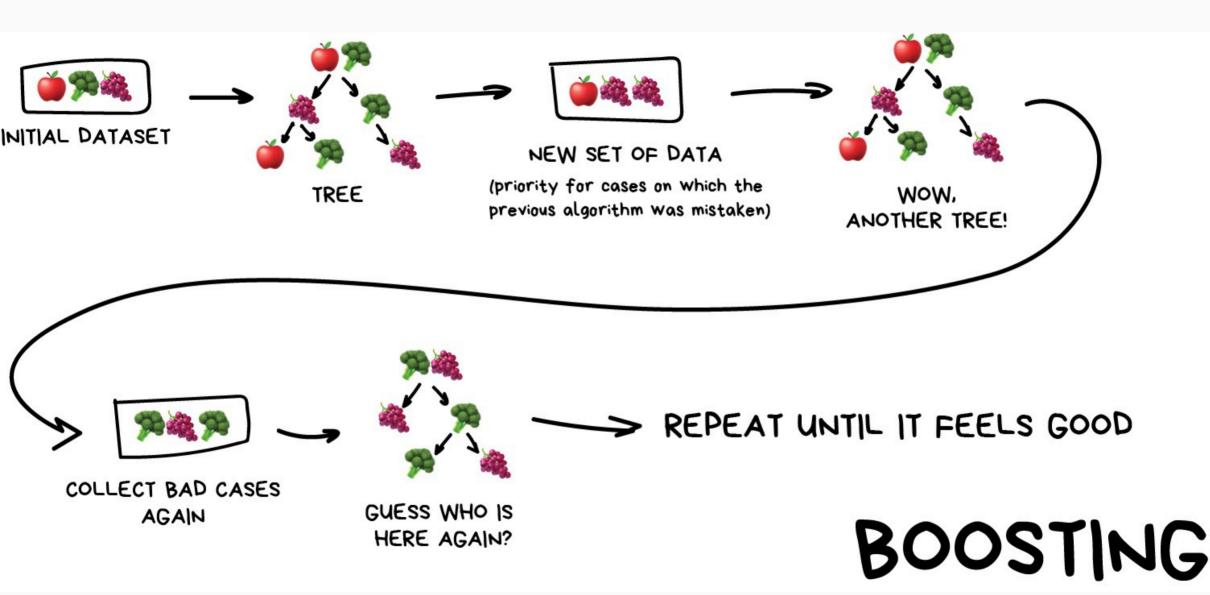
- no Poisson, Gamma or log-normal loss functions available
- bad news for actuaries.

The {distRforest} package on Roel's GitHub **?**:



- based on {rpart} which supports **Poisson** regression (as we have seen before)
- extended to support **Gamma** and **log-normal** deviance as loss function
- extended to support random forest generation
- used in Henckaerts et al. (2020).

(Stochastic) Gradient Boosting Machines



Boosting vs. Bagging

Similar to bagging, boosting is a **general technique** to create an **ensemble** of any type of base learner.

With bagging

- strong base learners
 - low bias, high variance
 - for example: deep trees
- variance reduction through averaging
- parallel approach
 - trees not using information from each other
 - performance thanks to averaging
 - low risk for overfitting.

With boosting

- weak base learners
 - low variance, high bias
 - for example: stumps
- bias reduction in ensemble through updating
- sequential approach
 - current tree uses information from all past trees
 - performance thanks to rectifying past mistakes
 - high risk for overfitting.

GBM: stochastic gradient boosting with trees

We focus on **GBM**:

- with decision trees
- stochastic by subsampling in the rows (and columns) of the data
- gradient by optimizing the loss function via gradient descent.

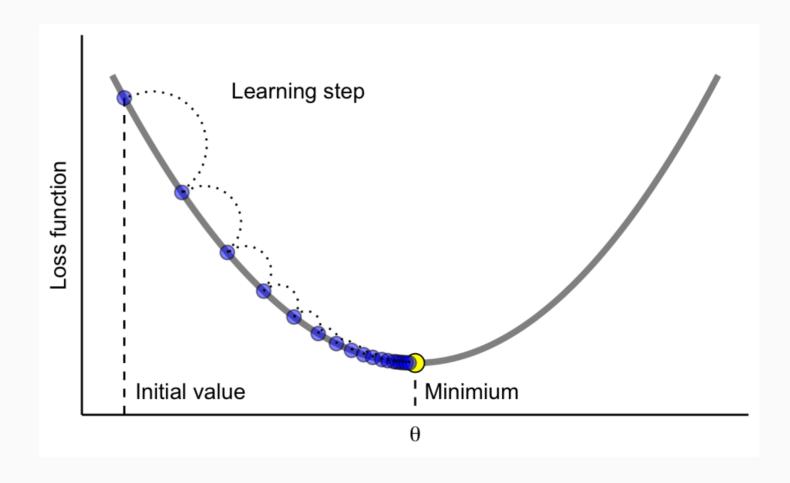


Figure 12.3 from Boehmke & Greenwell Hands-on machine learning with R.

