R Exercise 3

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1 Classification: Basic Concepts and Techniques

1.1 Install packages

```
if(!require(pacman))
  install.packages("pacman")
```

```
Loading required package: pacman
```

```
pacman::p_load(tidyverse, rpart, rpart.plot, caret,
  lattice, FSelector, sampling, pROC, mlbench)
```

1.2 The Zoo Dataset

```
data(Zoo, package="mlbench")
head(Zoo)
```

```
          hair feathers  eggs  milk airborne aquatic predator toothed backbone
aardvark  TRUE    FALSE FALSE  TRUE    FALSE   FALSE     TRUE    TRUE     TRUE
antelope  TRUE    FALSE FALSE  TRUE    FALSE   FALSE    FALSE    TRUE     TRUE
bass     FALSE    FALSE  TRUE FALSE    FALSE    TRUE     TRUE    TRUE     TRUE
bear      TRUE    FALSE FALSE  TRUE    FALSE   FALSE     TRUE    TRUE     TRUE
boar      TRUE    FALSE FALSE  TRUE    FALSE   FALSE     TRUE    TRUE     TRUE
buffalo   TRUE    FALSE FALSE  TRUE    FALSE   FALSE    FALSE    TRUE     TRUE
         breathes venomous  fins legs  tail domestic catsize   type
aardvark     TRUE    FALSE FALSE    4 FALSE    FALSE    TRUE mammal
```

```
antelope      TRUE     FALSE FALSE    4  TRUE     FALSE     TRUE mammal
bass         FALSE     FALSE  TRUE    0  TRUE     FALSE    FALSE   fish
bear          TRUE     FALSE FALSE    4 FALSE     FALSE     TRUE mammal
boar          TRUE     FALSE FALSE    4  TRUE     FALSE     TRUE mammal
buffalo       TRUE     FALSE FALSE    4  TRUE     FALSE     TRUE mammal
```

```
library(tidyverse)
as_tibble(Zoo, rownames = "animal")
```

```
# A tibble: 101 x 18
   animal  hair  feathers eggs  milk  airborne aquatic predator toothed backbone
   <chr>   <lgl> <lgl>    <lgl> <lgl> <lgl>    <lgl>   <lgl>    <lgl>   <lgl>
 1 aardva~ TRUE  FALSE    FALSE TRUE  FALSE    FALSE   TRUE     TRUE    TRUE
 2 antelo~ TRUE  FALSE    FALSE TRUE  FALSE    FALSE   FALSE    TRUE    TRUE
 3 bass    FALSE FALSE    TRUE  FALSE FALSE    TRUE    TRUE     TRUE    TRUE
 4 bear    TRUE  FALSE    FALSE TRUE  FALSE    FALSE   TRUE     TRUE    TRUE
 5 boar    TRUE  FALSE    FALSE TRUE  FALSE    FALSE   TRUE     TRUE    TRUE
 6 buffalo TRUE  FALSE    FALSE TRUE  FALSE    FALSE   FALSE    TRUE    TRUE
 7 calf    TRUE  FALSE    FALSE TRUE  FALSE    FALSE   FALSE    TRUE    TRUE
 8 carp    FALSE FALSE    TRUE  FALSE FALSE    TRUE    FALSE    TRUE    TRUE
 9 catfish FALSE FALSE    TRUE  FALSE FALSE    TRUE    TRUE     TRUE    TRUE
10 cavy    TRUE  FALSE    FALSE TRUE  FALSE    FALSE   FALSE    TRUE    TRUE
# i 91 more rows
# i 8 more variables: breathes <lgl>, venomous <lgl>, fins <lgl>, legs <int>,
#   tail <lgl>, domestic <lgl>, catsize <lgl>, type <fct>
```

```
Zoo <- Zoo |>
  mutate(across(where(is.logical), factor, levels = c(TRUE, FALSE))) |>
  mutate(across(where(is.character), factor))
```

```
Warning: There was 1 warning in `mutate()`.
i In argument: `across(where(is.logical), factor, levels = c(TRUE, FALSE))`.
Caused by warning:
! The `...` argument of `across()` is deprecated as of dplyr 1.1.0.
Supply arguments directly to `.fns` through an anonymous function instead.

  # Previously
  across(a:b, mean, na.rm = TRUE)

  # Now
  across(a:b, \(x) mean(x, na.rm = TRUE))
```

```r
summary(Zoo)
```

```
   hair        feathers       eggs          milk        airborne     aquatic      predator
 TRUE :43     TRUE :20     TRUE :59     TRUE :41     TRUE :24     TRUE :36     TRUE :56
 FALSE:58     FALSE:81     FALSE:42     FALSE:60     FALSE:77     FALSE:65     FALSE:45



  toothed      backbone     breathes     venomous       fins           legs
 TRUE :61     TRUE :83     TRUE :80     TRUE : 8     TRUE :17     Min.   :0.000
 FALSE:40     FALSE:18     FALSE:21     FALSE:93     FALSE:84     1st Qu.:2.000
                                                                  Median :4.000
                                                                  Mean   :2.842
                                                                  3rd Qu.:4.000
                                                                  Max.   :8.000
   tail        domestic     catsize                  type
 TRUE :75     TRUE :13     TRUE :44     mammal        :41
 FALSE:26     FALSE:88     FALSE:57     bird          :20
                                        reptile       : 5
                                        fish          :13
                                        amphibian     : 4
                                        insect        : 8
                                        mollusc.et.al:10
```

1.3 Decision Trees

```r
library(rpart)
```

1.3.1 Create Tree With Default Settings (uses pre-pruning)

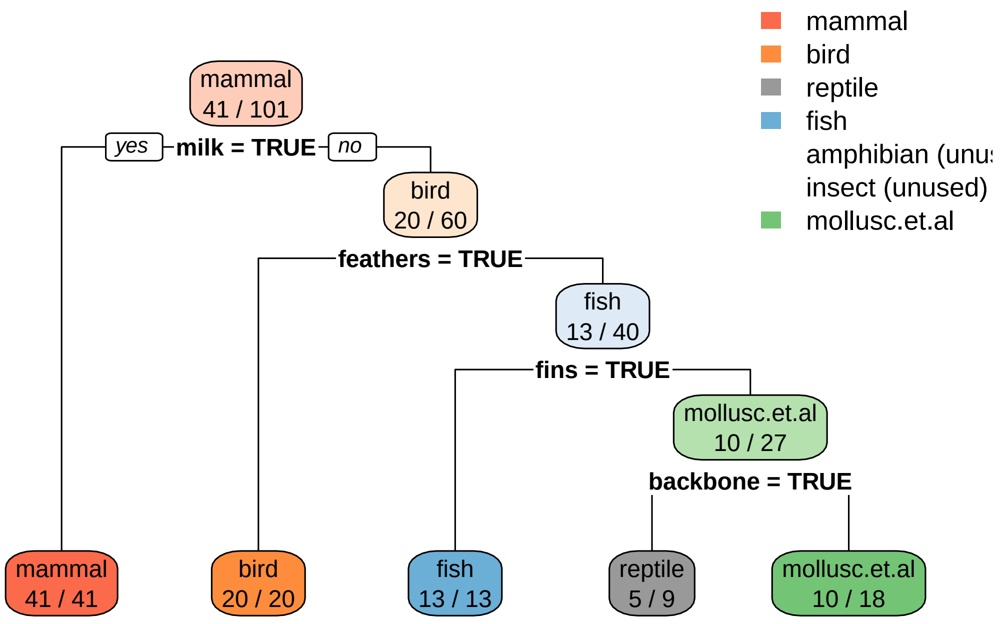
```r
tree_default <- Zoo |>
  rpart(type ~ ., data = _)
tree_default
```

```
n= 101
```

```
node), split, n, loss, yval, (yprob)
      * denotes terminal node

 1) root 101 60 mammal (0.41 0.2 0.05 0.13 0.04 0.079 0.099)
   2) milk=TRUE 41  0 mammal (1 0 0 0 0 0 0) *
   3) milk=FALSE 60 40 bird (0 0.33 0.083 0.22 0.067 0.13 0.17)
     6) feathers=TRUE 20  0 bird (0 1 0 0 0 0 0) *
     7) feathers=FALSE 40 27 fish (0 0 0.12 0.33 0.1 0.2 0.25)
      14) fins=TRUE 13  0 fish (0 0 0 1 0 0 0) *
      15) fins=FALSE 27 17 mollusc.et.al (0 0 0.19 0 0.15 0.3 0.37)
        30) backbone=TRUE 9  4 reptile (0 0 0.56 0 0.44 0 0) *
        31) backbone=FALSE 18  8 mollusc.et.al (0 0 0 0 0 0.44 0.56) *
```

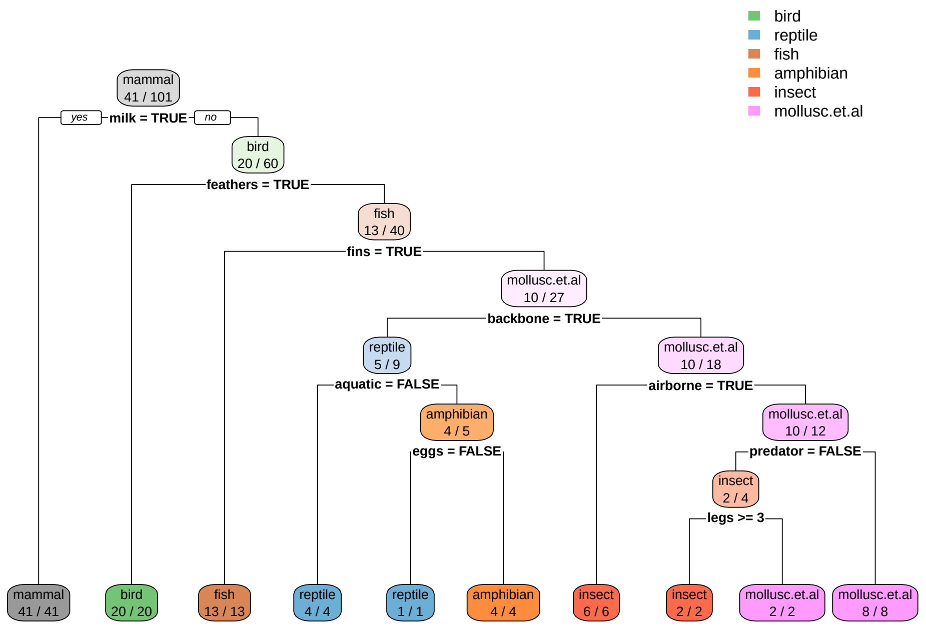
Plotting

```
library(rpart.plot)
rpart.plot(tree_default, extra = 2)
```



1.3.2 Create a Full Tree

```
tree_full <- Zoo |>
  rpart(type ~ . , data = _,
        control = rpart.control(minsplit = 2, cp = 0))
rpart.plot(tree_full, extra = 2,
           roundint=FALSE,
            box.palette = list("Gy", "Gn", "Bu", "Bn",
                               "Or", "Rd", "Pu")) # specify 7 colors
```



```
tree_full
```

```
n= 101

node), split, n, loss, yval, (yprob)
      * denotes terminal node

  1) root 101 60 mammal (0.41 0.2 0.05 0.13 0.04 0.079 0.099)
    2) milk=TRUE 41  0 mammal (1 0 0 0 0 0 0) *
    3) milk=FALSE 60 40 bird (0 0.33 0.083 0.22 0.067 0.13 0.17)
      6) feathers=TRUE 20  0 bird (0 1 0 0 0 0 0) *
      7) feathers=FALSE 40 27 fish (0 0 0.12 0.33 0.1 0.2 0.25)
    14) fins=TRUE 13  0 fish (0 0 0 1 0 0 0) *
    15) fins=FALSE 27 17 mollusc.et.al (0 0 0.19 0 0.15 0.3 0.37)
      30) backbone=TRUE 9  4 reptile (0 0 0.56 0 0.44 0 0)
        60) aquatic=FALSE 4  0 reptile (0 0 1 0 0 0 0) *
        61) aquatic=TRUE 5  1 amphibian (0 0 0.2 0 0.8 0 0)
         122) eggs=FALSE 1  0 reptile (0 0 1 0 0 0 0) *
         123) eggs=TRUE 4  0 amphibian (0 0 0 0 1 0 0) *
      31) backbone=FALSE 18  8 mollusc.et.al (0 0 0 0 0 0.44 0.56)
        62) airborne=TRUE 6  0 insect (0 0 0 0 0 1 0) *
        63) airborne=FALSE 12  2 mollusc.et.al (0 0 0 0 0 0.17 0.83)
         126) predator=FALSE 4  2 insect (0 0 0 0 0 0.5 0.5)
           252) legs>=3 2  0 insect (0 0 0 0 0 1 0) *
           253) legs< 3 2  0 mollusc.et.al (0 0 0 0 0 0 1) *
         127) predator=TRUE 8  0 mollusc.et.al (0 0 0 0 0 0 1) *
```

Training error on tree with pre-pruning

```
predict(tree_default, Zoo) |> head ()
```

```
         mammal bird reptile fish amphibian insect mollusc.et.al
aardvark      1    0       0    0         0      0             0
antelope      1    0       0    0         0      0             0
bass          0    0       0    1         0      0             0
bear          1    0       0    0         0      0             0
boar          1    0       0    0         0      0             0
buffalo       1    0       0    0         0      0             0
```

```
pred <- predict(tree_default, Zoo, type="class")
head(pred)
```

```
aardvark antelope     bass     bear     boar  buffalo
  mammal   mammal     fish   mammal   mammal   mammal
Levels: mammal bird reptile fish amphibian insect mollusc.et.al
```

```
confusion_table <- with(Zoo, table(type, pred))
confusion_table
```

```
               pred
type             mammal bird reptile fish amphibian insect mollusc.et.al
```

```
mammal            41    0       0    0         0      0             0
bird               0   20       0    0         0      0             0
reptile            0    0       5    0         0      0             0
fish               0    0       0   13         0      0             0
amphibian          0    0       4    0         0      0             0
insect             0    0       0    0         0      0             8
mollusc.et.al      0    0       0    0         0      0            10
```

```
correct <- confusion_table |> diag() |> sum()
correct
```

```
[1] 89
```

```
error <- confusion_table |> sum() - correct
error
```

```
[1] 12
```

```
accuracy <- correct / (correct + error)
accuracy
```

```
[1] 0.8811881
```

Use a function for accuracy

```
accuracy <- function(truth, prediction) {
    tbl <- table(truth, prediction)
    sum(diag(tbl))/sum(tbl)
}

accuracy(Zoo |> pull(type), pred)
```

```
[1] 0.8811881
```

Training error of the full tree

```
accuracy(Zoo |> pull(type),
         predict(tree_full, Zoo, type = "class"))
```

```
[1] 1
```

Get a confusion table with more statistics (using caret)

```
library(caret)
confusionMatrix(data = pred,
                reference = Zoo |> pull(type))
```

```
Confusion Matrix and Statistics

               Reference
Prediction      mammal bird reptile fish amphibian insect mollusc.et.al
  mammal            41    0       0    0         0      0             0
  bird               0   20       0    0         0      0             0
  reptile            0    0       5    0         4      0             0
  fish               0    0       0   13         0      0             0
  amphibian          0    0       0    0         0      0             0
  insect             0    0       0    0         0      0             0
  mollusc.et.al      0    0       0    0         0      8            10

Overall Statistics

               Accuracy : 0.8812
                 95% CI : (0.8017, 0.9371)
    No Information Rate : 0.4059
    P-Value [Acc > NIR] : < 2.2e-16

                  Kappa : 0.8431

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: mammal Class: bird Class: reptile Class: fish
Sensitivity                 1.0000       1.000        1.00000      1.0000
Specificity                 1.0000       1.000        0.95833      1.0000
Pos Pred Value              1.0000       1.000        0.55556      1.0000
```

```
Neg Pred Value              1.0000       1.000        1.00000      1.0000
Prevalence                  0.4059       0.198        0.04950      0.1287
Detection Rate              0.4059       0.198        0.04950      0.1287
Detection Prevalence        0.4059       0.198        0.08911      0.1287
Balanced Accuracy           1.0000       1.000        0.97917      1.0000
                     Class: amphibian Class: insect Class: mollusc.et.al
Sensitivity                    0.0000       0.00000              1.00000
Specificity                    1.0000       1.00000              0.91209
Pos Pred Value                    NaN           NaN              0.55556
Neg Pred Value                 0.9604       0.92079              1.00000
Prevalence                     0.0396       0.07921              0.09901
Detection Rate                 0.0000       0.00000              0.09901
Detection Prevalence           0.0000       0.00000              0.17822
Balanced Accuracy              0.5000       0.50000              0.95604
```

1.3.3 Make Predictions for New Data

```
my_animal <- tibble(hair = TRUE, feathers = TRUE, eggs = FALSE,
  milk = TRUE, airborne = TRUE, aquatic = FALSE, predator = TRUE,
  toothed = TRUE, backbone = TRUE, breathes = TRUE, venomous = FALSE,
  fins = FALSE, legs = 4, tail = TRUE, domestic = FALSE,
  catsize = FALSE, type = NA)
```

```
my_animal <- my_animal |>
  mutate(across(where(is.logical), factor, levels = c(TRUE, FALSE)))
my_animal
```

```
# A tibble: 1 x 17
  hair  feathers eggs  milk  airborne aquatic predator toothed backbone breathes
  <fct> <fct>    <fct> <fct> <fct>    <fct>   <fct>    <fct>   <fct>    <fct>
1 TRUE  TRUE     FALSE TRUE  TRUE     FALSE   TRUE     TRUE    TRUE     TRUE
# i 7 more variables: venomous <fct>, fins <fct>, legs <dbl>, tail <fct>,
#   domestic <fct>, catsize <fct>, type <fct>
```

```
predict(tree_default , my_animal, type = "class")
```

```
     1
mammal
Levels: mammal bird reptile fish amphibian insect mollusc.et.al
```

