Hands-on Machine Learning with R - Module 2

Hands-on webinar

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hands-on-machine-learning-R-module-2 | September 9 & 10, 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

https://katrienantonio.github.io/ & https://jonascrevecoeur.github.io/ & https://henckr.github.io/

katrien.antonio@kuleuven.be & jonas.crevecoeur@kuleuven.be & roel.henckaerts@kuleuven.be

(Katrien) Professor in insurance data science

(Jonas) Postdoc and consultant in statistics and 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)?

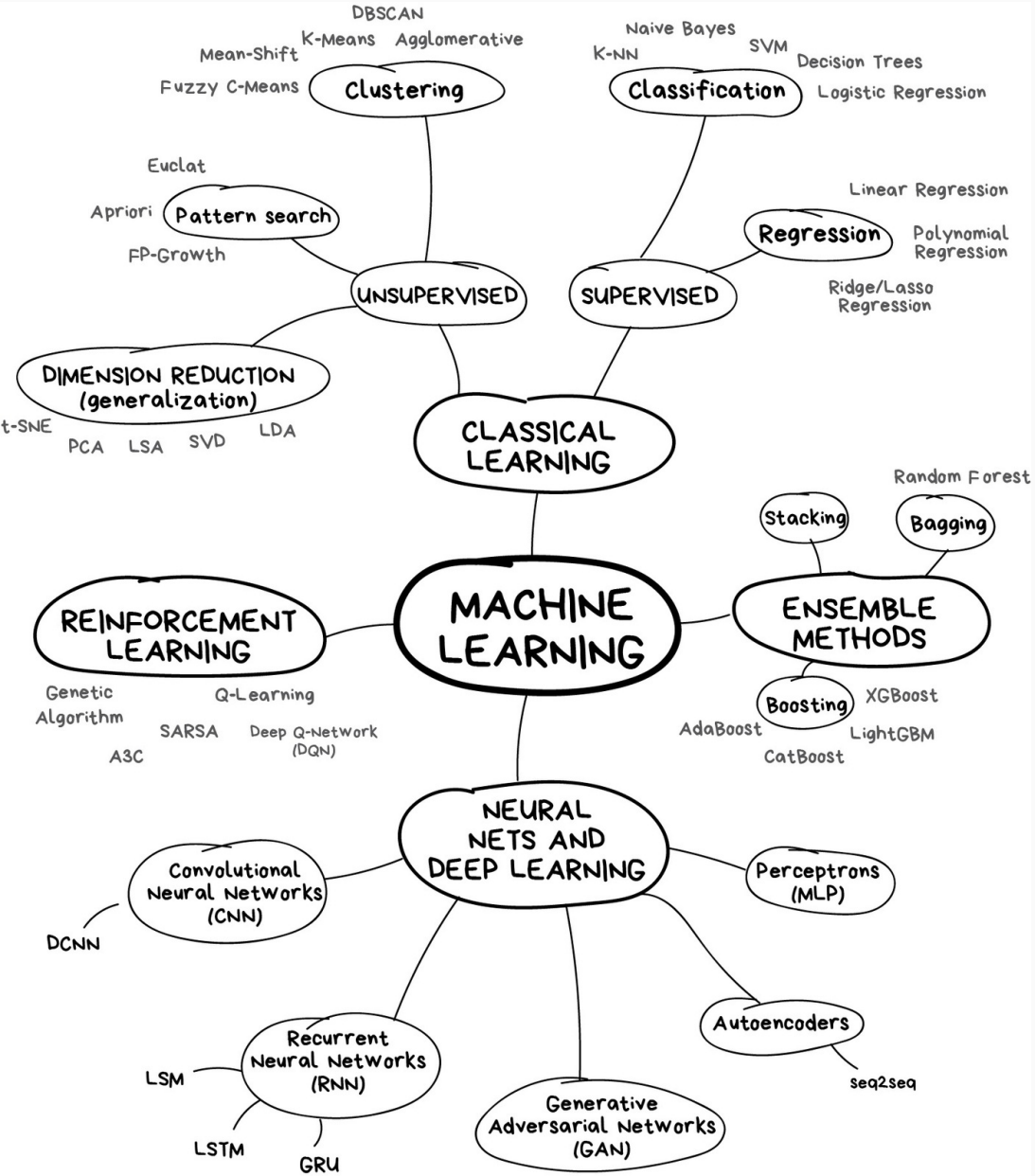
Why this course?

The goals of this module 🚀

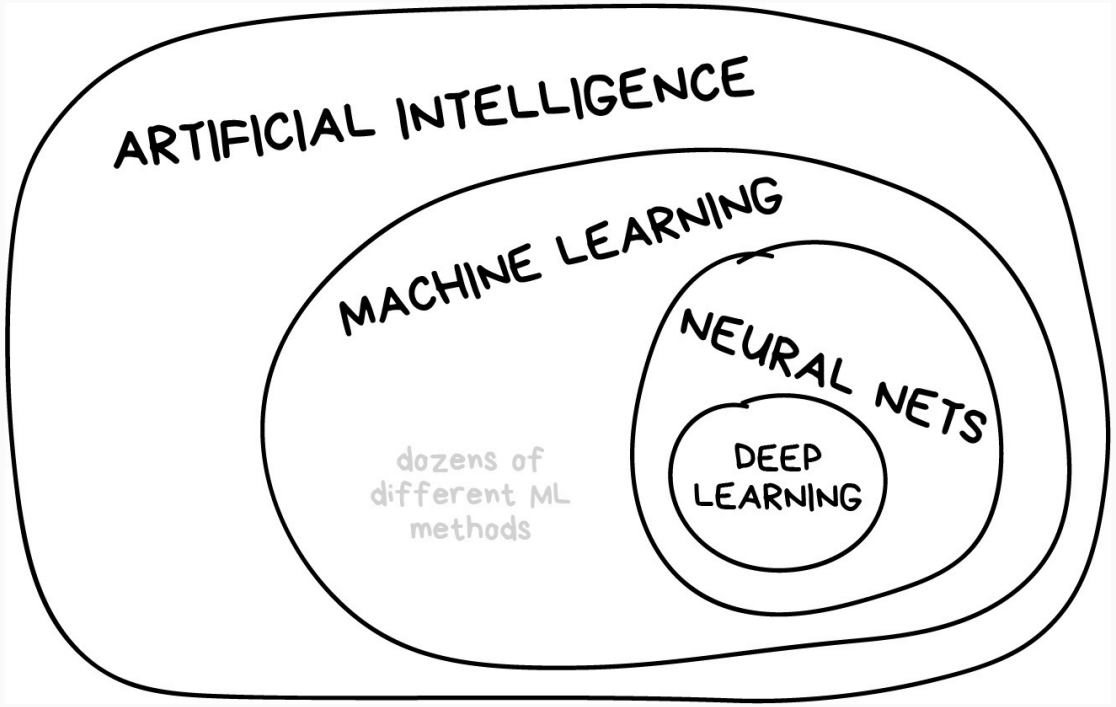
- develop foundations of working with regression and decision trees
- step from simple trees to ensembles of trees, with bagging and boosting
- focus on the use of these ML methods for the analysis of frequency + severity data
- discuss and construct some useful interpretation tools, e.g. variable importance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

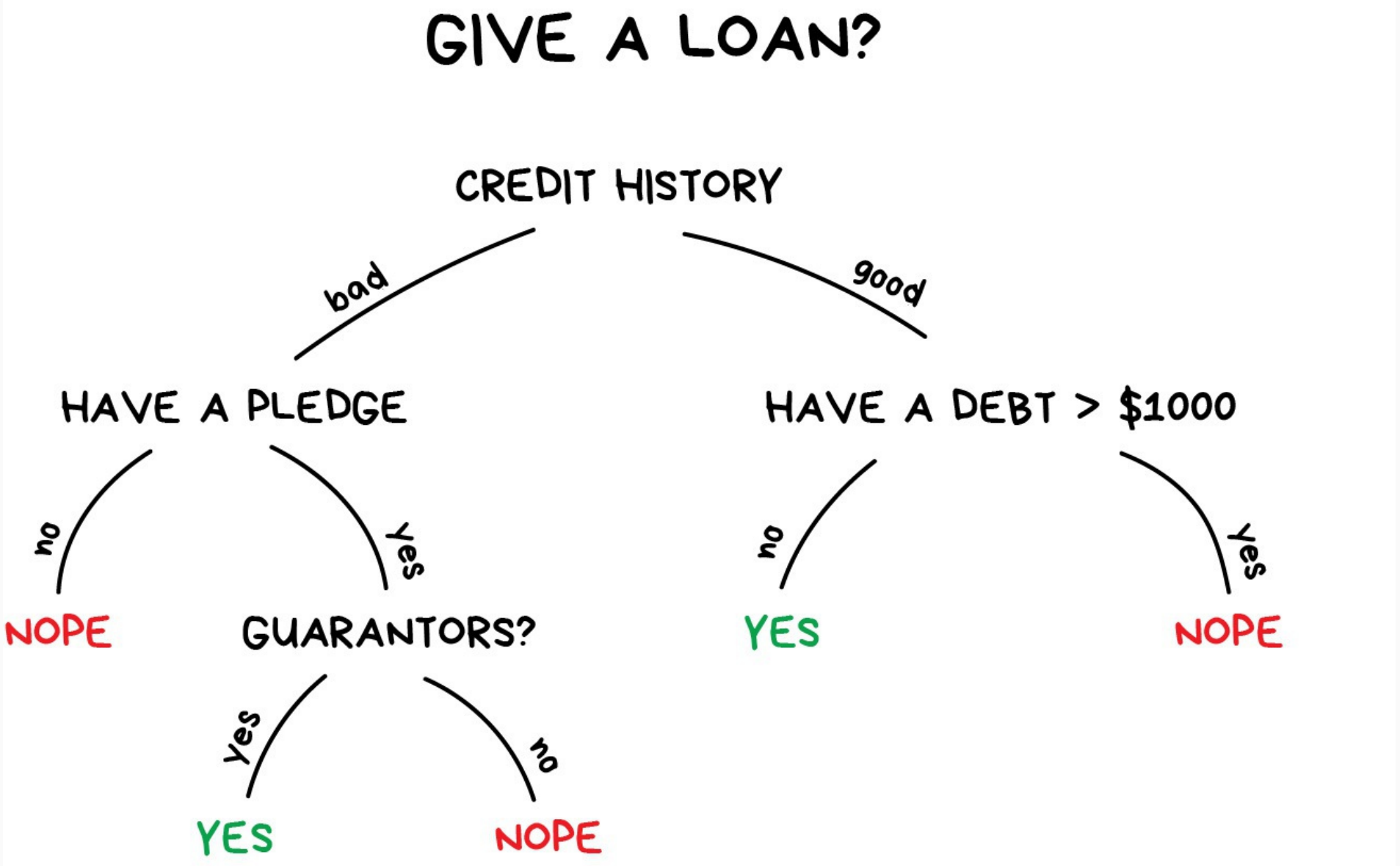
Machine learning (ML) according to Wikipedia:

> *"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



DECISION TREE

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

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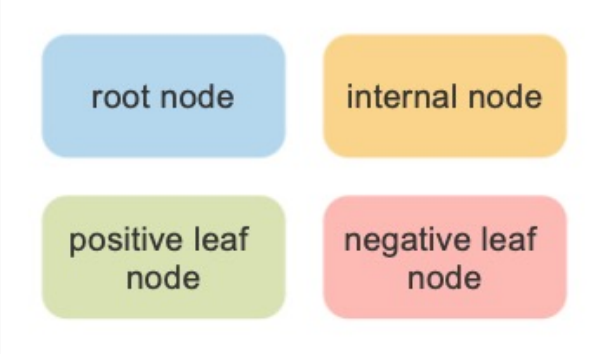
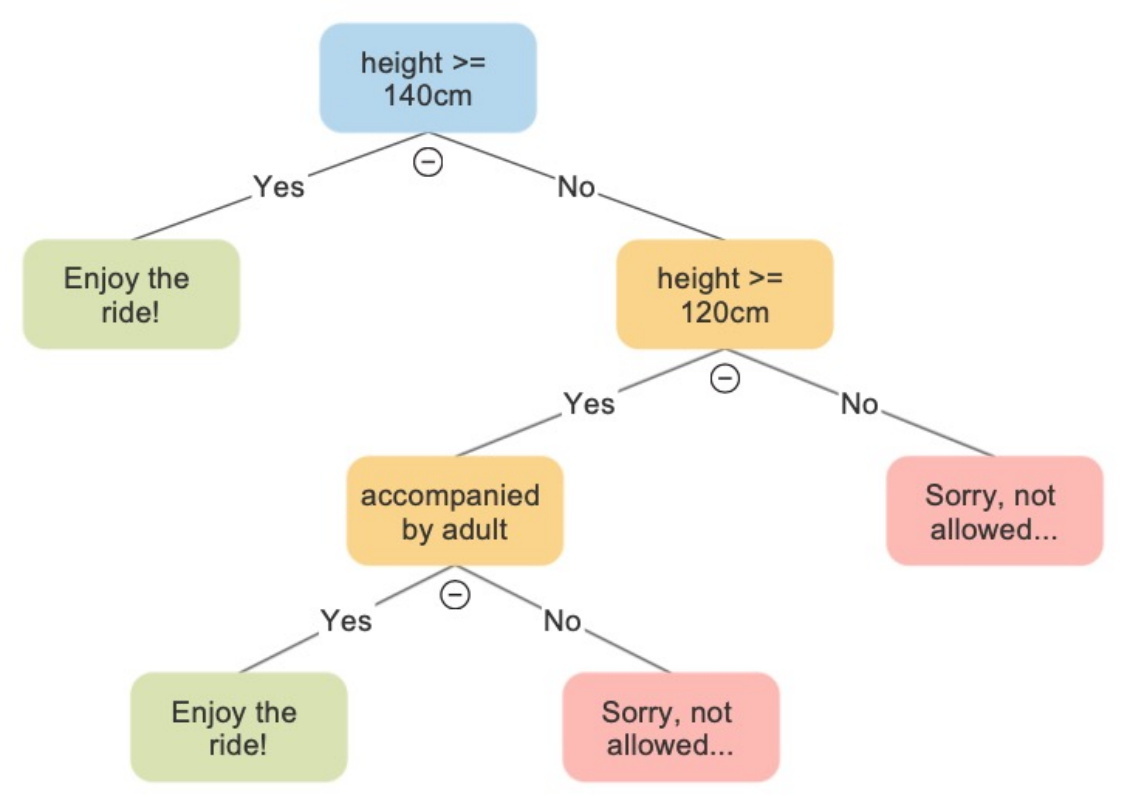
A tree then predicts the output in a **leaf node** as follows:

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

Different types of nodes:





Tree growing process

A golden standard is the **C**lassification **A**nd **R**egression **T**ree 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 R_1 + loss in region R_2
- 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}

```
rpart(formula, data, method,
      control = rpart.control(cp, maxdepth, minsplit, minbucket))
```

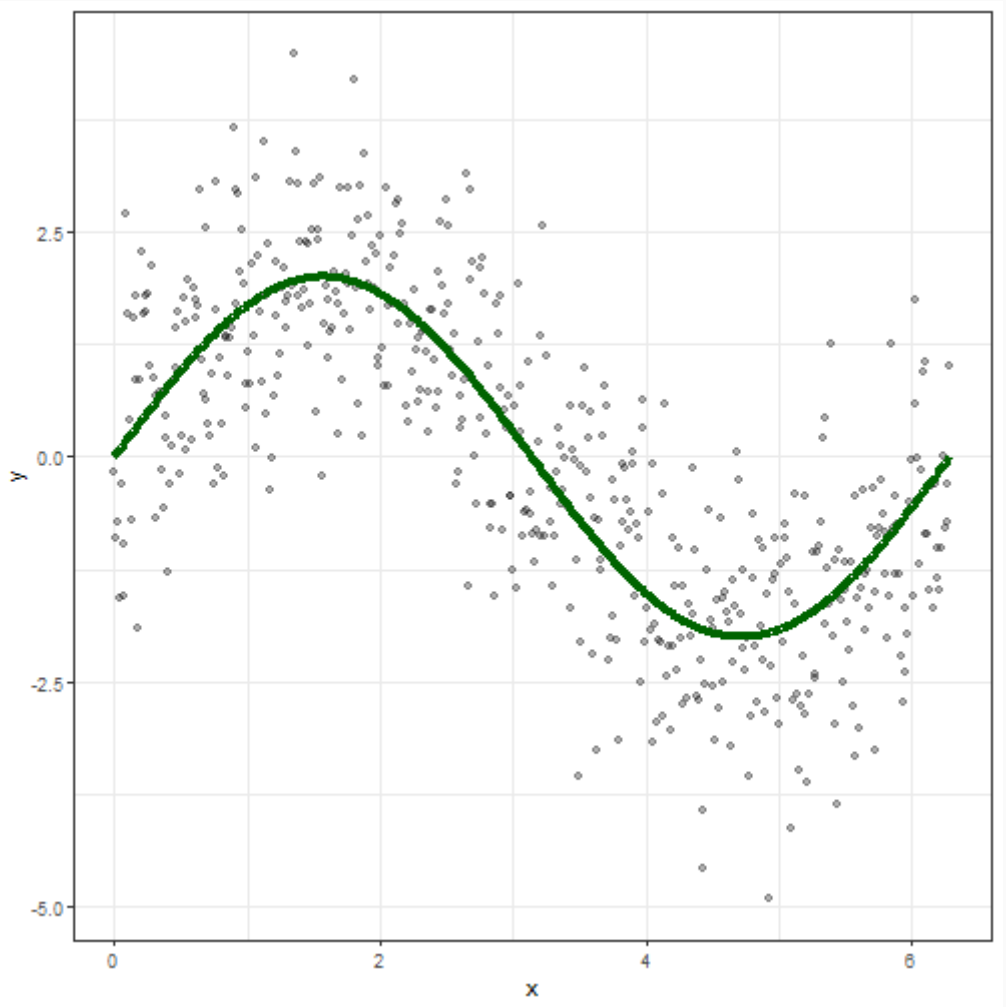
- `formula`: a formula as *response ~ feature1 + feature2 + ...*  no need to include the interactions!
- `data`: the observation data containing the response and features
- `method`: a string specifying which **loss function** to use
  - "anova" for regression (SSE as loss)
  - "class" for classification (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 ← tibble::tibble(
  x = seq(0, 2 * pi, length.out = 500),
  m = 2 * sin(x),
  y = m + rnorm(length(x), sd = 1)
  )
```

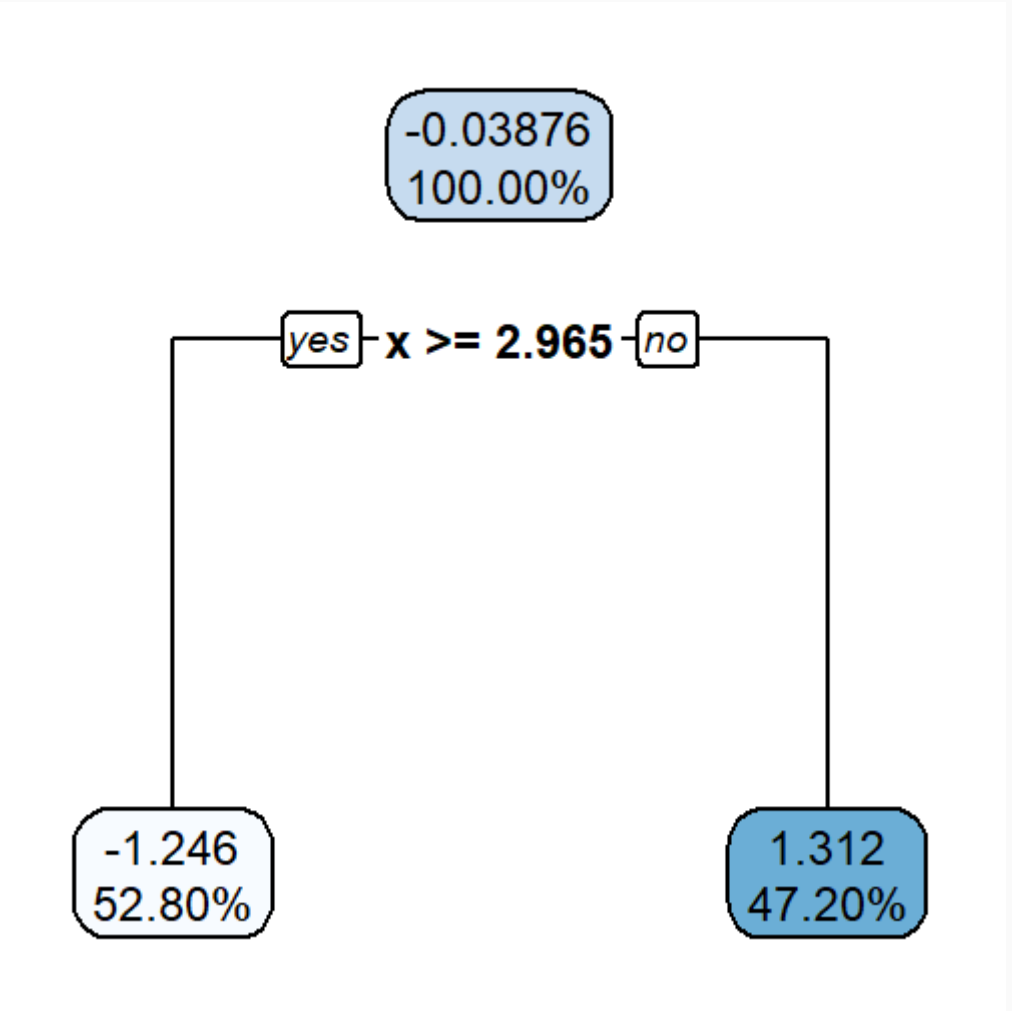
```
##             x          m          y
## 1  0.00000000 0.00000000 -0.1789007
## 2  0.01259155 0.02518244 -0.9028617
## 3  0.02518311 0.05036089 -0.7336728
## 4  0.03777466 0.07553136 -1.5750691
## 5  0.05036621 0.10068985 -0.3073767
## 6  0.06295777 0.12583237 -0.9696970
## 7  0.07554932 0.15095495 -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 ← rpart(formula = y ~ 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)
```



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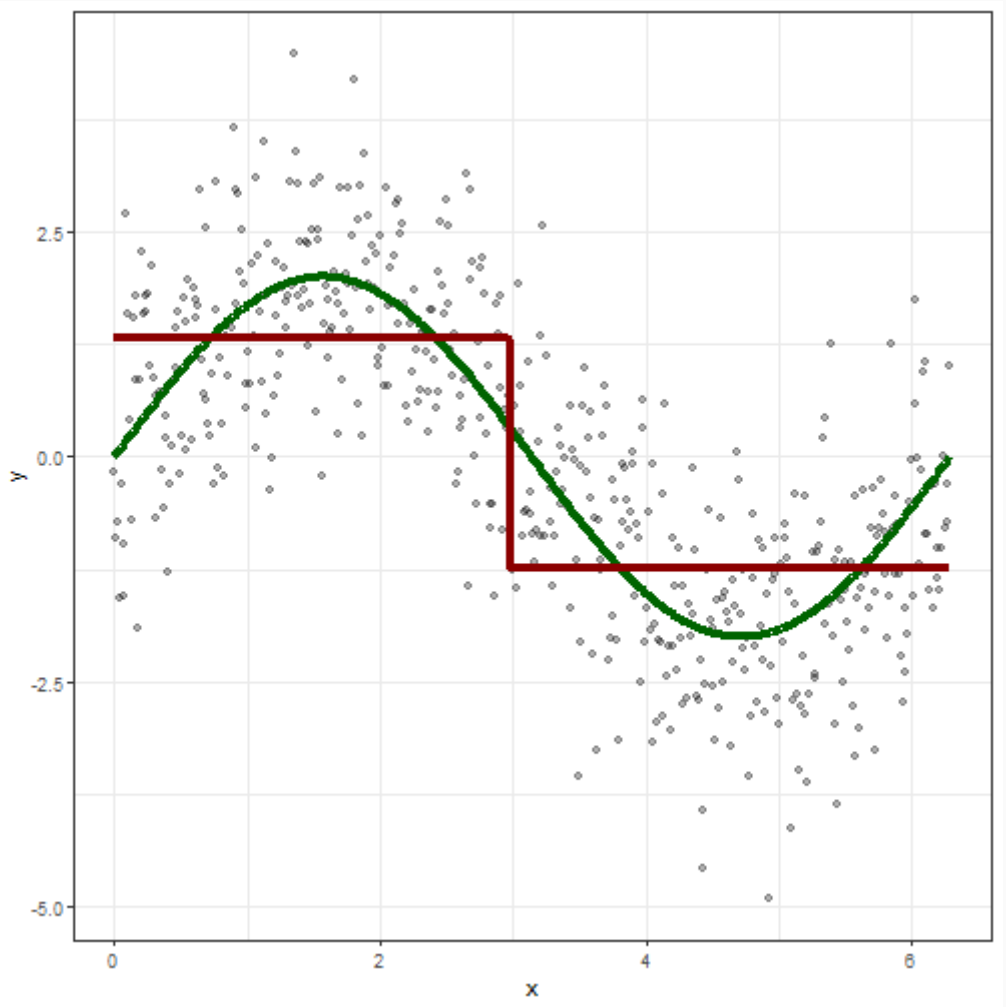
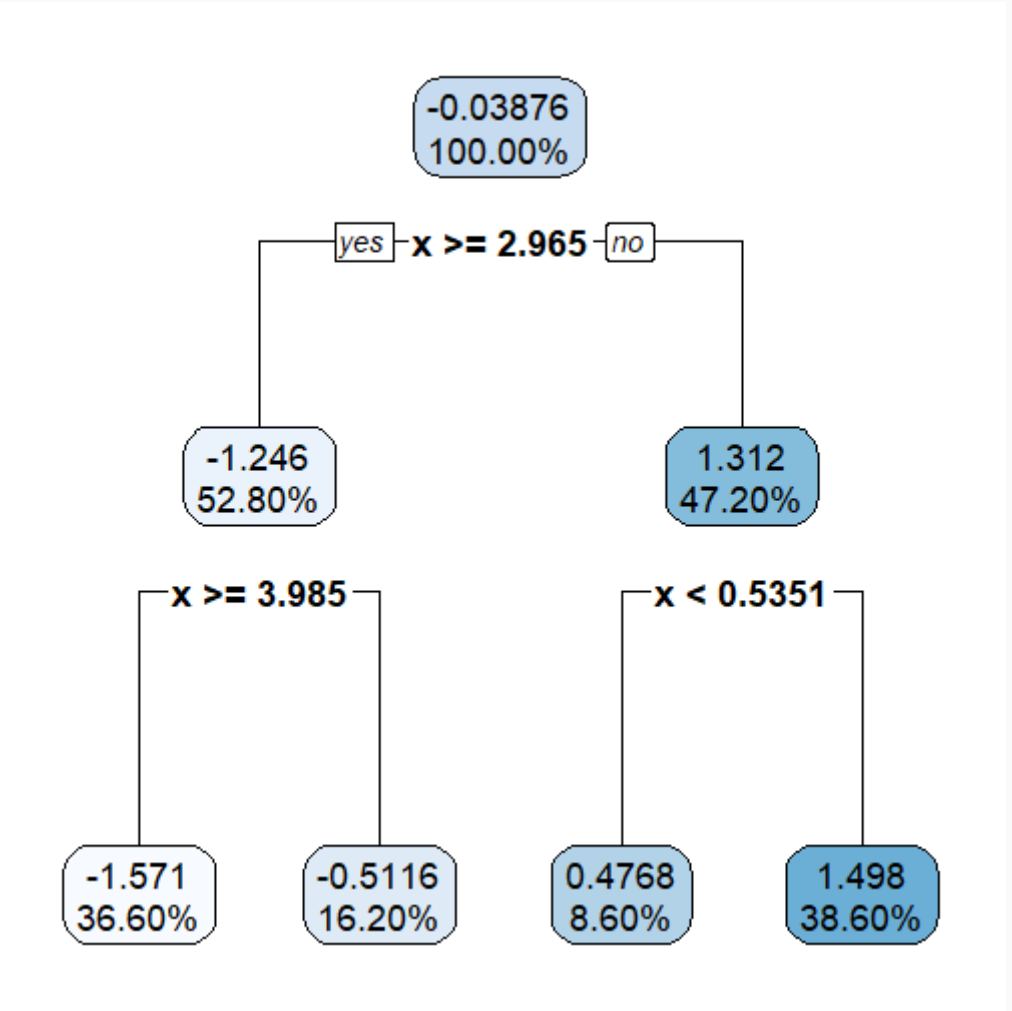
##   3) x< 2.965311 236  298.8888  1.31176200 *
```