Stochastic gradient descent

The **learning rate** (also called step size) is very important in gradient descent

- if too big → likely to overshoot the optimal solution
- if too small → slow process to reach the optimal solution

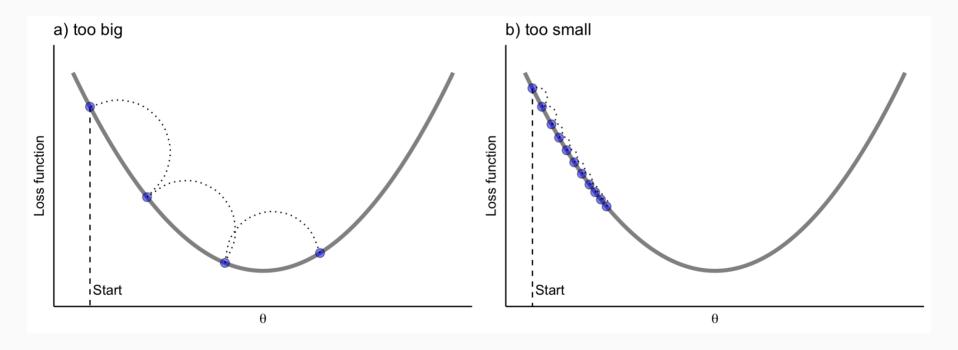


Figure 12.4 from Boehmke & Greenwell Hands-on machine learning with R.

Subsampling allows to escape plateaus or local minima for non-convex loss functions.

GBM training process

Initialize the model fit with a global average and calculate pseudo-residuals.

Do the following B times:

- fit a tree of a pre-specified depth to the **pseudo-residuals**
- update the model fit and pseudo-residuals with a shrunken version
- shrinkage to slow down learning and prevent overfitting.

The model fit after B iterations is the **end product**.

Some popular packages for stochastic gradient boosting

- {gbm}: standard for regression and classification, but not the fastest
- {gbm3}: faster version of {gbm} via parallel processing, but not backwards compatible
- {xgboost}: efficient implementation with some **extra** elements, for example regularization.

Using {gbm}

```
gbm(formula, data, distribution, var.monotone, n.trees,
   interaction.depth, shrinkage, n.minobsinnode, bag.fraction, cv.folds)
```

- formula: a formula as response ~ feature1 + feature2 + ...
- can contain an **offset!**
- data: the observation data containing the response and features
- distribution: a string specifying which loss function to use (gaussian, laplace, tdist, bernoulli, poisson, coxph,...)
- var.monotone: vector indicating a monotone increasing (+1), decreasing (-1), or arbitrary (0) relationship
- n.trees: the number of trees in the ensemble
- interaction.depth and n.minobsinnode: the maximum tree depth and minimum number of leaf node observations
- shrinkage: shrinkage parameter applied to each tree in the expansion (also called: learning rate or step size)
- bag.fraction: fraction of observations to sample for building the next tree
- cv.folds: number of cross-validation folds to perform.

GBM parameters

A lot of parameters at our disposal to **tweak** the GBM.

Some have a **big impact** on the performance and should therefore be **properly tuned**:

- n.trees: depends very much on the use case, ranging from 100's to 10 000's
- interaction.depth: low values are preferred for boosting to obtain weak base learners
- shrinkage: typically set to the lowest possible value that is **computationally** feasible.

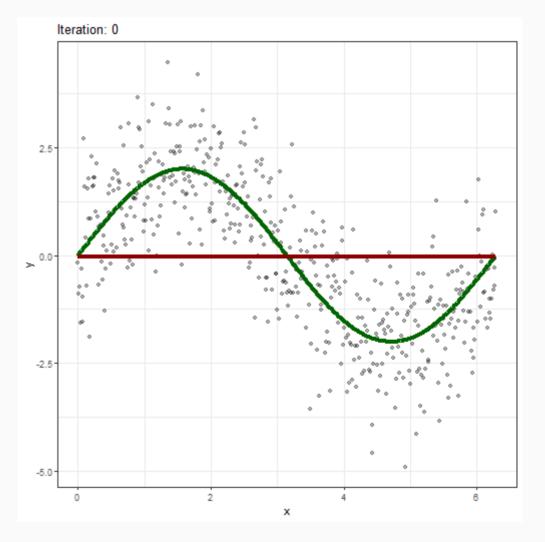
Rule of thumb: if shrinkage then ntrees .

Let's have a look at the **impact** of these tuning parameters!

GBM parameters (cont.)