1.4 Model Evaluation with Caret

```r
library(caret)
```

Set random number generator seed to make results reproducible

```r
set.seed(2000)
```

1.4.1 Hold out Test Data

```r
inTrain <- createDataPartition(y = Zoo$type, p = .8, list = FALSE)
Zoo_train <- Zoo |> slice(inTrain)
```

```
Warning: Slicing with a 1-column matrix was deprecated in dplyr 1.1.0.
```

```r
Zoo_test <- Zoo |> slice(-inTrain)
```

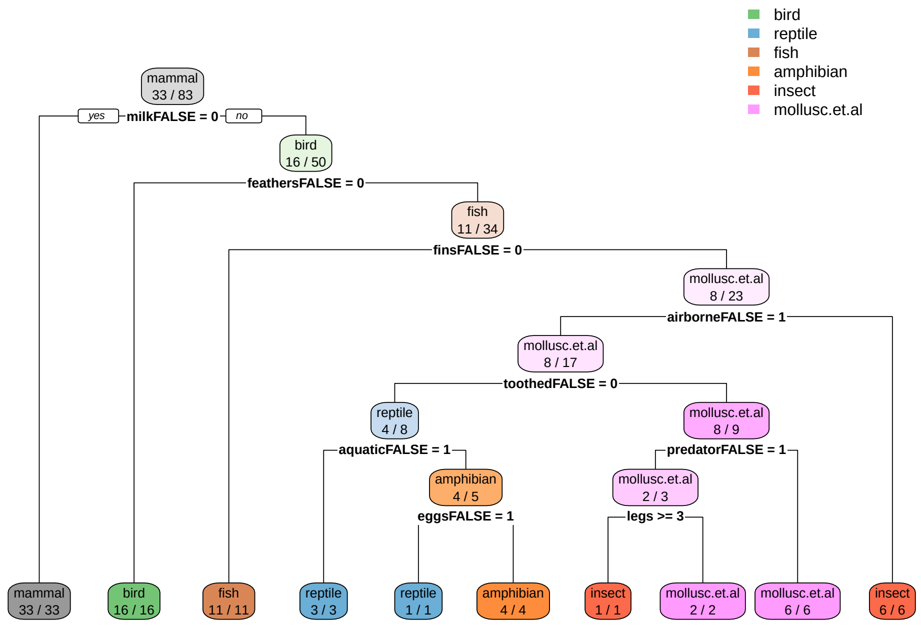
1.4.2 Learn a Model and Tune Hyperparameters on the Training Data

```r
fit <- Zoo_train |>
  train(type ~ .,
    data = _ ,
    method = "rpart",
    control = rpart.control(minsplit = 2),
    trControl = trainControl(method = "cv", number = 10),
    tuneLength = 5)

fit
```

```
CART

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'

No pre-processing
Resampling: Cross-Validated (10 fold)
```

```
Summary of sample sizes: 77, 74, 75, 73, 74, 76, ...
Resampling results across tuning parameters:

  cp    Accuracy   Kappa
  0.00  0.9384921  0.9188571
  0.08  0.8973810  0.8681837
  0.16  0.7447619  0.6637060
  0.22  0.6663095  0.5540490
  0.32  0.4735317  0.1900043

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was cp = 0.
```

```
rpart.plot(fit$finalModel, extra = 2,
  box.palette = list("Gy", "Gn", "Bu", "Bn", "Or", "Rd", "Pu"))
```



```
varImp(fit)
```

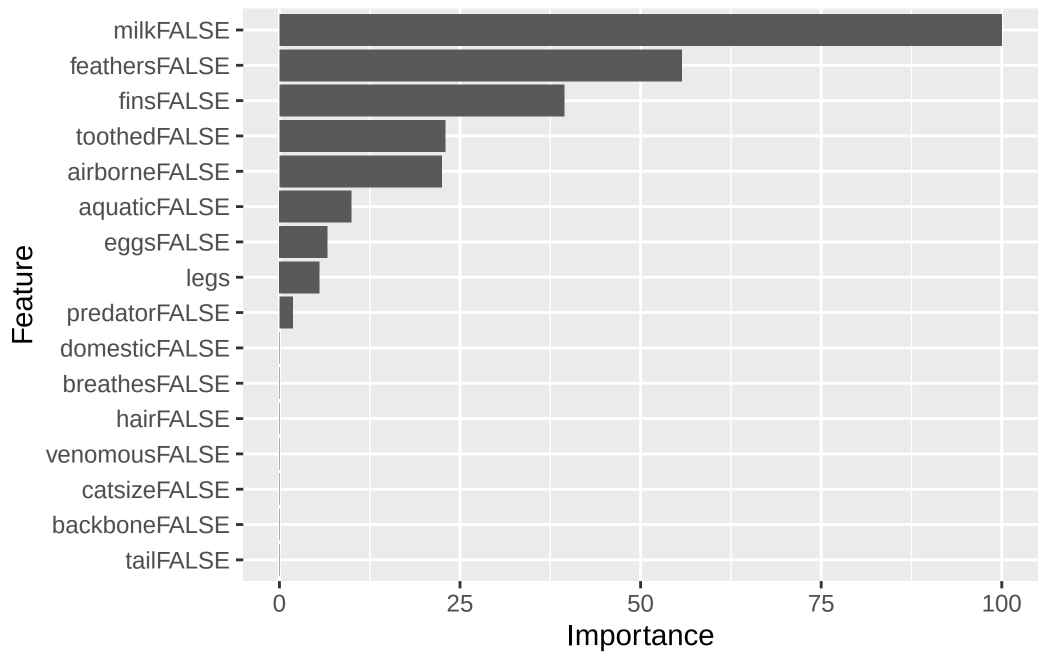
```
rpart variable importance

              Overall
toothedFALSE  100.000
```

```
feathersFALSE  69.814
backboneFALSE  63.084
milkFALSE      55.555
eggsFALSE      53.614
hairFALSE      50.518
finsFALSE      46.984
tailFALSE      28.447
breathesFALSE  28.128
airborneFALSE  26.272
legs           25.859
aquaticFALSE    5.960
predatorFALSE   2.349
venomousFALSE   1.387
catsizeFALSE    0.000
domesticFALSE   0.000
```

```r
imp <- varImp(fit, compete = FALSE)
imp
```

```
rpart variable importance

              Overall
milkFALSE     100.000
feathersFALSE  55.694
finsFALSE      39.453
toothedFALSE   22.956
airborneFALSE  22.478
aquaticFALSE    9.987
eggsFALSE       6.658
legs            5.549
predatorFALSE   1.850
domesticFALSE   0.000
breathesFALSE   0.000
catsizeFALSE    0.000
tailFALSE       0.000
hairFALSE       0.000
backboneFALSE   0.000
venomousFALSE   0.000
```

```r
ggplot(imp)
```



1.5 Testing: Confusion Matrix and Confidence Interval for Accuracy

Use the best model on the test data

```
pred <- predict(fit, newdata = Zoo_test)
pred
```

```
 [1] mammal        mammal        mollusc.et.al insect        mammal
 [6] mammal        mammal        bird          mammal        mammal
[11] bird          fish          fish          mammal        mollusc.et.al
[16] bird          insect        bird
Levels: mammal bird reptile fish amphibian insect mollusc.et.al
```

```
confusionMatrix(data = pred,
                ref = Zoo_test |> pull(type))
```

```
Confusion Matrix and Statistics

               Reference
Prediction      mammal bird reptile fish amphibian insect mollusc.et.al
  mammal             8    0       0    0         0      0             0
  bird              0    4       0    0          0      0             0
  reptile           0    0       0    0          0      0             0
  fish              0    0       0    2          0      0             0
  amphibian         0    0       0    0          0      0             0
  insect            0    0       1    0          0      1             0
  mollusc.et.al     0    0       0    0          0      0             2

Overall Statistics

               Accuracy : 0.9444
                 95% CI : (0.7271, 0.9986)
    No Information Rate : 0.4444
    P-Value [Acc > NIR] : 1.076e-05

                  Kappa : 0.9231

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: mammal Class: bird Class: reptile Class: fish
Sensitivity                 1.0000      1.0000        0.00000      1.0000
Specificity                 1.0000      1.0000        1.00000      1.0000
Pos Pred Value              1.0000      1.0000            NaN      1.0000
Neg Pred Value              1.0000      1.0000        0.94444      1.0000
Prevalence                  0.4444      0.2222        0.05556      0.1111
Detection Rate              0.4444      0.2222        0.00000      0.1111
Detection Prevalence        0.4444      0.2222        0.00000      0.1111
Balanced Accuracy           1.0000      1.0000        0.50000      1.0000
                     Class: amphibian Class: insect Class: mollusc.et.al
Sensitivity                        NA       1.00000               1.0000
Specificity                         1       0.94118               1.0000
Pos Pred Value                     NA       0.50000               1.0000
Neg Pred Value                     NA       1.00000               1.0000
Prevalence                          0       0.05556               0.1111
Detection Rate                      0       0.05556               0.1111
Detection Prevalence                0       0.11111               0.1111
Balanced Accuracy                  NA       0.97059               1.0000
```

1.6 Model Comparison

```r
train_index <- createFolds(Zoo_train$type, k = 10)
```

```r
rpartFit <- Zoo_train |>
  train(type ~ .,
        data = _,
        method = "rpart",
        tuneLength = 10,
        trControl = trainControl(method = "cv", indexOut = train_index)
  )
```

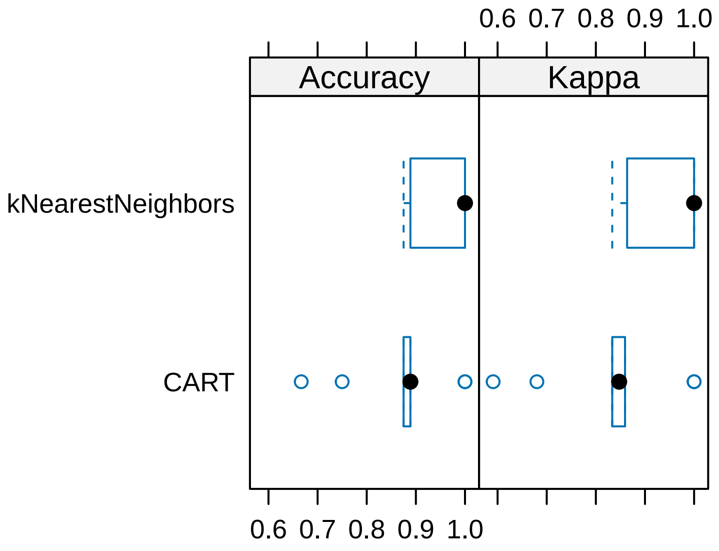
```r
knnFit <- Zoo_train |>
  train(type ~ .,
        data = _,
        method = "knn",
        preProcess = "scale",
          tuneLength = 10,
          trControl = trainControl(method = "cv", indexOut = train_index)
  )
```

```r
resamps <- resamples(list(
        CART = rpartFit,
        kNearestNeighbors = knnFit
        ))

summary(resamps)
```

```

Call:
summary.resamples(object = resamps)

Models: CART, kNearestNeighbors
Number of resamples: 10

Accuracy
                       Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
CART              0.6666667 0.8750000 0.8888889 0.8722222 0.8888889    1    0
kNearestNeighbors 0.8750000 0.9166667 1.0000000 0.9652778 1.0000000    1    0

Kappa
```

```
                       Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
CART              0.5909091 0.8333333 0.8474576 0.8341866 0.8570312    1    0
kNearestNeighbors 0.8333333 0.8977273 1.0000000 0.9546970 1.0000000    1    0
```

```
library(lattice)
bwplot(resamps, layout = c(3, 1))
```



```
difs <- diff(resamps)
difs
```

```
Call:
diff.resamples(x = resamps)

Models: CART, kNearestNeighbors
Metrics: Accuracy, Kappa
Number of differences: 1
p-value adjustment: bonferroni
```

```
summary(difs)
```

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

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

Accuracy
                   CART    kNearestNeighbors
CART                       -0.09306
kNearestNeighbors 0.01151

Kappa
                   CART   kNearestNeighbors
CART                      -0.1205
kNearestNeighbors 0.0104
```

1.7 Feature Selection and Feature Preparation

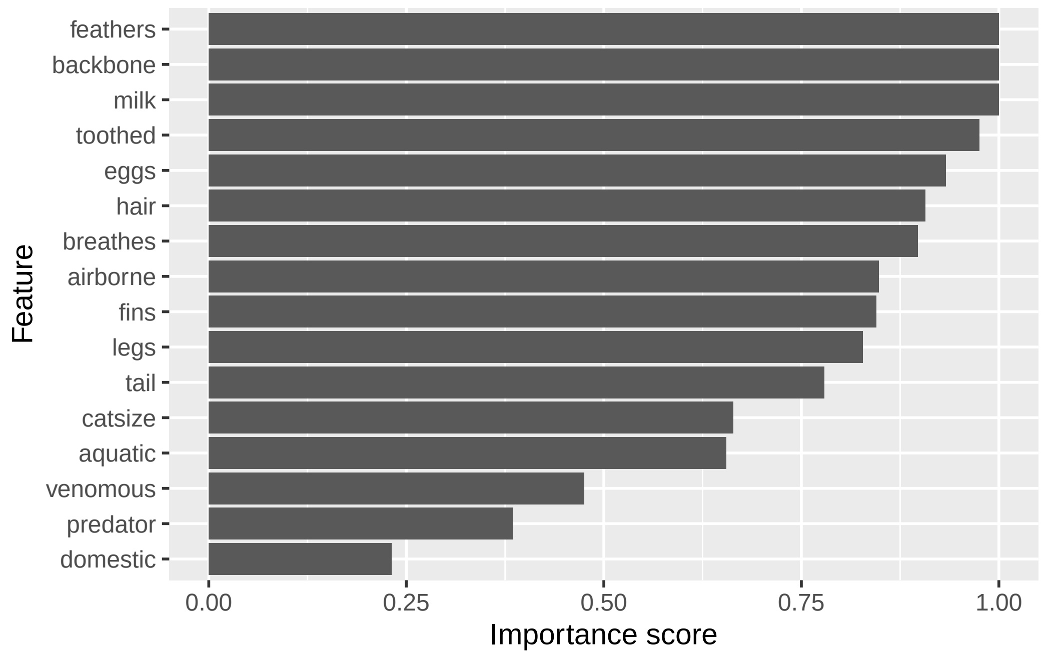
```
library(FSelector)
```

```
weights <- Zoo_train |>
  chi.squared(type ~ ., data = _) |>
  as_tibble(rownames = "feature") |>
  arrange(desc(attr_importance))

weights
```

```
# A tibble: 16 x 2
   feature  attr_importance
   <chr>              <dbl>
 1 feathers           1
 2 backbone           1
 3 milk               1
 4 toothed            0.975
 5 eggs               0.933
 6 hair               0.907
 7 breathes           0.898
 8 airborne           0.848
 9 fins               0.845
10 legs               0.828
11 tail               0.779
12 catsize            0.664
```

```
13 aquatic            0.655
14 venomous           0.475
15 predator           0.385
16 domestic           0.231
```

```r
ggplot(weights,
  aes(x = attr_importance, y = reorder(feature, attr_importance))) +
  geom_bar(stat = "identity") +
  xlab("Importance score") +
  ylab("Feature")
```



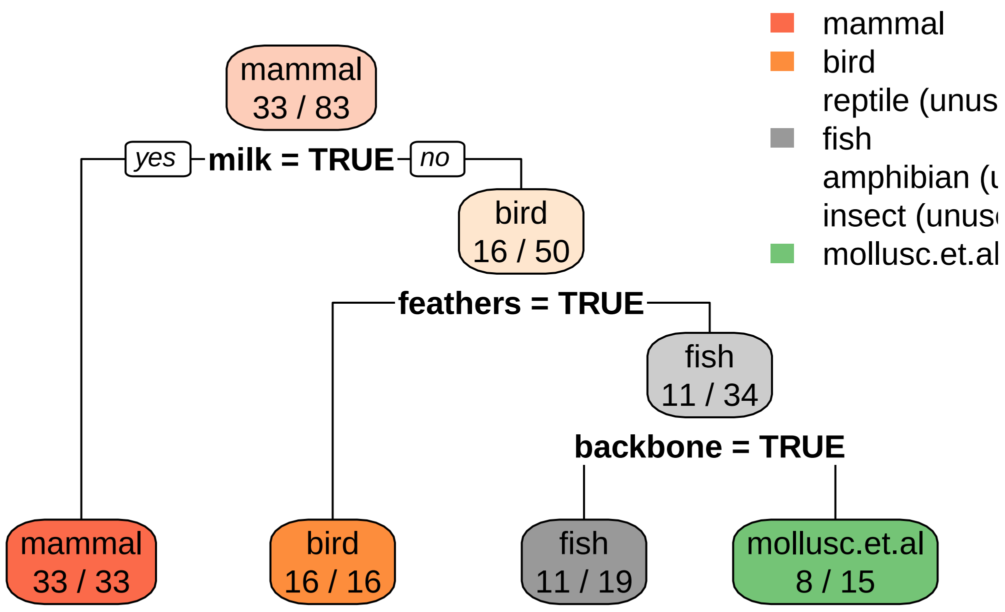
```r
# Get the 5 best features


subset <- cutoff.k(weights |>
                   column_to_rownames("feature"), 5)
subset
```

```
[1] "feathers" "backbone" "milk"     "toothed"  "eggs"
```

```
# Use only the best 5 features to build a model (Fselector provides as.simple.formula)

f <- as.simple.formula(subset, "type")
f
```

```
type ~ feathers + backbone + milk + toothed + eggs
<environment: 0x12c3a2c50>
```

```
m <- Zoo_train |> rpart(f, data = _)
rpart.plot(m, extra = 2, roundint = FALSE)
```