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



Adding splits

```
fit ← rpart(formula = y ~ 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≥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≥0.535141 193  206.99550  1.49779000 *
```



Adding splits (cont.)

```
fit ← rpart(formula = y ~ x,
            data = dfr,
            method = 'anova',
            control = rpart.control(
              maxdepth = 2
              )
            )
print(fit)
## n= 500
##
## node), split, n, deviance, yval
##       * denotes terminal node
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## 1) root 500 1498.45700 -0.03876172
##   2) x≥2.965311 264  384.33360 -1.24604800
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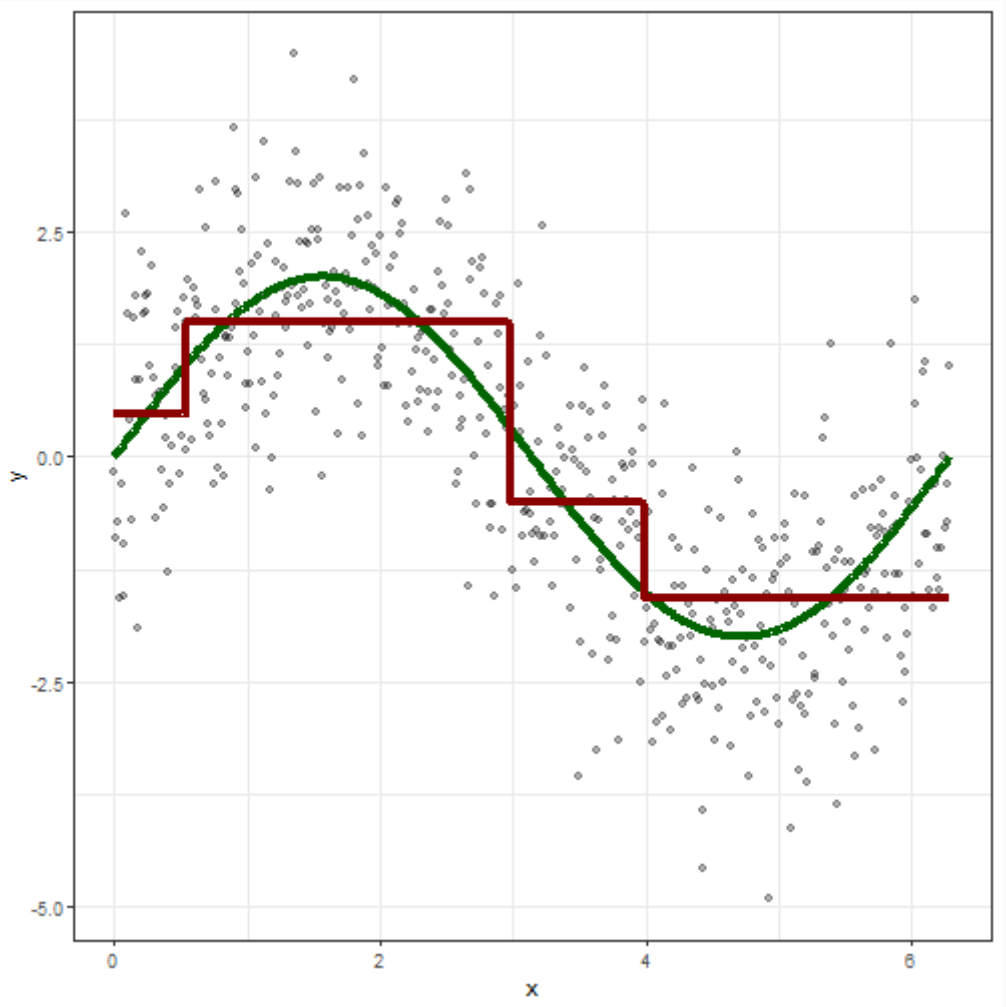


Your turn

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)**:

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

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 *
##     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≥0.535141 193  206.99550  1.49779000 *
```

Let's predict the values for leaf node 6.

Q.1: calculate the prediction

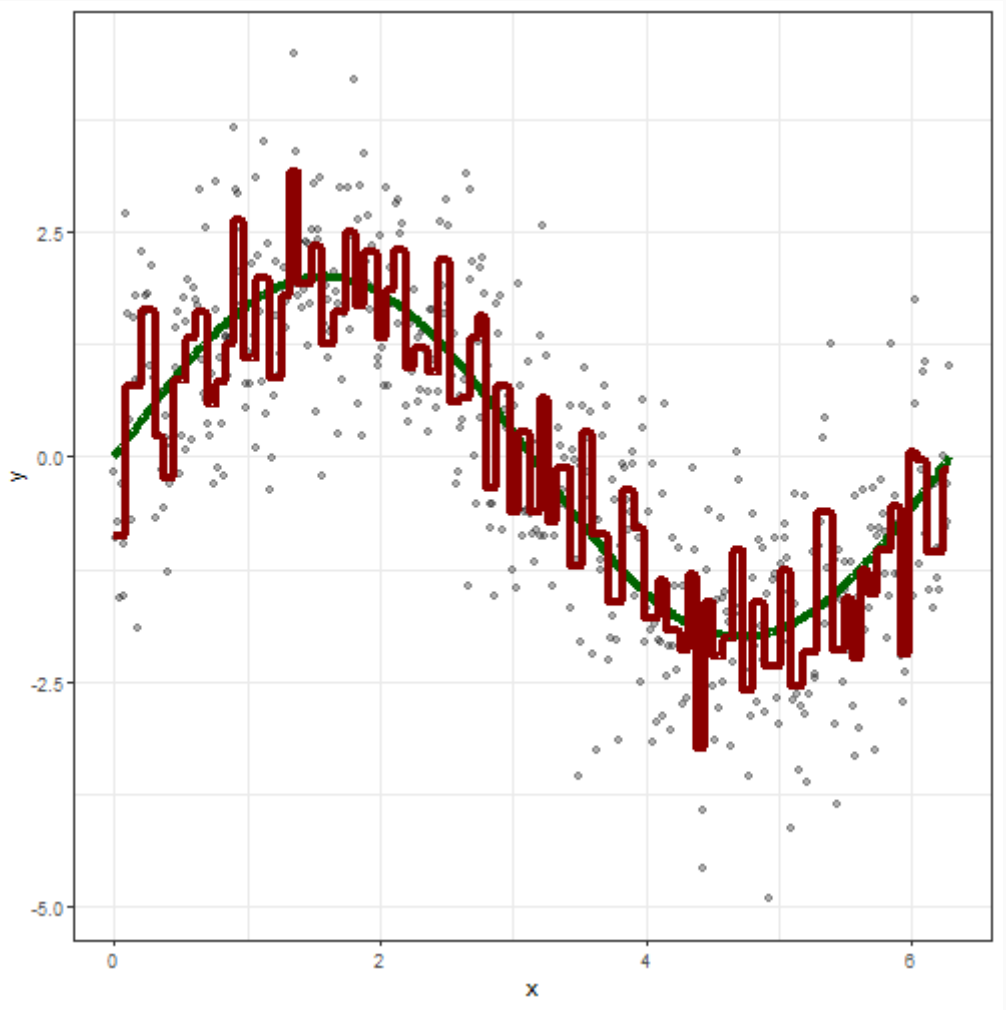
```
# Subset observations in node 6
obs ← dfr %>% dplyr::filter(x < 0.535141)

# 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 ← rpart(formula = y ~ x,
            data = dfr,
            method = 'anova',
            control = rpart.control(
              maxdepth = 20,
              minsplit = 10,
              minbucket = 5,
              cp = 0
              )
            )
```



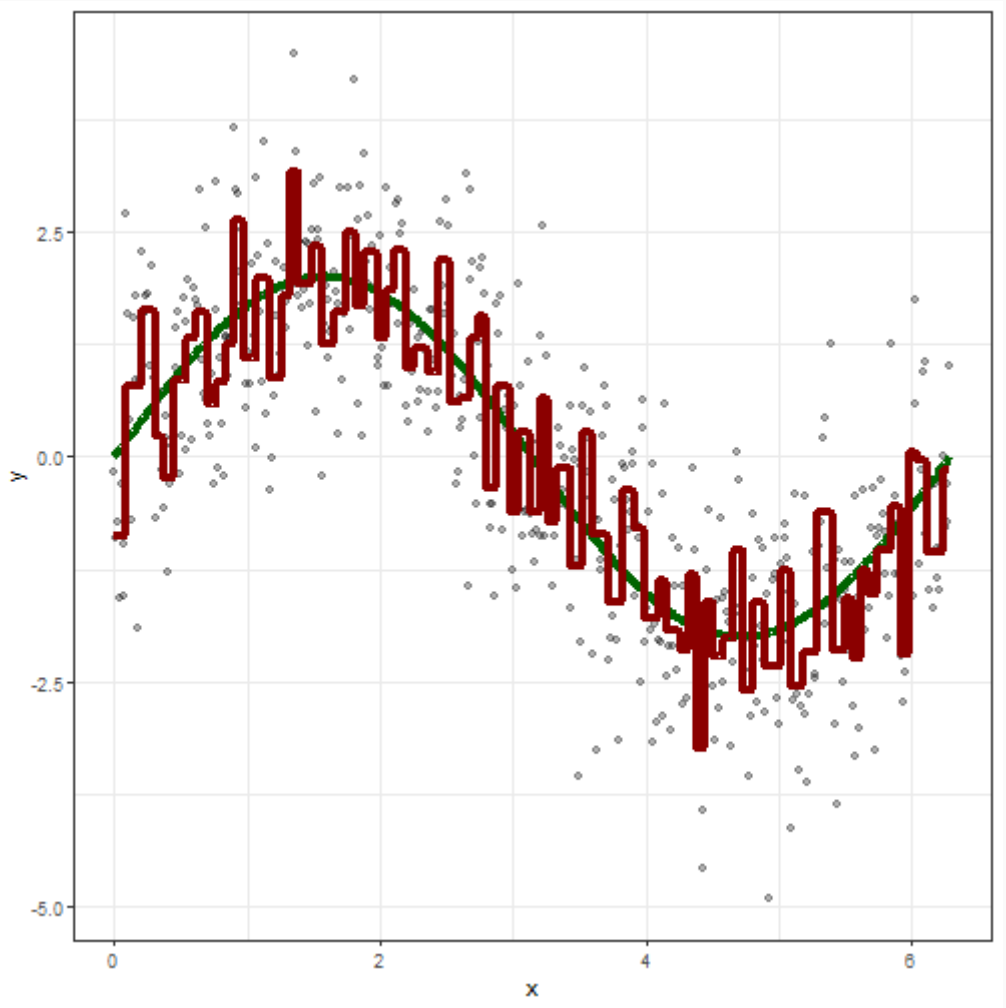
Take-away 📢 - understanding the `cp` parameter:

- 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.)

```
fit ← rpart(formula = y ~ x,
            data = dfr,
            method = 'anova',
            control = rpart.control(
              maxdepth = 20,
              minsplit = 10,
              minbucket = 5,
              cp = 0
              )
            )
```

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 ↑ and variance ↓
- a **deep** tree will overfit:

  bias ↓ 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 ↑ and variance ↓
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  bias ↓ 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?

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

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

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

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

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

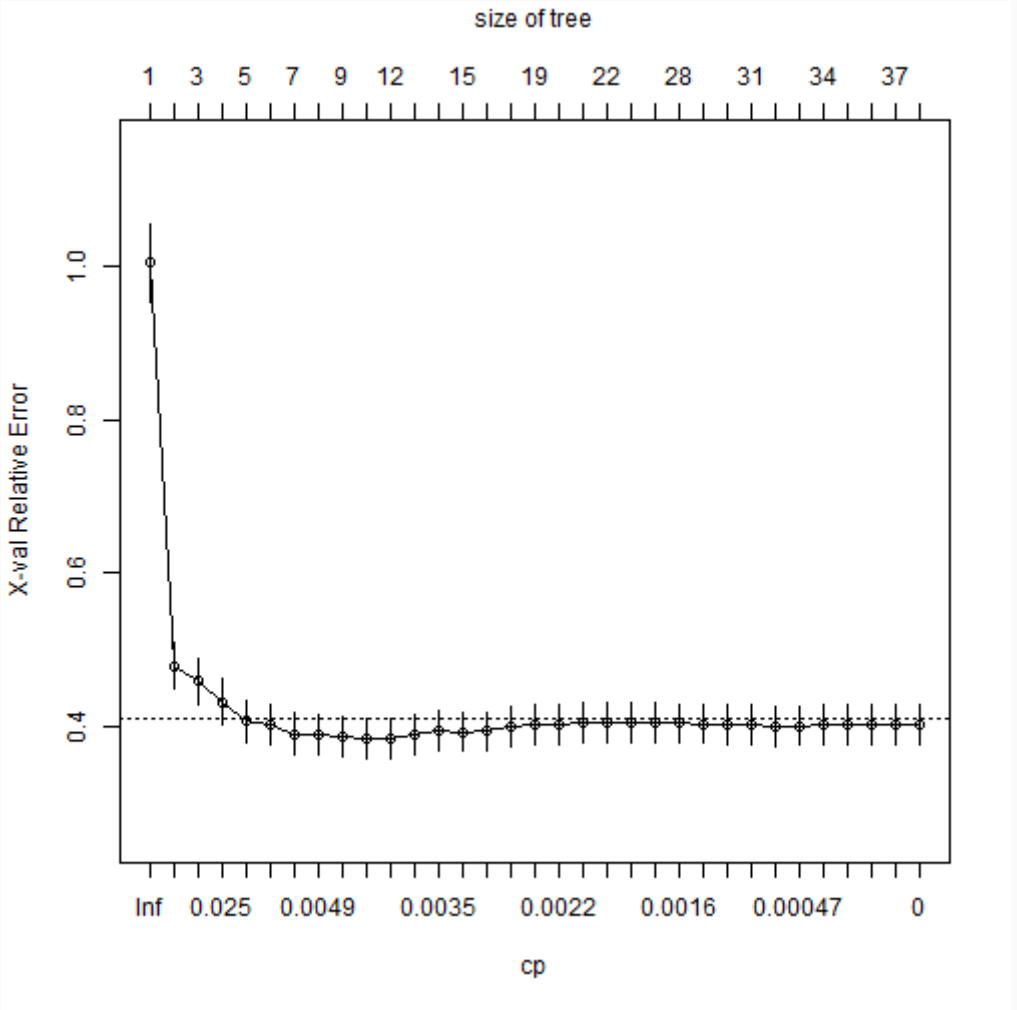
- `cp` is the complexity parameter in {rpart}
- `cp` is α divided by f_{loss} evaluated in root node.

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

Pruning via cross-validation

```
set.seed(87654) # reproducibility
fit ← rpart(formula = y ~ x,
            data = dfr,
            method = 'anova',
            control = rpart.control(
              maxdepth = 10,
              minsplit = 20,
              minbucket = 10,
              cp = 0,
              xval = 5
              )
            )
```

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



Pruning via cross-validation

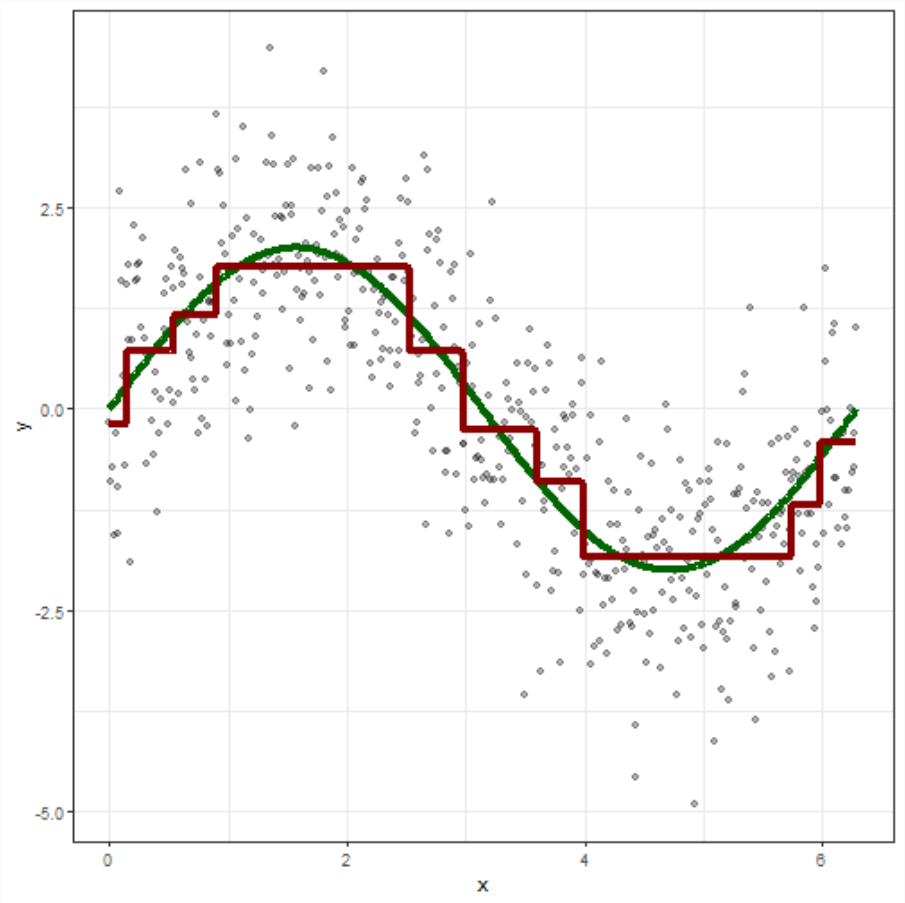
```
set.seed(87654) # reproducibility
fit ← rpart(formula = y ~ x,
            data = dfr,
            method = 'anova',
            control = rpart.control(
              maxdepth = 10,
              minsplit = 20,
              minbucket = 10,
              cp = 0,
              xval = 5
         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

```
print(cpt[1:20,])
# Which cp value do we choose?
min_xerr ← which.min(cpt[,'xerror'])
se_rule ← min(which(cpt[, 'xerror'] <
  (cpt[min_xerr, 'xerror'] + cpt[min_xerr, 'xstd'])))
```

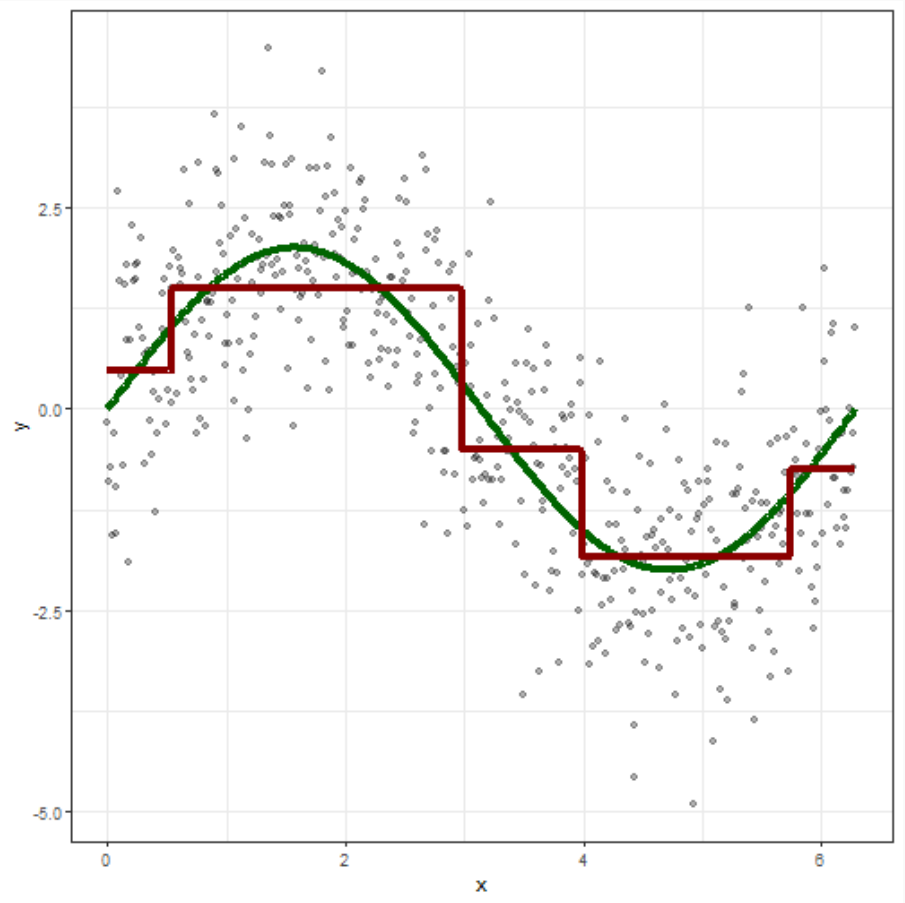
```
##            CP nsplit rel error   xerror      xstd
## 1  0.54404922      0  1.000000 1.004726 0.0514072
## 2  0.04205955      1  0.455951 0.479691 0.0306899
## 3  0.02638545      2  0.413891 0.459565 0.0303987
## 4  0.02446313      3  0.387506 0.432619 0.0288631
## 5  0.01686947      4  0.363043 0.407090 0.0271596
## 6  0.00556730      5  0.346173 0.402555 0.0269263
## 7  0.00537029      6  0.340606 0.390939 0.0263032
## 8  0.00455035      7  0.335236 0.389550 0.0259170
## 9  0.00438010      8  0.330685 0.387857 0.0262972
## 10 0.00437052      9  0.326305 0.384689 0.0262569
## 11 0.00417651     11  0.317564 0.384689 0.0262569
## 12 0.00413572     12  0.313388 0.389304 0.0264134
## 13 0.00288842     13  0.309252 0.394634 0.0263896
## 14 0.00248513     14  0.306363 0.393097 0.0255738
## 15 0.00230656     16  0.301393 0.394084 0.0254549
## 16 0.00227479     17  0.299087 0.401089 0.0260820
## 17 0.00222192     18  0.296812 0.403132 0.0258395
## 18 0.00218218     19  0.294590 0.403132 0.0258395
## 19 0.00189012     20  0.292408 0.405123 0.0258289
## 20 0.00177060     21  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

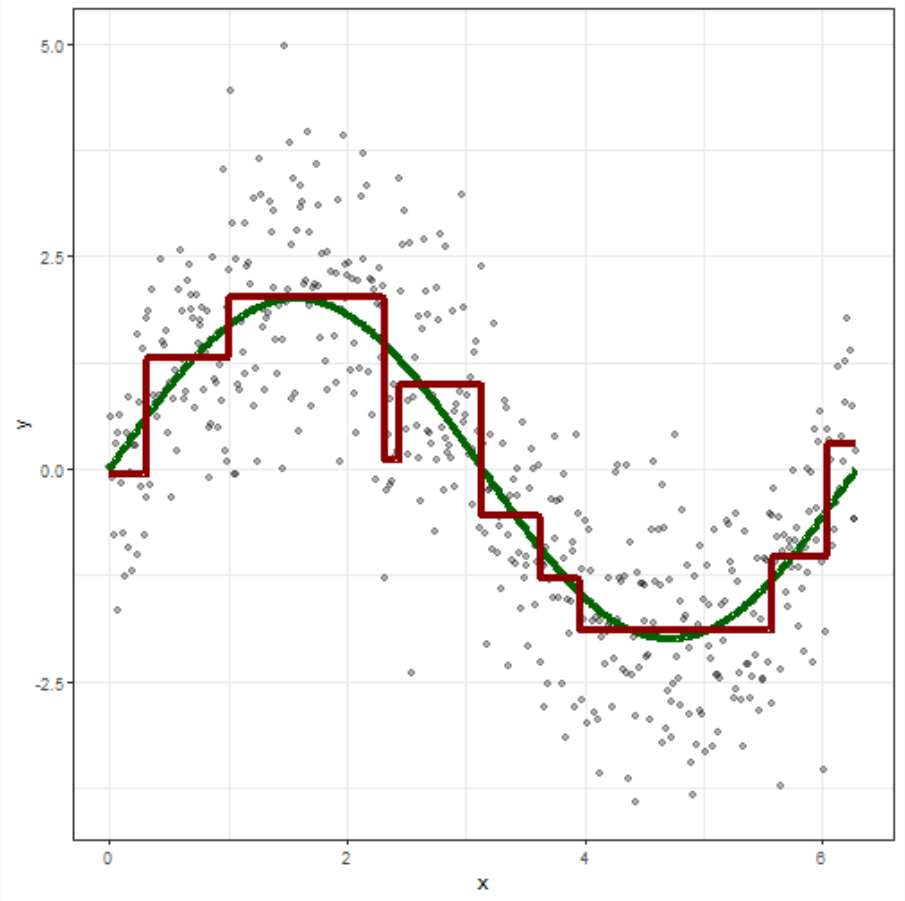
Q: Trees are often associated with high variance, meaning that the resulting model can be very sensitive to the input data. Let's explore this statement!

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?