Fit a GBM of 10 **stumps**, **without** applying shrinkage:

```
library(gbm)
# Fit the GBM
fit \leftarrow gbm(formula = y \sim x,
           data = dfr,
           distribution = 'gaussian',
           n.trees = 10,
           interaction.depth = 1,
           shrinkage = 1
# Predict from the GBM
pred ← predict(fit,
                n.trees = fit$n.trees,
                 type = 'response')
```

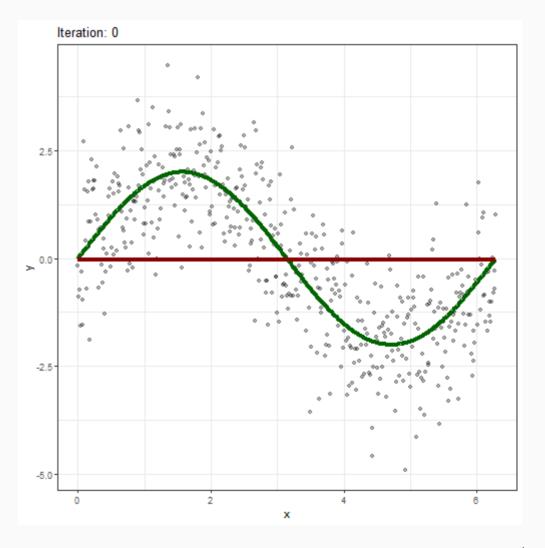


GBM parameters (cont.)

Fit a GBM of 10 **stumps**, **with** shrinkage:

Applying shrinkage **slows down** the learning process:

- avoids overfitting
- but we need more trees and longer training time.



GBM parameters (cont.)

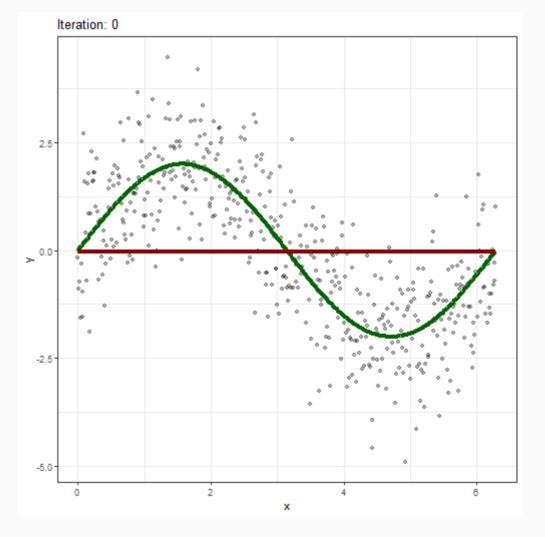
Fit a GBM of 10 **shallow** trees, **with** shrinkage:

Increasing tree **depth** allows more versatile splits:

- faster learning
- risk of **overfitting** (shrinkage important!)



interaction.depth > 1 allows for interactions!



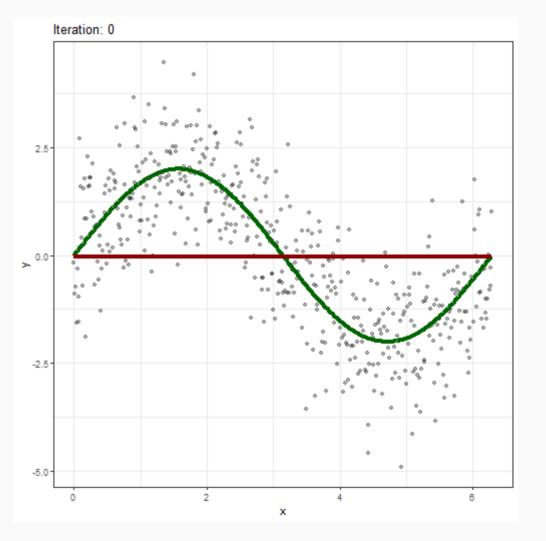
GBM parameters (cont.)

Fit a GBM of 10 **shallow** trees, **without** shrinkage:

The **danger** for overfitting is real!

Rule of thumb:

• set shrinkage ≤ 0.01 and adjust n.trees accordingly (computational constraint).



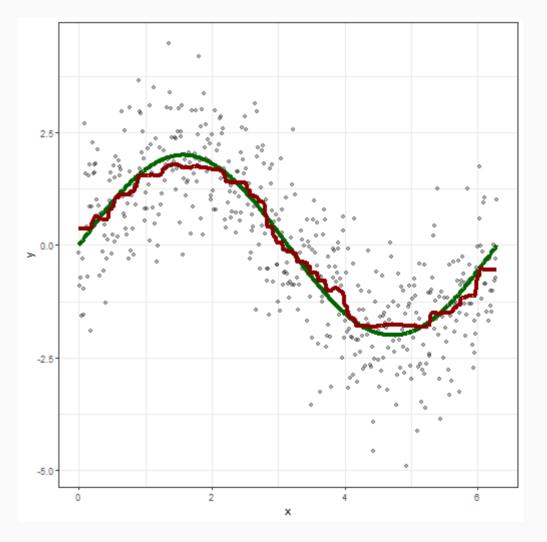
Adding trees to the ensemble

Fit a GBM of 300 shallow trees, with shrinkage:

Hi, that's a nice fit!



Always **beware** of **overfitting** when adding trees!