```
Zoo_train |>
  gain.ratio(type ~ ., data = _) |>
  as_tibble(rownames = "feature") |>
  arrange(desc(attr_importance))
```

```
# A tibble: 16 x 2
   feature  attr_importance
   <chr>              <dbl>
 1 backbone           1
 2 milk               1.00
 3 feathers           1.00
 4 toothed           0.919
 5 eggs              0.827
 6 breathes          0.821
 7 hair              0.782
 8 fins              0.689
 9 legs              0.682
10 airborne          0.671
11 tail              0.573
12 aquatic           0.391
13 catsize           0.383
14 venomous          0.351
15 predator          0.125
16 domestic          0.0975
```

1.7.1 Feature Subset Selection

```
Zoo_train |>
  cfs(type ~ ., data = _)
```

```
 [1] "hair"     "feathers" "eggs"     "milk"     "toothed"  "backbone"
 [7] "breathes" "fins"     "legs"     "tail"
```

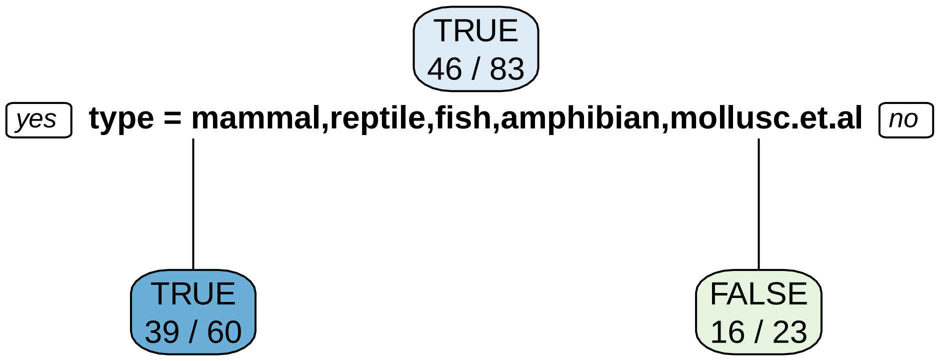
```
evaluator <- function(subset) {
  model <- Zoo_train |>
    train(as.simple.formula(subset, "type"),
          data = _,
          method = "rpart",
          trControl = trainControl(method = "boot", number = 5),
          tuneLength = 0)
  results <- model$resample$Accuracy
  cat("Trying features:", paste(subset, collapse = " + "), "\n")
  m <- mean(results)
  cat("Accuracy:", round(m, 2), "\n\n")
  m
}
```

```
features <- Zoo_train |> colnames() |> setdiff("type")
```

```
##subset <- backward.search(features, evaluator)
##subset <- forward.search(features, evaluator)
##subset <- best.first.search(features, evaluator)
##subset <- hill.climbing.search(features, evaluator)
##subset
```

1.7.2 Using Dummy Variables for Factors

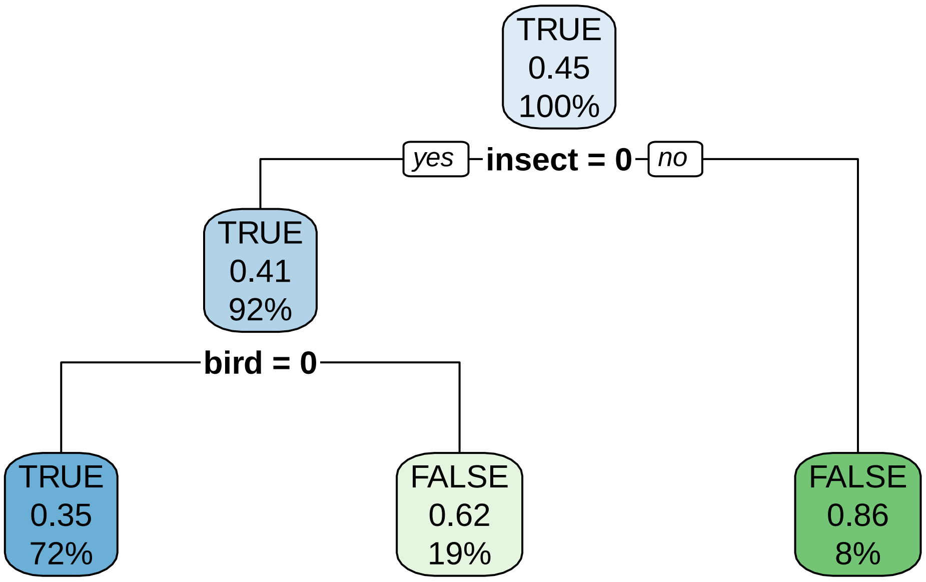
```
tree_predator <- Zoo_train |>
  rpart(predator ~ type, data = _)
rpart.plot(tree_predator, extra = 2, roundint = FALSE)
```



```
Zoo_train_dummy <- as_tibble(class2ind(Zoo_train$type)) |>
  mutate(across(everything(), as.factor)) |>
  add_column(predator = Zoo_train$predator)
Zoo_train_dummy
```

```
# A tibble: 83 x 8
   mammal bird  reptile fish  amphibian insect mollusc.et.al predator
   <fct>  <fct> <fct>   <fct> <fct>     <fct>  <fct>         <fct>
 1 1      0     0       0     0         0      0             TRUE
 2 1      0     0       0     0         0      0             FALSE
 3 0      0     0       1     0         0      0             TRUE
 4 1      0     0       0     0         0      0             TRUE
 5 1      0     0       0     0         0      0             FALSE
 6 1      0     0       0     0         0      0             FALSE
 7 0      0     0       1     0         0      0             FALSE
 8 0      0     0       1     0         0      0             TRUE
 9 1      0     0       0     0         0      0             FALSE
10 0      1     0       0     0         0      0             FALSE
# i 73 more rows
```

```
tree_predator <- Zoo_train_dummy |>
  rpart(predator ~ .,
        data = _,
        control = rpart.control(minsplit = 2, cp = 0.01))
rpart.plot(tree_predator, roundint = FALSE)
```

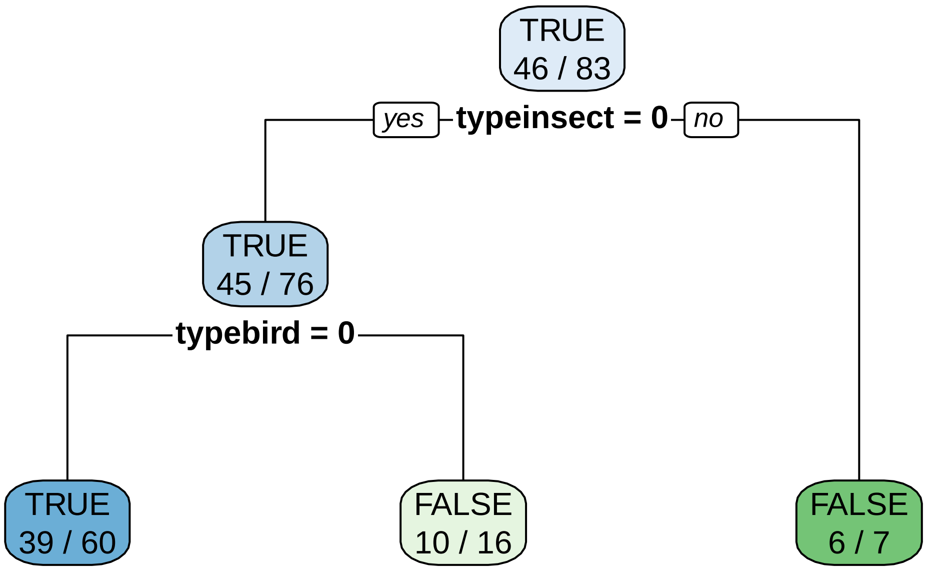


```
fit <- Zoo_train |>
  train(predator ~ type,
        data = _,
        method = "rpart",
        control = rpart.control(minsplit = 2),
        tuneGrid = data.frame(cp = 0.01))
fit
```

```
CART

83 samples
 1 predictor
 2 classes: 'TRUE', 'FALSE'
```

```
No pre-processing
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 83, 83, 83, 83, 83, 83, ...
Resampling results:

  Accuracy   Kappa
  0.6060423  0.2034198

Tuning parameter 'cp' was held constant at a value of 0.01
```

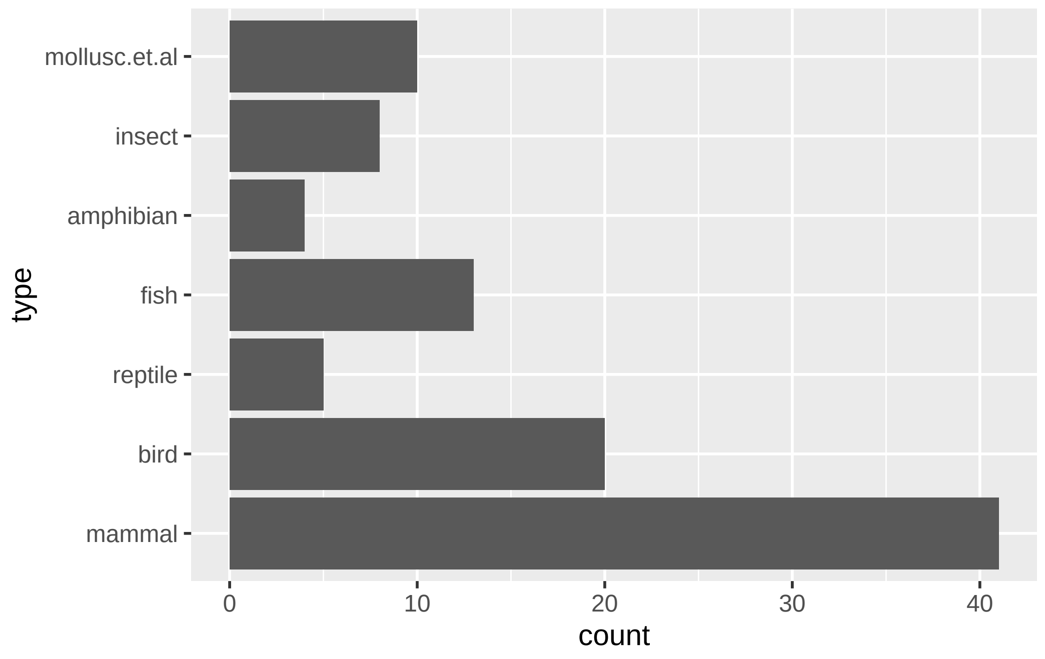
```r
rpart.plot(fit$finalModel, extra = 2)
```



1.8 Class Imbalance

```r
library(rpart)
library(rpart.plot)
data(Zoo, package="mlbench")
```

```r
#Class distribution

ggplot(Zoo, aes(y = type)) + geom_bar()
```



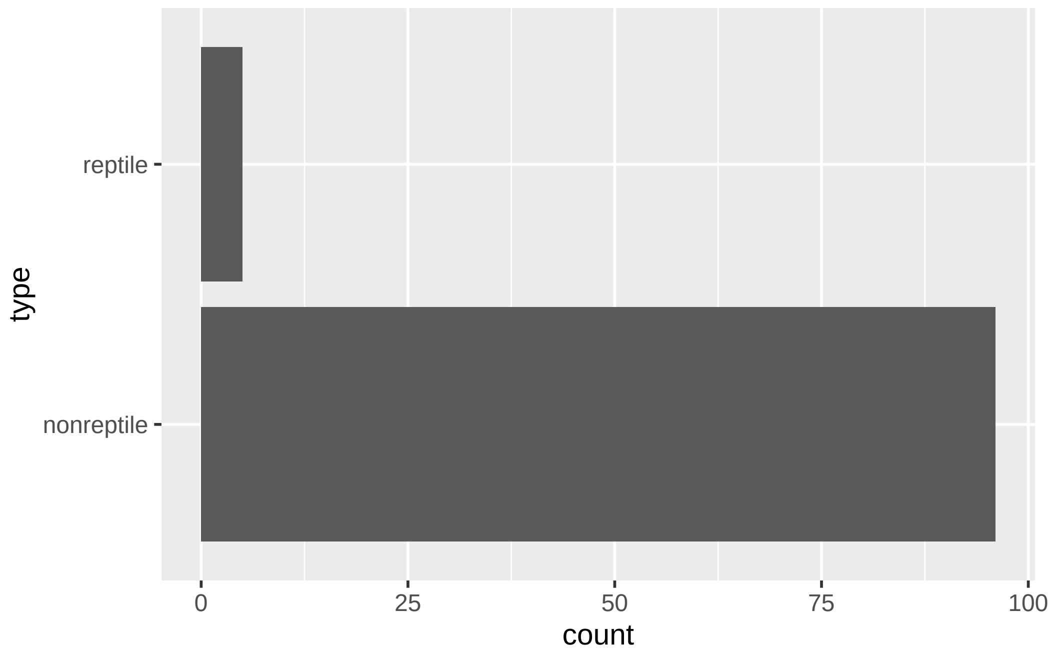
```
Zoo_reptile <- Zoo |>
  mutate(type = factor(Zoo$type == "reptile",
                       levels = c(FALSE, TRUE),
                       labels = c("nonreptile", "reptile")))
```

```
summary(Zoo_reptile)
```

```
    hair          feathers          eggs            milk
 Mode :logical   Mode :logical   Mode :logical   Mode :logical
 FALSE:58        FALSE:81        FALSE:42        FALSE:60
 TRUE :43        TRUE :20        TRUE :59        TRUE :41



  airborne        aquatic         predator        toothed
 Mode :logical   Mode :logical   Mode :logical   Mode :logical
 FALSE:77        FALSE:65        FALSE:45        FALSE:40
 TRUE :24        TRUE :36        TRUE :56        TRUE :61



  backbone        breathes        venomous          fins
```

```
Mode :logical   Mode :logical   Mode :logical   Mode :logical
FALSE:18        FALSE:21        FALSE:93        FALSE:84
TRUE :83        TRUE :80        TRUE :8         TRUE :17


     legs           tail          domestic         catsize
Min.   :0.000   Mode :logical   Mode :logical   Mode :logical
1st Qu.:2.000   FALSE:26        FALSE:88        FALSE:57
Median :4.000   TRUE :75        TRUE :13        TRUE :44
Mean   :2.842
3rd Qu.:4.000
Max.   :8.000
        type
nonreptile:96
reptile   : 5
```

```
ggplot(Zoo_reptile, aes(y = type)) + geom_bar()
```



```
set.seed(1234)

inTrain <- createDataPartition(y = Zoo_reptile$type, p = .5, list = FALSE)
training_reptile <- Zoo_reptile |> slice(inTrain)
testing_reptile <- Zoo_reptile |> slice(-inTrain)
```

1.8.1 Option 1: Use the Data As Is and Hope For The Best

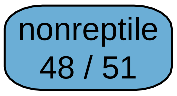
```
fit <- training_reptile |>
  train(type ~ .,
        data = _,
        method = "rpart",
        trControl = trainControl(method = "cv"))
```

```
Warning in nominalTrainWorkflow(x = x, y = y, wts = weights, info = trainInfo,
: There were missing values in resampled performance measures.
```

```
fit
```

```
CART

51 samples
16 predictors
 2 classes: 'nonreptile', 'reptile'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 46, 47, 46, 46, 45, 46, ...
Resampling results:

  Accuracy   Kappa
  0.9466667  0

Tuning parameter 'cp' was held constant at a value of 0
```

```
rpart.plot(fit$finalModel, extra = 2)
```



```r
confusionMatrix(data = predict(fit, testing_reptile),
                ref = testing_reptile$type, positive = "reptile")
```

```
Confusion Matrix and Statistics

            Reference
Prediction   nonreptile reptile
  nonreptile         48       2
  reptile             0       0

               Accuracy : 0.96
                 95% CI : (0.8629, 0.9951)
    No Information Rate : 0.96
    P-Value [Acc > NIR] : 0.6767

                  Kappa : 0

 Mcnemar's Test P-Value : 0.4795

            Sensitivity : 0.00
            Specificity : 1.00
         Pos Pred Value :  NaN
         Neg Pred Value : 0.96
             Prevalence : 0.04
         Detection Rate : 0.00
   Detection Prevalence : 0.00
      Balanced Accuracy : 0.50

       'Positive' Class : reptile
```

1.8.2 Option 2: Balance Data With Resampling

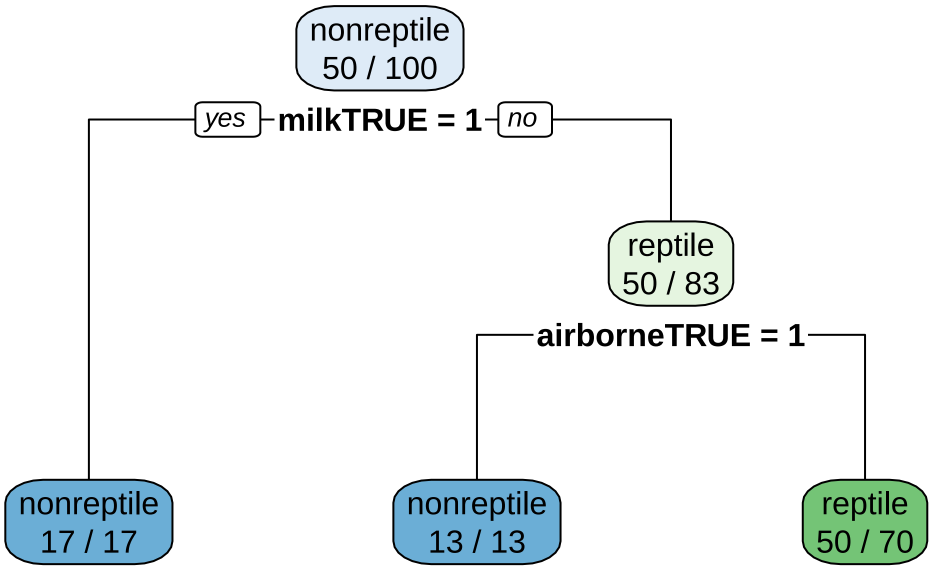
```r
library(sampling)
set.seed(1000) # for repeatability

id <- strata(training_reptile, stratanames = "type", size = c(50, 50), method = "srswr")
training_reptile_balanced <- training_reptile |>
  slice(id$ID_unit)
table(training_reptile_balanced$type)
```