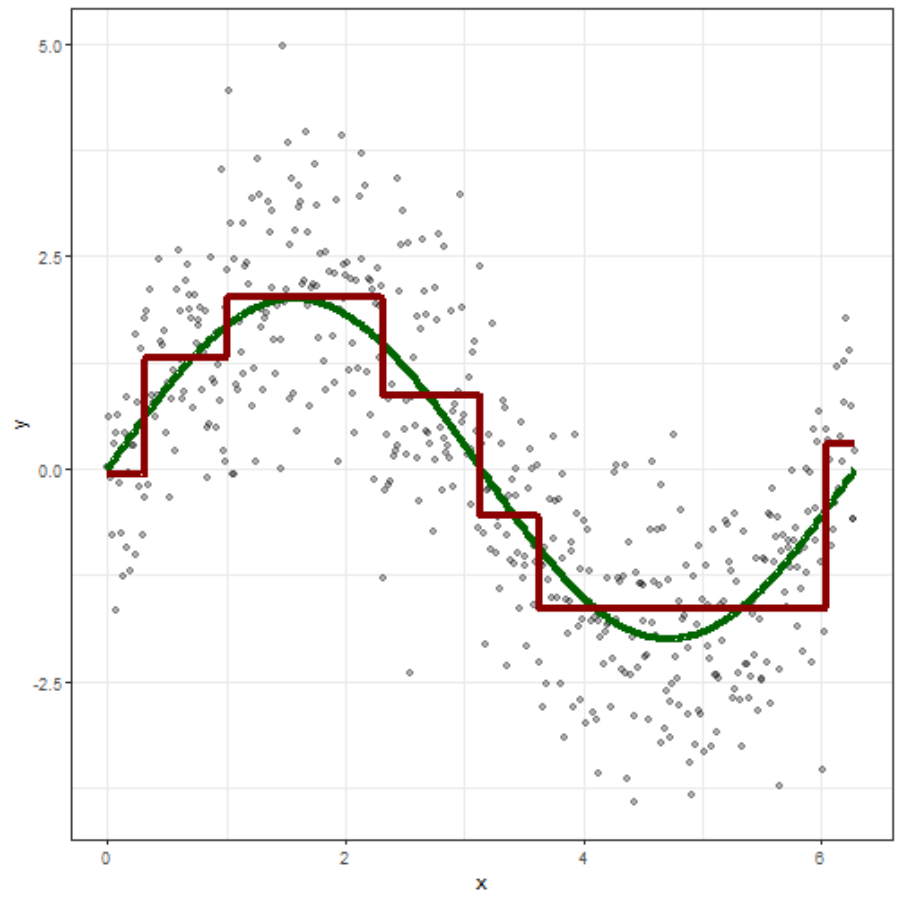
Q.1: a brand new data set

```
# 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

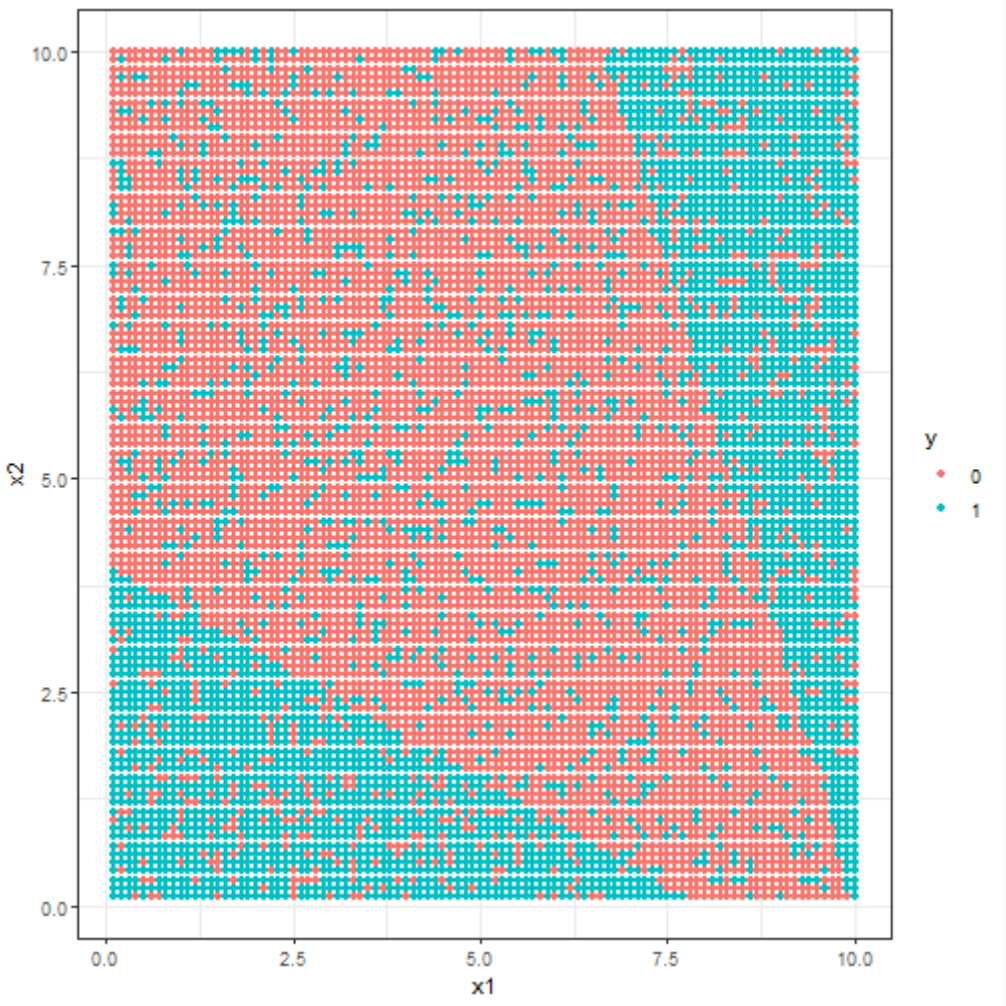


Q.3: trees look rather different compared to those from before, even though they try to approximate the same function.

Toy example of a classification tree

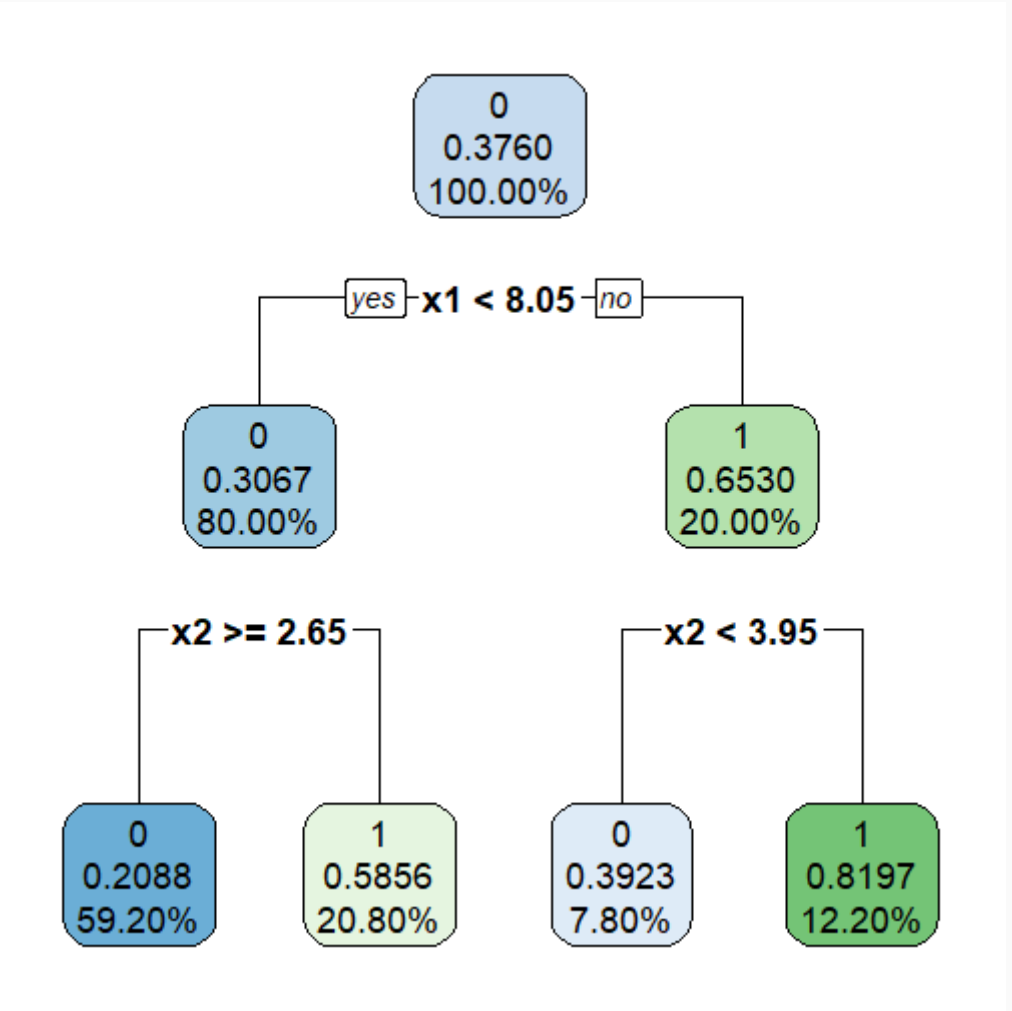
Simulated data

```
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))
              )
         )
    )
)
```



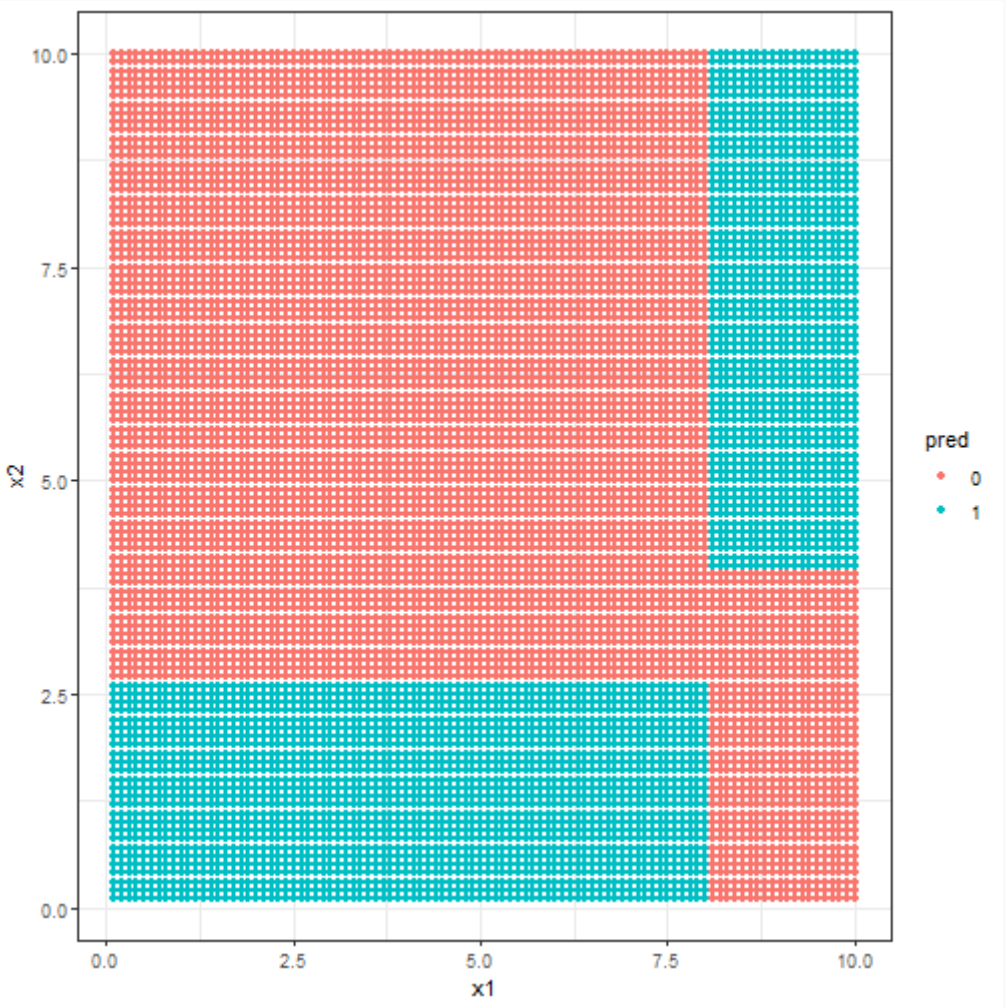
Fitting a simple tree

```
fit ← rpart(formula = y ~ 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≥8.05 2000  694 1 (0.3470000 0.6530000)
##     6) x2< 3.95 780  306 0 (0.6076923 0.3923077) *
##     7) x2≥3.95 1220  220 1 (0.1803279 0.8196721) *
```



Fitting a simple tree (cont.)

```
fit ← rpart(formula = y ~ 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≥8.05 2000  694 1 (0.3470000 0.6530000)
##     6) x2< 3.95 780  306 0 (0.6076923 0.3923077) *
##     7) x2≥3.95 1220  220 1 (0.1803279 0.8196721) *
```



What about an overly complex tree?

```
fit ← rpart(formula = y ~ x1 + x2,
            data = dfc,
            method = 'class',
            control = rpart.control(
              maxdepth = 20,
              minsplit = 10,
              minbucket = 5,
              cp = 0
              )
            )
```

What about an overly complex tree?

```
fit ← rpart(formula = y ~ x1 + x2,
            data = dfc,
            method = 'class',
            control = rpart.control(
              maxdepth = 20,
              minsplit = 10,
              minbucket = 5,
              cp = 0
              )
            )
```

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.

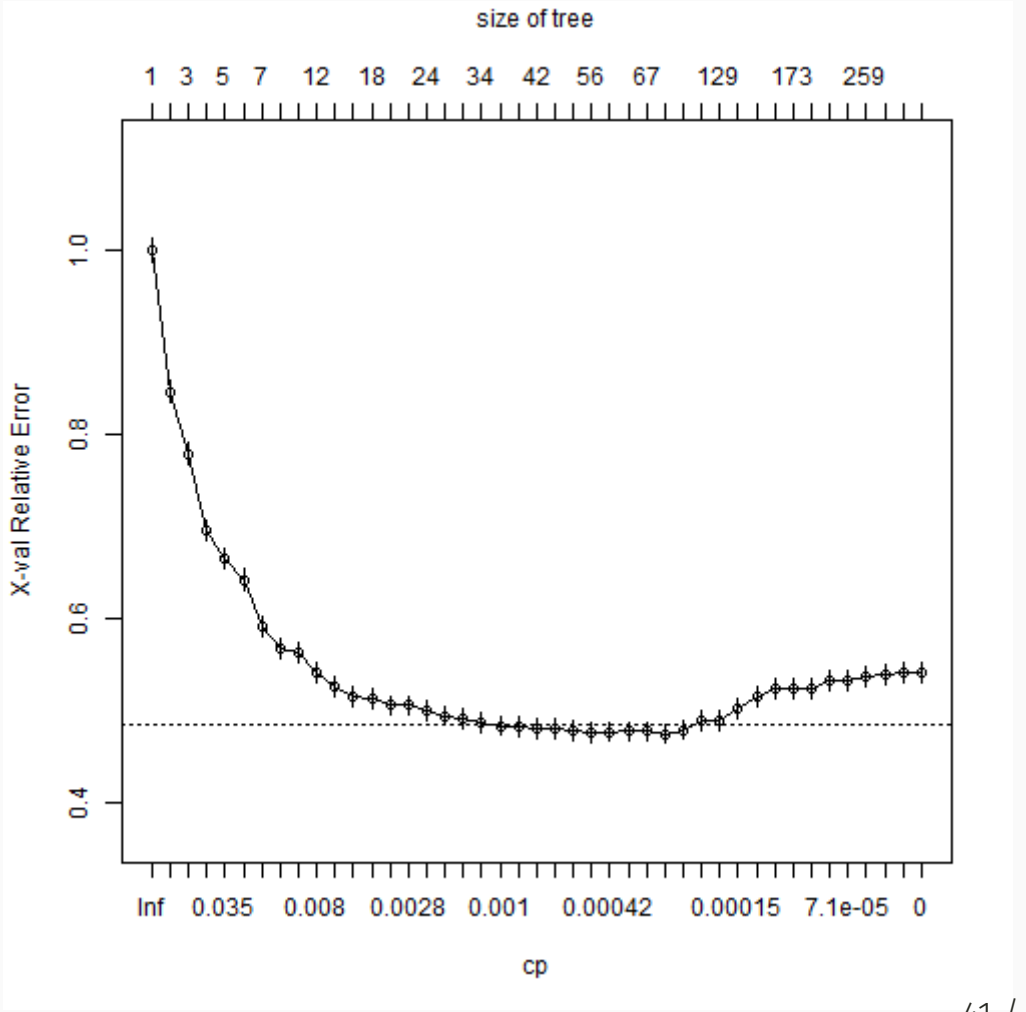
1. Set `xval = 5` in `rpart.control()` (do not forget to set a **seed** beforehand).
2. Graphically inspect the xval results via `plotcp()`.
3. Extract the xval results via `$cptable`.
4. Apply the min xerror and/or the one SE rule to find the **optimal** `cp`.
5. Show the resulting classifier graphically.

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

```
set.seed(87654) # reproducibility
fit ← rpart(formula = y ~ 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

```
# Which cp value do we choose?
min_xerr ← which.min(cpt[,'xerror'])

se_rule ← min(which(cpt[, 'xerror'] <
  (cpt[min_xerr, 'xerror'] + cpt[min_xerr, 'xstd'])))
```

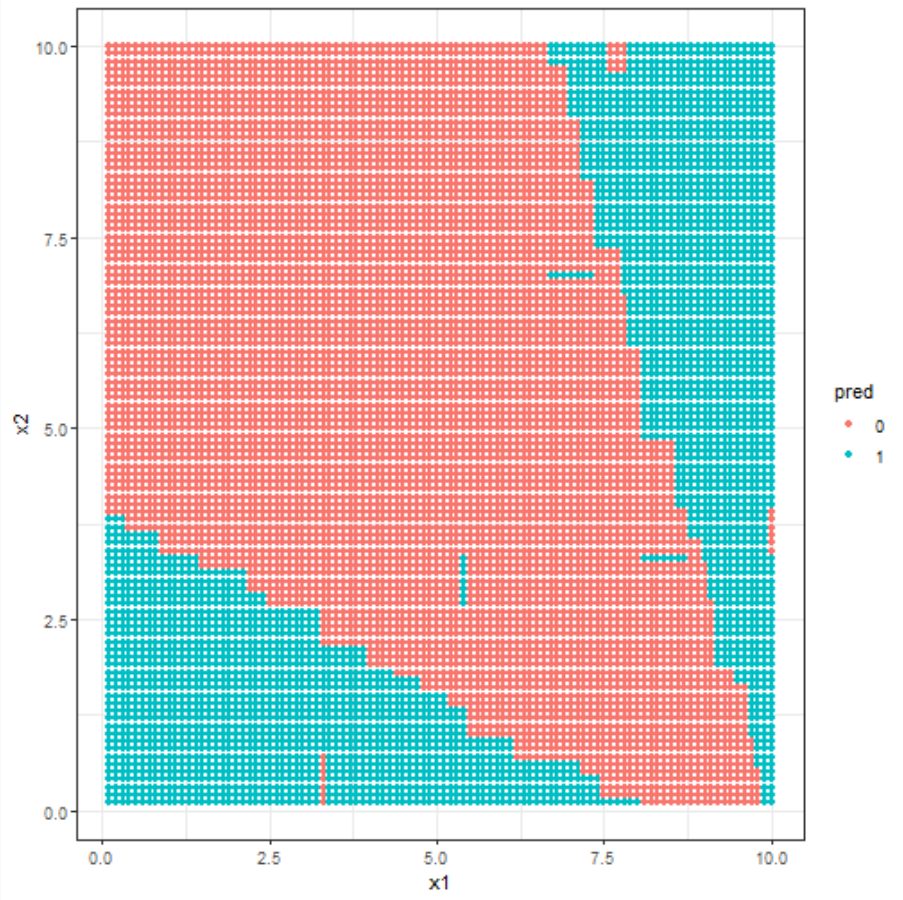
```
unname(min_xerr)
## [1] 29
```

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

```
print(cpt[16:35,], digits = 6)
##             CP nsplit rel error   xerror      xstd
## 16 0.001861702     23  0.471543 0.500000 0.0103913
## 17 0.001595745     25  0.467819 0.494149 0.0103443
## 18 0.001329787     26  0.466223 0.490957 0.0103184
## 19 0.001063830     33  0.456915 0.487234 0.0102880
## 20 0.000930851     34  0.455851 0.483245 0.0102552
## 21 0.000797872     36  0.453989 0.482713 0.0102508
## 22 0.000709220     41  0.450000 0.480319 0.0102310
## 23 0.000664894     44  0.447872 0.480319 0.0102310
## 24 0.000531915     50  0.443883 0.478457 0.0102155
## 25 0.000443262     55  0.441223 0.476330 0.0101978
## 26 0.000398936     58  0.439894 0.476596 0.0102000
## 27 0.000354610     60  0.439096 0.477660 0.0102089
## 28 0.000332447     66  0.436968 0.477660 0.0102089
## 29 0.000265957     74  0.434309 0.474734 0.0101844
## 30 0.000199468    103  0.426330 0.478989 0.0102200
## 31 0.000177305    112  0.424468 0.488830 0.0103011
## 32 0.000166223    128  0.421543 0.488830 0.0103011
## 33 0.000132979    139  0.419681 0.502128 0.0104082
## 34 0.000113982    153  0.417819 0.515160 0.0105105
## 35 0.000106383    167  0.416223 0.523936 0.0105780
```

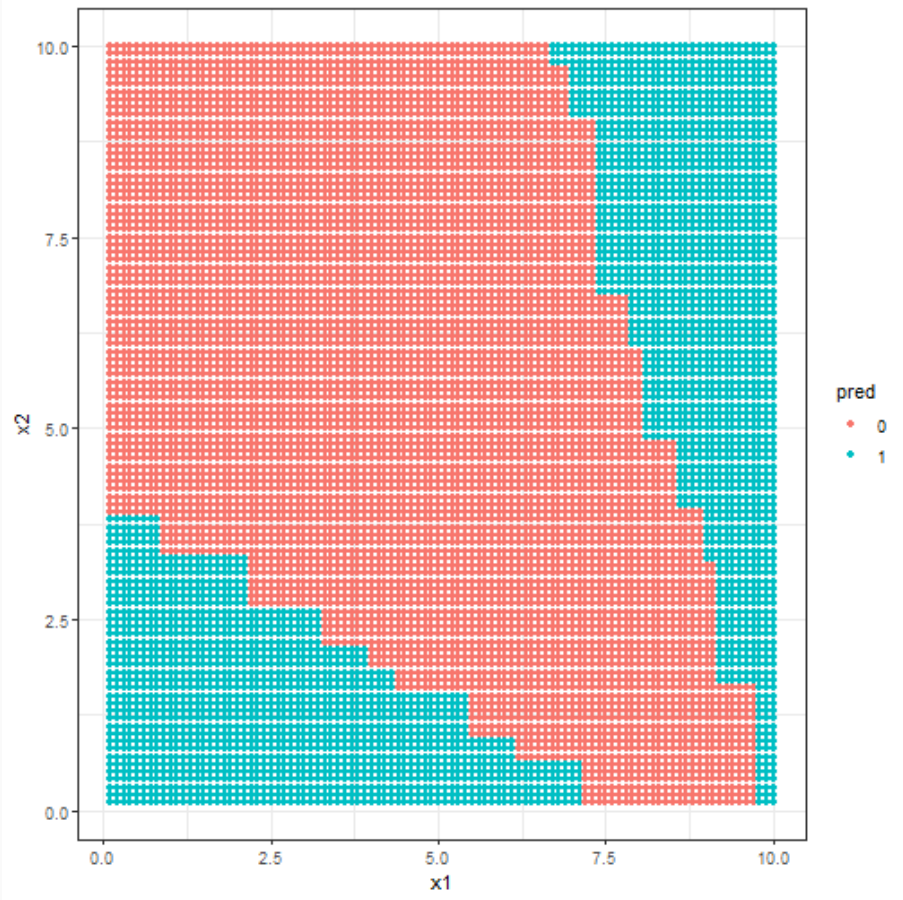
Q.5a: optimal subtree via min CV error

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



Q.5b: optimal subtree via one SE rule

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



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**:

$$D^{\text{Poi}} = 2 \cdot \sum_{i=1}^{n} y_i \cdot \ln \frac{y_i}{\text{expo}_i \cdot \hat{f}(x_i)} - \{y_i - \text{expo}_i \cdot \hat{f}(x_i)\},$$

with expo the exposure measure.

Here we go:

```
# Read the MTPL data
#setwd(dirname(rstudioapi::getActiveDocumentContext()$path))
mtpl ← read.table('../data/PC_data.txt',
                  header = TRUE, stringsAsFactors = TRUE) %>%
  as_tibble() %>% rename_all(tolower) %>% rename(expo = exp)
```

Fitting a simple tree to the MTPL data

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

```
print(fit)
```

```
## 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 *
```

Take-away - Poisson tree in {rpart}:

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

Fitting a simple tree to the MTPL data

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

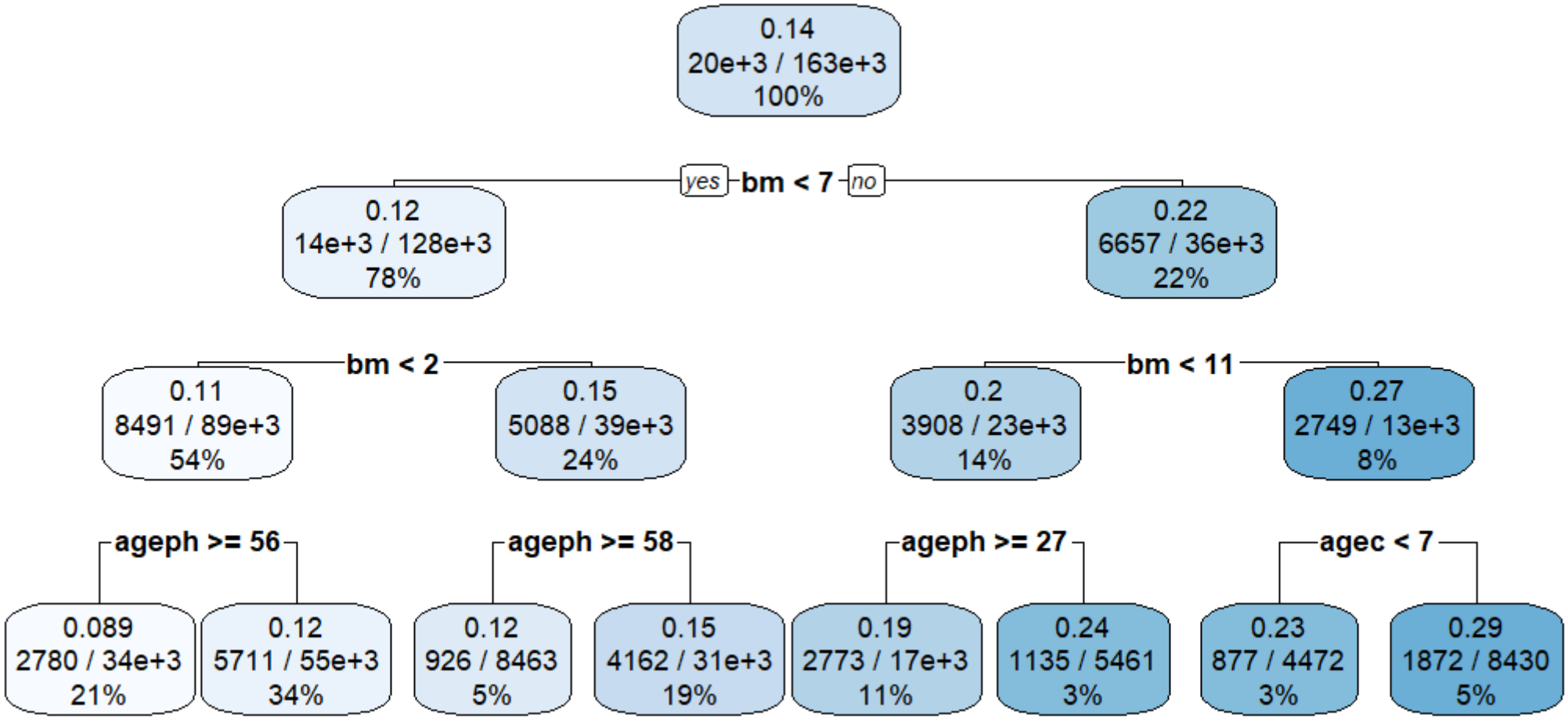
```
print(fit)
```

```
## 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 *
```

Easier way to understand this tree?