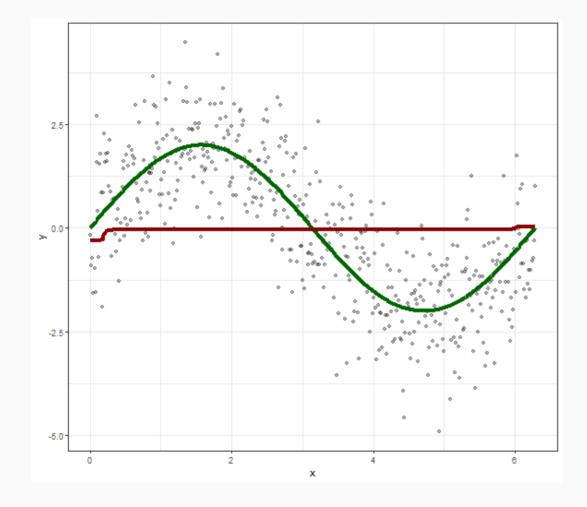




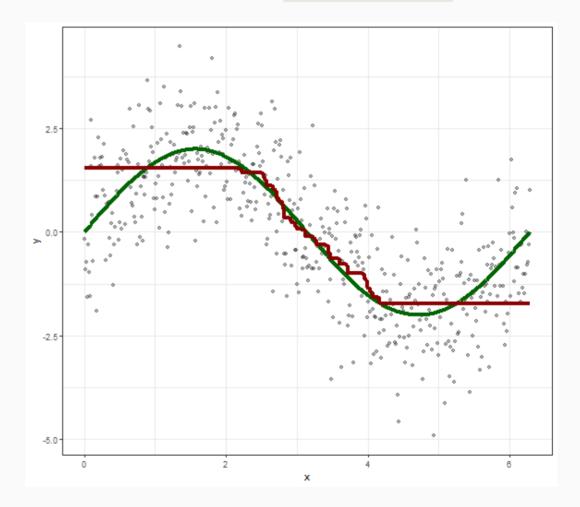
Q: use the previous code to **experiment** with your **GBM parameters** of choice (see ?gbm).

Your turn

Monotonic increasing fit via var.monotone = 1:



Monotonic decreasing fit via var.monotone = -1:



Tuning GBMs

Classification with {gbm}

Let's **experiment** with the classification example (data = dfc) to get even more grip on the tuning of **GBM parameters**.

Which distribution to specify for classification?

- "bernoulli": logistic regression for 0-1 outcomes
- "huberized": huberized hinge loss for 0-1 outcomes
- "adaboost": the AdaBoost exponential loss for 0-1 outcomes

Watch out: {gbm} does not take factors as response so you need to recode y

- either to a **numeric** in the range [0,1]
- or a **boolean** TRUE / FALSE

```
dfc ← dfc %>% dplyr::mutate(y_recode = as.integer(as.character(y)))
```

Classification - parameter combinations

Set up a grid for the parameters and list to save results:

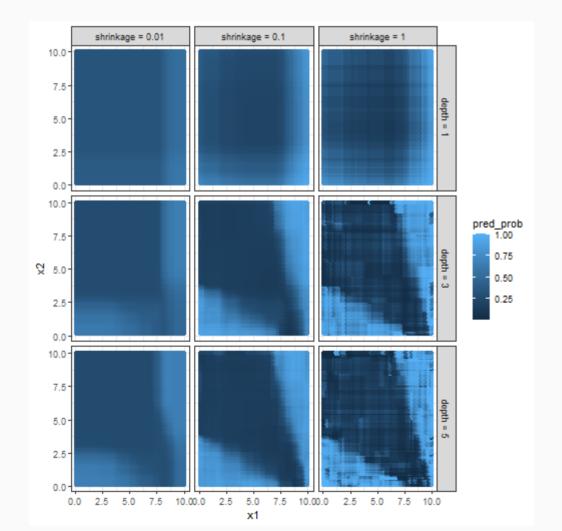
```
 \text{ctrl\_grid} \leftarrow \text{expand.grid(depth} = c(1,3,5), \\ \text{shrinkage} = c(0.01,0.1,1))   \text{results} \leftarrow \text{vector('list', length} = \text{nrow(ctrl\_grid)})
```

Fit different a GBM with 100 trees for each parameter combination:

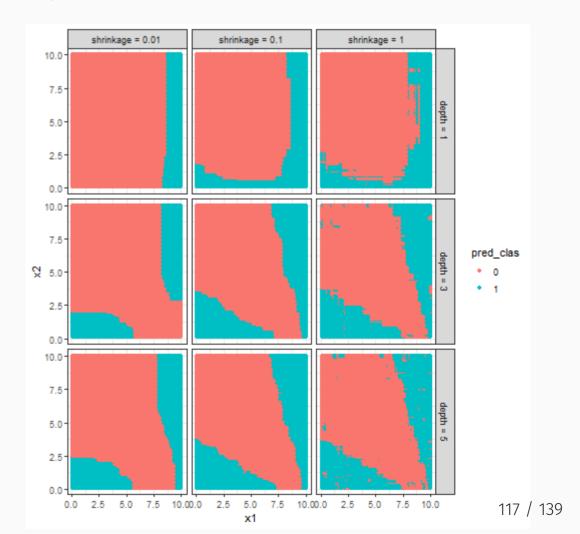
```
for(i in seq len(nrow(ctrl grid))) {
 fit \leftarrow gbm(y_recode \sim x1 + x2,
             data = dfc.
             distribution = 'bernoulli',
             n.trees = 100,
             interaction.depth = ctrl grid$depth[i],
             shrinkage = ctrl grid$shrinkage[i])
 # Save predictions, both the probabilities and the class
 results[[i]] ← dfc %>% mutate(
   depth = factor(paste('depth =',ctrl grid$depth[i]), ordered =TRUE),
   shrinkage = factor(paste('shrinkage =',ctrl grid$shrinkage[i]), ordered = TRUE),
   pred_prob = predict(fit, n.trees = fit$n.trees, type = 'response'),
   pred_clas = factor(1*(predict(fit, n.trees = fit$n.trees, type = 'response') ≥ 0.5)))
                                                                                                                   116 / 139
```

Classification - resulting fits

The predicted **probabilities**



The predicted classes





Your turn

Q: complete the code below to find the **optimal combination** of **tuning parameters**.

- 1. Set up a search grid.
- 2. Fit a GBM for each combination op parameters.
- 3. Extract the OOB performance for each GBM.

Beware: a fitted gbm object returns the improvements in OOB error via \$00bag.improve.

Performing the grid search:

The results:

```
my grid %>% dplyr::arrange(desc(oob improv))
    depth shrinkage oob improv
## 1
               0.10 0.179728774
## 2
               0.10 0.175448387
## 3
               0.01 0.123874131
## 4
               0.01 0.100252315
## 5
               0.10 0.067270554
## 6
               0.01 0.039404600
## 7
               1.00 0.036592026
## 8
          1.00 0.006891027
## 9
        5 1.00 -0.094434251
```

Another tuning option is to set cv.folds > 0 and track the cross-validation error via fit\$cv.error.

That would be a more general approach but also more time-consuming.

Claim frequency and severity modeling with {gbm}

Claim frequency modeling

```
set.seed(76539) # reproducibility
fit ← gbm(formula = nclaims ~
              ageph + agec + bm + power +
              coverage + fuel + sex + fleet + use +
             offset(log(expo)),
           data = mtpl,
            distribution = 'poisson',
            var.monotone = c(0,0,1,0,0,0,0,0,0),
           n.trees = 200,
           interaction.depth = 3,
            n.minobsinnode = 1000,
            shrinkage = 0.1,
            bag.fraction = 0.75,
            cv.folds = 0
```

- Include the log of exposure as an offset.
- Specify the **Poisson** distribution for the target.
- Impose a monotonically increasing constraint on bm.
- Perform **stochastic** gradient boosting with bag.fraction < 1.

Inspecting the individual trees

```
fit %>%
 pretty.gbm.tree(i.tree = 1) %>%
  print(digits = 4)
    SplitVar SplitCodePred LeftNode RightNode MissingNode ErrorReduction Weight
                                                                     164.94 122423
## 0
                   6.500000
## 1
                   1.500000
                                                                             95743
                  -0.027378
                                                                       0.00
                                                                             66472
                  0.004986
                                                                       0.00
                                                                             29271
                  -0.017484
                                                                       0.00
                                                                             95743
## 5
                  10.500000
                                                                      15.42
                                                                             26680
                                                           8
                   0.035538
                                                                       0.00
## 6
                                                                             17014
                   0.065038
                                                                       0.00
                                                                              9666
## 8
                   0.046226
                                                                             26680
                                                          -1
                                                                       0.00
                  -0.003599
                                                                       0.00 122423
## 9
     Prediction
     -0.003599
     -0.017484
     -0.027378
## 3
      0.004986
     -0.017484
      0.046226
## 6
      0.035538
      0.065038
```

Feature importance

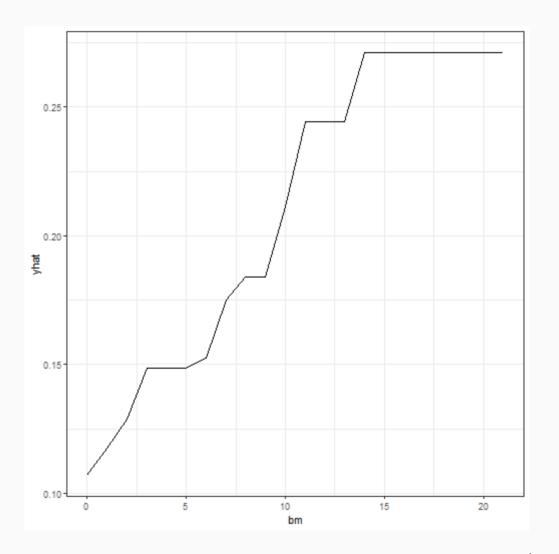
Applying the summary function on a object of class gbm shows built-in feature importance results:

Partial dependence plot

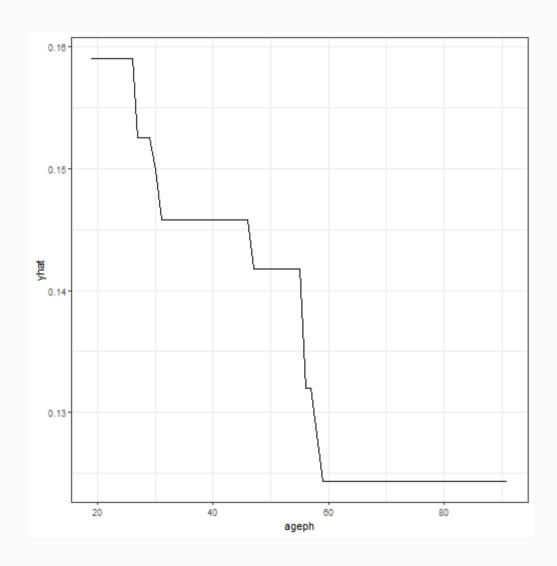
Use the following **helper function** for the PDPs:

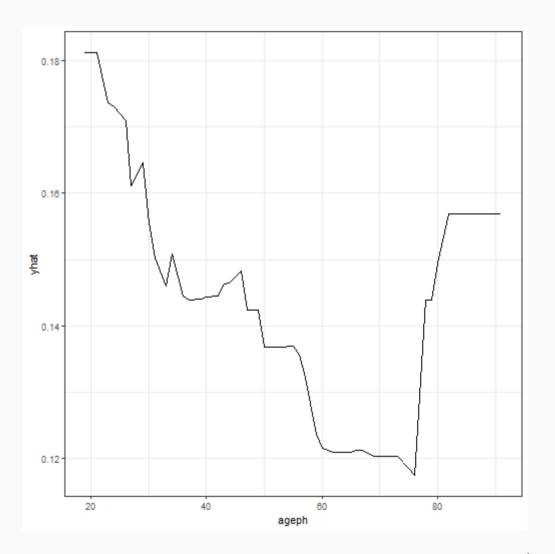
Partial dependence of the **bonus-malus level**:

Notice that the monotonic constraint is satisfied.



The age effect in a single tree and a gbm





Claim severity modeling

From the gbm help on the distribution argument:

Currently available options are "gaussian" (squared error), "laplace" (absolute loss), "tdist" (t-distribution loss), "bernoulli" (logistic regression for 0-1 outcomes), "huberized" (huberized hinge loss for 0-1 outcomes), "adaboost" (the AdaBoost exponential loss for 0-1 outcomes), "poisson" (count outcomes), "coxph" (right censored observations), "quantile", or "pairwise" (ranking measure using the LambdaMart algorithm).

Which one to choose for claim severity?

Possible solution: the {gbm} version on Harry Southworth's GitHub 😯

```
install.packages("devtools")
devtools::install_github("harrysouthworth/gbm")
```

XGBoost

XGBoost

XGBoost stands for eXtreme Gradient Boosting.

Optimized gradient boosting library: efficient, flexible and portable across multiple languages.

XGBoost follows the same general boosting approach as GBM, but adds some extra elements:

- regularization: extra protection against overfitting (see Lasso and glmnet on Day 1)
- early stopping: stop model tuning when improvement slows down
- parallel processing: can deliver huge speed gains
- different base learners: boosted GLMs are a possibility
- multiple languages: implemented in R, Python, C++, Java, Scala and Julia

XGBoost also allows to **subsample columns** in the data, much like the random forest did

- GBM only allowed subsampling of rows
- XGBoost therefore unites boosting and random forest to some extent.

Very **flexible** method with many many parameters, full list can be found here.

Using {xgboost}

```
xgboost(data, nrounds, early_stopping_rounds, params)
```

- data: training data, preferably an xgb.DMatrix (also accepts matrix, dgCMatrix, or name of a local data file)
- nrounds: max number of boosting iterations
- early_stopping_rounds: training with a validation set will stop if the performance doesn't improve for k rounds
- params: the list of parameters
 - booster: gbtree, gblinear or dart
 - objective: reg:squarederror, binary:logistic, count:poisson, survival:cox, reg:gamma, reg:tweedie, ...
 - eval_metric: rmse, mae, logloss, auc, poisson-nloglik, gamma-nloglik, gamma-deviance, tweedie-nloglik, ...
 - base_score: initial prediction for all observations (global bias)
 - nthread: number of parallel threads used to run XGBoost (defaults to max available)
 - eta: learning rate or step size used in update to prevent overfitting
 - o gamma: minimum loss reduction required to make a further partition on a leaf node
 - max_depth and min_child_weight: maximum depth and minimum leaf node observations
 - subsample and colsample_by*: subsample rows and columns (bytree, bylevel or bynode)
 - lambda and alpha: L2 an L1 regularization term to prevent overfitting
 - monotone_constraints: constraint on variable monotonicity.