```
nonreptile    reptile 
        50         50 
```

```r
fit <- training_reptile_balanced |>
  train(type ~ .,
        data = _,
        method = "rpart",
        trControl = trainControl(method = "cv"),
        control = rpart.control(minsplit = 5))

fit
```

```
CART 

100 samples
 16 predictor
  2 classes: 'nonreptile', 'reptile' 

No pre-processing
Resampling: Cross-Validated (10 fold) 
Summary of sample sizes: 90, 90, 90, 90, 90, 90, ... 
Resampling results across tuning parameters:

  cp    Accuracy  Kappa
  0.22  0.78      0.56 
  0.26  0.67      0.34 
  0.34  0.54      0.08 

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was cp = 0.22.
```

```r
rpart.plot(fit$finalModel, extra = 2)
```



```r
confusionMatrix(data = predict(fit, testing_reptile),
                ref = testing_reptile$type, positive = "reptile")
```

```
Confusion Matrix and Statistics

            Reference
Prediction   nonreptile reptile
  nonreptile         33       0
  reptile            15       2

               Accuracy : 0.7
                 95% CI : (0.5539, 0.8214)
    No Information Rate : 0.96
    P-Value [Acc > NIR] : 1.0000000

                  Kappa : 0.1497

 Mcnemar's Test P-Value : 0.0003006

            Sensitivity : 1.0000
            Specificity : 0.6875
         Pos Pred Value : 0.1176
         Neg Pred Value : 1.0000
             Prevalence : 0.0400
         Detection Rate : 0.0400
   Detection Prevalence : 0.3400
      Balanced Accuracy : 0.8438

       'Positive' Class : reptile
```

```
id <- strata(training_reptile, stratanames = "type", size = c(50, 100), method = "srswr")
training_reptile_balanced <- training_reptile |>
  slice(id$ID_unit)
table(training_reptile_balanced$type)
```

```
nonreptile    reptile
        50        100
```

```
fit <- training_reptile_balanced |>
  train(type ~ .,
        data = _,
        method = "rpart",
        trControl = trainControl(method = "cv"),
        control = rpart.control(minsplit = 5))

confusionMatrix(data = predict(fit, testing_reptile),
                ref = testing_reptile$type, positive = "reptile")
```

```
Confusion Matrix and Statistics

            Reference
Prediction   nonreptile reptile
  nonreptile         33       0
  reptile            15       2

               Accuracy : 0.7
                 95% CI : (0.5539, 0.8214)
    No Information Rate : 0.96
    P-Value [Acc > NIR] : 1.0000000

                  Kappa : 0.1497
```

```
 Mcnemar's Test P-Value : 0.0003006

            Sensitivity : 1.0000
            Specificity : 0.6875
         Pos Pred Value : 0.1176
         Neg Pred Value : 1.0000
             Prevalence : 0.0400
         Detection Rate : 0.0400
   Detection Prevalence : 0.3400
      Balanced Accuracy : 0.8438

       'Positive' Class : reptile
```

1.8.3 Option 3: Build A Larger Tree and use Predicted Probabilities

```
fit <- training_reptile |>
  train(type ~ .,
        data = _,
        method = "rpart",
        tuneLength = 10,
        trControl = trainControl(method = "cv",
        classProbs = TRUE,  ## necessary for predict with type="prob"
        summaryFunction=twoClassSummary),  ## necessary for ROC
        metric = "ROC",
        control = rpart.control(minsplit = 3))
```

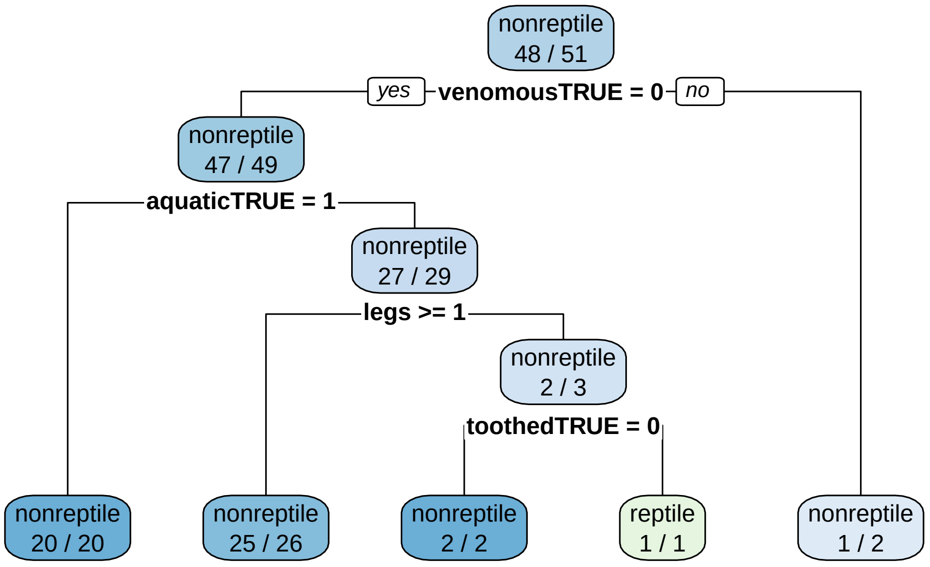
```
Warning in nominalTrainWorkflow(x = x, y = y, wts = weights, info = trainInfo,
: There were missing values in resampled performance measures.
```

```
fit
```

```
CART

51 samples
16 predictors
 2 classes: 'nonreptile', 'reptile'
```

```
No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 46, 47, 46, 46, 46, 45, ...
Resampling results:

  ROC        Sens   Spec
  0.3583333  0.975  0

Tuning parameter 'cp' was held constant at a value of 0
```

```
rpart.plot(fit$finalModel, extra = 2)
```



```
confusionMatrix(data = predict(fit, testing_reptile),
                ref = testing_reptile$type, positive = "reptile")
```

```
Confusion Matrix and Statistics

            Reference
Prediction   nonreptile reptile
  nonreptile         48       2
  reptile             0       0

               Accuracy : 0.96
                 95% CI : (0.8629, 0.9951)
```

```
    No Information Rate : 0.96
    P-Value [Acc > NIR] : 0.6767

                  Kappa : 0

 Mcnemar's Test P-Value : 0.4795

            Sensitivity : 0.00
            Specificity : 1.00
         Pos Pred Value :  NaN
         Neg Pred Value : 0.96
             Prevalence : 0.04
         Detection Rate : 0.00
   Detection Prevalence : 0.00
      Balanced Accuracy : 0.50

       'Positive' Class : reptile
```

```
prob <- predict(fit, testing_reptile, type = "prob")
tail(prob)
```

```
     nonreptile    reptile
tuna  1.0000000 0.00000000
vole  0.9615385 0.03846154
wasp  0.5000000 0.50000000
wolf  0.9615385 0.03846154
worm  1.0000000 0.00000000
wren  0.9615385 0.03846154
```

```
pred <- as.factor(ifelse(prob[,"reptile"]>=0.01, "reptile", "nonreptile"))

confusionMatrix(data = pred,
                ref = testing_reptile$type, positive = "reptile")
```

```
Confusion Matrix and Statistics

            Reference
Prediction   nonreptile reptile
  nonreptile         13       0
  reptile            35      2

               Accuracy : 0.3
                 95% CI : (0.1786, 0.4461)
    No Information Rate : 0.96
    P-Value [Acc > NIR] : 1

                  Kappa : 0.0289

 Mcnemar's Test P-Value : 9.081e-09

            Sensitivity : 1.00000
            Specificity : 0.27083
         Pos Pred Value : 0.05405
         Neg Pred Value : 1.00000
             Prevalence : 0.04000
         Detection Rate : 0.04000
   Detection Prevalence : 0.74000
      Balanced Accuracy : 0.63542

       'Positive' Class : reptile
```

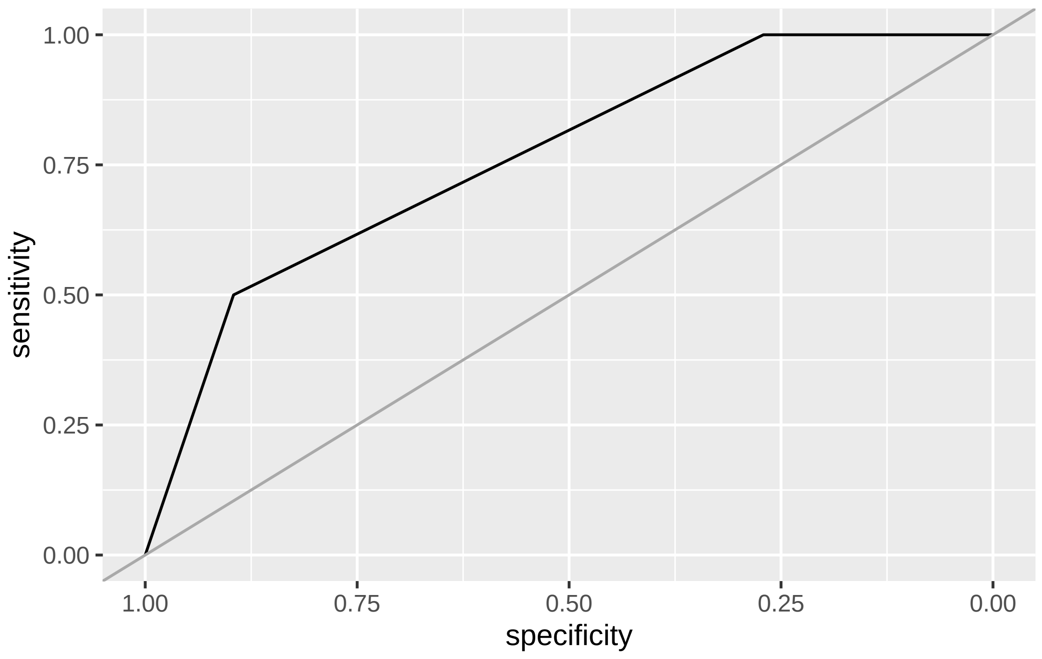
```r
library("pROC")
r <- roc(testing_reptile$type == "reptile", prob[,"reptile"])
```

```
Setting levels: control = FALSE, case = TRUE

Setting direction: controls < cases
```

```r
r
```

```
Call:
roc.default(response = testing_reptile$type == "reptile", predictor = prob[,     "reptile"])

Data: prob[, "reptile"] in 48 controls (testing_reptile$type == "reptile" FALSE) < 2 cases (
Area under the curve: 0.7656
```

```r
ggroc(r) + geom_abline(intercept = 1, slope = 1, color = "darkgrey")
```



1.8.4 Option 4: Use a Cost-Sensitive Classifier

```
cost <- matrix(c(
  0,   1,
  100, 0
), byrow = TRUE, nrow = 2)
cost
```

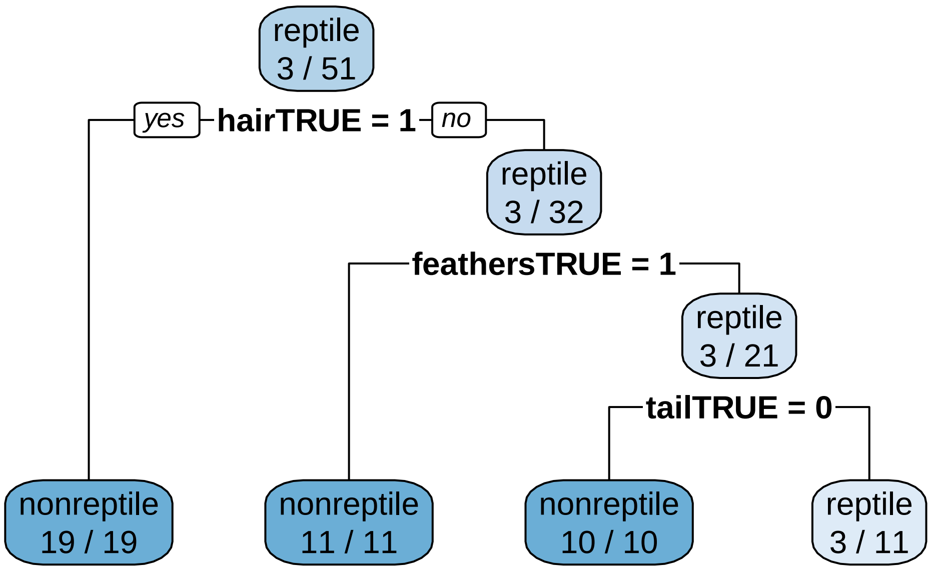
```
     [,1] [,2]
[1,]    0    1
[2,]  100    0
```

```
fit <- training_reptile |>
  train(type ~ .,
        data = _,
        method = "rpart",
        parms = list(loss = cost),
        trControl = trainControl(method = "cv"))
```

```
fit
```

```
CART

51 samples
16 predictors
 2 classes: 'nonreptile', 'reptile'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 46, 46, 46, 45, 46, 45, ...
Resampling results:

  Accuracy   Kappa
  0.4766667  -0.03038961

Tuning parameter 'cp' was held constant at a value of 0
```

```r
rpart.plot(fit$finalModel, extra = 2)
```



```r
confusionMatrix(data = predict(fit, testing_reptile),
                ref = testing_reptile$type, positive = "reptile")
```

```
Confusion Matrix and Statistics
```

```
            Reference
Prediction   nonreptile reptile
  nonreptile         39       0
  reptile             9       2

               Accuracy : 0.82
                 95% CI : (0.6856, 0.9142)
    No Information Rate : 0.96
    P-Value [Acc > NIR] : 0.999975

                  Kappa : 0.2574

 Mcnemar's Test P-Value : 0.007661

            Sensitivity : 1.0000
            Specificity : 0.8125
         Pos Pred Value : 0.1818
         Neg Pred Value : 1.0000
             Prevalence : 0.0400
         Detection Rate : 0.0400
   Detection Prevalence : 0.2200
      Balanced Accuracy : 0.9062

       'Positive' Class : reptile
```

2 Classification: Alternative Techniques

2.1 Install packages

```
if(!require(pacman))
  install.packages("pacman")

pacman::p_load(
  C50,                # C5.0 Decision Trees and Rule-Based Models
  caret,              # Classification and Regression Training
  e1071,              # Misc Functions of the Department of Statistics (e1071), TU Wien
  keras,              # R Interface to 'Keras'
  kernlab,            # Kernel-Based Machine Learning Lab
  lattice,            # Trellis Graphics for R
  MASS,                # Support Functions and Datasets for Venables and Ripley's MASS
  mlbench,             # Machine Learning Benchmark Problems
  nnet,                # Feedforward Neural Networks and Multinomial Log-Linear Models
  palmerpenguins,      # Palmer Archipelago (Antarctica) Penguin Data
  party,               # A Laboratory for Recursive Partytioning
  partykit,            # A Toolkit for Recursive Partytioning
  randomForest,        # Breiman and Cutler's Random Forests for Classification and Regress
  rpart,               # Recursive partitioning models
  RWeka,               # R/Weka Interface
  scales,              # Scale Functions for Visualization
  tidymodels,          # Tidy machine learning framework
  tidyverse,           # Tidy data wrangling and visualization
  xgboost              # Extreme Gradient Boosting
)
```

```
options(digits=3)
```

2.2 Training and Test Data

```
data(Zoo, package="mlbench")
Zoo <- as.data.frame(Zoo)
Zoo |> glimpse()
```

```
Rows: 101
Columns: 17
$ hair     <lgl> TRUE, TRUE, FALSE, TRUE, TRUE, TRUE, TRUE, FALSE, FALSE, TRUE~
$ feathers <lgl> FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE~
$ eggs     <lgl> FALSE, FALSE, TRUE, FALSE, FALSE, FALSE, FALSE, TRUE, TRUE, F~
$ milk     <lgl> TRUE, TRUE, FALSE, TRUE, TRUE, TRUE, TRUE, FALSE, FALSE, TRUE~
$ airborne <lgl> FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE~
$ aquatic  <lgl> FALSE, FALSE, TRUE, FALSE, FALSE, FALSE, FALSE, TRUE, TRUE, F~
$ predator <lgl> TRUE, FALSE, TRUE, TRUE, TRUE, FALSE, FALSE, FALSE, TRUE, FAL~
$ toothed  <lgl> TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, T~
$ backbone <lgl> TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, T~
$ breathes <lgl> TRUE, TRUE, FALSE, TRUE, TRUE, TRUE, TRUE, FALSE, FALSE, TRUE~
$ venomous <lgl> FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE~
$ fins     <lgl> FALSE, FALSE, TRUE, FALSE, FALSE, FALSE, FALSE, TRUE, TRUE, F~
$ legs     <int> 4, 4, 0, 4, 4, 4, 4, 0, 0, 4, 4, 2, 0, 0, 4, 6, 2, 4, 0, 0, 2~
$ tail     <lgl> FALSE, TRUE, TRUE, FALSE, TRUE, TRUE, TRUE, TRUE, TRUE, FALSE~
$ domestic <lgl> FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, TRUE, TRUE, FALSE, ~
$ catsize  <lgl> TRUE, TRUE, FALSE, TRUE, TRUE, TRUE, TRUE, FALSE, FALSE, FALS~
$ type     <fct> mammal, mammal, fish, mammal, mammal, mammal, mammal, fish, f~
```