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

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 ⩾ 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

```
mtpl %>%
  dplyr::filter(bm < 2,
                ageph ⩾ 56) %>%
  dplyr::summarise(claim_freq =
                     sum(nclaims)/sum(expo))
```

```
##   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 $\mu = \sum y_i / \sum \text{expo}_i$
- use coefficient of variation $k = \sigma/\mu$ as **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:

$$\frac{\alpha + \sum y_i}{\beta + \sum \text{expo}_i}, \quad \alpha = 1/k^2, \quad \beta = \alpha/\mu.$$

```
k ← 1

alpha ← 1/k^2

mu ← mtpl %>%
  with(sum(nclaims)/sum(expo))

beta ← alpha/mu

mtpl %>%
  dplyr::filter(bm < 2, ageph ⩾ 56) %>%
  dplyr::summarise(prediction =
            (alpha + sum(nclaims))/(beta + sum(expo)))
```

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

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

Coefficient of variation very low

```
fit ← rpart(formula =
              cbind(expo,nclaims) ~
              ageph + agec + bm + power +
              coverage + fuel + sex + fleet + use,
            data = mtpl,
            method = 'poisson',
            control = rpart.control(
              maxdepth = 3,
              cp = 0),
            parms = list(shrink = 10^-5)
            )
```

```
## 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
##      4) 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 *
##       11) ageph< 57.5 30588 17537.510 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

```
fit ← rpart(formula =
              cbind(expo,nclaims) ~
              ageph + agec + bm + power +
              coverage + fuel + sex + fleet + use,
            data = mtpl,
            method = 'poisson',
            control = rpart.control(
              maxdepth = 3,
              cp = 0),
            parms = list(shrink = 10^5)
            )
```

```
# Remember this number?
mtpl %>%
  dplyr::filter(bm < 2, ageph ⩾ 56) %>%
  dplyr::summarise(claim_freq =
                     sum(nclaims)/sum(expo))
```

```
##   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⩾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.

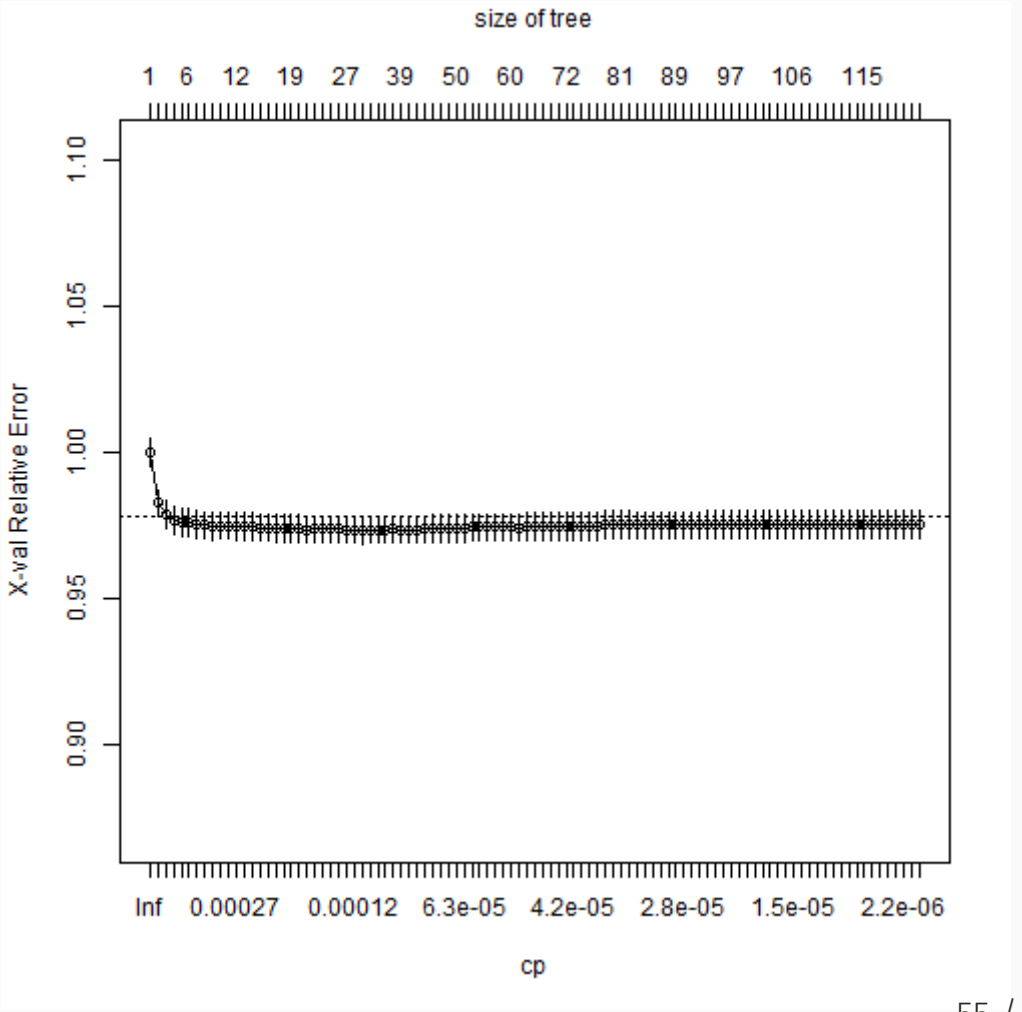
1. Start from an overly complex tree. Do not forget your favorite random **seed** upfront!
2. Inspect the cross-validation results.
3. Choose the `cp` value minimizing `xerror` for pruning.
4. Visualize the pruned tree with `rpart.plot`.

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

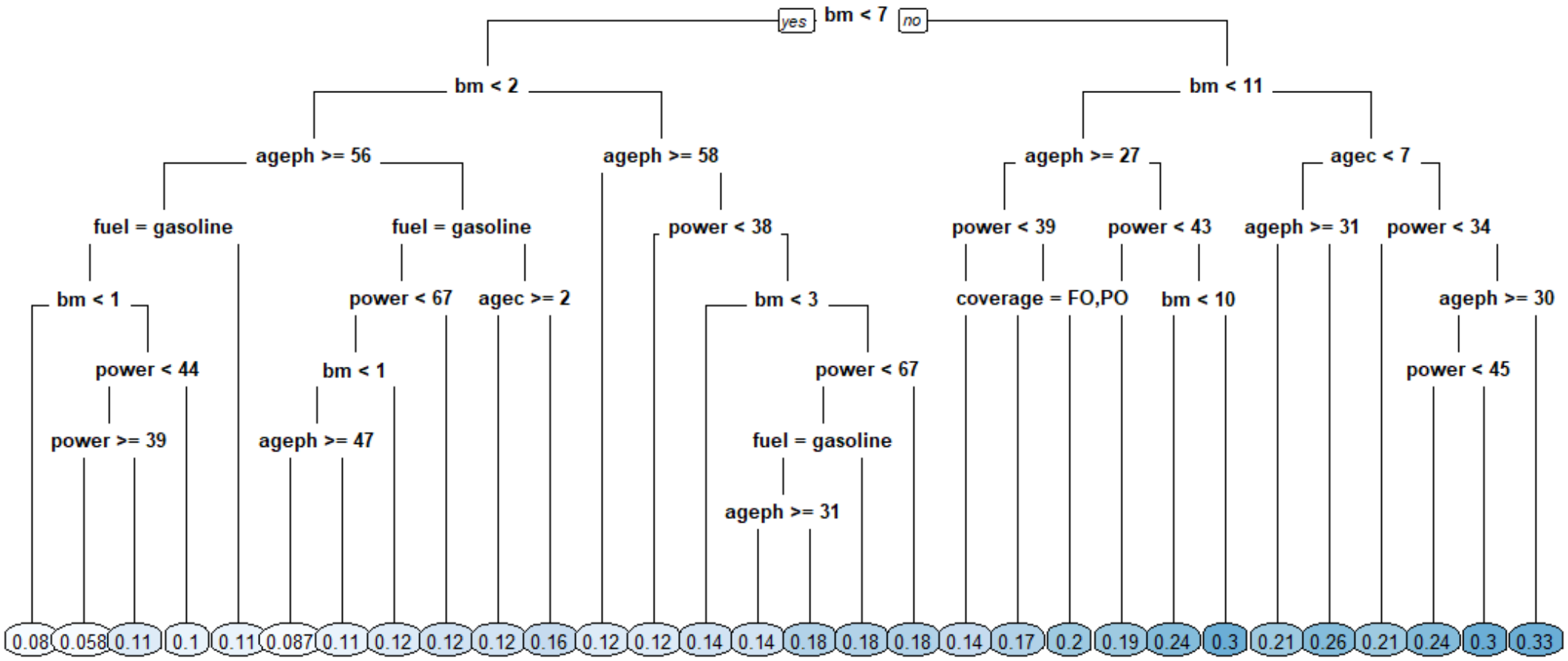
```
plotcp(fit)
```



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

```
# Get the cross-validation results
cpt ← fit$cptable

# Look for the minimal xerror
min_xerr ← which.min(cpt[,'xerror'])
cpt[min_xerr,]
##           CP       nsplit    rel error       xerror         xstd
## 1.152833e-04 2.900000e+01 9.693815e-01 9.735286e-01 4.668765e-03

# Prune the tree
fit_srt ← prune(fit,
                cp = cpt[min_xerr, 'CP'])
```

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**

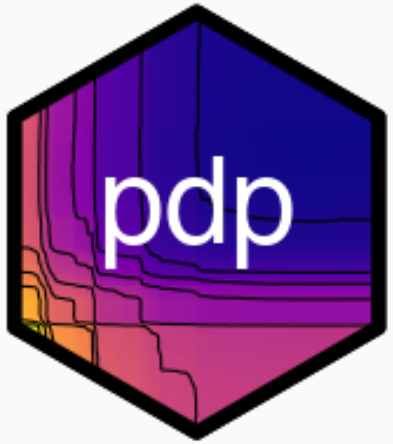
- is easy with a **shallow** tree but hard with a **deep** tree
- luckily there are some **tools** to aid you.

Feature importance

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

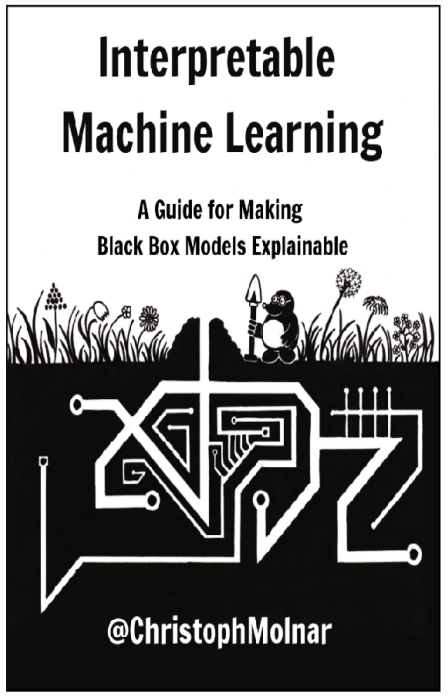
Partial dependence plot

- 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:

- 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

$$\bar{f}_\ell(x_\ell) = \frac{1}{n}\sum_{i=1}^{n} f_{\text{tree}}(x_\ell, \boldsymbol{x}^i_{-\ell})$$

- bivariate

$$\bar{f}_{k,\ell}(x_k, x_\ell) = \frac{1}{n}\sum_{i=1}^{n} f_{\text{tree}}(x_k, x_\ell, \boldsymbol{x}^i_{-k,\ell})$$

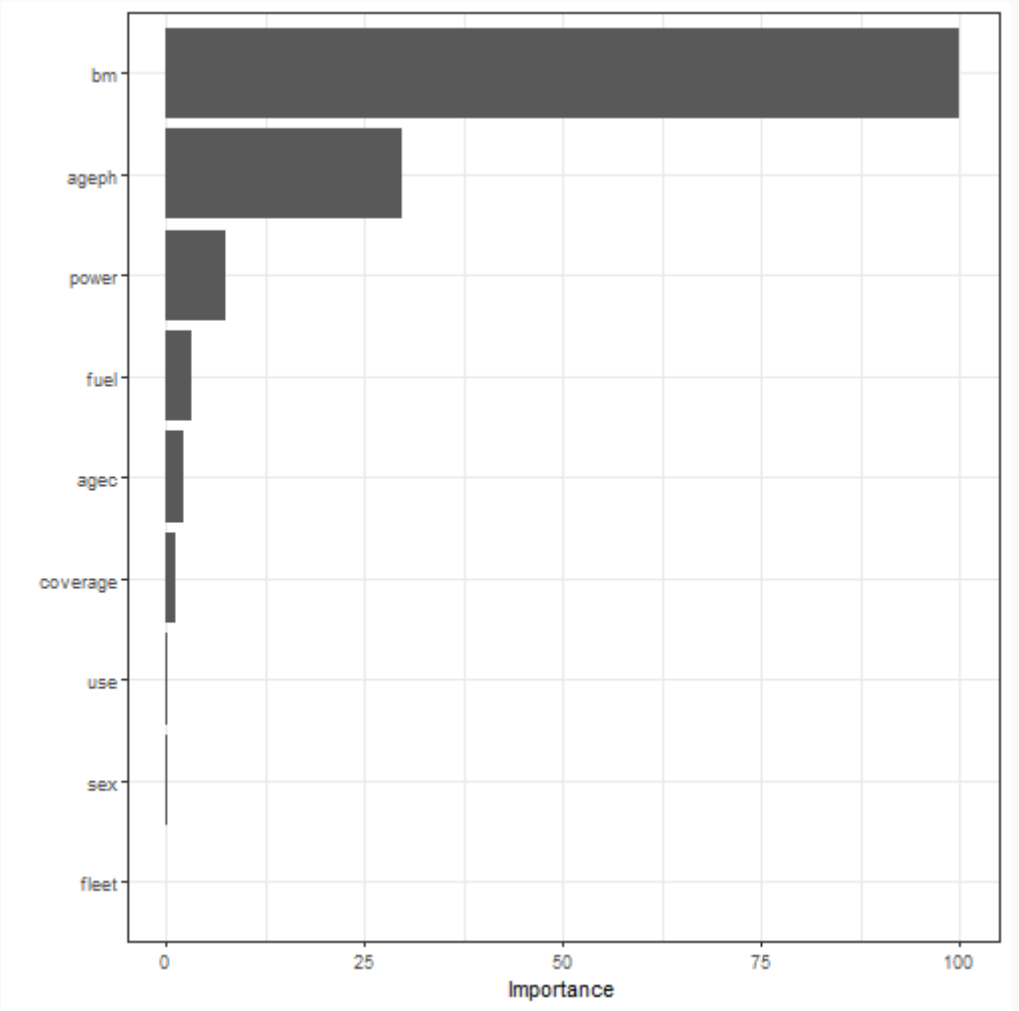
- marginal effects, interactions can stay hidden!

Feature importance

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

```
##   Variable   Importance
## 1       bm 2186.5664729
## 2    ageph  651.1768792
## 3    power  164.2502735
## 4     fuel   70.5542003
## 5     agec   45.8086193
## 6 coverage   24.9202279
## 7      use    2.2088357
## 8      sex    0.7547625
## 9    fleet    0.2642045
```

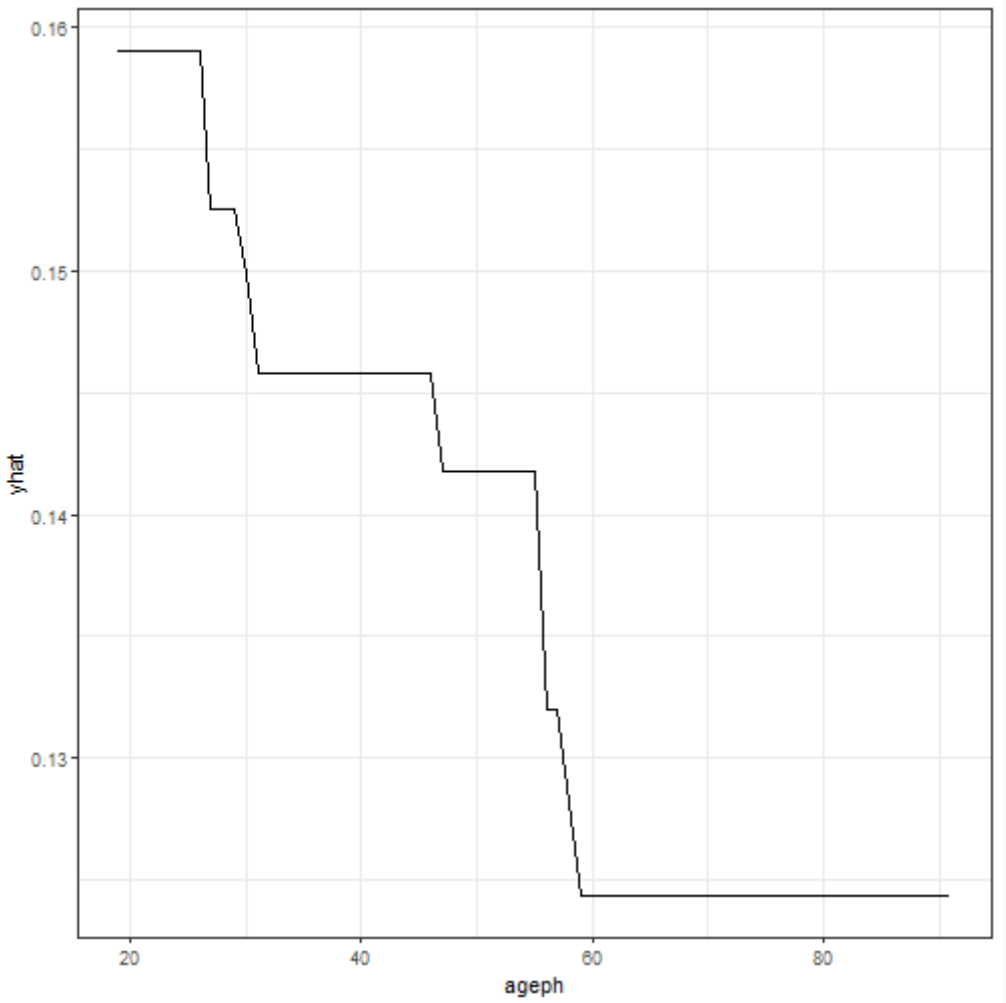
```r
# Function vip makes the plot
vip::vip(fit_srt, scale = TRUE)
```



Partial dependence plot

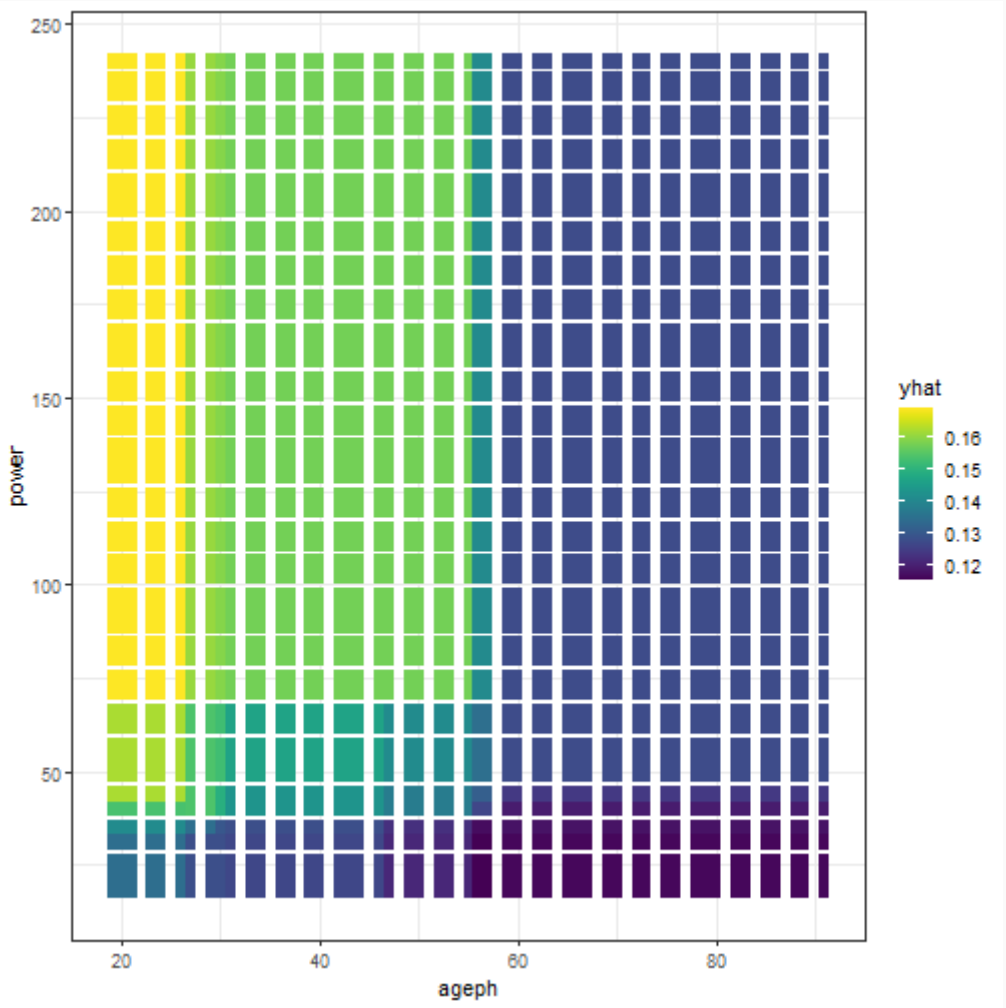
```r
library(pdp)
# Need to define this helper function for Poisson
pred.fun ← function(object,newdata){
  mean(predict(object, newdata))
}

# Sample 5000 observations to speed up pdp generation
set.seed(48927)
pdp_ids ← mtpl %>% nrow %>% sample(size = 5000)
```

```r
# partial: computes the marginal effect
# autoplot: creates the graph using ggplot2
fit_srt %>%
  pdp::partial(pred.var = 'ageph',
               pred.fun = pred.fun,
               train = mtpl[pdp_ids,]) %>%
  autoplot()
```



Partial dependence plot in two dimensions

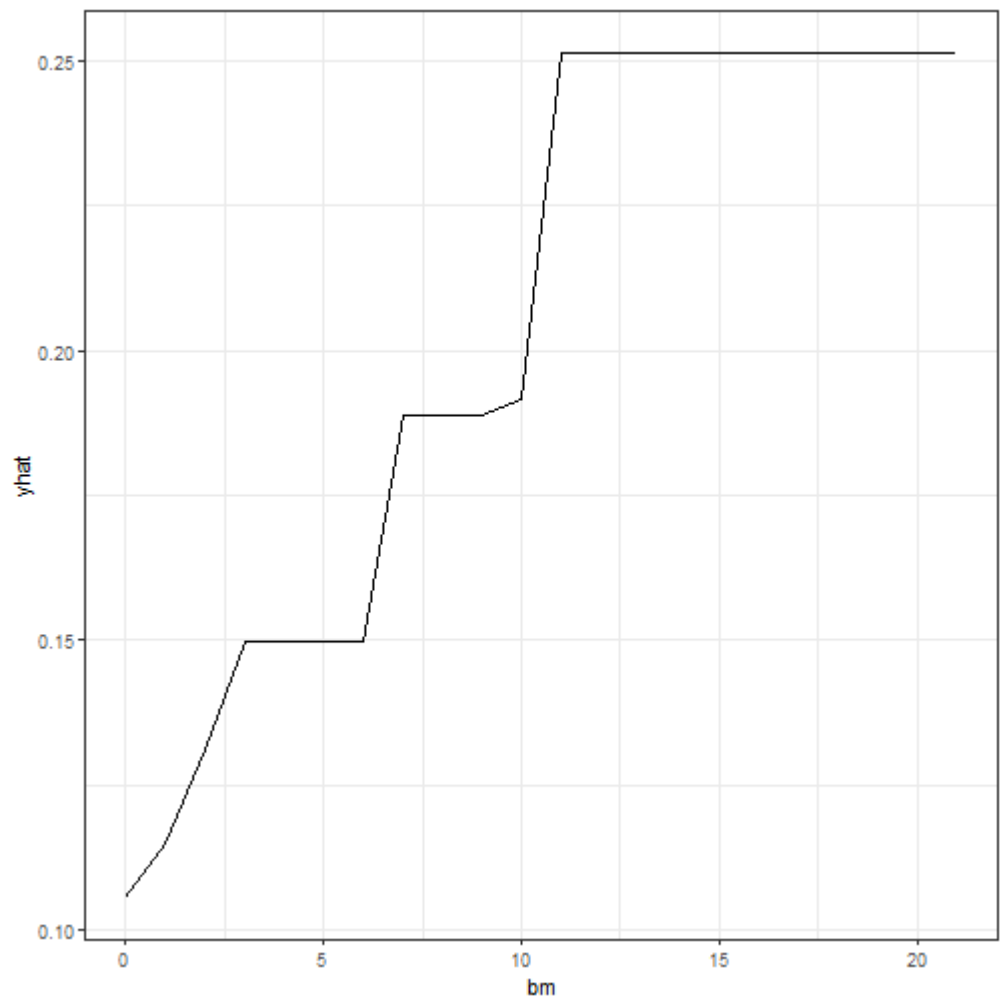
```
# partial: computes the marginal effect
# autoplot: creates the graph using ggplot2
fit_srt %>%
  pdp::partial(pred.var = c('ageph','power'),
               pred.fun = pred.fun,
               train = mtpl[pdp_ids,]) %>%
  autoplot()
```



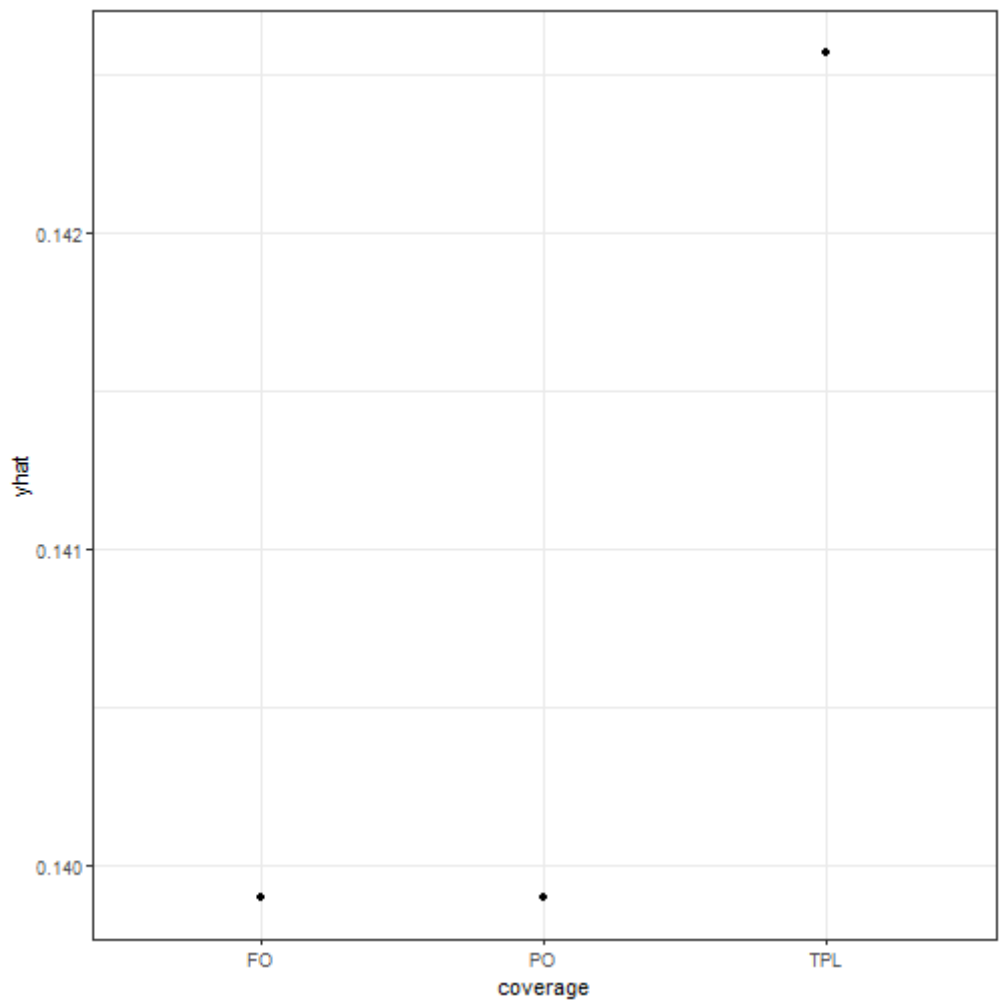
Use partial dependence plots for **other features** to gain understanding of your model.

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.

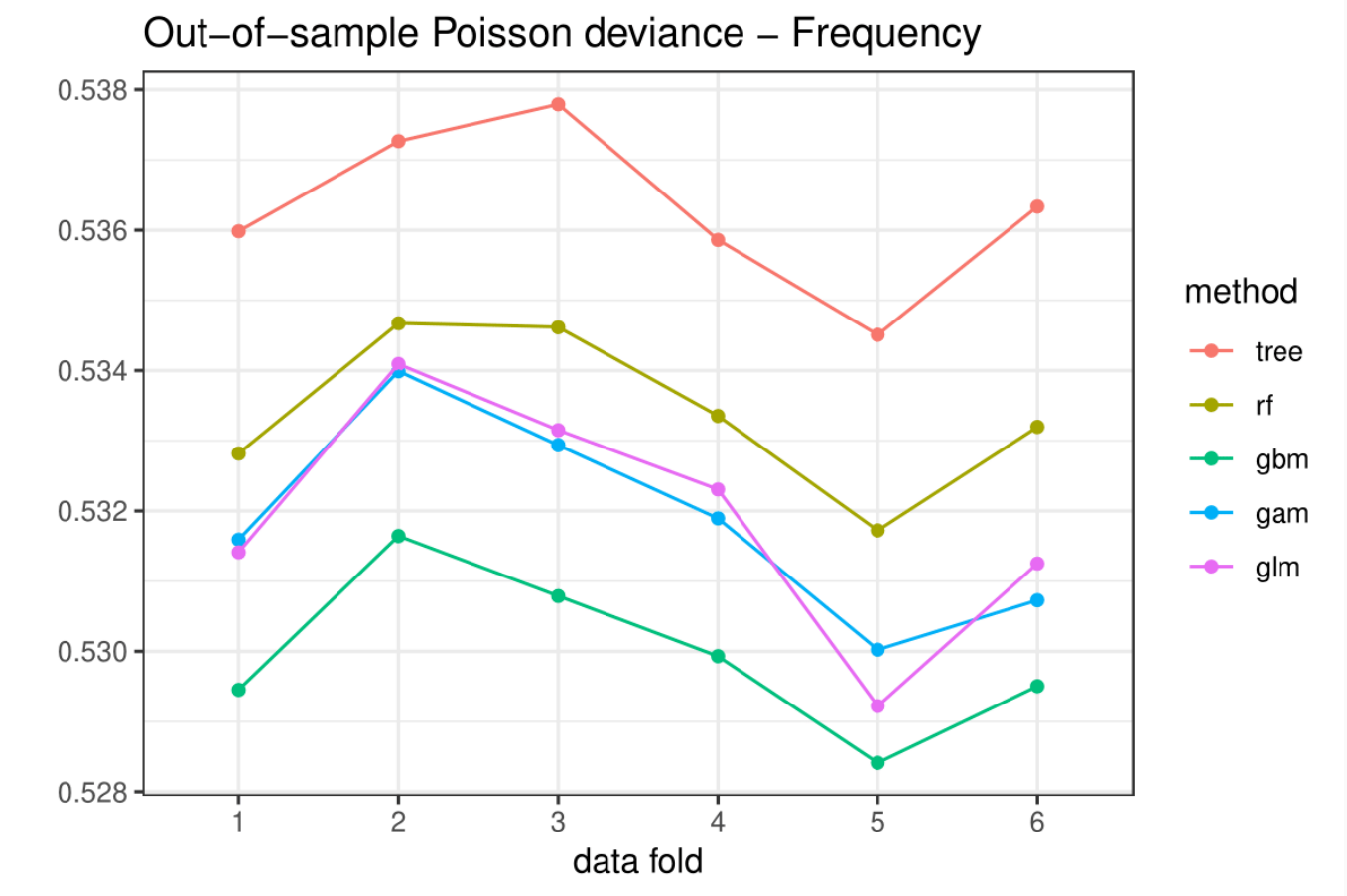
Model comparison on claim frequency data

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

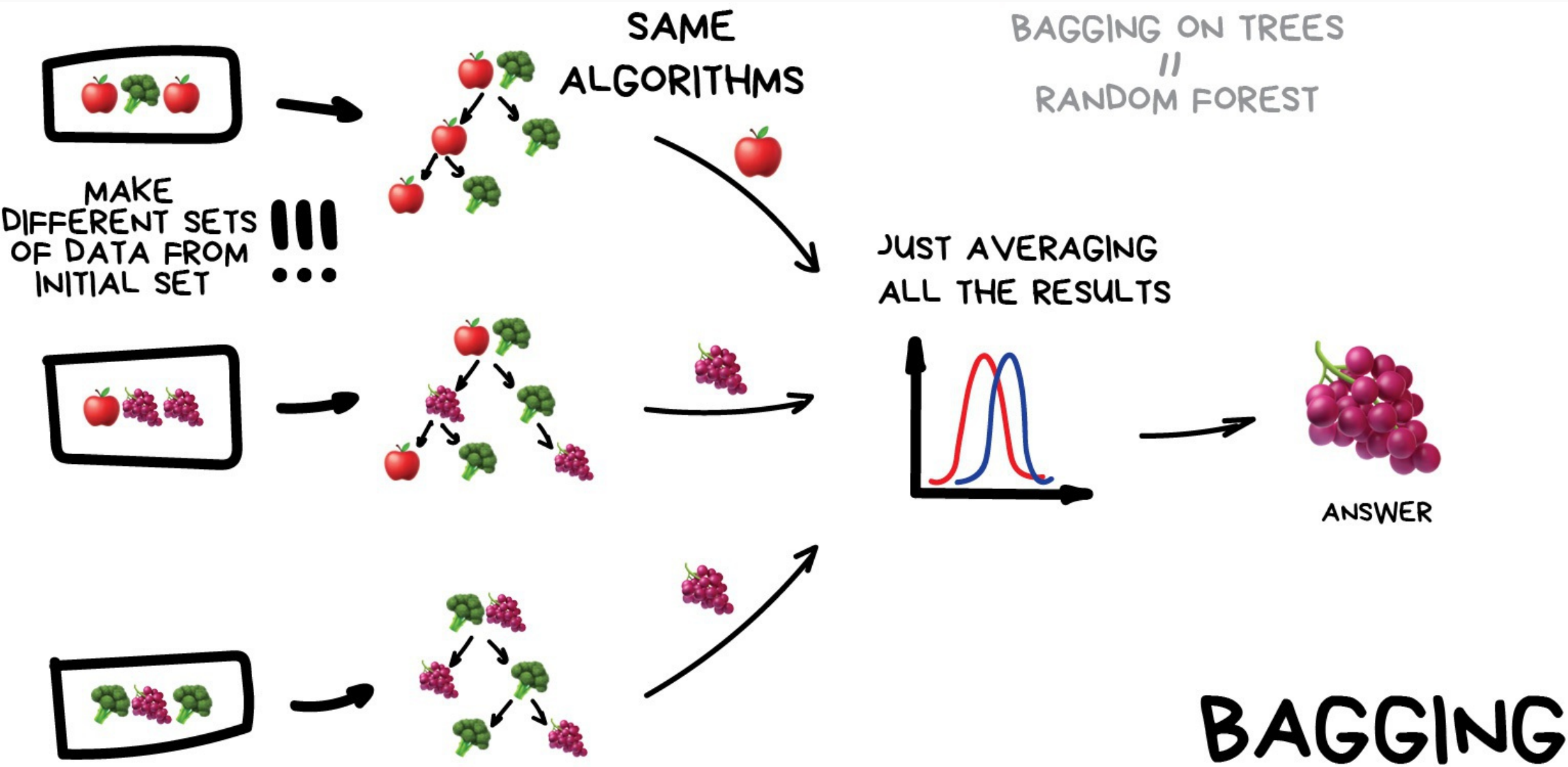
Analyzing frequency as well as severity data.

Picture taken from Henckaerts et al. (2020).

Boosting > Random forest > Bagging > Decision tree



Introducing bagging


SAME
ALGORITHMS
BAGGING ON TREES
=
RANDOM FOREST
MAKE
DIFFERENT SETS
OF DATA FROM
INITIAL SET
!!!
JUST AVERAGING
ALL THE RESULTS
ANSWER
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
```