Supplying the data to XGBoost

```
xgb.DMatrix(data, info = list())
```

- data: a matrix object
- info: a named list of additional information

- Features go into the **data** argument (needs to be converted to a matrix)
- The target and offset are specified via label and base_margin in info respectively

This results in an xgb.DMatrix object:

```
print(mtpl_xgb)
## xgb.DMatrix dim: 163231 x 9 info: label base_margin colnames: yes
```

A simple XGBoost model

```
set.seed(86493) # reproducibility
fit ← xgboost(
 data = mtpl_xgb,
 nrounds = 200,
 early_stopping_rounds = 20,
 verbose = FALSE,
 params = list(
   booster = 'gbtree',
   objective = 'count:poisson',
   eval metric = 'poisson-nloglik',
   eta = 0.1, nthread = 1,
   subsample = 0.75, colsample_bynode = 0.5,
   max_depth = 3, min_child_weight = 1000,
   gamma = 0, lambda = 1, alpha = 1
```

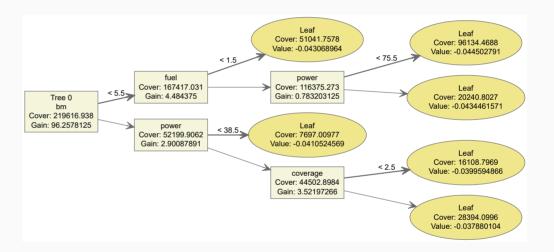
- Fit an XGBoost model to the xgb.DMatrix data
- Perform early stopping after 20 iterations without improvement
- Use a **decision tree** as base learner
- Choose the **Poisson** distribution for the target
- Stochastic boosting in rows and random split candidates in columns (like random forest)
- Apply **regularization** comparable to the elastic net penalty in {glmnet}.

Inspecting single trees

Possible to inspect **single trees** via xgb.plot.tree:

- note that the trees are 0-indexed
- 0 returns first tree, 1 returns second tree,...
- can also supply a vector of indexes

```
xgb.plot.tree(
  feature_names = colnames(mtpl_xgb),
  model = fit,
  trees = 0
)
```



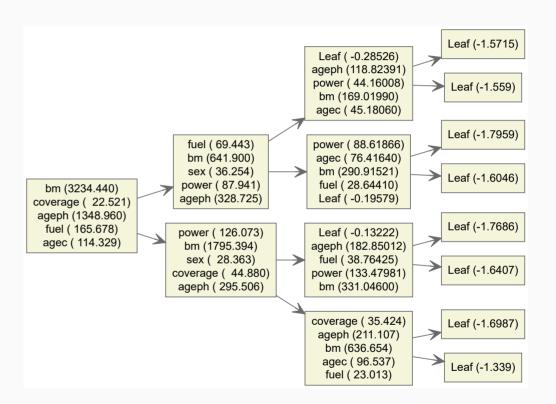
XGBoost in one tree

Get a compressed view of an XGBoost model via

```
xgb.plot.multi.trees:
```

- compressing an ensemble of trees into a single treegraph representation
- goal is to improve the interpretability

```
xgb.plot.multi.trees(
  model = fit,
  feature_names = colnames(mtpl_xgb)
)
```



Further built-in interpretations

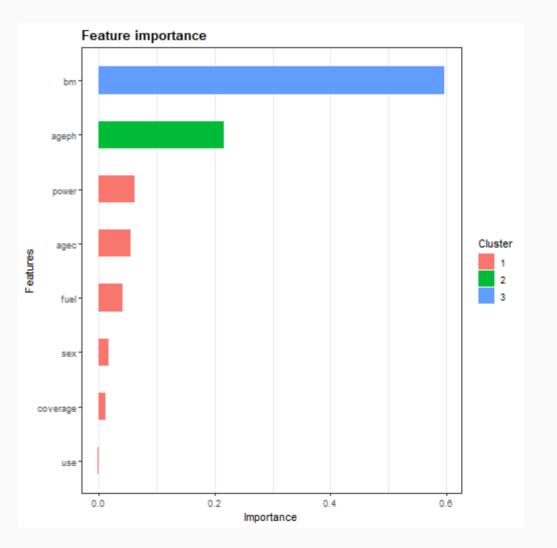
Built-in feature importance:

- xgb.importance: calculates values
- xgb.ggplot.importance: **visual** representation

```
xgb.ggplot.importance(
   importance_matrix = xgb.importance(
    feature_names = colnames(mtpl_xgb),
   model = fit
)
)
```

Packages such as {vip} and {pdp} can also be used on xgboost models

• even a vignette dedicated to this.