```
set.seed(123)  # for reproducibility
inTrain <- createDataPartition(y = Zoo$type, p = .8)[[1]]
Zoo_train <- dplyr::slice(Zoo, inTrain)
Zoo_test <- dplyr::slice(Zoo, -inTrain)
```

2.3 Fitting Different Classification Models to the Training Data

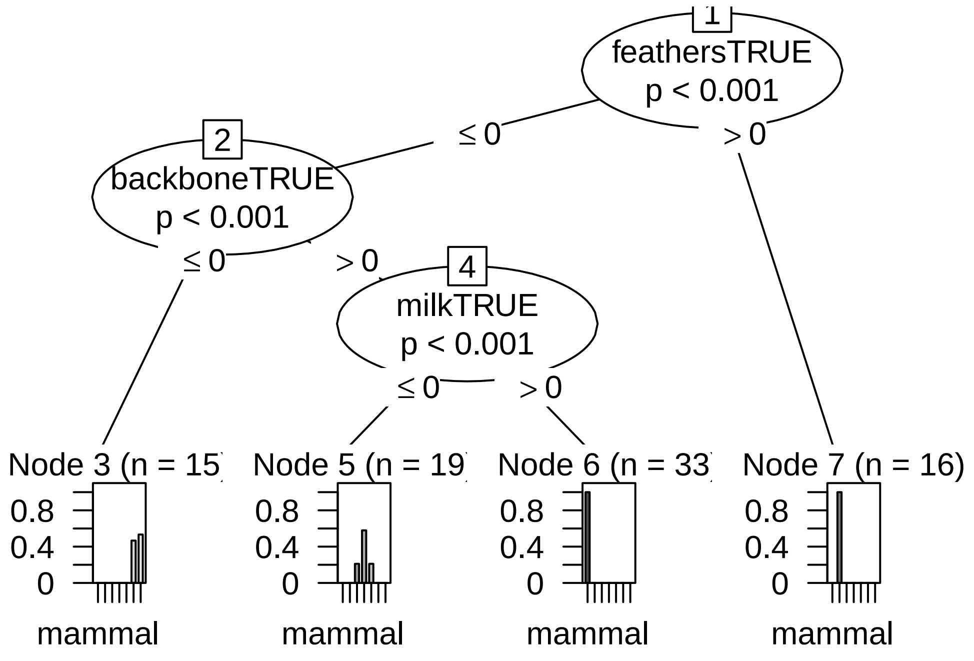
```
train_index <- createFolds(Zoo_train$type, k = 10)
```

2.3.1 Conditional Inference Tree (Decision Tree)

```
ctreeFit <- Zoo_train |> train(type ~ .,
  method = "ctree",
  data = _,
    tuneLength = 5,
    trControl = trainControl(method = "cv", indexOut = train_index))
ctreeFit
```

```
Conditional Inference Tree

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 76, 72, 73, 76, 75, 75, ...
Resampling results across tuning parameters:

  mincriterion  Accuracy  Kappa
  0.010         0.827     0.772
  0.255         0.827     0.772
  0.500         0.827     0.772
  0.745         0.827     0.772
  0.990         0.827     0.772

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was mincriterion = 0.99.
```

```
plot(ctreeFit$finalModel)
```



2.3.2 C 4.5 Decision Tree

```
C45Fit <- Zoo_train |> train(type ~ .,
  method = "J48",
  data = _,
    tuneLength = 5,
    trControl = trainControl(method = "cv", indexOut = train_index))
C45Fit
```

```
C4.5-like Trees

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'
```

```
No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 76, 75, 73, 76, 74, 74, ...
Resampling results across tuning parameters:

  C      M  Accuracy  Kappa
  0.010  1  0.975     0.967
  0.010  2  0.965     0.954
  0.010  3  0.953     0.940
  0.010  4  0.959     0.948
  0.010  5  0.970     0.962
  0.133  1  1.000     1.000
  0.133  2  0.976     0.968
  0.133  3  0.965     0.954
  0.133  4  0.959     0.948
  0.133  5  0.970     0.962
  0.255  1  1.000     1.000
  0.255  2  0.976     0.968
  0.255  3  0.965     0.954
  0.255  4  0.959     0.948
  0.255  5  0.970     0.962
  0.378  1  1.000     1.000
  0.378  2  0.976     0.968
  0.378  3  0.965     0.954
  0.378  4  0.959     0.948
  0.378  5  0.970     0.962
  0.500  1  1.000     1.000
  0.500  2  0.976     0.968
  0.500  3  0.965     0.954
  0.500  4  0.959     0.948
  0.500  5  0.970     0.962

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were C = 0.133 and M = 1.
```

```r
C45Fit$finalModel
```

```
J48 pruned tree
------------------

feathersTRUE <= 0
```

```
|   milkTRUE <= 0
|   |   backboneTRUE <= 0
|   |   |   predatorTRUE <= 0
|   |   |   |   legs <= 2: mollusc.et.al (1.0)
|   |   |   |   legs > 2: insect (6.0)
|   |   |   predatorTRUE > 0: mollusc.et.al (8.0/1.0)
|   |   backboneTRUE > 0
|   |   |   finsTRUE <= 0
|   |   |   |   aquaticTRUE <= 0: reptile (3.0)
|   |   |   |   aquaticTRUE > 0
|   |   |   |   |   eggsTRUE <= 0: reptile (1.0)
|   |   |   |   |   eggsTRUE > 0: amphibian (4.0)
|   |   |   finsTRUE > 0: fish (11.0)
|   milkTRUE > 0: mammal (33.0)
feathersTRUE > 0: bird (16.0)

Number of Leaves  :     9

Size of the tree :  17
```

2.3.3 K-Nearest Neighbors

```
knnFit <- Zoo_train |> train(type ~ .,
  method = "knn",
  data = _,
  preProcess = "scale",
    tuneLength = 5,
  tuneGrid=data.frame(k = 1:10),
    trControl = trainControl(method = "cv", indexOut = train_index))
knnFit
```

```
k-Nearest Neighbors

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'

Pre-processing: scaled (16)
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 77, 74, 75, 75, 74, 74, ...
Resampling results across tuning parameters:
  k   Accuracy  Kappa
   1  1.000     1.000
   2  0.965     0.954
   3  0.963     0.951
   4  0.942     0.925
   5  0.941     0.921
   6  0.963     0.951
   7  0.963     0.951
   8  0.941     0.921
   9  0.908     0.883
  10  0.918     0.892

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was k = 1.
```

```
knnFit$finalModel
```

```
1-nearest neighbor model
Training set outcome distribution:

       mammal           bird        reptile           fish      amphibian
           33             16              4             11              4
       insect mollusc.et.al
            7              8
```

2.3.4 PART (Rule-based classifier)

```
rulesFit <- Zoo_train |> train(type ~ .,
  method = "PART",
  data = _,
  tuneLength = 5,
  trControl = trainControl(method = "cv", indexOut = train_index))
rulesFit
```

```
Rule-Based Classifier

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'
```

```
No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 73, 74, 76, 76, 75, 74, ...
Resampling results across tuning parameters:

  threshold  pruned  Accuracy  Kappa
  0.010      yes     0.979     0.973
  0.010      no      0.979     0.973
  0.133      yes     0.990     0.987
  0.133      no      0.979     0.973
  0.255      yes     0.990     0.987
  0.255      no      0.979     0.973
  0.378      yes     0.990     0.987
  0.378      no      0.979     0.973
  0.500      yes     0.990     0.987
  0.500      no      0.979     0.973

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were threshold = 0.5 and pruned = yes.
```

```
rulesFit$finalModel
```

```
PART decision list
------------------

feathersTRUE <= 0 AND
milkTRUE > 0: mammal (33.0)

feathersTRUE > 0: bird (16.0)

backboneTRUE <= 0 AND
airborneTRUE <= 0 AND
predatorTRUE > 0: mollusc.et.al (7.0)

backboneTRUE > 0 AND
finsTRUE > 0: fish (11.0)

backboneTRUE <= 0: insect (8.0/1.0)

aquaticTRUE > 0: amphibian (5.0/1.0)
```

```
: reptile (3.0)

Number of Rules  :  7
```

2.3.5 Linear Support Vector Machines

```r
svmFit <- Zoo_train |> train(type ~.,
  method = "svmLinear",
  data = _,
    tuneLength = 5,
    trControl = trainControl(method = "cv", indexOut = train_index))
svmFit
```

```
Support Vector Machines with Linear Kernel

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 74, 74, 77, 75, 74, 77, ...
Resampling results:

  Accuracy  Kappa
  1         1

Tuning parameter 'C' was held constant at a value of 1
```

```r
svmFit$finalModel
```

```
Support Vector Machine object of class "ksvm"

SV type: C-svc  (classification)
 parameter : cost C = 1

Linear (vanilla) kernel function.
```

```
Number of Support Vectors : 39

Objective Function Value : -0.143 -0.217 -0.15 -0.175 -0.0934 -0.0974 -0.292 -0.0835 -0.154 
Training error : 0
```

2.3.6 Random Forest

```r
randomForestFit <- Zoo_train |> train(type ~ .,
  method = "rf",
  data = _,
    tuneLength = 5,
    trControl = trainControl(method = "cv", indexOut = train_index))
randomForestFit
```

```
Random Forest

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 75, 76, 75, 76, 74, 73, ...
Resampling results across tuning parameters:

  mtry  Accuracy  Kappa
   2    1         1
   5    1         1
   9    1         1
  12    1         1
  16    1         1

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was mtry = 2.
```

```r
randomForestFit$finalModel
```

```
Call:
 randomForest(x = x, y = y, mtry = param$mtry)
               Type of random forest: classification
```

```
                     Number of trees: 500
No. of variables tried at each split: 2

        OOB estimate of  error rate: 7.23%
Confusion matrix:
              mammal bird reptile fish amphibian insect mollusc.et.al
mammal            33    0       0    0         0      0             0
bird               0   16       0    0         0      0             0
reptile            0    1       0    2         1      0             0
fish               0    0       0   11         0      0             0
amphibian          0    0       0    0         4      0             0
insect             0    0       0    0         0      7             0
mollusc.et.al      1    0       0    0         0      1             6
              class.error
mammal               0.00
bird                 0.00
reptile              1.00
fish                 0.00
amphibian            0.00
insect               0.00
mollusc.et.al        0.25
```

2.3.7 Gradient Boosted Decision Trees (xgboost)

```
xgboostFit <- Zoo_train |> train(type ~ .,
  method = "xgbTree",
  data = _,
  tuneLength = 5,
  trControl = trainControl(method = "cv", indexOut = train_index),
  tuneGrid = expand.grid(
    nrounds = 20,
    max_depth = 3,
    colsample_bytree = .6,
    eta = 0.1,
    gamma=0,
    min_child_weight = 1,
    subsample = .5
  ))
xgboostFit
```

```
eXtreme Gradient Boosting
```

```
83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 77, 73, 74, 75, 75, 75, ...
Resampling results:

  Accuracy  Kappa
  0.973     0.964

Tuning parameter 'nrounds' was held constant at a value of 20
Tuning
 held constant at a value of 1
Tuning parameter 'subsample' was held
 constant at a value of 0.5
```

```
xgboostFit$finalModel
```

```
##### xgb.Booster
raw: 112.4 Kb
call:
  xgboost::xgb.train(params = list(eta = param$eta, max_depth = param$max_depth,
    gamma = param$gamma, colsample_bytree = param$colsample_bytree,
    min_child_weight = param$min_child_weight, subsample = param$subsample),
    data = x, nrounds = param$nrounds, num_class = length(lev),
    objective = "multi:softprob")
params (as set within xgb.train):
  eta = "0.1", max_depth = "3", gamma = "0", colsample_bytree = "0.6", min_child_weight = "1
xgb.attributes:
  niter
callbacks:
  cb.print.evaluation(period = print_every_n)
# of features: 16
niter: 20
nfeatures : 16
xNames : hairTRUE feathersTRUE eggsTRUE milkTRUE airborneTRUE aquaticTRUE predatorTRUE toothe
problemType : Classification
tuneValue :
      nrounds max_depth eta gamma colsample_bytree min_child_weight subsample
1      20         3 0.1     0                0.6                1       0.5
obsLevels : mammal bird reptile fish amphibian insect mollusc.et.al
param :
    list()
```

2.3.8 Artificial Neural Network

```
nnetFit <- Zoo_train |> train(type ~ .,
  method = "nnet",
  data = _,
    tuneLength = 5,
    trControl = trainControl(method = "cv", indexOut = train_index),
  trace = FALSE)
nnetFit
```

```
Neural Network

83 samples
16 predictors
 7 classes: 'mammal', 'bird', 'reptile', 'fish', 'amphibian', 'insect', 'mollusc.et.al'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 75, 74, 74, 74, 74, 75, ...
Resampling results across tuning parameters:

  size  decay  Accuracy  Kappa
  1     0e+00  0.776     0.681
  1     1e-04  0.789     0.709
  1     1e-03  0.911     0.882
  1     1e-02  0.832     0.781
  1     1e-01  0.722     0.621
  3     0e+00  0.963     0.950
  3     1e-04  0.976     0.968
  3     1e-03  0.986     0.979
  3     1e-02  0.986     0.981
  3     1e-01  0.976     0.968
  5     0e+00  0.965     0.953
  5     1e-04  0.986     0.981
  5     1e-03  0.986     0.981
  5     1e-02  0.986     0.981
  5     1e-01  0.986     0.981
  7     0e+00  0.976     0.968
  7     1e-04  0.986     0.981
  7     1e-03  0.986     0.981
  7     1e-02  0.986     0.981
  7     1e-01  0.986     0.981
  9     0e+00  0.986     0.981
  9     1e-04  0.986     0.981
  9     1e-03  0.986     0.981
  9     1e-02  0.986     0.981
  9     1e-01  0.986     0.981

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were size = 3 and decay = 0.01.
```

```
nnetFit$finalModel
```

```
a 16-3-7 network with 79 weights
inputs: hairTRUE feathersTRUE eggsTRUE milkTRUE airborneTRUE aquaticTRUE predatorTRUE toothe
output(s): .outcome
options were - softmax modelling  decay=0.01
```

2.4 Comparing Models

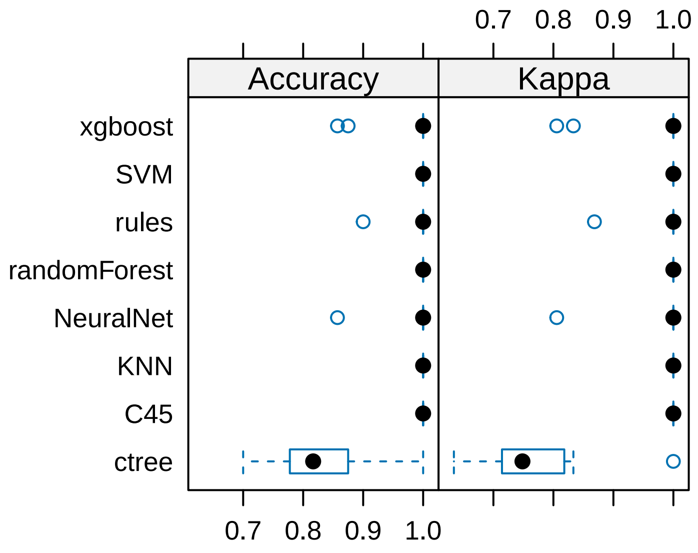
```
resamps <- resamples(list(
  ctree = ctreeFit,
  C45 = C45Fit,
  SVM = svmFit,
  KNN = knnFit,
  rules = rulesFit,
  randomForest = randomForestFit,
  xgboost = xgboostFit,
  NeuralNet = nnetFit
    ))
resamps
```

```
Call:
resamples.default(x = list(ctree = ctreeFit, C45 = C45Fit, SVM = svmFit, KNN
 = knnFit, rules = rulesFit, randomForest = randomForestFit, xgboost
 = xgboostFit, NeuralNet = nnetFit))

Models: ctree, C45, SVM, KNN, rules, randomForest, xgboost, NeuralNet
Number of resamples: 10
Performance metrics: Accuracy, Kappa
Time estimates for: everything, final model fit
```

```r
summary(resamps)
```

```

Call:
summary.resamples(object = resamps)

Models: ctree, C45, SVM, KNN, rules, randomForest, xgboost, NeuralNet
Number of resamples: 10

Accuracy
              Min. 1st Qu. Median  Mean 3rd Qu. Max. NA's
ctree        0.700   0.778  0.817 0.827   0.871    1    0
C45          1.000   1.000  1.000 1.000   1.000    1    0
SVM          1.000   1.000  1.000 1.000   1.000    1    0
KNN          1.000   1.000  1.000 1.000   1.000    1    0
rules        0.900   1.000  1.000 0.990   1.000    1    0
randomForest 1.000   1.000  1.000 1.000   1.000    1    0
xgboost      0.857   1.000  1.000 0.973   1.000    1    0
NeuralNet    0.857   1.000  1.000 0.986   1.000    1    0

Kappa
              Min. 1st Qu. Median  Mean 3rd Qu. Max. NA's
ctree        0.634   0.715  0.748 0.772   0.815    1    0
C45          1.000   1.000  1.000 1.000   1.000    1    0
SVM          1.000   1.000  1.000 1.000   1.000    1    0
KNN          1.000   1.000  1.000 1.000   1.000    1    0
rules        0.868   1.000  1.000 0.987   1.000    1    0
randomForest 1.000   1.000  1.000 1.000   1.000    1    0
xgboost      0.806   1.000  1.000 0.964   1.000    1    0
NeuralNet    0.806   1.000  1.000 0.981   1.000    1    0
```

```r
library(lattice)
bwplot(resamps, layout = c(3, 1))
```



```r
difs <- diff(resamps)
difs
```

```

Call:
diff.resamples(x = resamps)

Models: ctree, C45, SVM, KNN, rules, randomForest, xgboost, NeuralNet
Metrics: Accuracy, Kappa
Number of differences: 28
p-value adjustment: bonferroni
```

```r
summary(difs)
```

```

Call:
summary.diff.resamples(object = difs)