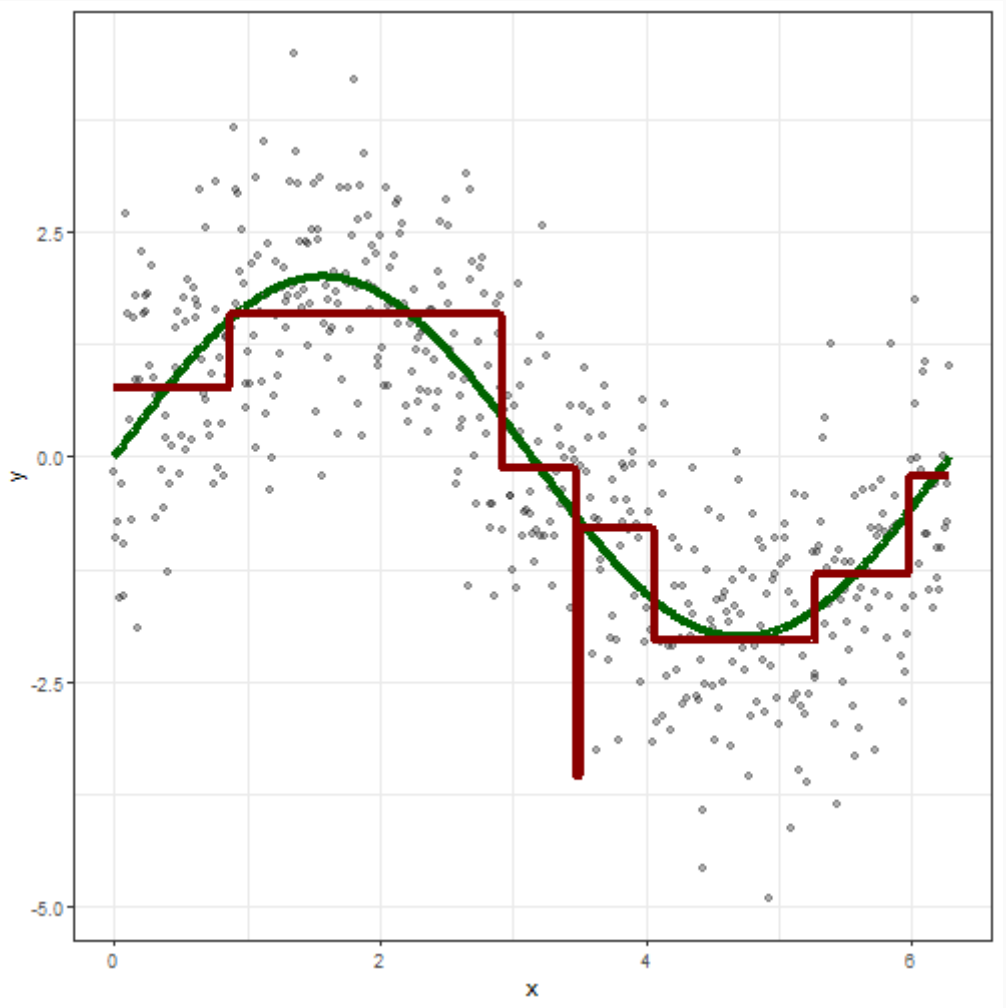
Sample 2:

```
##            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

```
fit_b1 ← rpart(formula = y ~ x,
               data = dfr_b1,
               method = 'anova',
               control = rpart.control(
                 maxdepth = 30,
                 minsplit = 20,
                 minbucket = 3,
                 cp = 0.01
                 )
               )
```

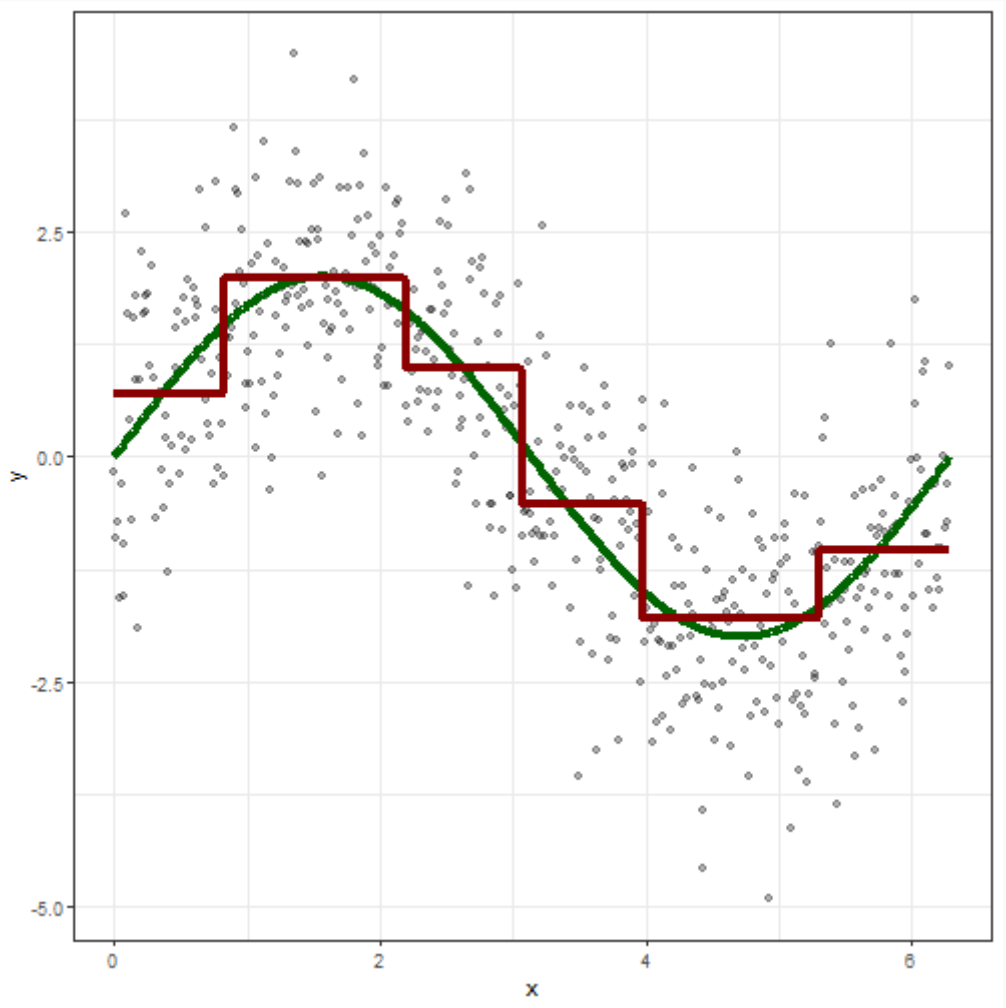
On it's own, this is a noisy prediction with very high variance!



Decision tree on sample 2

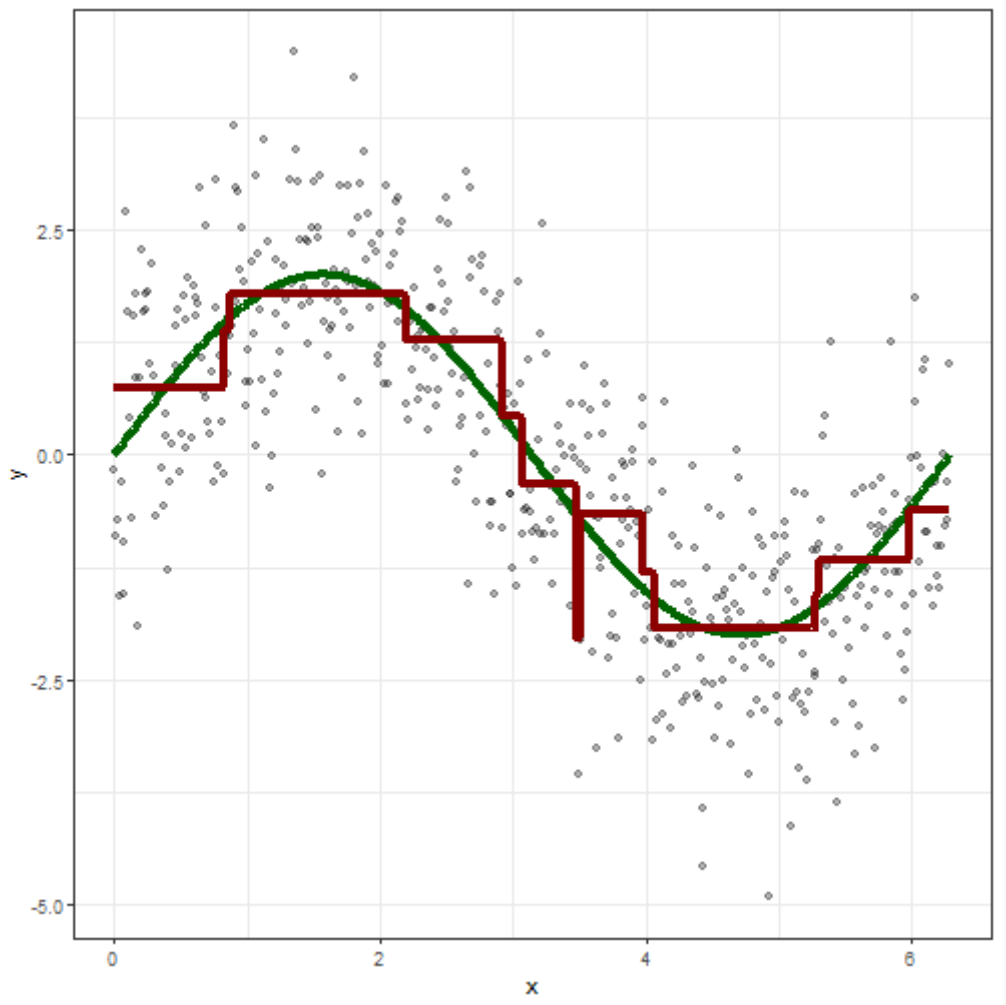
```
fit_b2 ← rpart(formula = y ~ x,
               data = dfr_b2,
               method = 'anova',
               control = rpart.control(
                 maxdepth = 30,
                 minsplit = 20,
                 minbucket = 3,
                 cp = 0.01
                 )
               )
```

Again, very high variance on it's own!



Combining the predictions of both trees

```
# Predictions for the first tree
pred_b1 ← fit_b1 %>% predict(dfr)
# Predictions for the first tree
pred_b2 ← fit_b2 %>% predict(dfr)

# Average the predictions
pred ← rowMeans(cbind(pred_b1,
                      pred_b2))
```



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

```
# Generate the third bootstrapped sample
set.seed(28726)
bsample_3 ← dfr %>% nrow %>%
                sample(replace = TRUE)
# Use the indices to sample the data
dfr_b3 ← dfr %>% dplyr::slice(bsample_3)
```

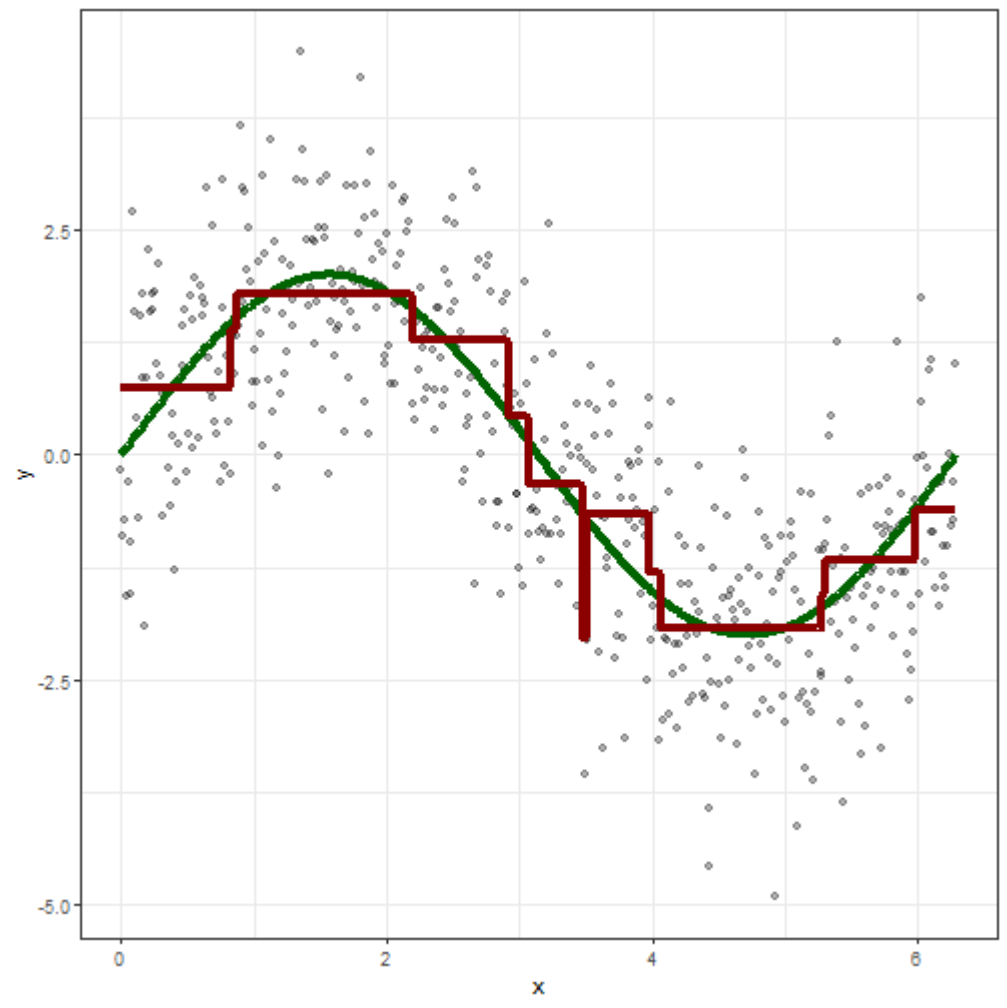
Q.2: fit a deep tree

```
# Fit an unpruned tree
fit_b3 ← rpart(formula = y ~ x,
             data = dfr_b3,
             method = 'anova',
             control = rpart.control(
               maxdepth = 30,
               minsplit = 20,
               minbucket = 3,
               cp = 0.01))
```

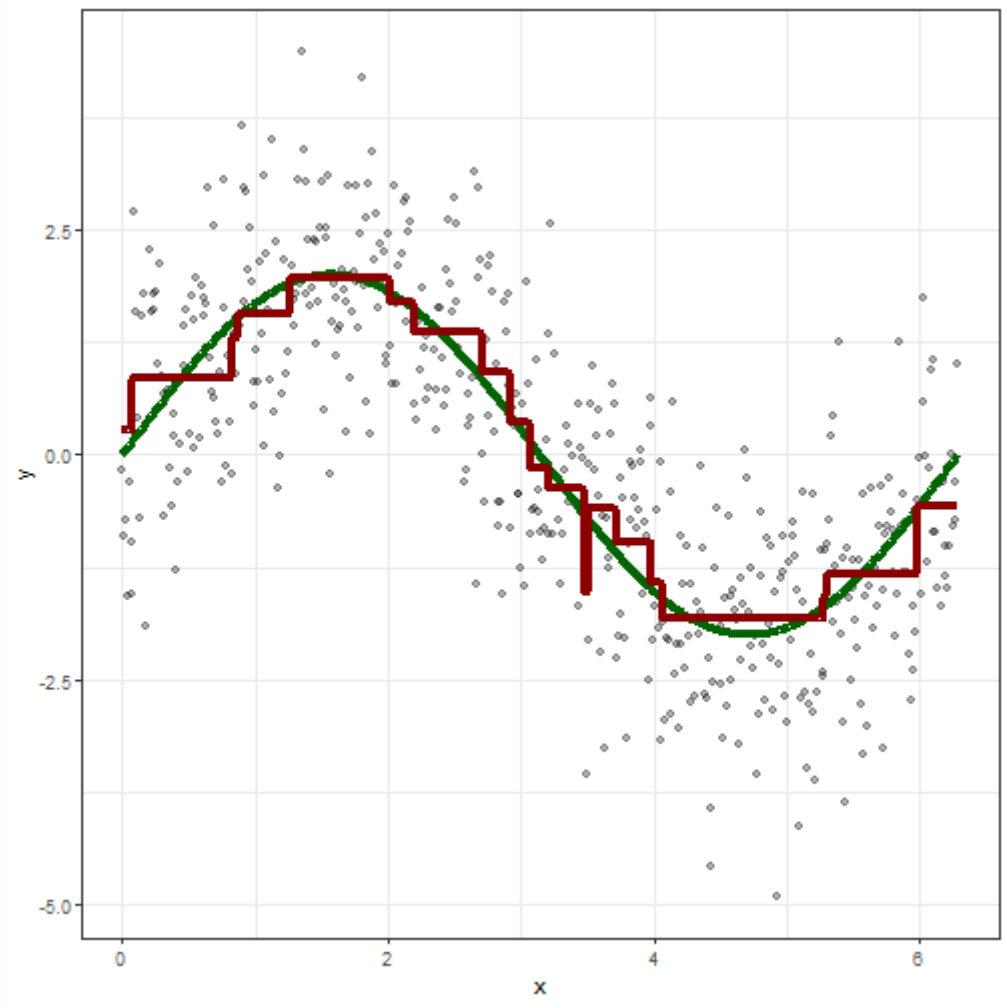
Q.3: average the predictions

```
# Predictions for the third tree
pred_b3 ← fit_b3 %>% predict(dfr)
# Average the predictions
pred_new ← rowMeans(cbind(pred_b1,
                          pred_b2,
                          pred_b3))
```

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}

```
bagging(formula, data, control = rpart.control(___),
        nbagg, ns, coob)
```

- `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 size of training data - say 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.

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- 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?