Cross-validation with XGBoost

Built-in cross-validation with xgb.cv

- same interface as the xgboost function
- add nfolds to define the number of folds
- add stratified for **stratification**

```
set.seed(86493) # reproducibility
xval \leftarrow xgb.cv(data = mtpl xgb,
               nrounds = 200,
               early stopping rounds = 20,
               verbose = FALSE,
               nfold = 5,
               stratified = TRUE,
               params = list(booster = 'gbtree',
                              objective = 'count:poisson',
                              eval metric = 'poisson-nloglik',
                              eta = 0.1, nthread = 1,
                              subsample = 0.75, colsample bynode = 0.5,
                             max depth = 3, min child weight = 1000,
                             gamma = 0, lambda = 1, alpha = 1)
```

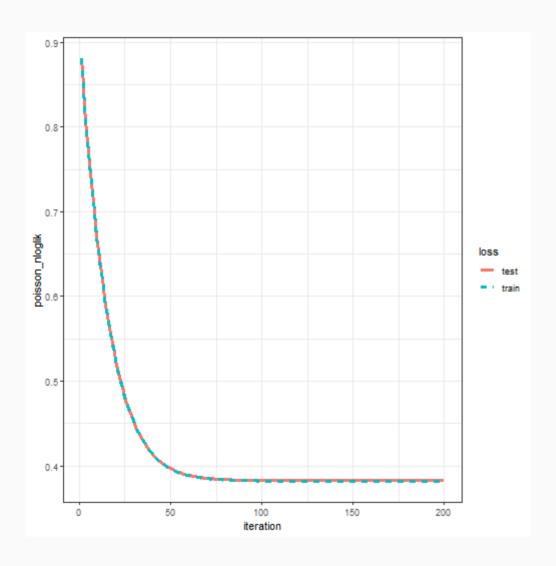
Cross-validation results

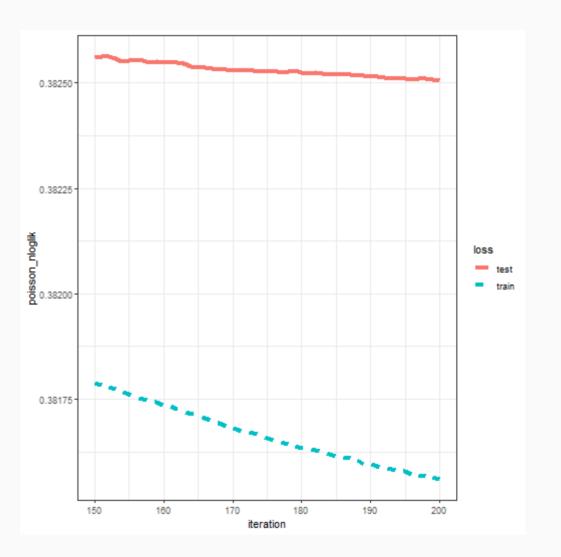
Get the cross-validation results via \$evaluation log:

```
xval$evaluation log %>% print(digits = 5)
        iter train poisson nloglik mean train poisson nloglik std
##
    1:
                                 0.88048
                                                         0.00017649
    2:
                                 0.84983
                                                         0.00016304
    3:
                                 0.82167
                                                         0.00020066
    4:
                                 0.79477
                                                         0.00028473
     5:
                                 0.76935
                                                         0.00019933
   196:
         196
                                 0.38157
                                                         0.00097562
  197:
         197
                                 0.38157
                                                         0.00097635
   198:
         198
                                 0.38157
                                                         0.00097577
  199:
         199
                                 0.38156
                                                         0.00097688
  200:
        200
                                 0.38156
                                                         0.00097555
        test poisson nloglik mean test poisson nloglik std
##
    1:
                           0.88052
                                                 0.00071933
    2:
                          0.85029
                                                 0.00083193
    3:
                          0.82171
                                                 0.00083297
    4:
                          0.79471
                                                 0.00083522
     5:
                          0.76925
                                                 0.00086406
## 196:
                           0.38251
                                                 0.00381020
```

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Cross-validation results







Your turn

That's a wrap on tree-based ML! Now it's your time to experiment.

Below are some **suggestions**, but feel free to **get creative**.

- 1. Perform a **tuning** exercise for your favorite tree-based algorithm. Beware that tuning can take up a lot of time, so do not overdo this.
- 2. Apply your favorite algorithm on a classification problem, for example to predict the **occurence** of a claim.
- 3. Use a **gamma** deviance to build a **severity** XGBoost model. The <code>mtpl</code> data contains the average claim amount in the feature <code>average</code>. Remember: if you want to develop a GBM with a gamma loss, you need the implementation available at Harry Southworth's Github.
- 4. Develop a boosting or random forest model for the **Ames Housing** data (see module 1) and extract **insights** in the form of feature importance and partial dependence plots.
- 5. Compare the performance of a regression tree, random forest and boosting model. Which model performs **best**?

Thanks!



Slides created with the R package xaringan.

Course material available via

• https://github.com/katrienantonio/hands-on-machine-learning-R-module-2