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

Accuracy
             ctree    C45      SVM      KNN      rules    randomForest xgboost
ctree                 -0.17262 -0.17262 -0.17262 -0.16262 -0.17262     -0.14583
C45          0.00193           0.00000  0.00000  0.01000  0.00000       0.02679
```

```
SVM          0.00193 NA                0.00000  0.01000  0.00000      0.02679
KNN          0.00193 NA       NA                0.01000  0.00000      0.02679
rules        0.00376 1.00000  1.00000  1.00000          -0.01000      0.01679
randomForest 0.00193 NA       NA       NA       1.00000               0.02679
xgboost      0.05129 1.00000  1.00000  1.00000  1.00000  1.00000
NeuralNet    0.01405 1.00000  1.00000  1.00000  1.00000  1.00000      1.00000
             NeuralNet
ctree        -0.15833
C45           0.01429
SVM           0.01429
KNN           0.01429
rules         0.00429
randomForest  0.01429
xgboost      -0.01250
NeuralNet

Kappa
             ctree   C45      SVM      KNN      rules    randomForest xgboost
ctree                -0.22840 -0.22840 -0.22840 -0.21524 -0.22840     -0.19229
C45          0.00116           0.00000  0.00000  0.01316  0.00000      0.03611
SVM          0.00116 NA                 0.00000  0.01316  0.00000      0.03611
KNN          0.00116 NA       NA                 0.01316  0.00000      0.03611
rules        0.00238 1.00000  1.00000  1.00000          -0.01316      0.02295
randomForest 0.00116 NA       NA       NA       1.00000               0.03611
xgboost      0.04216 1.00000  1.00000  1.00000  1.00000  1.00000
NeuralNet    0.01055 1.00000  1.00000  1.00000  1.00000  1.00000      1.00000
             NeuralNet
ctree        -0.20895
C45           0.01944
SVM           0.01944
KNN           0.01944
rules         0.00629
randomForest  0.01944
xgboost      -0.01667
NeuralNet
```

2.5 Applying the Chosen Model to the Test Data

```r
pr <- predict(randomForestFit, Zoo_test)
pr
```

```
 [1] mammal        mammal        mammal        fish          fish         
 [6] bird          bird          mammal        mammal        mammal       
[11] mammal        mollusc.et.al reptile       mammal        bird         
[16] mollusc.et.al bird          insect       
Levels: mammal bird reptile fish amphibian insect mollusc.et.al
```

```r
confusionMatrix(pr, reference = Zoo_test$type)
```

```
Confusion Matrix and Statistics

               Reference
Prediction       mammal bird reptile fish amphibian insect mollusc.et.al
  mammal              8    0       0    0         0      0             0
  bird                0    4       0    0         0      0             0
  reptile             0    0       1    0         0      0             0
  fish                0    0       0    2         0      0             0
  amphibian           0    0       0    0         0      0             0
  insect              0    0       0    0         0      1             0
  mollusc.et.al       0    0       0    0         0      0             2

Overall Statistics
                                     
               Accuracy : 1          
                 95% CI : (0.815, 1)
    No Information Rate : 0.444      
    P-Value [Acc > NIR] : 4.58e-07   
                                     
                  Kappa : 1          
                                     
 Mcnemar's Test P-Value : NA         

Statistics by Class:

                     Class: mammal Class: bird Class: reptile Class: fish
Sensitivity                  1.000       1.000         1.0000       1.000
```

```
Specificity                 1.000       1.000         1.0000        1.000
Pos Pred Value              1.000       1.000         1.0000        1.000
Neg Pred Value              1.000       1.000         1.0000        1.000
Prevalence                  0.444       0.222         0.0556        0.111
Detection Rate              0.444       0.222         0.0556        0.111
Detection Prevalence        0.444       0.222         0.0556        0.111
Balanced Accuracy           1.000       1.000         1.0000        1.000
                     Class: amphibian Class: insect Class: mollusc.et.al
Sensitivity                        NA        1.0000                1.000
Specificity                         1        1.0000                1.000
Pos Pred Value                     NA        1.0000                1.000
Neg Pred Value                     NA        1.0000                1.000
Prevalence                          0        0.0556                0.111
Detection Rate                      0        0.0556                0.111
Detection Prevalence                0        0.0556                0.111
Balanced Accuracy                  NA        1.0000                1.000
```

2.6 Comparing Decision Boundaries of Popular Classification Techniques

```r
library(scales)
library(tidyverse)
library(ggplot2)
library(caret)

decisionplot <- function(model, data, class_var,
  predict_type = c("class", "prob"), resolution = 3 * 72) {
  # resolution is set to 72 dpi if the image is rendered  3 inches wide.

  y <- data |> pull(class_var)
  x <- data |> dplyr::select(-all_of(class_var))

  # resubstitution accuracy
  prediction <- predict(model, x, type = predict_type[1])
  # LDA returns a list
  if(is.list(prediction)) prediction <- prediction$class
  prediction <- factor(prediction, levels = levels(y))

  cm <- confusionMatrix(data = prediction,
                        reference = y)
  acc <- cm$overall["Accuracy"]
```

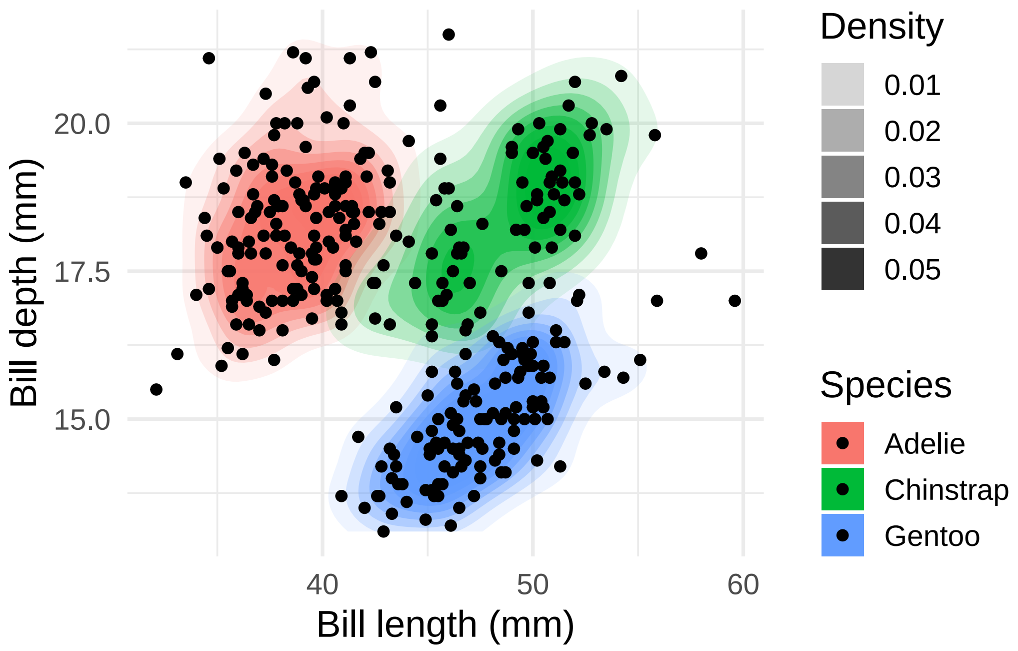
```r
# evaluate model on a grid
r <- sapply(x[, 1:2], range, na.rm = TRUE)
xs <- seq(r[1,1], r[2,1], length.out = resolution)
ys <- seq(r[1,2], r[2,2], length.out = resolution)
g <- cbind(rep(xs, each = resolution), rep(ys, time = resolution))
colnames(g) <- colnames(r)
g <- as_tibble(g)

### guess how to get class labels from predict
### (unfortunately not very consistent between models)
cl <- predict(model, g, type = predict_type[1])

# LDA returns a list
prob <- NULL
if(is.list(cl)) {
  prob <- cl$posterior
  cl <- cl$class
} else
  if(!is.na(predict_type[2]))
    try(prob <- predict(model, g, type = predict_type[2]))

# we visualize the difference in probability/score between the
# winning class and the second best class.
# don't use probability if predict for the classifier does not support it.
max_prob <- 1
if(!is.null(prob))
  try({
    max_prob <- t(apply(prob, MARGIN = 1, sort, decreasing = TRUE))
    max_prob <- max_prob[,1] - max_prob[,2]
  }, silent = TRUE)

cl <- factor(cl, levels = levels(y))

g <- g |> add_column(prediction = cl, probability = max_prob)

ggplot(g, mapping = aes(
  x = .data[[colnames(g)[1]]], y = .data[[colnames(g)[2]]])) +
  geom_raster(mapping = aes(fill = prediction, alpha = probability)) +
  geom_contour(mapping = aes(z = as.numeric(prediction)),
    bins = length(levels(cl)), linewidth = .5, color = "black") +
  geom_point(data = data, mapping =  aes(
        x = .data[[colnames(data)[1]]],
        y = .data[[colnames(data)[2]]],
        shape = .data[[class_var]]), alpha = .7) +
      scale_alpha_continuous(range = c(0,1), limits = c(0,1), guide = "none") +
      labs(subtitle = paste("Training accuracy:", round(acc, 2))) +
       theme_minimal(base_size = 14)
}
```

2.6.1 Penguins Dataset

```
set.seed(1000)
data("penguins")
penguins <- as_tibble(penguins) |>
  drop_na()

### Three classes
### (note: MASS also has a select function which hides dplyr's select)
x <- penguins |> dplyr::select(bill_length_mm, bill_depth_mm, species)
x
```

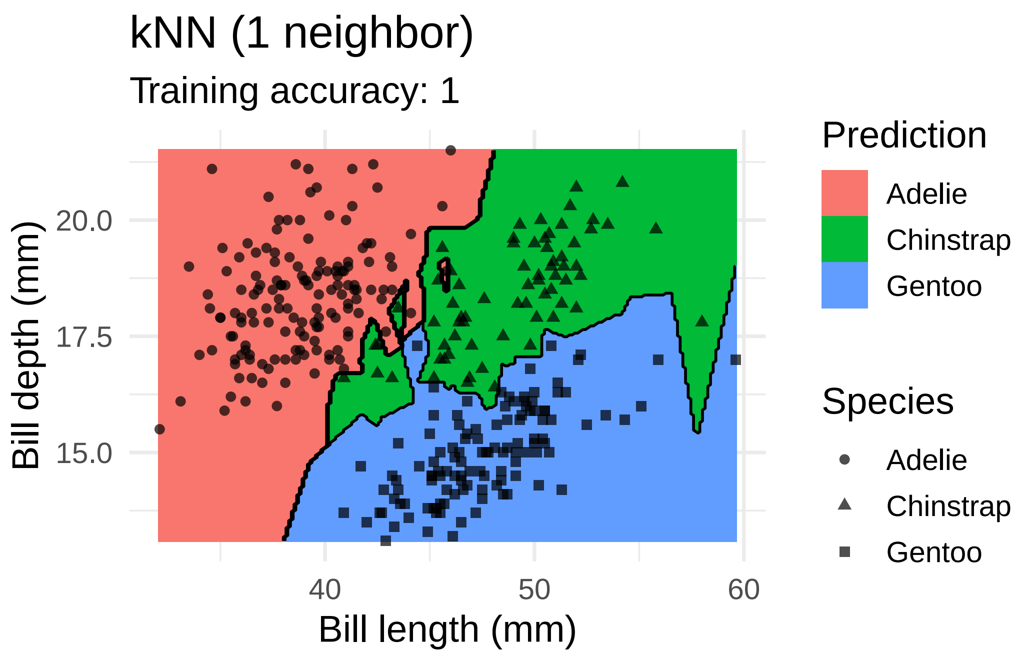
```
# A tibble: 333 x 3
   bill_length_mm bill_depth_mm species
            <dbl>         <dbl> <fct>  
 1           39.1          18.7 Adelie 
 2           39.5          17.4 Adelie 
 3           40.3          18   Adelie 
 4           36.7          19.3 Adelie 
 5           39.3          20.6 Adelie 
 6           38.9          17.8 Adelie 
 7           39.2          19.6 Adelie 
 8           41.1          17.6 Adelie 
 9           38.6          21.2 Adelie 
10           34.6          21.1 Adelie 
# i 323 more rows
```

```
ggplot(x, aes(x = bill_length_mm, y = bill_depth_mm, fill = species)) +
  stat_density_2d(geom = "polygon", aes(alpha = after_stat(level))) +
  geom_point() +
  theme_minimal(base_size = 14) +
  labs(x = "Bill length (mm)",
       y = "Bill depth (mm)",
       fill = "Species",
       alpha = "Density")
```

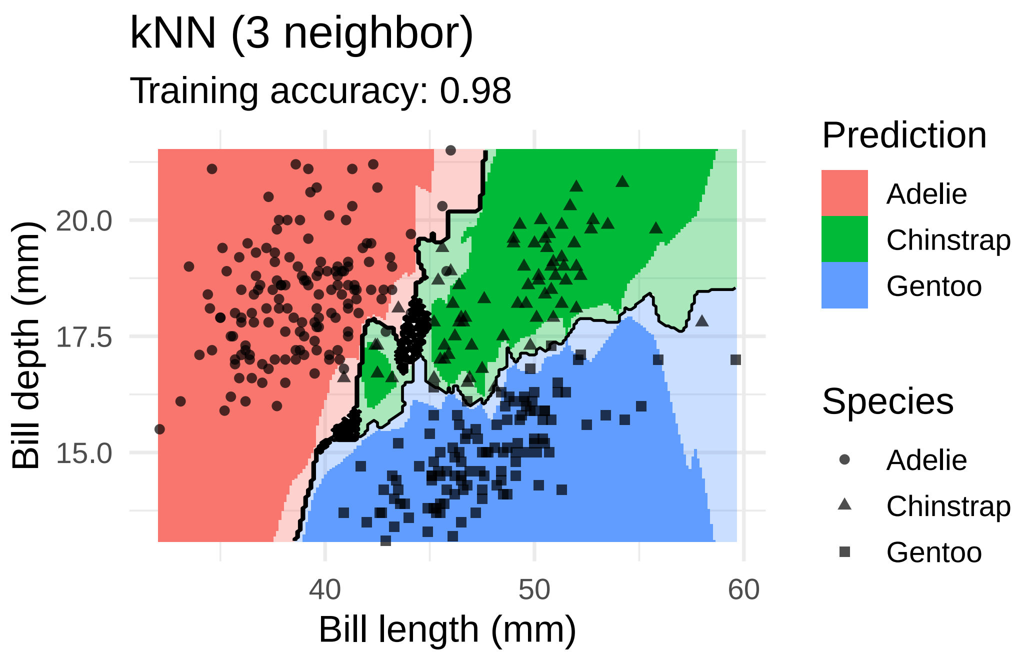


2.6.1.1 K-Nearest Neighbors Classifier

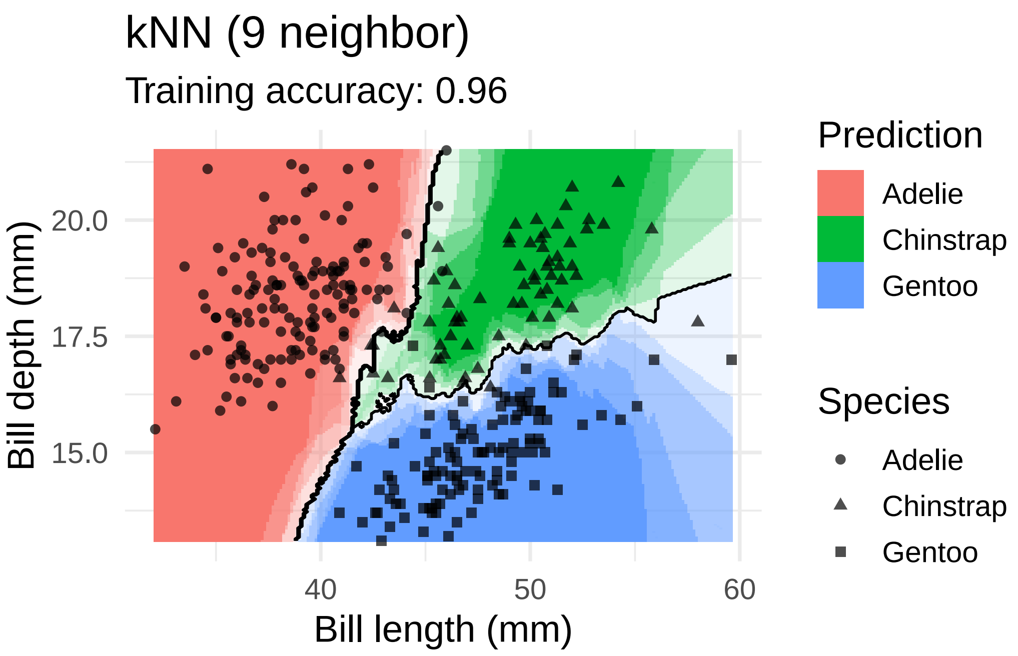
```
model <- x |> caret::knn3(species ~ ., data = _, k = 1)
decisionplot(model, x, class_var = "species") +
  labs(title = "kNN (1 neighbor)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



```r
model <- x |> caret::knn3(species ~ ., data = _, k = 3)
decisionplot(model, x, class_var = "species") +
  labs(title = "kNN (3 neighbor)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

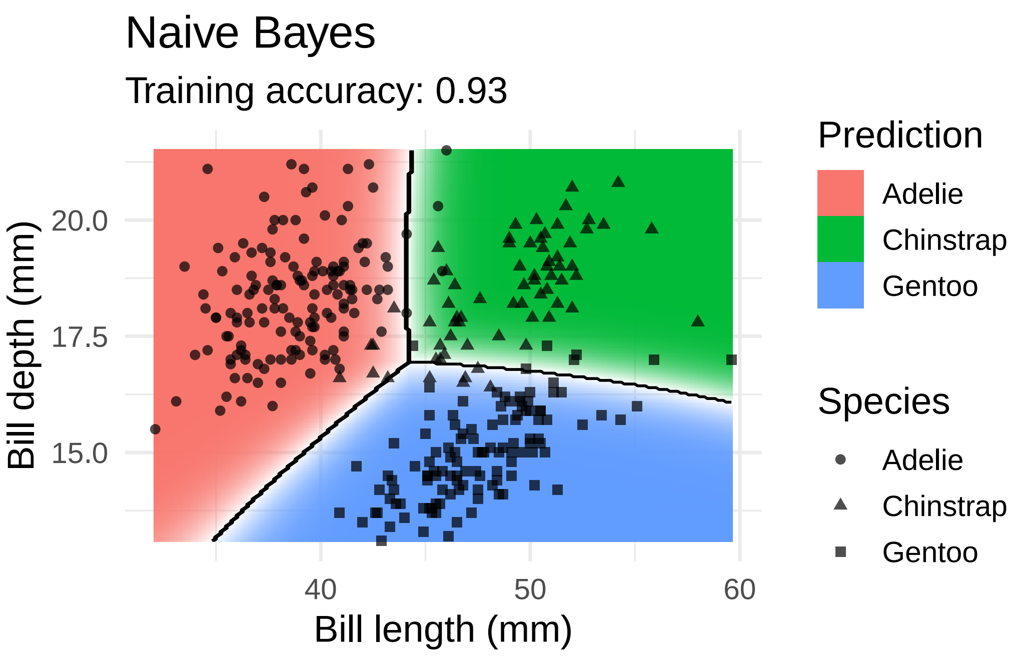