```
set.seed(12345)
N ← 100000 ; x ← 1:N
mean(x %in% sample(N,
                   replace = TRUE))
## [1] 0.63349
```

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

Even more when we sample **< N** observations

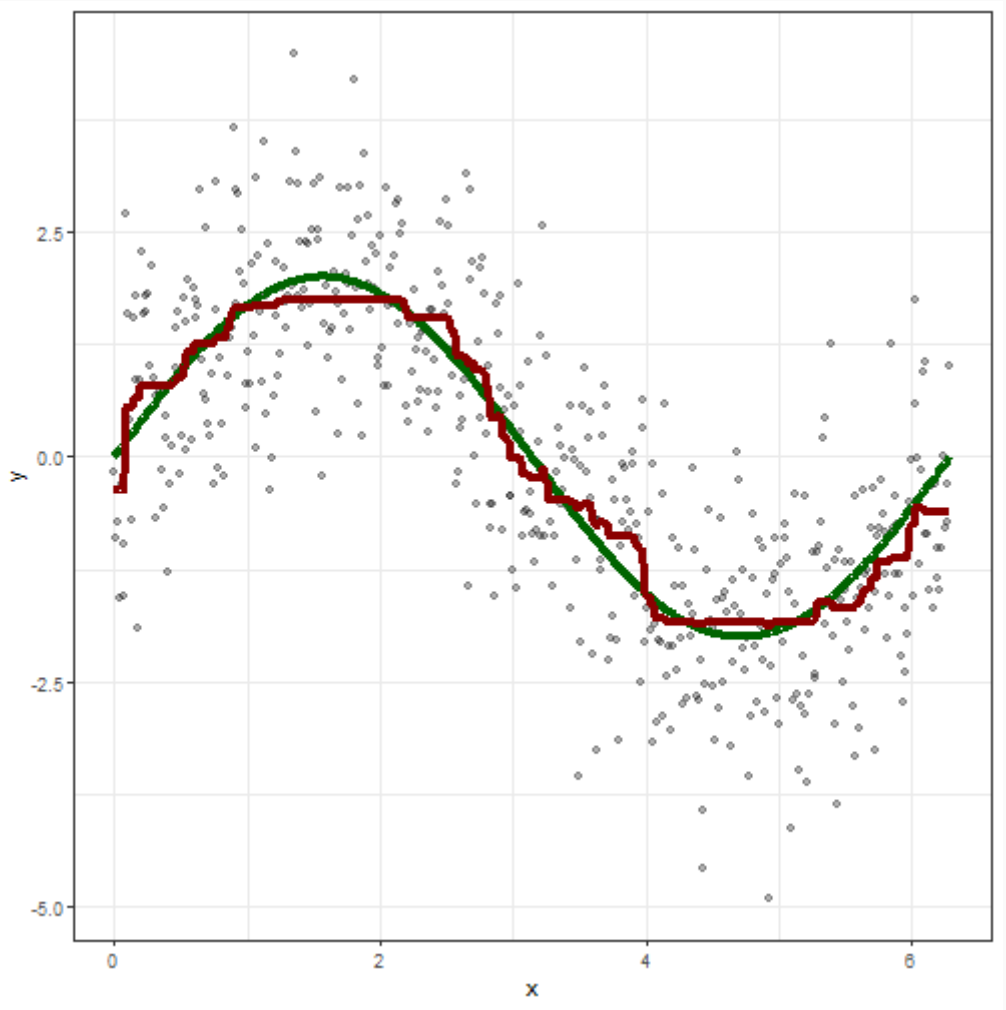
```
mean(x %in% sample(N,
                   size = 0.75*N,
                   replace = TRUE))
## [1] 0.52837
```

Bagging properly

```
library(ipred)
set.seed(83946) # reproducibility

# Fit a bagged tree model
fit ← ipred::bagging(formula = y ~ x,
                     data = dfr,
                     nbagg = 200,
                     ns = nrow(dfr),
                     coob = TRUE,
                     control = rpart.control(
                       maxdepth = 30,
                       minsplit = 20,
                       minbucket = 3,
                       cp = 0.01)
                     )
```

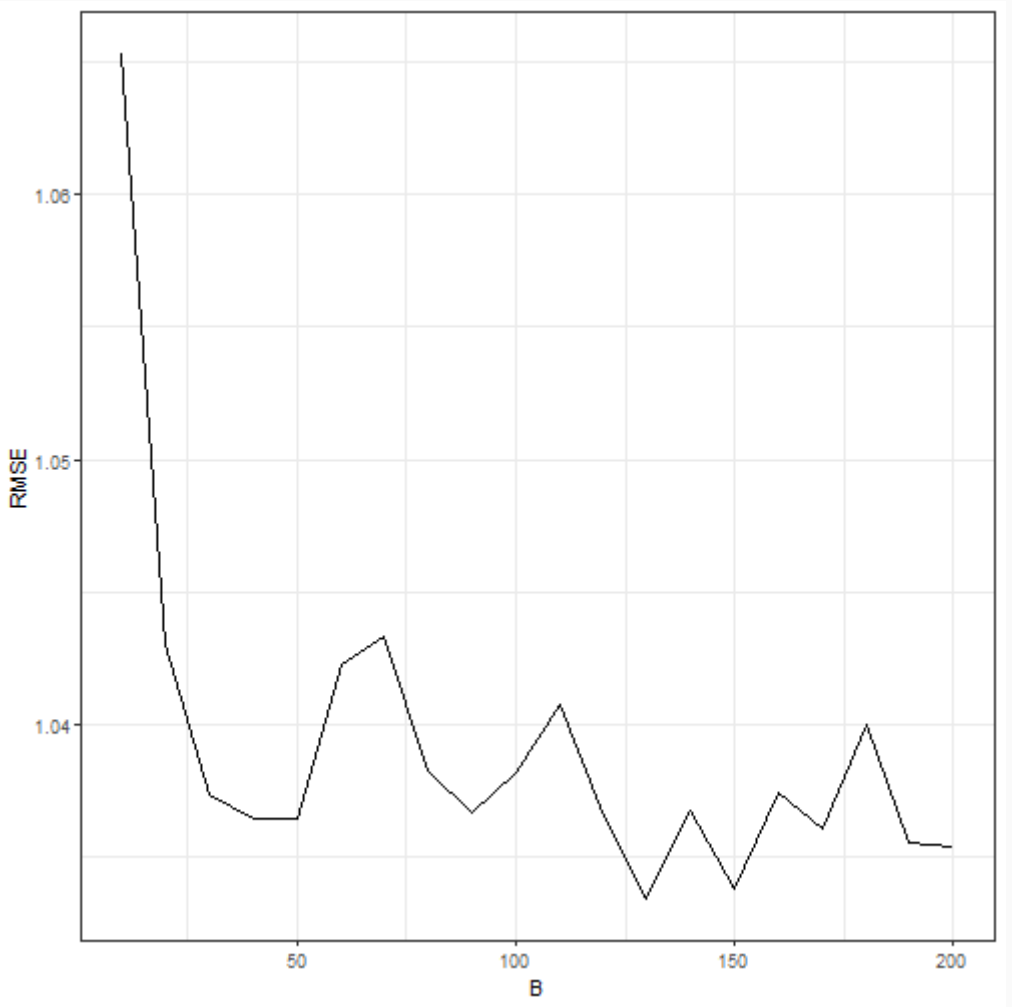
```
# Predict from this model
pred ← predict(fit, dfr)
```

With 200 trees we can see the variance reduction!



Evolution of the OOB error

```r
set.seed(98765) # reproducibility
# Define a grid for B
nbags ← 10*(1:20)
oob ← rep(0, length(nbags))
# Fit a bagged tree model
for(i in 1:length(nbags)){
  fit ← ipred::bagging(formula = y ~ x,
                data = dfr,
                nbagg = nbags[i],
                ns = nrow(dfr),
                coob = TRUE,
                control = rpart.control(
                  maxdepth = 30,
                  minsplit = 20,
                  minbucket = 3,
                  cp = 0.01)
                )
  oob[i] ← fit$err
}
```



Your turn

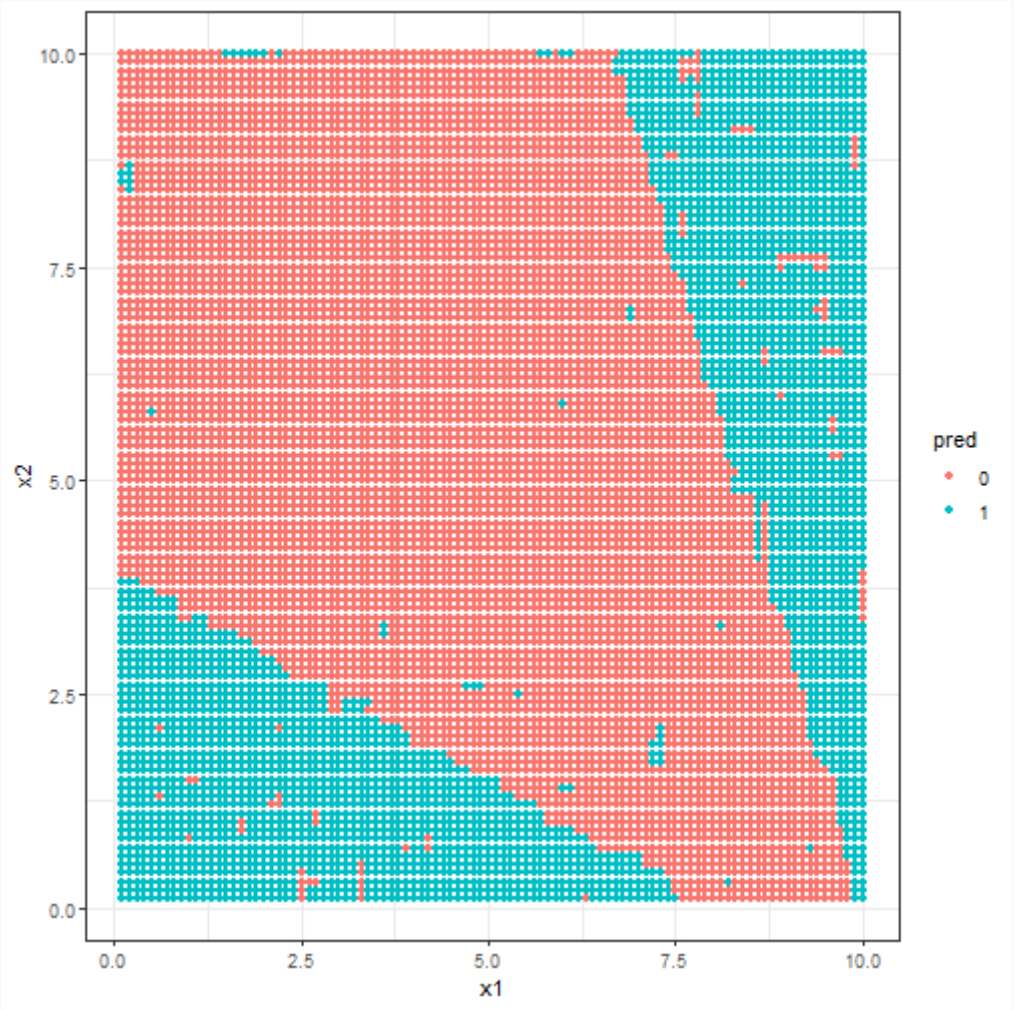
Use {ipred} to fit a bagged tree ensemble for the toy **classification** problem with data `dfc`.

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.

```
set.seed(98765) # reproducibility

# Fit a bagged tree model
fit ← ipred::bagging(formula = y ~ x1 + x2,
                     data = dfc,
                     nbagg = 100,
                     ns = nrow(dfc),
                     control = rpart.control(
                       maxdepth = 20,
                       minsplit = 10,
                       minbucket = 5,
                       cp = 0)
                     )
```

```
# Predict from this model
pred ← predict(fit,
                      newdata = dfc,
                      type = 'class',
                      aggregation = 'majority'
                      )
```



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.

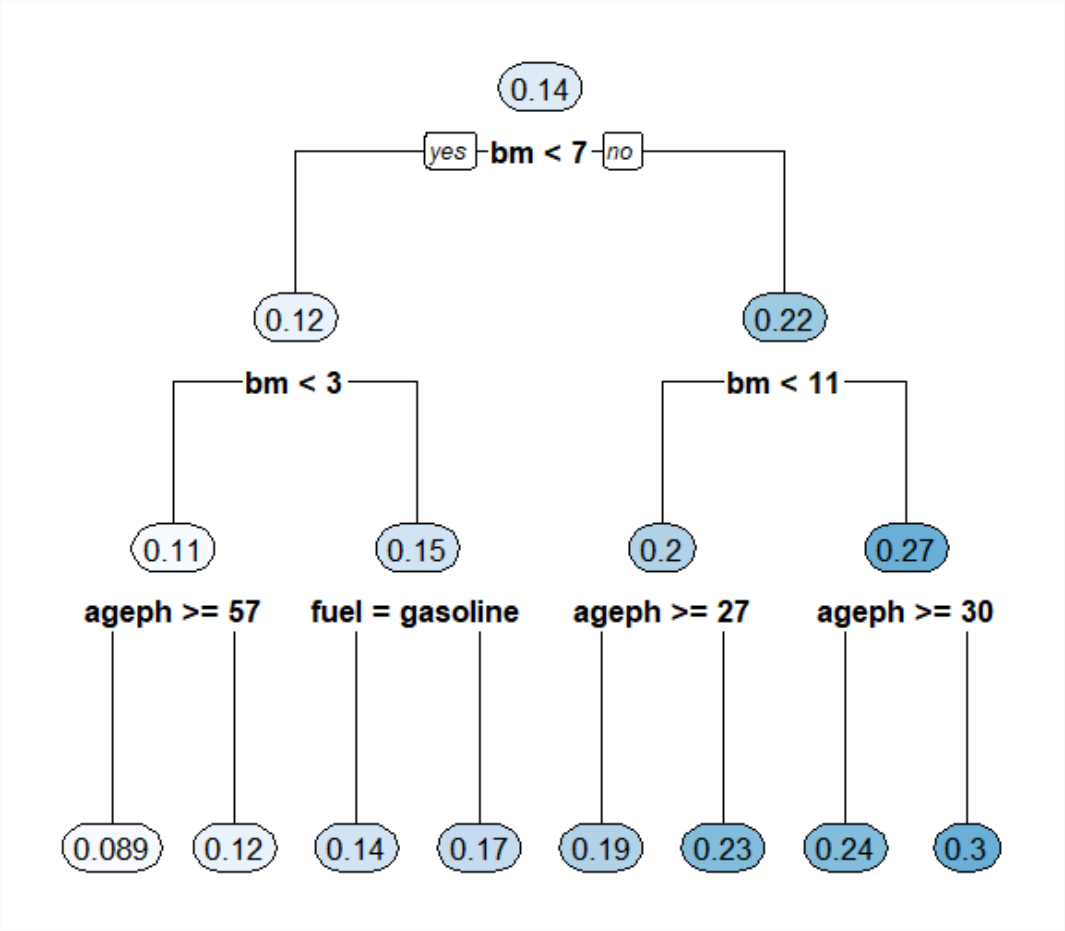
Q.1: two bootstrap samples

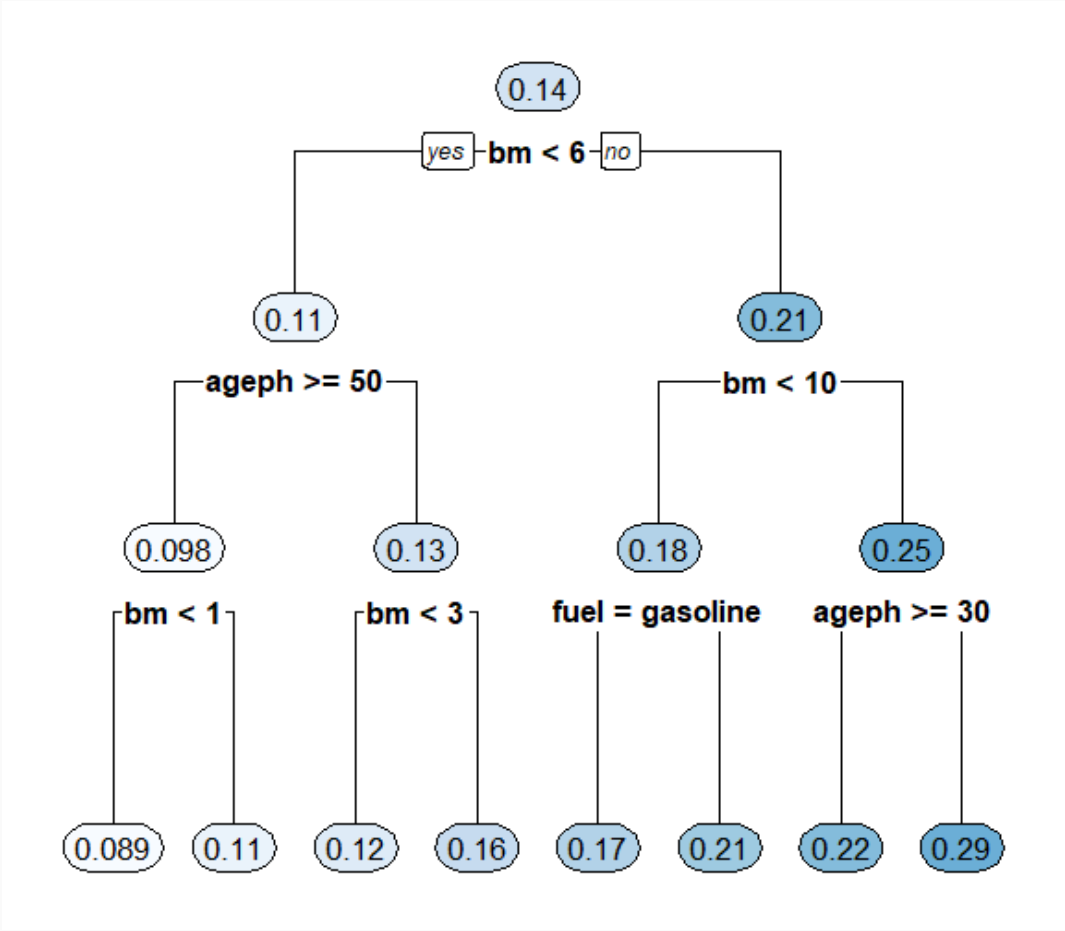
```
set.seed(486291) # reproducibility

# Generate the first bootstrapped sample
bsample_1 ← mtpl %>% nrow %>%
                sample(replace = TRUE)

# Generate another bootstrapped sample
bsample_2 ← mtpl %>% nrow %>%
                sample(replace = TRUE)

# Use the indices to sample the data
mtpl_b1 ← mtpl %>% dplyr::slice(bsample_1)
mtpl_b2 ← mtpl %>% dplyr::slice(bsample_2)
```

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 ← 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 mtry min.node.size error
## 1        100    3        163.231    NA
## 2        200    3        163.231    NA
## 3        100    6        163.231    NA
## 4        200    6        163.231    NA
## 5        100    9        163.231    NA
## 6        200    9        163.231    NA
## 7        100    3       1632.310    NA
## 8        200    3       1632.310    NA
## 9        100    6       1632.310    NA
## 10       200    6       1632.310    NA
## 11       100    9       1632.310    NA
## 12       200    9       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 ← 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 mtry min.node.size     error
## 1        200    3      1632.310 0.1332844
## 2        100    3      1632.310 0.1333003
## 3        200    6      1632.310 0.1333551
## 4        200    9      1632.310 0.1333689
## 5        100    6      1632.310 0.1333754
## 6        100    9      1632.310 0.1333862
## 7        200    3       163.231 0.1337361
## 8        100    3       163.231 0.1338148
## 9        200    6       163.231 0.1341431
## 10       100    6       163.231 0.1342326
## 11       200    9       163.231 0.1343189
## 12       100    9       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

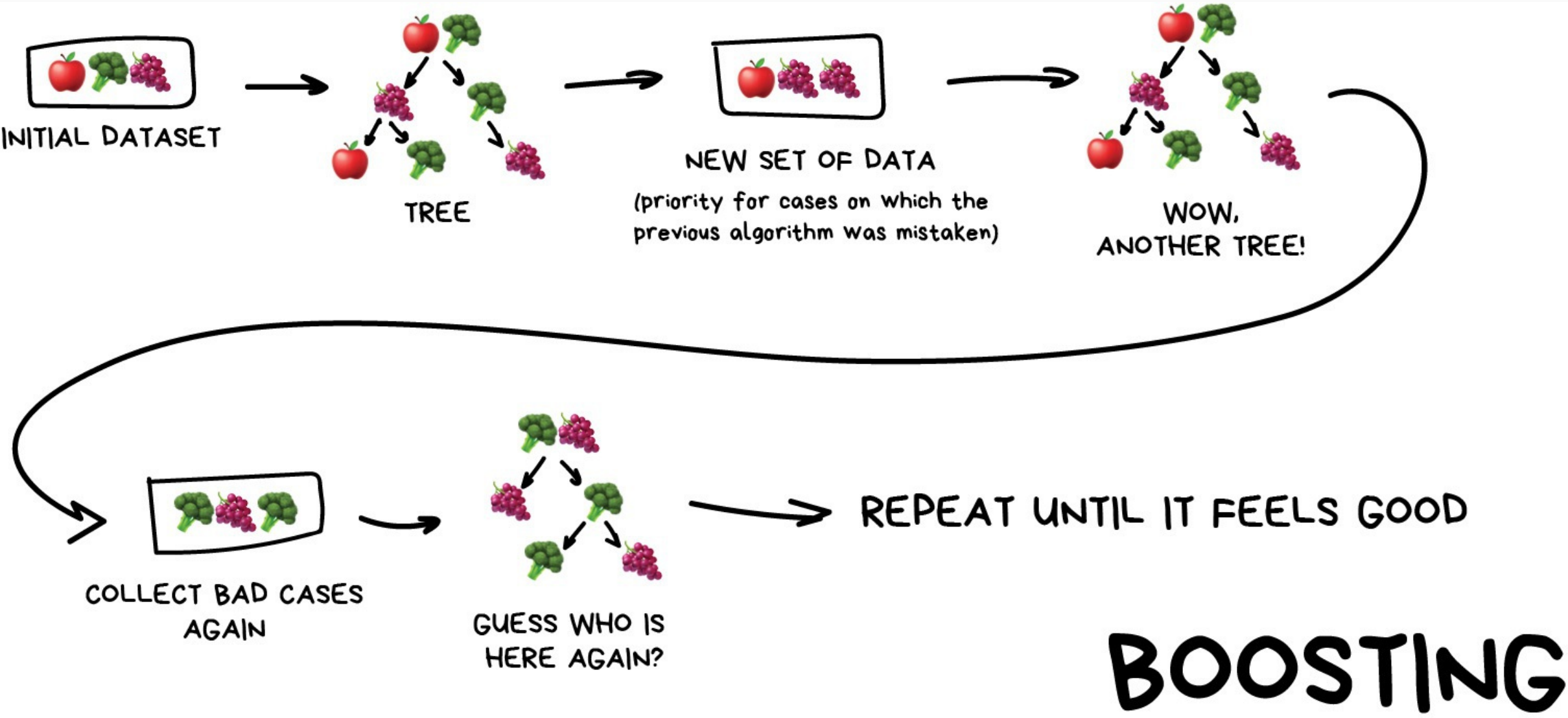
All available random forest packages (in R) only support standard regression based on the **Mean Squared Error**:

- 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


INITIAL DATASET
TREE
NEW SET OF DATA
(priority for cases on which the previous algorithm was mistaken)
WOW, ANOTHER TREE!
REPEAT UNTIL IT FEELS GOOD
GUESS WHO IS HERE AGAIN?
COLLECT BAD CASES AGAIN
BOOSTING

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**.

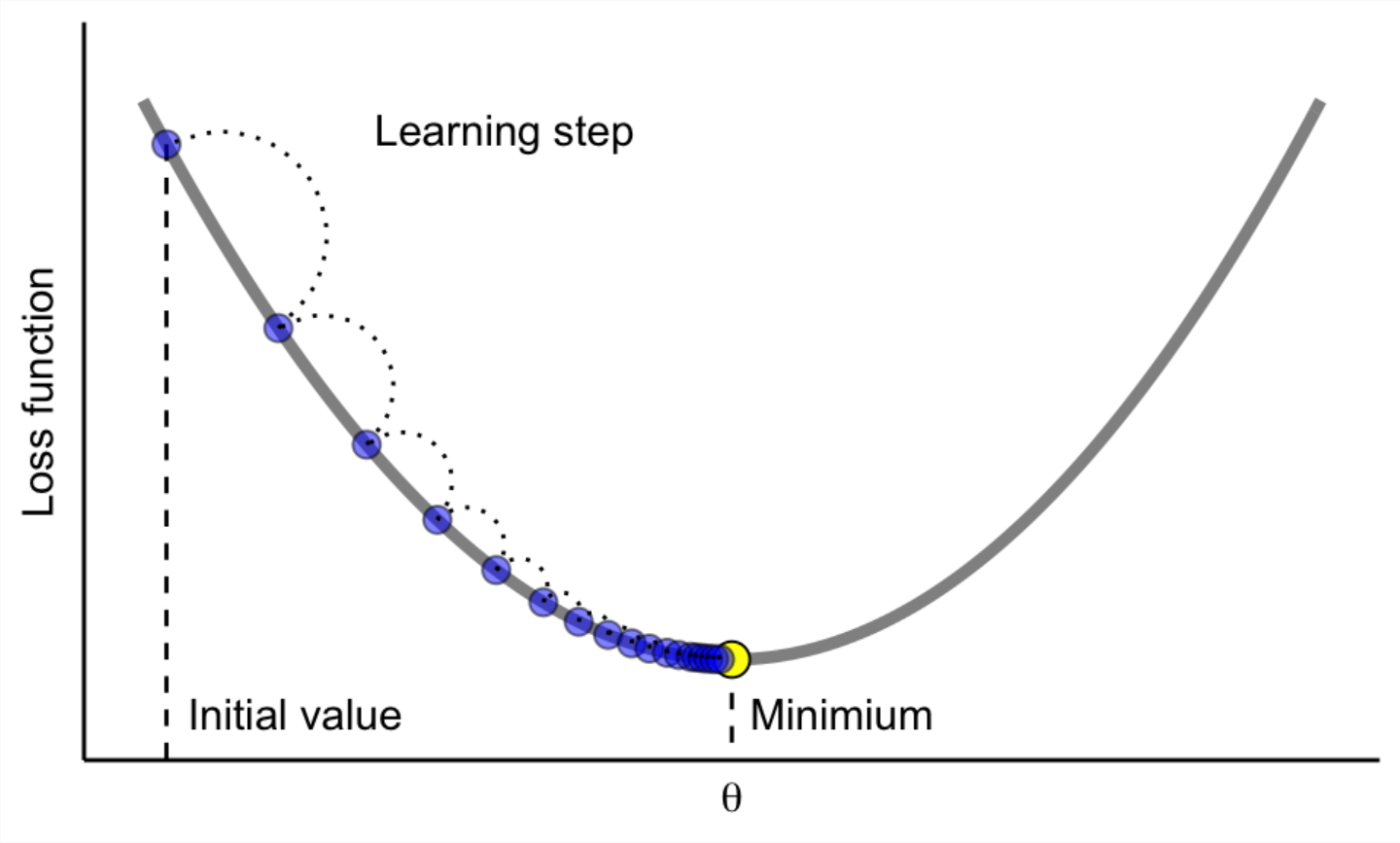


Figure 12.3 from Boehmke & Greenwell Hands-on machine learning with R.

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

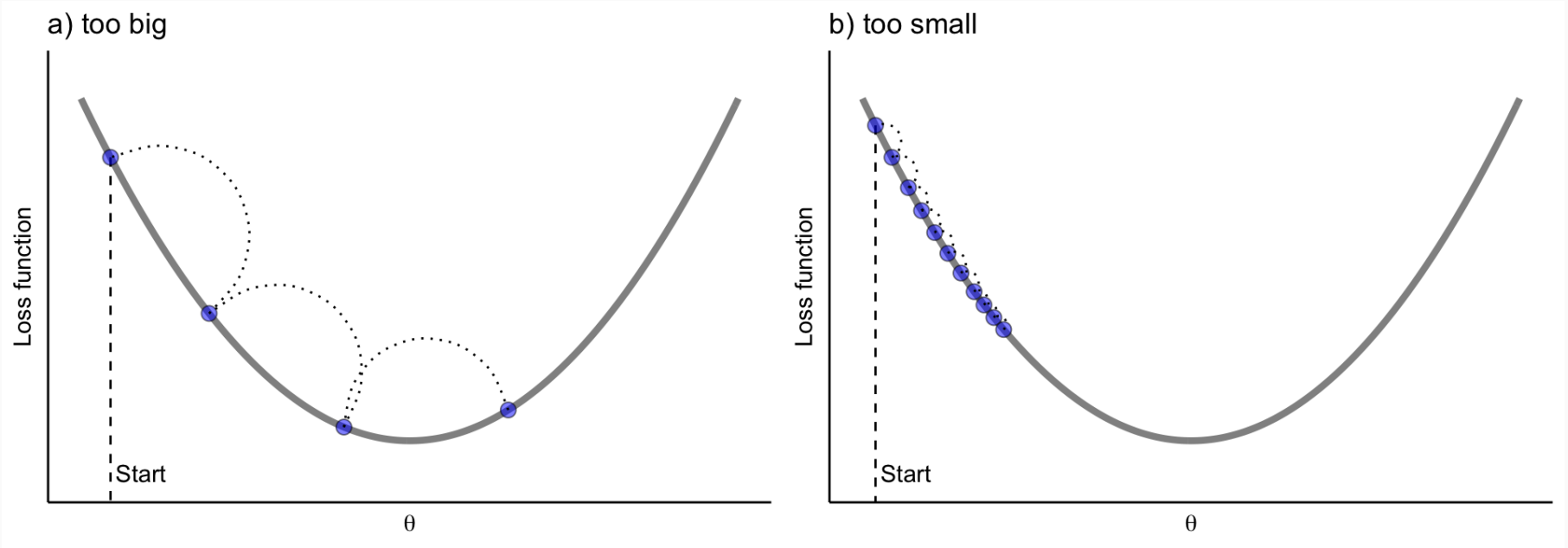


Figure 12.4 from Boehmke & Greenwell Hands-on machine learning with R.

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.

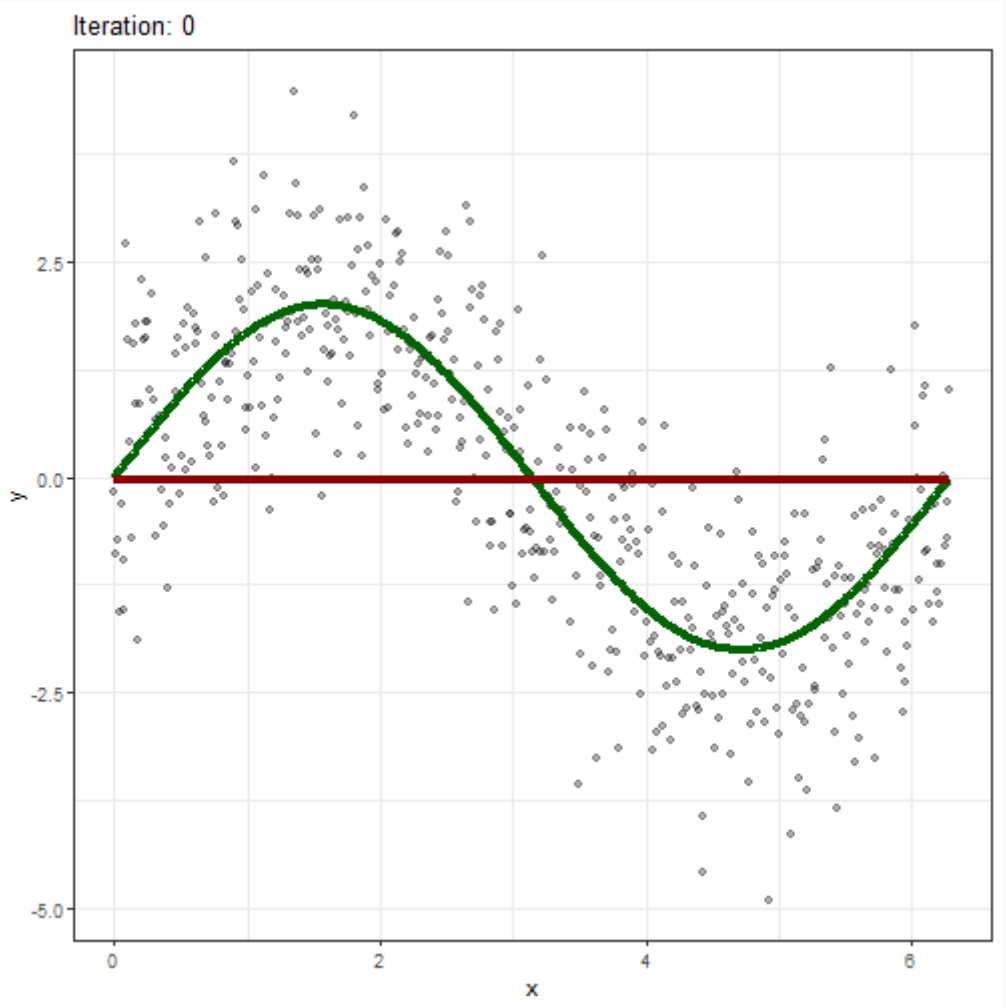
Rule of thumb: if `shrinkage` ⬇ then `ntrees` ⬆.

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 ← gbm(formula = y ~ 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')
```



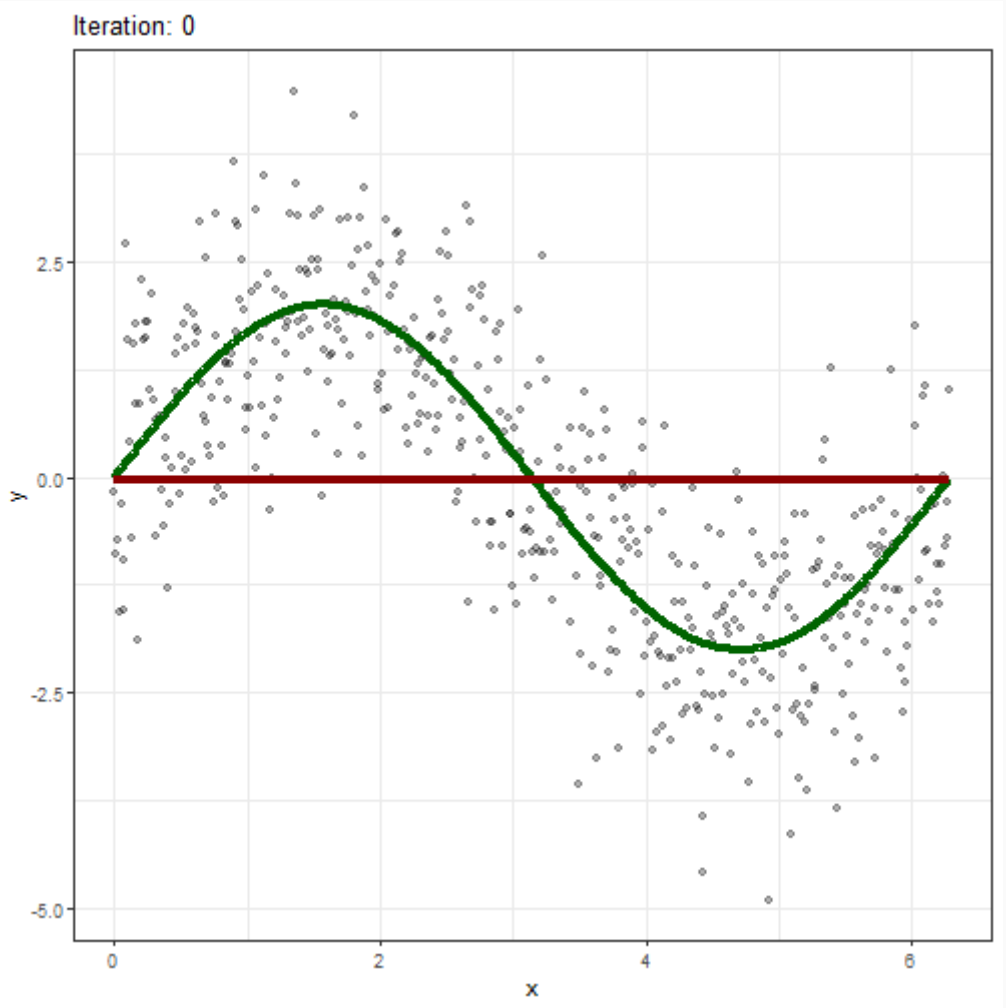
GBM parameters (cont.)

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

```
# Fit the GBM
fit ← gbm(formula = y ~ x,
          data = dfr,
          distribution = 'gaussian',
          n.trees = 10,
          interaction.depth = 1,
          shrinkage = 0.1
          )
```

Applying shrinkage slows down the learning process:

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



GBM parameters (cont.)

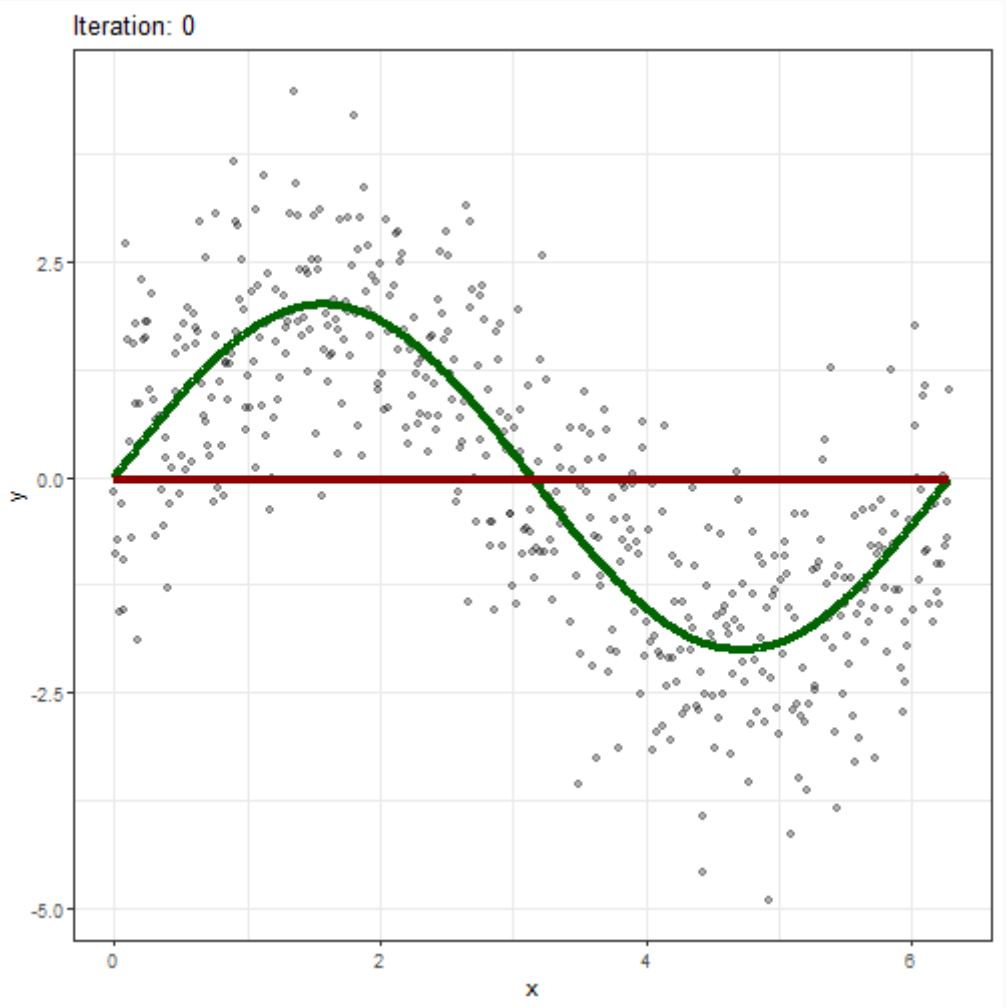
Fit a GBM of 10 shallow trees, **with** shrinkage:

```
# Fit the GBM
fit ← gbm(formula = y ~ x,
          data = dfr,
          distribution = 'gaussian',
          n.trees = 10,
          interaction.depth = 3,
          shrinkage = 0.1
          )
```

Increasing tree depth allows more versatile splits:

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

`interaction.depth > 1` allows for interactions!



GBM parameters (cont.)

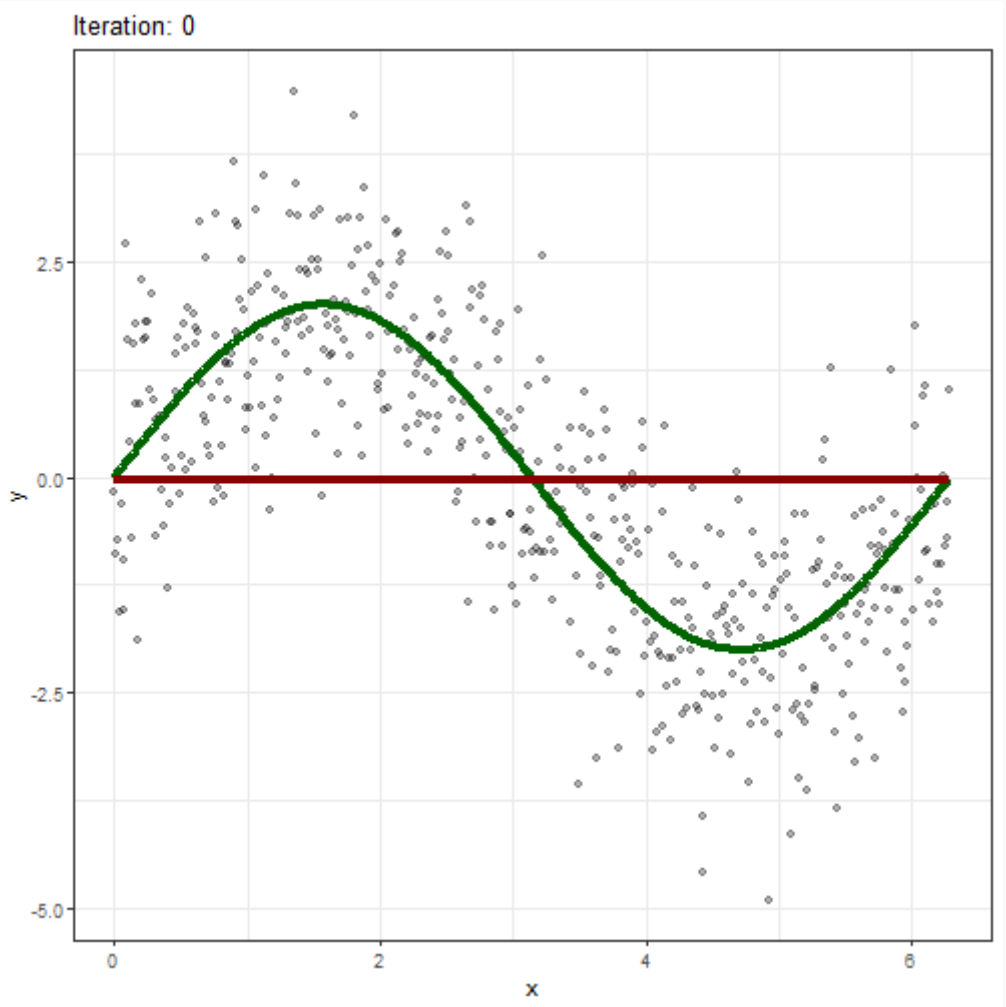
Fit a GBM of 10 shallow trees, **without** shrinkage:

```
# Fit the GBM
fit ← gbm(formula = y ~ x,
          data = dfr,
          distribution = 'gaussian',
          n.trees = 10,
          interaction.depth = 3,
          shrinkage = 1
          )
```

The **danger** for overfitting is real!

Rule of thumb:

- set `shrinkage ⩽ 0.01` and adjust `n.trees` accordingly (**computational constraint**).



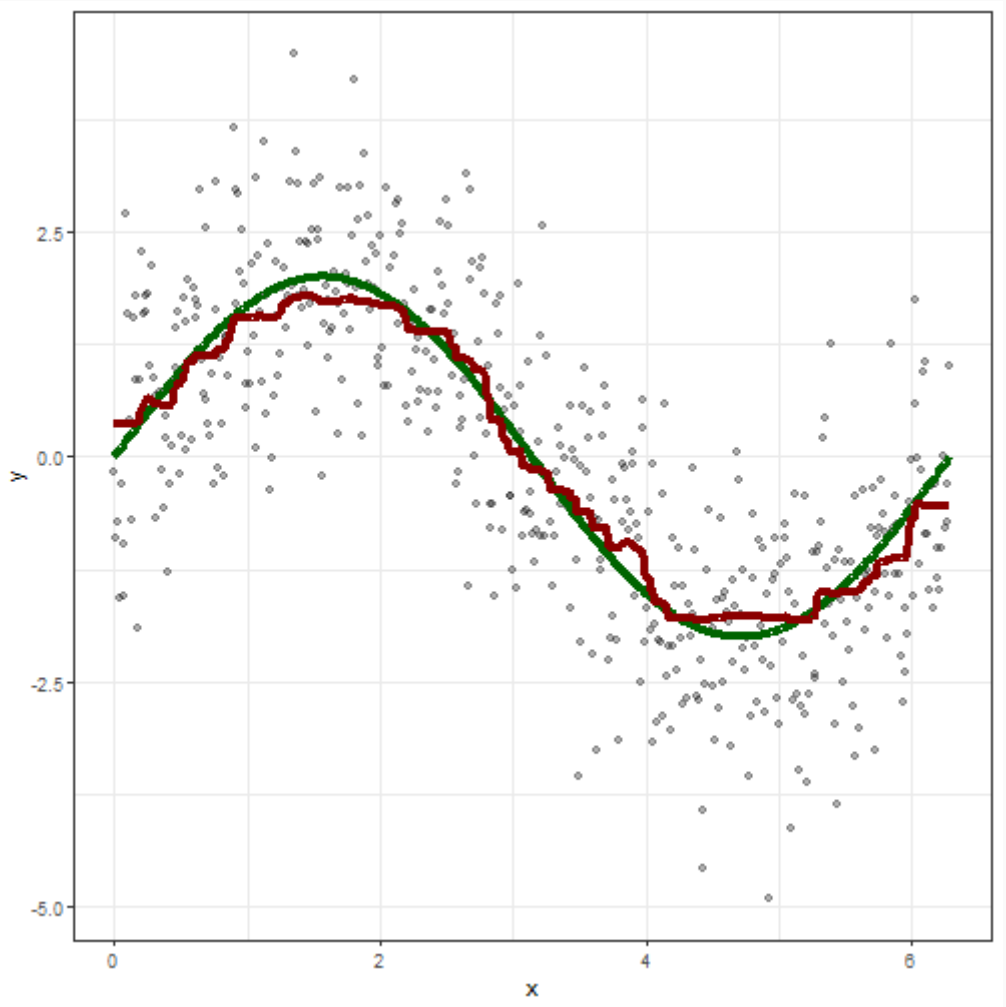
Adding trees to the ensemble

Fit a GBM of 300 shallow trees, with shrinkage:

```
# Fit the GBM
fit ← gbm(formula = y ~ x,
          data = dfr,
          distribution = 'gaussian',
          n.trees = 300,
          interaction.depth = 3,
          shrinkage = 0.01
          )
```

Hi, that's a nice fit!

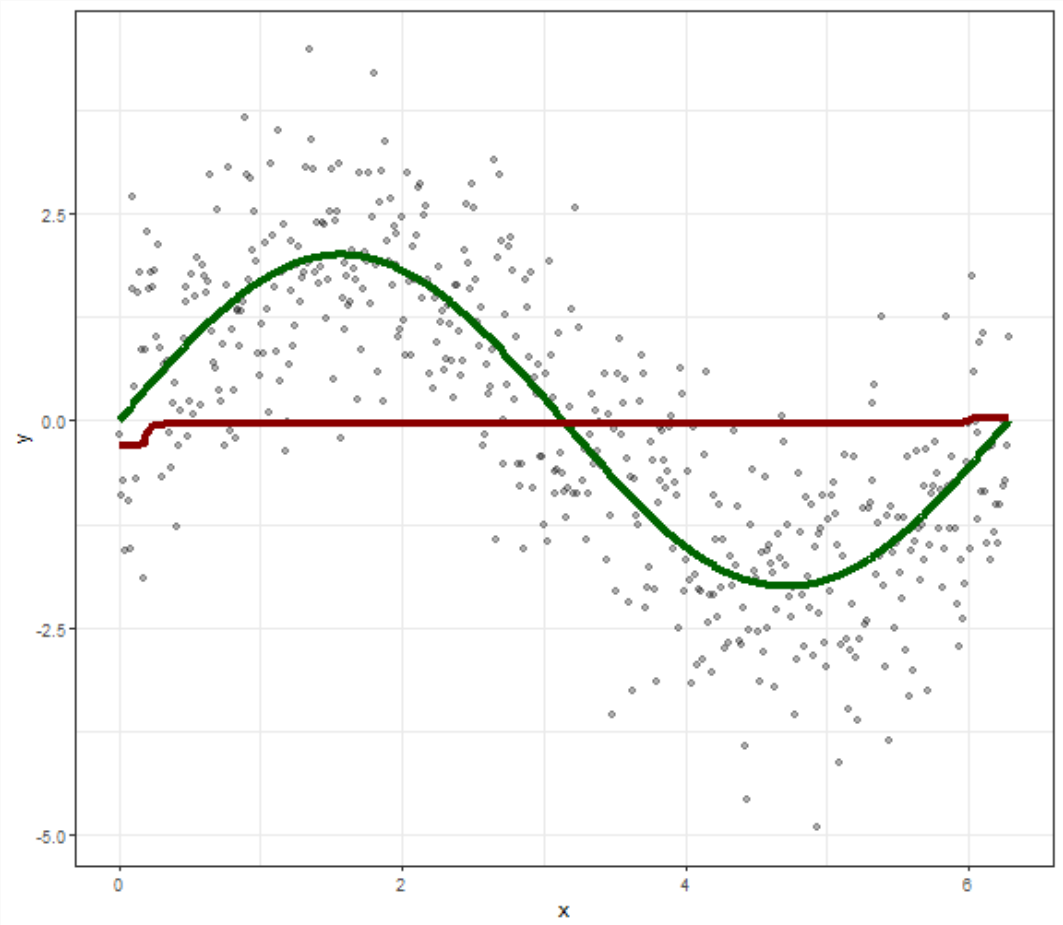
Always beware of **overfitting** when adding trees!



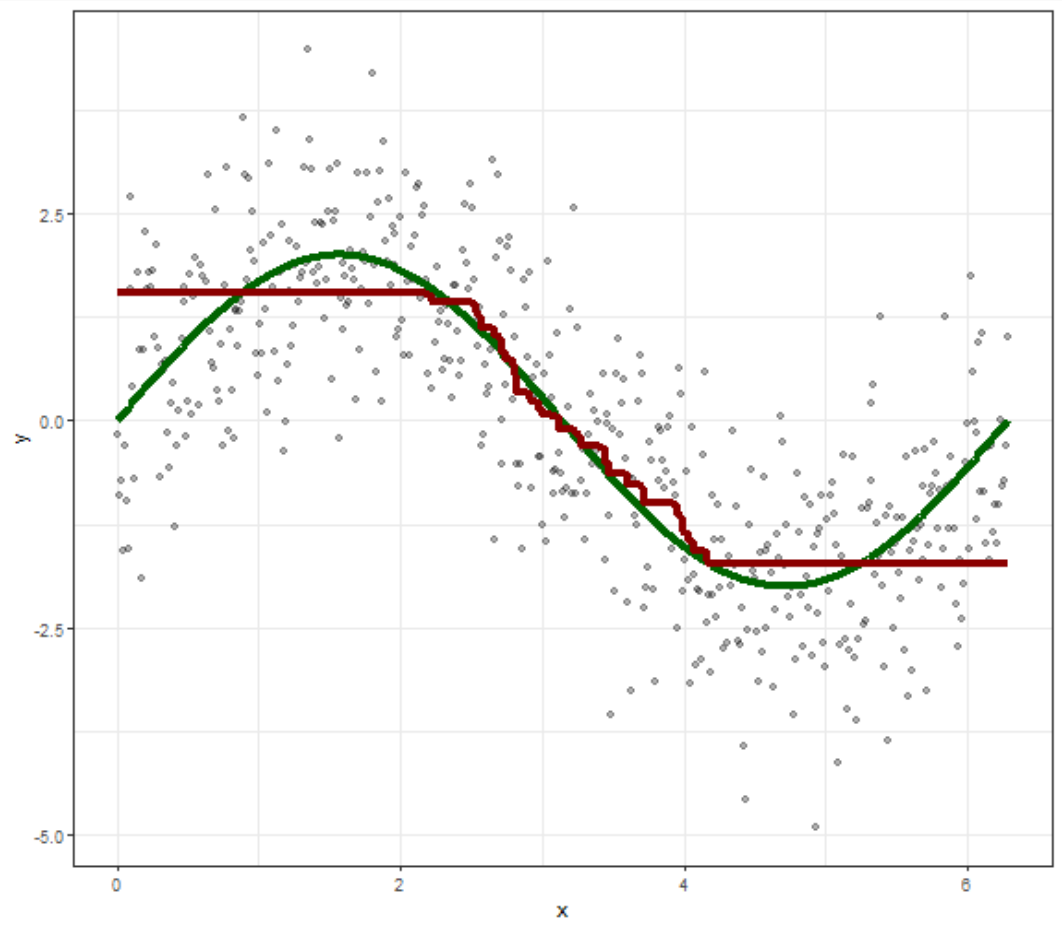
Q: use the previous code to **experiment** with your GBM parameters of choice (see `?gbm`).

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:

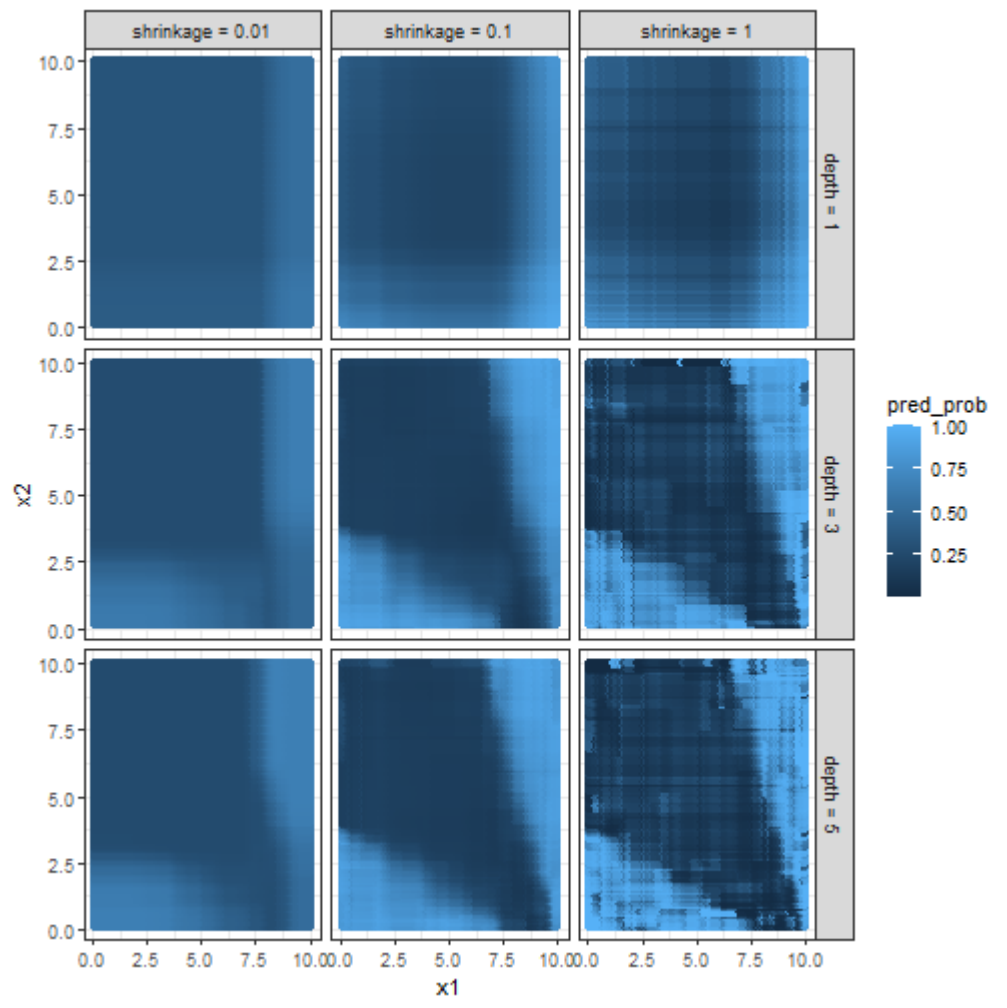
```
ctrl_grid ← expand.grid(depth = c(1,3,5),
                        shrinkage = c(0.01,0.1,1))
results ← vector('list', length = nrow(ctrl_grid))
```

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

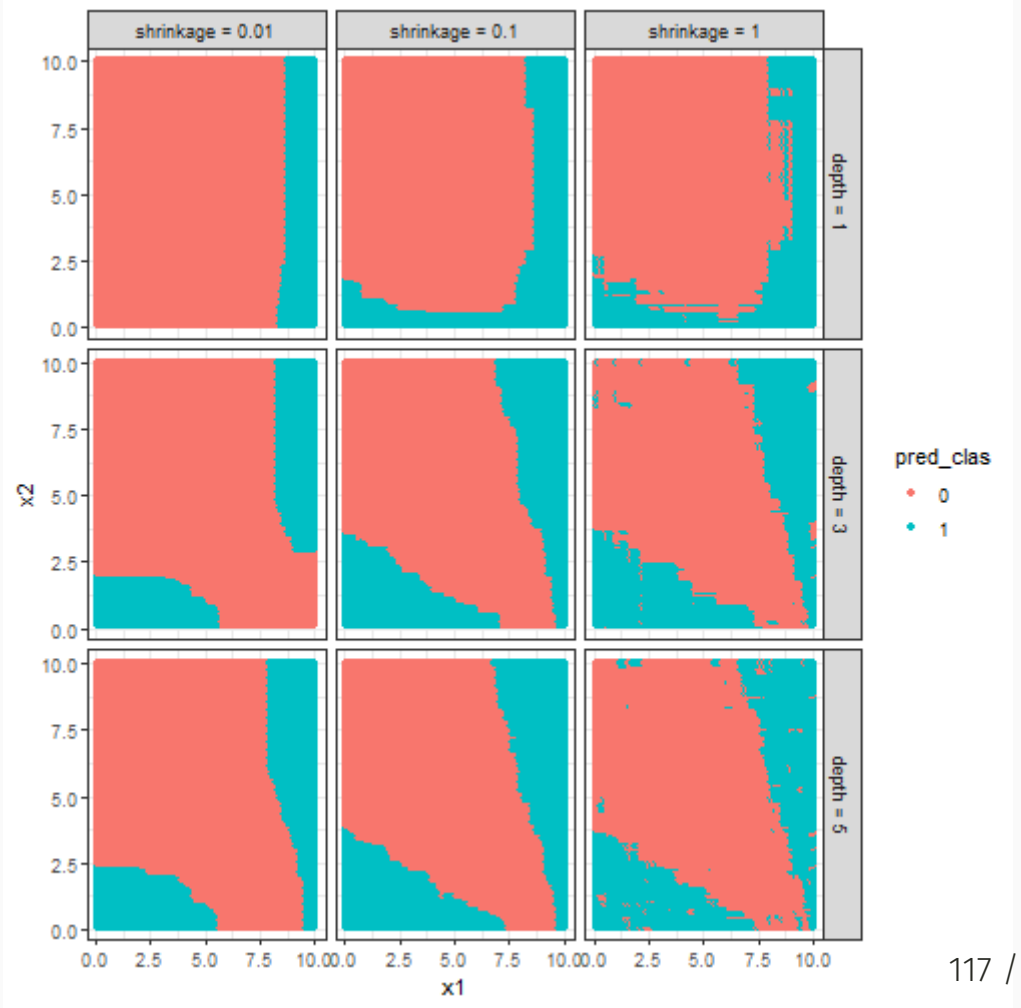
```
for(i in seq_len(nrow(ctrl_grid))) {
  fit ← gbm(y_recode ~ x1 + x2,
            data = dfc,
            distribution = 'bernoulli',
            n.trees = 100,
            interaction.depth = ctrl_grid$depth[i],
            shrinkage = ctrl_grid$shrinkage[i])

  # 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)))
}
```