```
model <- x |> caret::knn3(species ~ ., data = _, k = 9)
decisionplot(model, x, class_var = "species") +
  labs(title = "kNN (9 neighbor)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



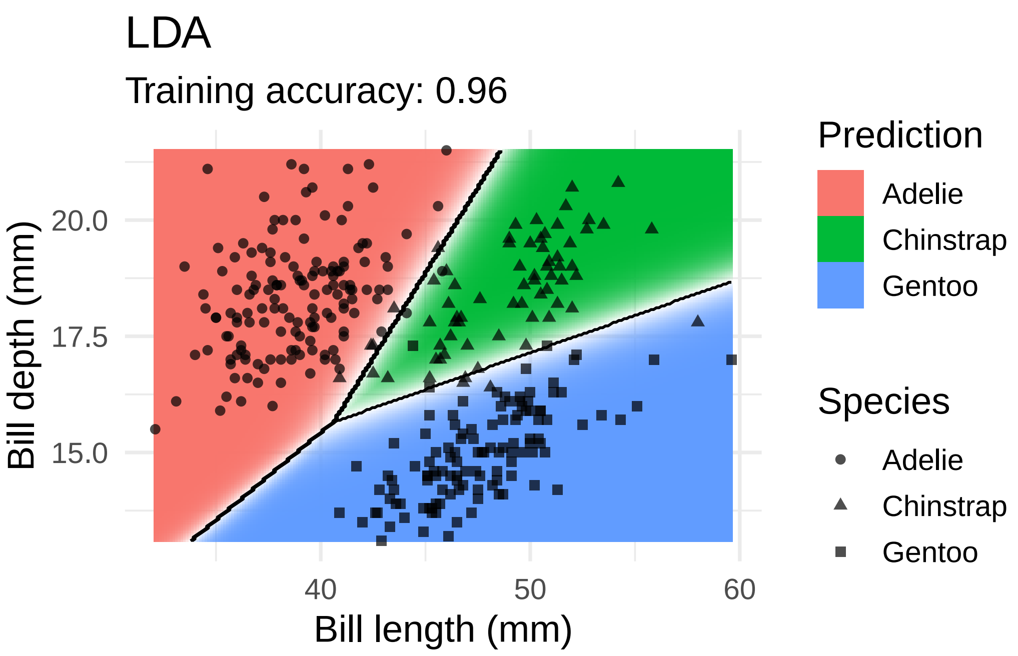
2.6.1.2 Naive Bayes Classifier

```
model <- x |> e1071::naiveBayes(species ~ ., data = _)
decisionplot(model, x, class_var = "species",
             predict_type = c("class", "raw")) +
  labs(title = "Naive Bayes",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



2.6.1.3 Linear Discriminant Analysis

```r
model <- x |> MASS::lda(species ~ ., data = _)
decisionplot(model, x, class_var = "species") +
  labs(title = "LDA",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

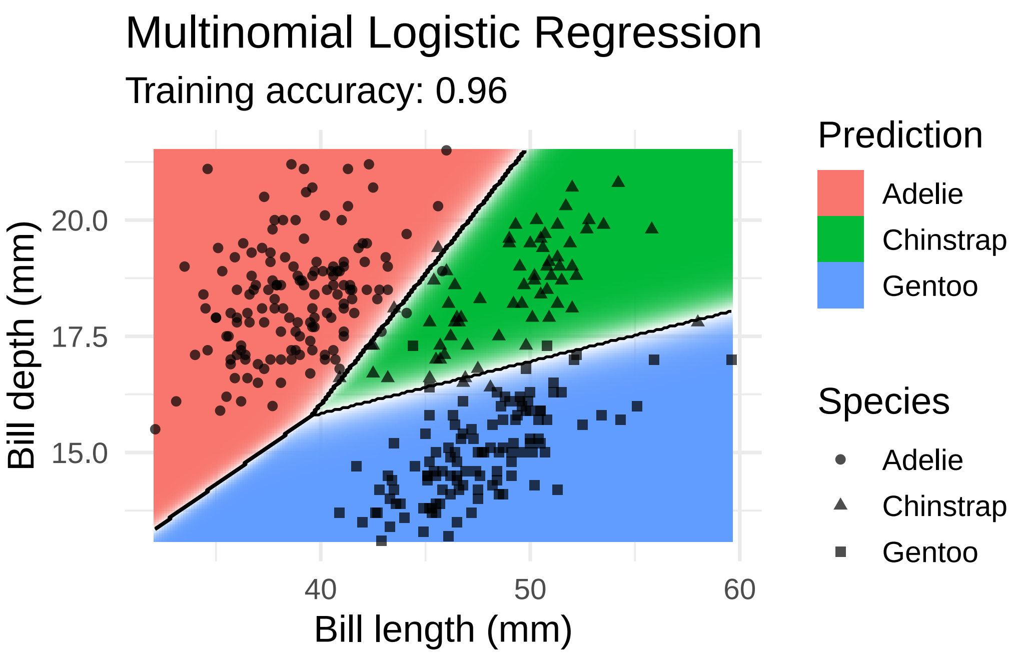


2.6.1.4 Multinomial Logistic Regression (implemented in nnet)

```
model <- x |> nnet::multinom(species ~., data = _)
```

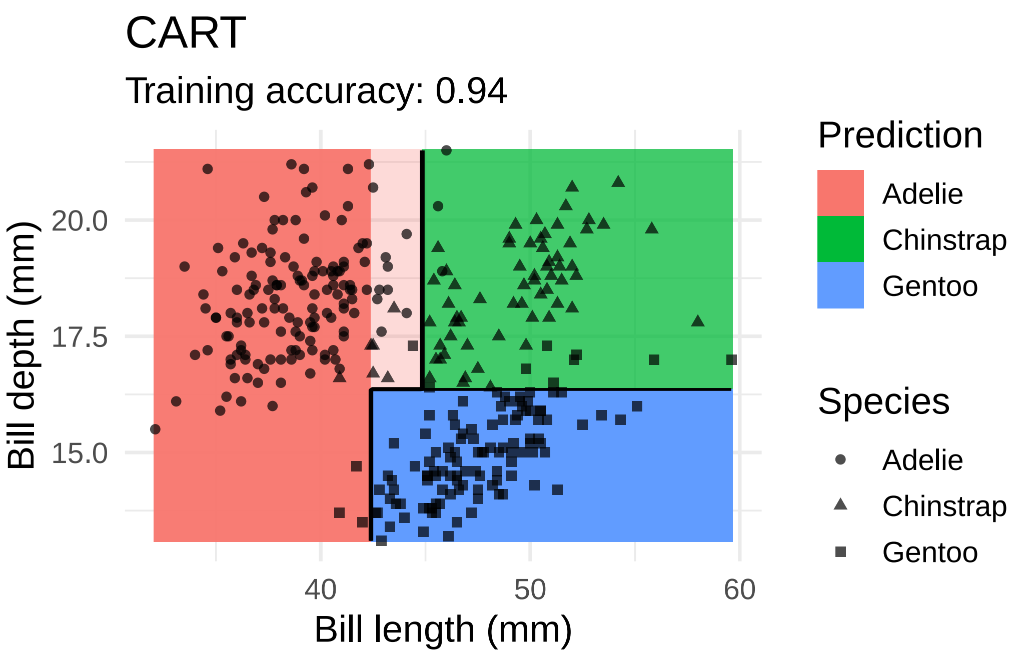
```
# weights:  12 (6 variable)
initial  value 365.837892
iter  10 value 26.650783
iter  20 value 23.943597
iter  30 value 23.916873
iter  40 value 23.901339
iter  50 value 23.895442
iter  60 value 23.894251
final  value 23.892065
converged
```

```
decisionplot(model, x, class_var = "species") +
  labs(title = "Multinomial Logistic Regression",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

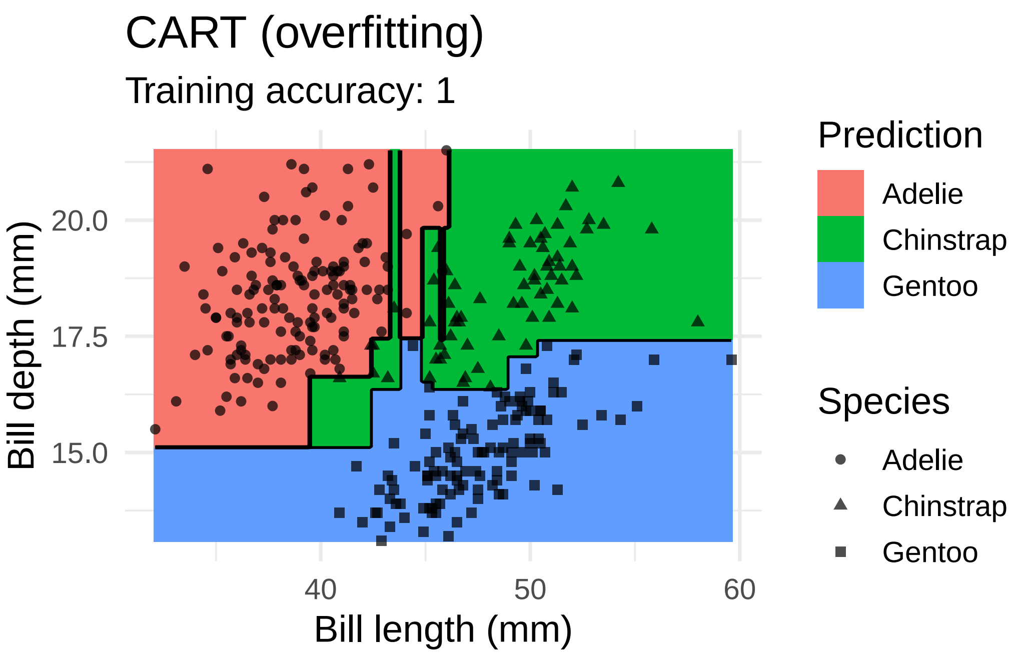


2.6.1.5 Decision Trees

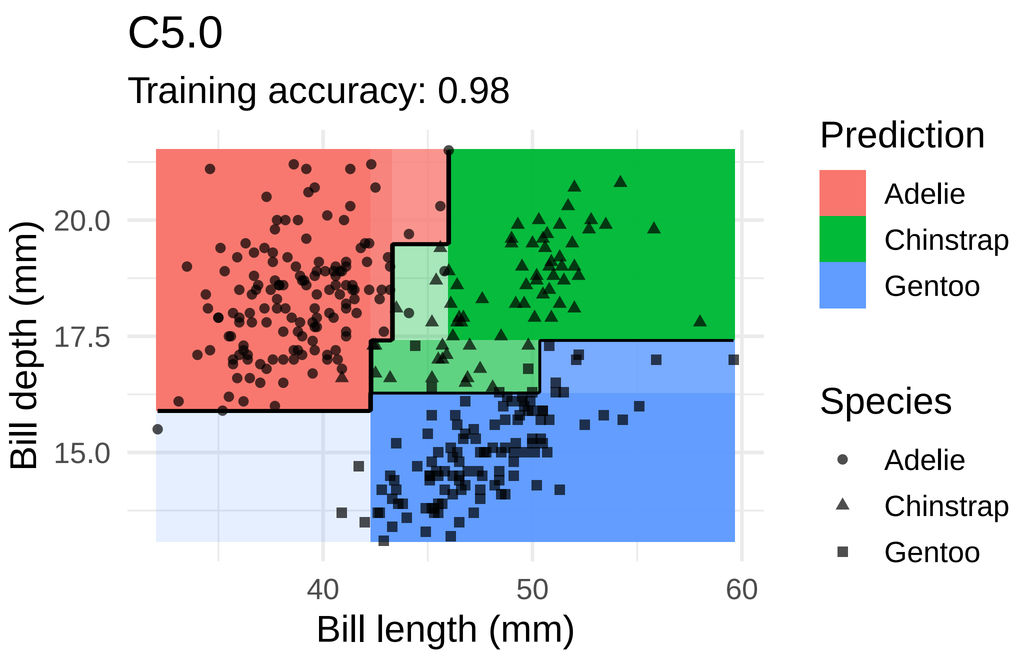
```
model <- x |> rpart::rpart(species ~ ., data = _)
decisionplot(model, x, class_var = "species") +
  labs(title = "CART",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



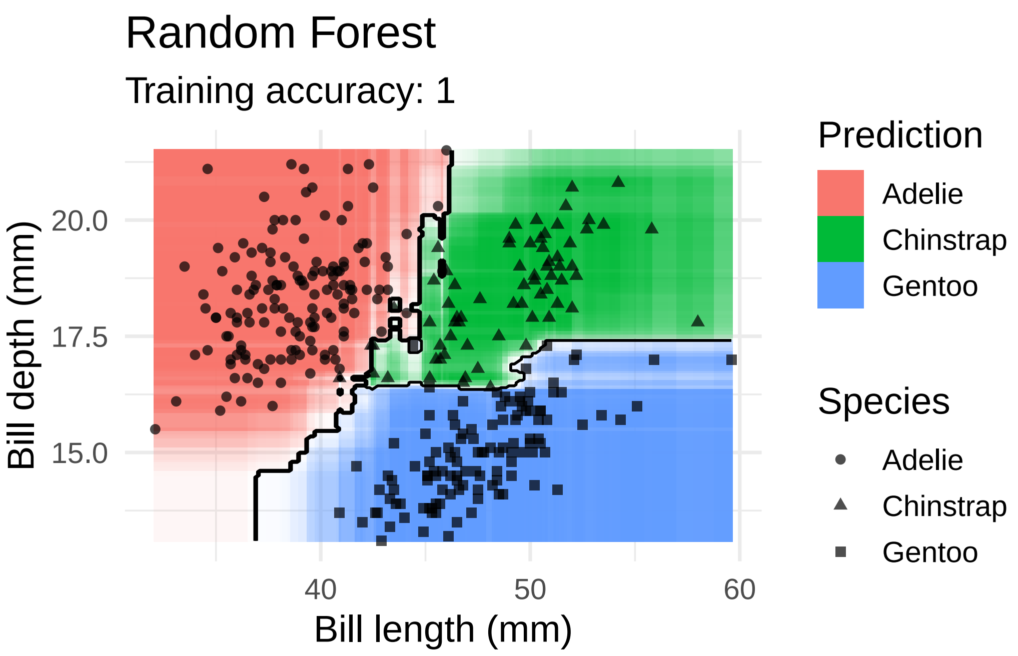
```r
model <- x |> rpart::rpart(species ~ ., data = _,
  control = rpart.control(cp = 0.001, minsplit = 1))
decisionplot(model, x, class_var = "species") +
  labs(title = "CART (overfitting)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



```
model <- x |> C50::C5.0(species ~ ., data = _)
decisionplot(model, x, class_var = "species") +
  labs(title = "C5.0",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