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 `$oobag.improve`.

```
my_grid ← expand.grid(___)
my_grid ← my_grid %>% dplyr::mutate(oob_improv = NA)

for(i in seq_len(nrow(my_grid))) {
  fit ← gbm(y_recode ~ x1 + x2,
            data = dfc,
            distribution = 'bernoulli',
            n.trees = ___,
            interaction.depth = ___,
            shrinkage = ___,
            ___)
  my_grid$oob_improv[i] ← sum(fit$oobag.improve)
}
```

Performing the grid search:

```
my_grid ← expand.grid(depth = c(1,3,5),
                      shrinkage = c(0.01,0.1,1))
my_grid ← my_grid %>% dplyr::mutate(oob_improv = NA)

for(i in seq_len(nrow(my_grid))) {
  fit ← gbm(y_recode ~ x1 + x2,
            data = dfc,
            distribution = 'bernoulli',
            n.trees = 100,
            interaction.depth = my_grid$depth[i],
            shrinkage = my_grid$shrinkage[i])
  my_grid$oob_improv[i] ← sum(fit$oobag.improve)
}
```

The results:

```
my_grid %>% dplyr::arrange(desc(oob_improv))
##   depth shrinkage   oob_improv
## 1     5      0.10  0.179728774
## 2     3      0.10  0.175448387
## 3     5      0.01  0.123874131
## 4     3      0.01  0.100252315
## 5     1      0.10  0.067270554
## 6     1      0.01  0.039404600
## 7     3      1.00  0.036592026
## 8     1      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
## 0        2      6.500000        1         5           9         164.94 122423
## 1        2      1.500000        2         3           4          27.29  95743
## 2       -1     -0.027378       -1        -1          -1           0.00  66472
## 3       -1      0.004986       -1        -1          -1           0.00  29271
## 4       -1     -0.017484       -1        -1          -1           0.00  95743
## 5        2     10.500000        6         7           8          15.42  26680
## 6       -1      0.035538       -1        -1          -1           0.00  17014
## 7       -1      0.065038       -1        -1          -1           0.00   9666
## 8       -1      0.046226       -1        -1          -1           0.00  26680
## 9       -1     -0.003599       -1        -1          -1           0.00 122423
##   Prediction
## 0  -0.003599
## 1  -0.017484
## 2  -0.027378
## 3   0.004986
## 4  -0.017484
## 5   0.046226
## 6   0.035538
## 7   0.065038
```

Feature importance

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

```
summary(fit, plotit = FALSE)
##                var    rel.inf
## bm              bm 61.3816154
## ageph       ageph 15.5230257
## power       power  8.4368204
## agec         agec  6.7923989
## fuel         fuel  3.2694791
## sex           sex  2.7324191
## coverage coverage  1.3318440
## fleet       fleet  0.3382497
## use           use  0.1941476
```

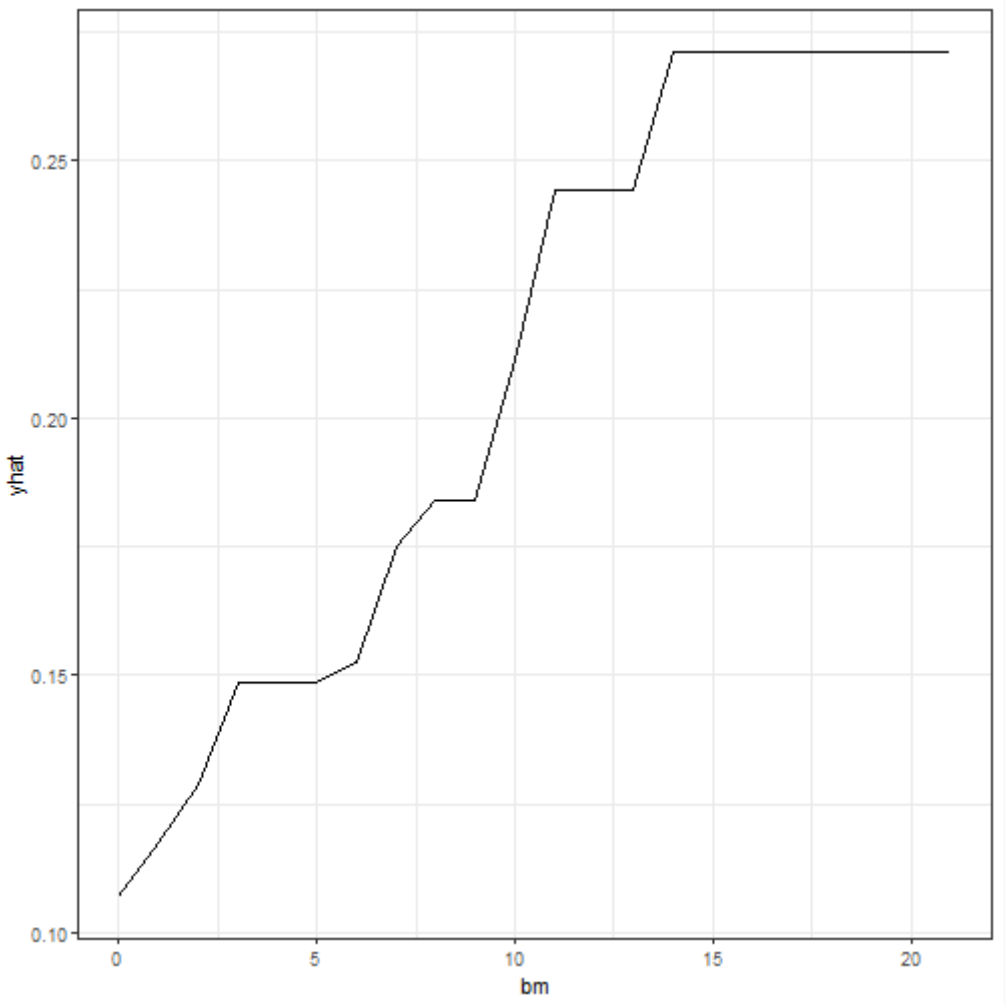
Partial dependence plot

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

```
pred.fun ← function(object,newdata){
  mean(predict(object, newdata,
               n.trees = object$n.trees,
               type = 'response'))
}
```

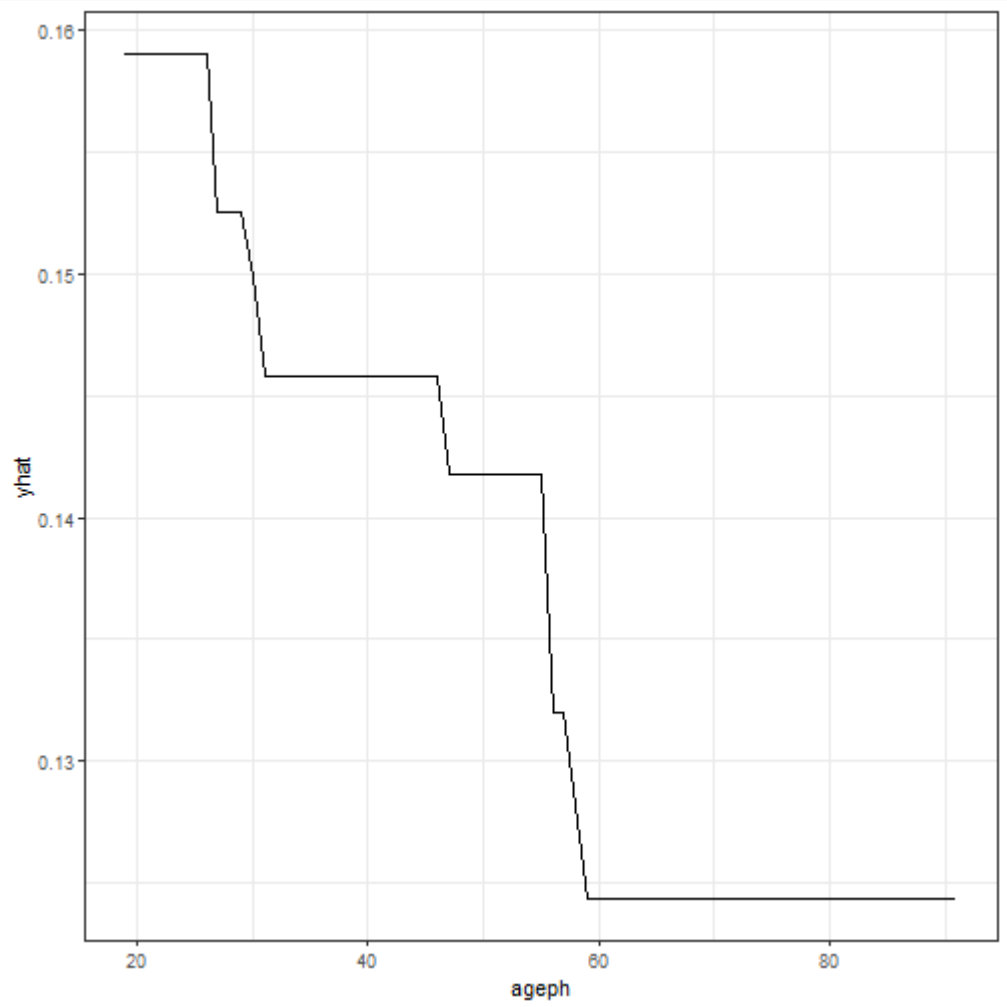
Partial dependence of the **bonus-malus level**:

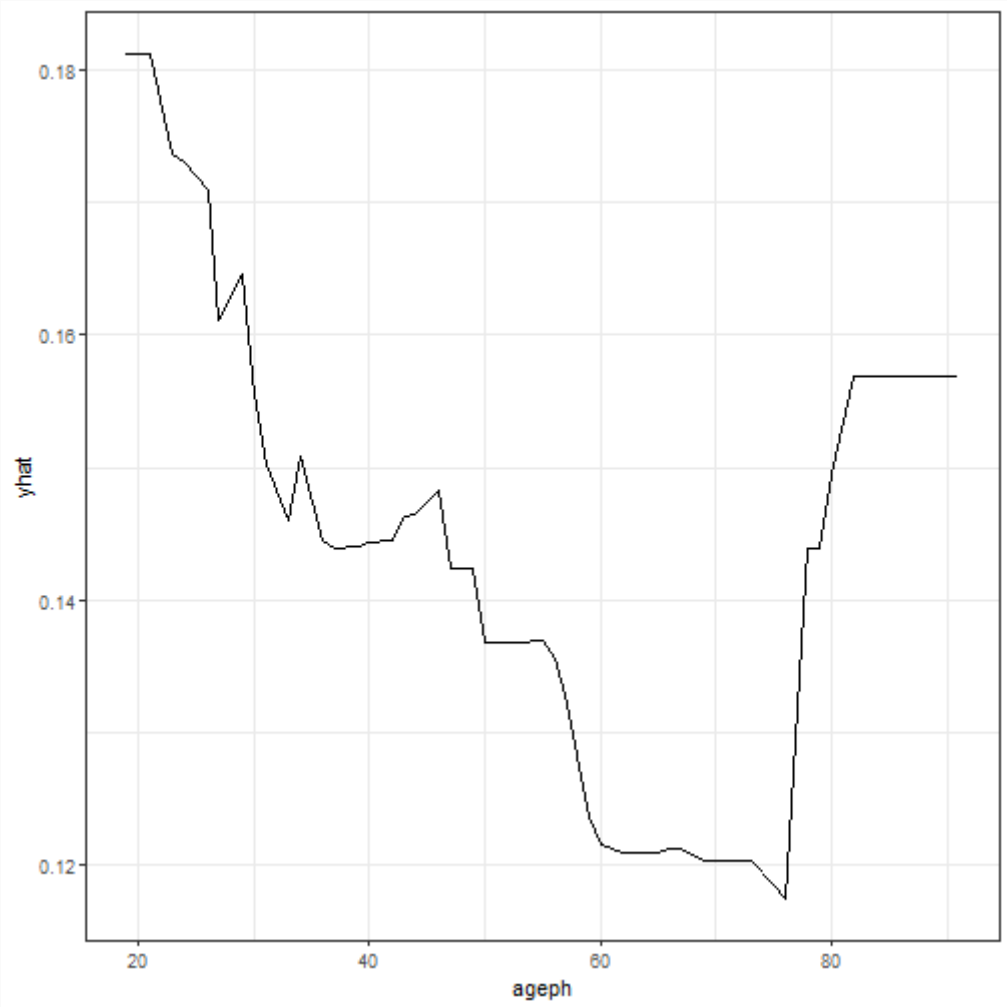
```
set.seed(48927)
pdp_ids ← mtpl %>% nrow %>% sample(size = 5000)
fit %>%
  partial(pred.var = 'bm',
          pred.fun = pred.fun,
          train = mtpl[pdp_ids,],
          recursive= FALSE) %>%
  autoplot()
```



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
  - `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

```
library(xgboost)
mtpl_xgb ← xgb.DMatrix(data = mtpl %>%
                         select(ageph,power,bm,agec,coverage,fuel,sex,fleet,use) %>%
                         data.matrix,
                       info = list(
                         'label' = mtpl$nclaims,
                         'base_margin' = log(mtpl$expo)))
```

- 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
    )
  )
```

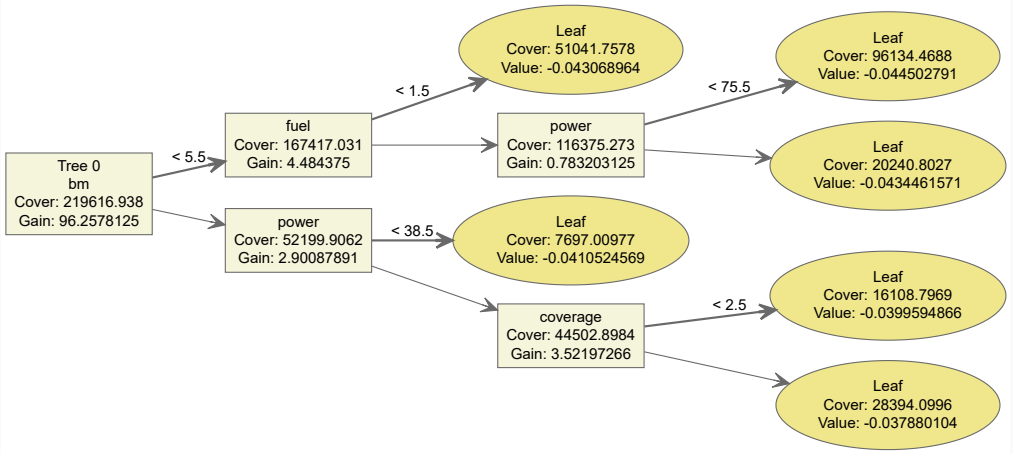
- Fit an XGBoost model to the **xgb.DMatrix** data
- Perform **early stopping** after 20 iterations without improvement
- Use a **decision tree** as base learner
- Choose the **Poisson** distribution for the target
- Stochastic boosting in **rows** and random split candidates in **columns** (like random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

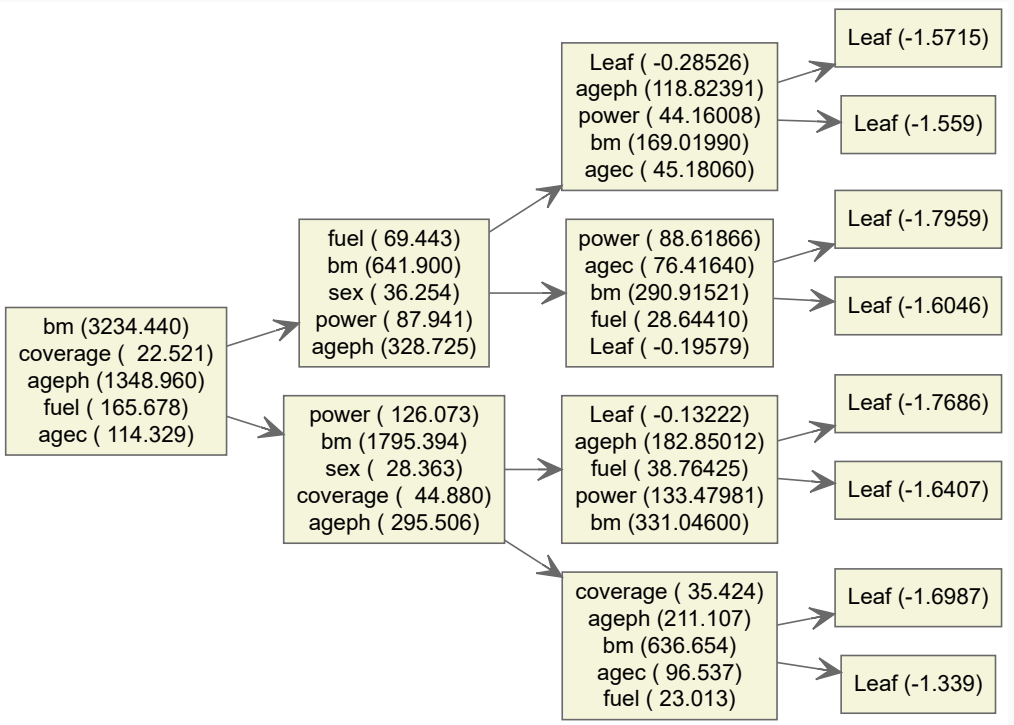


XGBoost in one tree

Get a compressed view of an XGBoost model via `xgb.plot.multi.trees`:

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

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



Further built-in interpretations

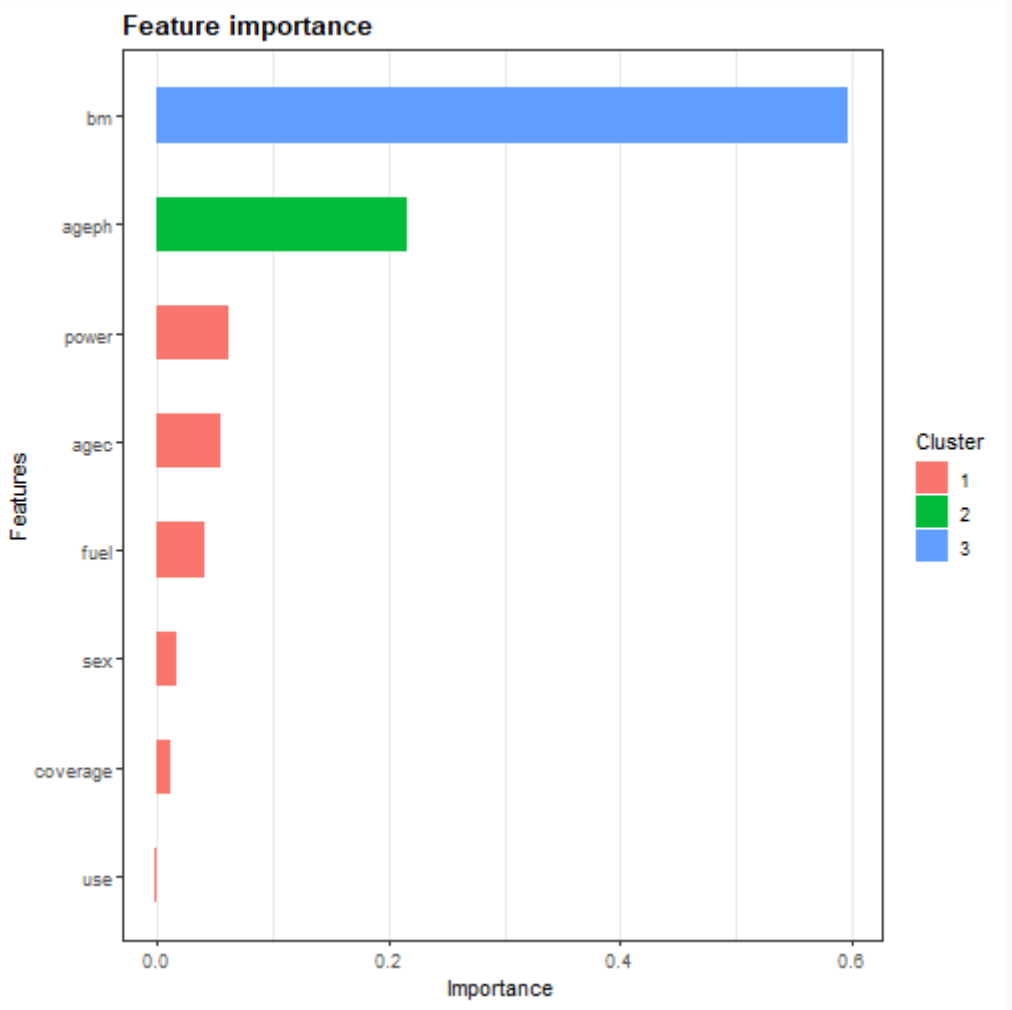
Built-in feature importance:

- `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**

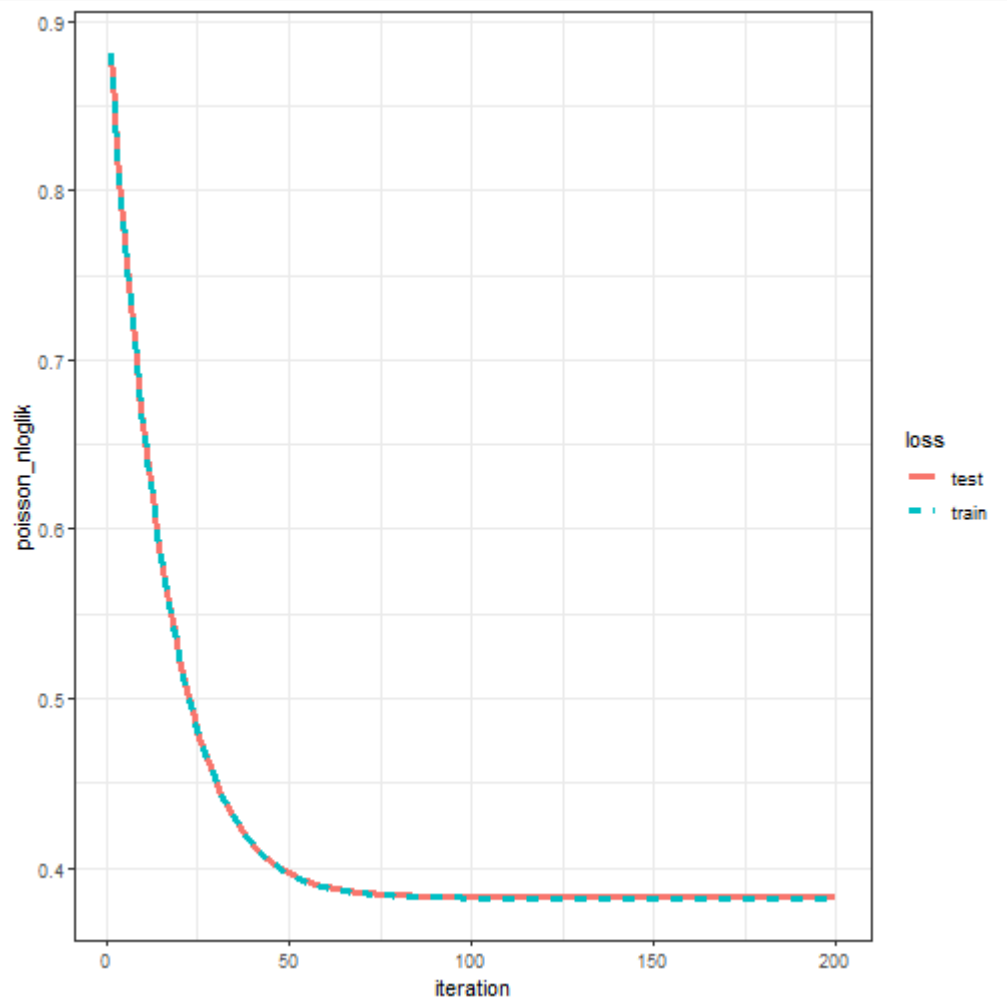
```
set.seed(86493) # reproducibility
xval ← xgb.cv(data = mtpl_xgb,
              nrounds = 200,
              early_stopping_rounds = 20,
              verbose = FALSE,
              nfold = 5,
              stratified = TRUE,
              params = list(booster = 'gbtree',
                            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))
```

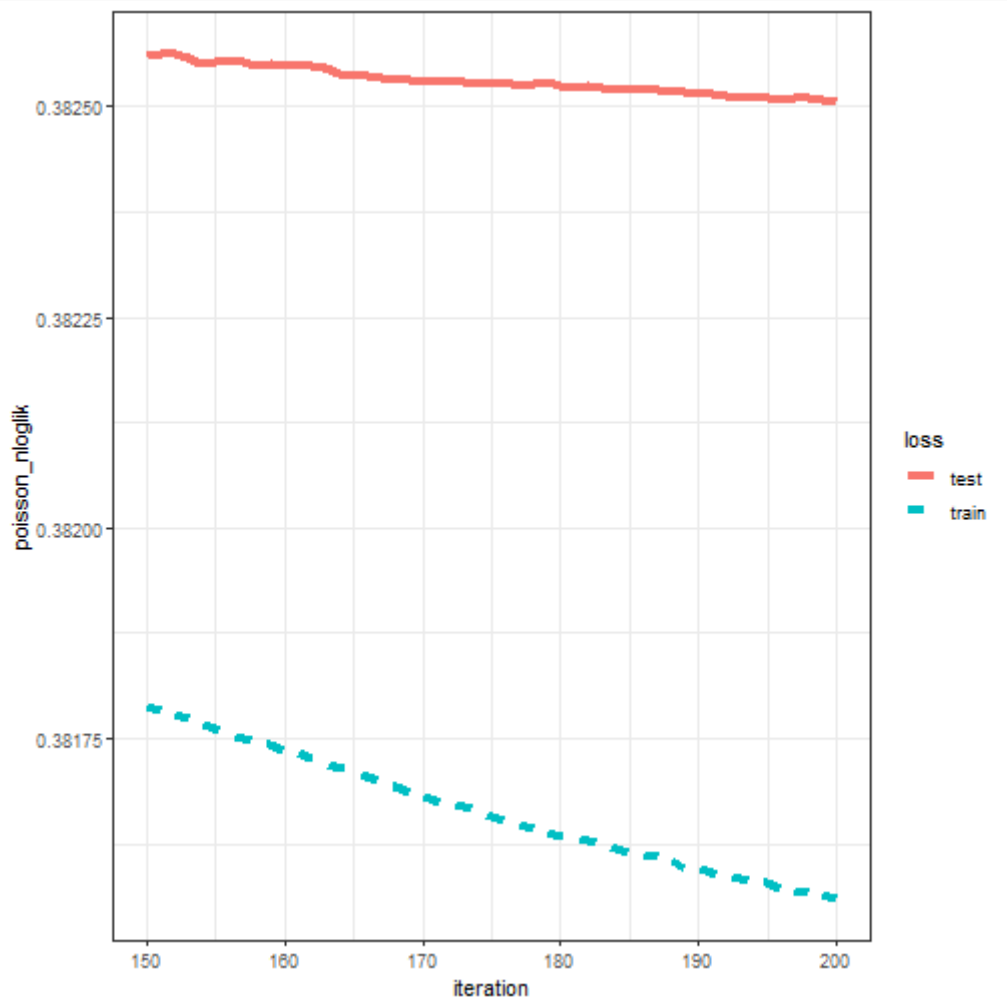
Cross-validation results

Get the cross-validation **results** via `$evaluation_log`:

```
xval$evaluation_log %>% print(digits = 5)
##      iter train_poisson_nloglik_mean train_poisson_nloglik_std
##   1:    1                    0.88048                 0.00017649
##   2:    2                    0.84983                 0.00016304
##   3:    3                    0.82167                 0.00020066
##   4:    4                    0.79477                 0.00028473
##   5:    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
```

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 `mtpl` data contains the average claim amount in the feature `average`. 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