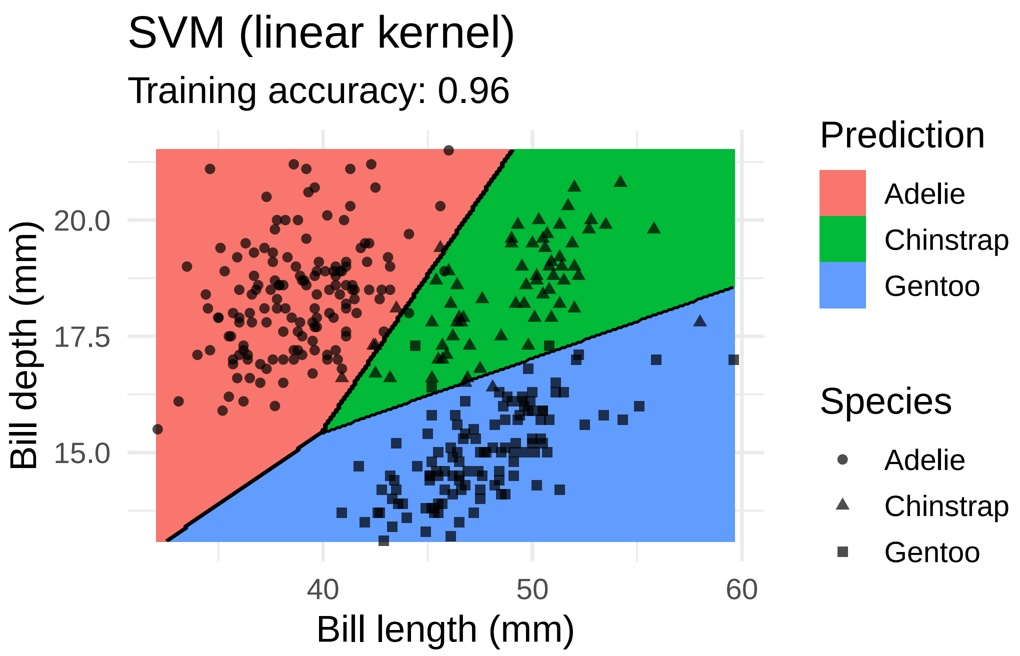


```r
model <- x |> randomForest::randomForest(species ~ ., data = _)
decisionplot(model, x, class_var = "species") +
  labs(title = "Random Forest",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

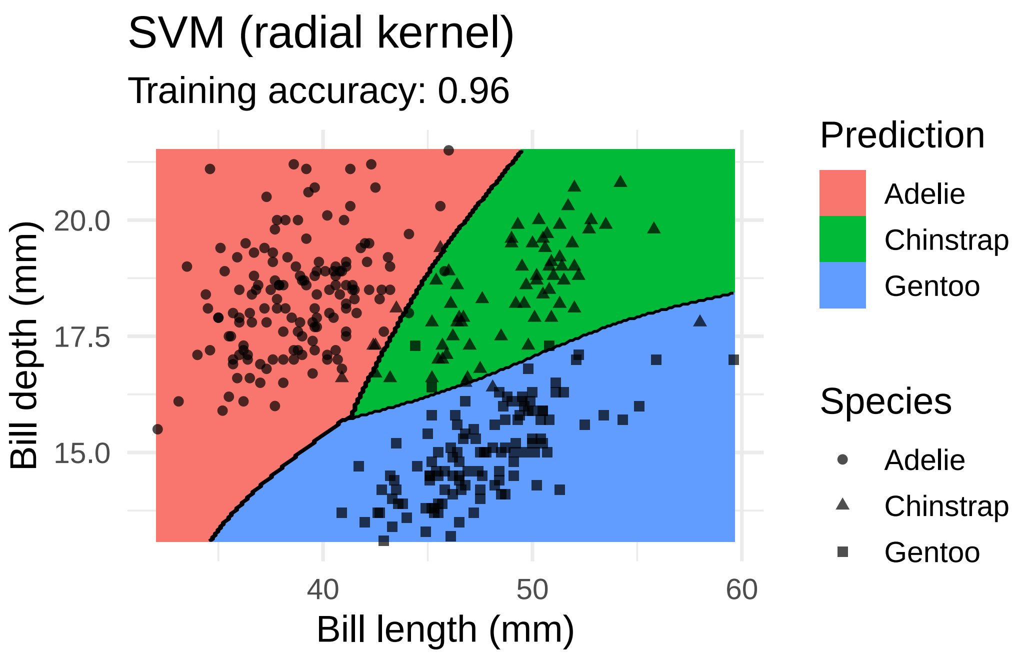


2.6.1.6 SVM

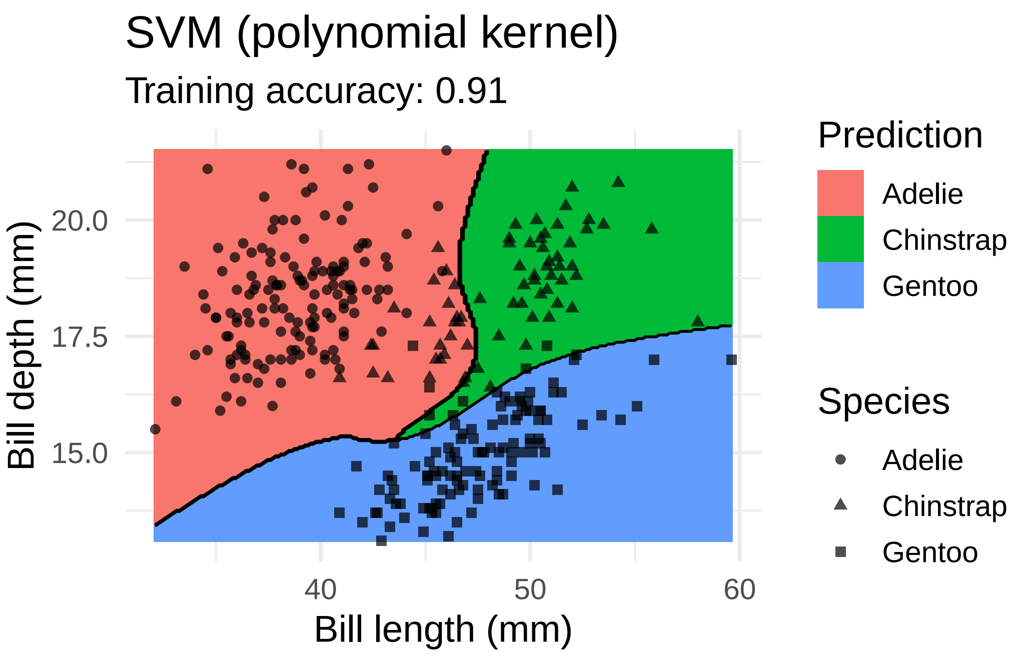
```
model <- x |> e1071::svm(species ~ ., data = _, kernel = "linear")
decisionplot(model, x, class_var = "species") +
  labs(title = "SVM (linear kernel)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



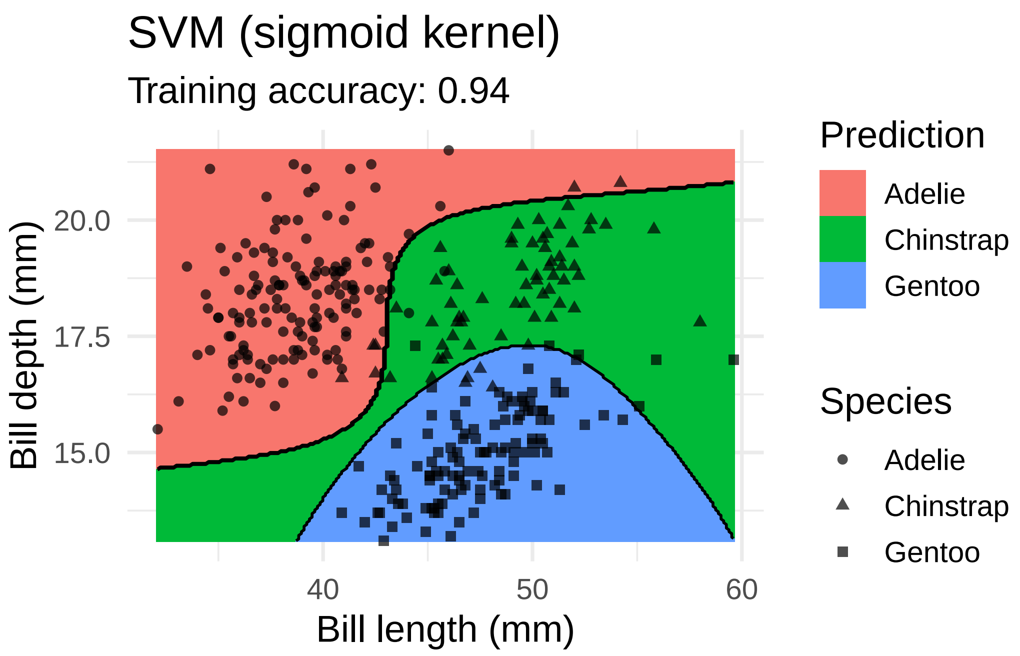
```r
model <- x |> e1071::svm(species ~ ., data = _, kernel = "radial")
decisionplot(model, x, class_var = "species") +
  labs(title = "SVM (radial kernel)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



```r
model <- x |> e1071::svm(species ~ ., data = _, kernel = "polynomial")
decisionplot(model, x, class_var = "species") +
  labs(title = "SVM (polynomial kernel)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



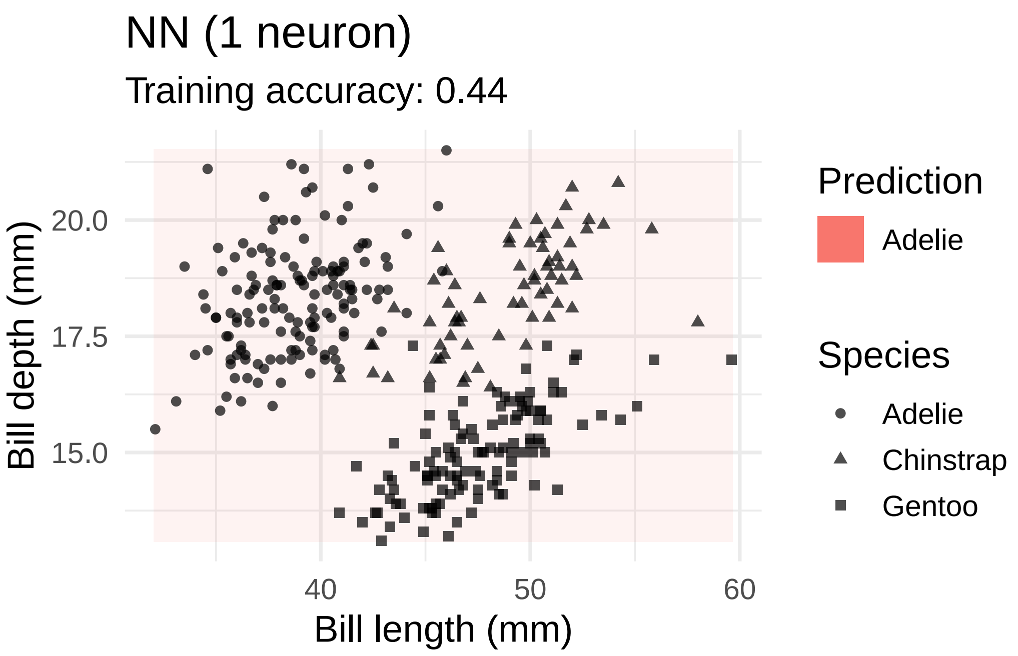
```
model <- x |> e1071::svm(species ~ ., data = _, kernel = "sigmoid")
decisionplot(model, x, class_var = "species") +
  labs(title = "SVM (sigmoid kernel)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



2.6.1.7 Single Layer Feed-forward Neural Networks

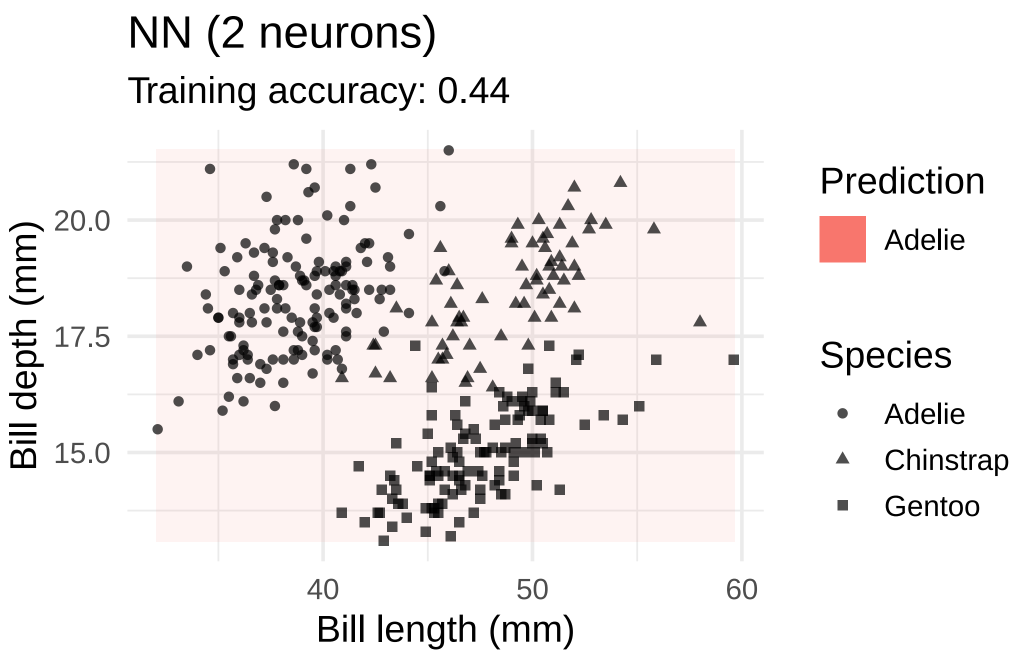
```
model <-x |> nnet::nnet(species ~ ., data = _, size = 1, trace = FALSE)
decisionplot(model, x, class_var  = "species",
  predict_type = c("class", "raw")) +
  labs(title = "NN (1 neuron)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

```
Warning: Computation failed in `stat_contour()`
Caused by error in `if (zero_range(range)) ...`:
! missing value where TRUE/FALSE needed
```

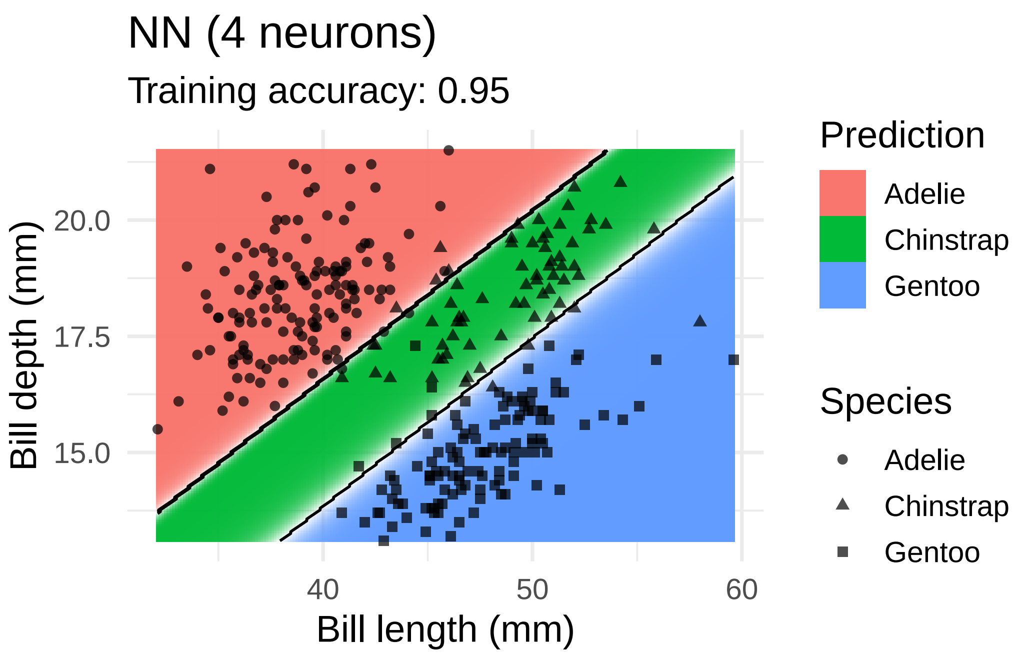


```
model <-x |> nnet::nnet(species ~ ., data = _, size = 2, trace = FALSE)
decisionplot(model, x, class_var  = "species",
  predict_type = c("class", "raw")) +
  labs(title = "NN (2 neurons)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

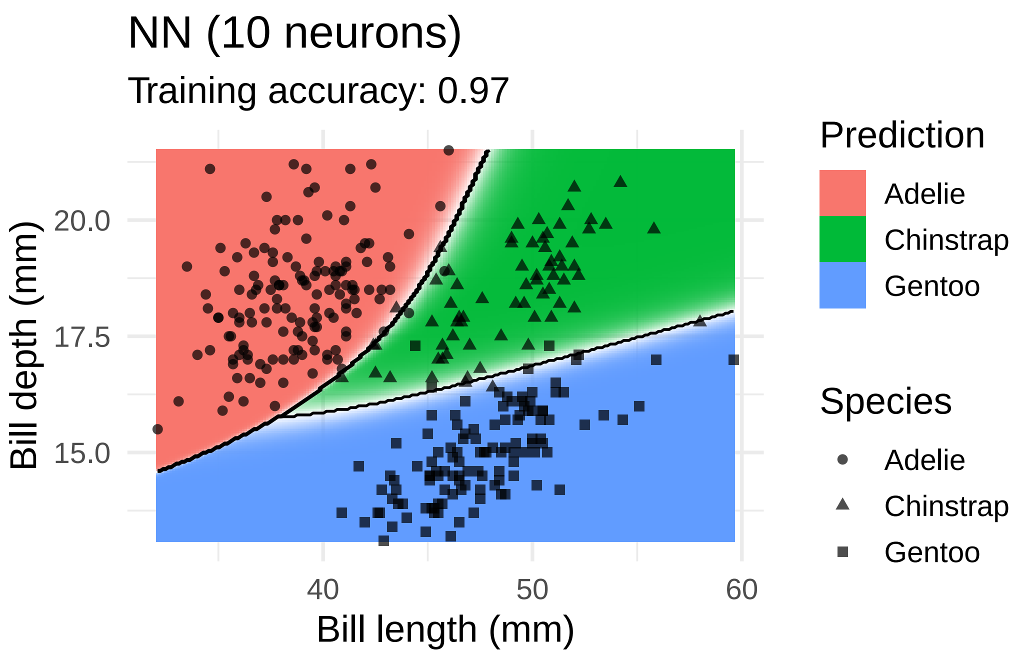
```
Warning: Computation failed in `stat_contour()`
Caused by error in `if (zero_range(range)) ...`:
! missing value where TRUE/FALSE needed
```



```
model <-x |> nnet::nnet(species ~ ., data = _, size = 4, trace = FALSE)
decisionplot(model, x, class_var  = "species",
  predict_type = c("class", "raw")) +
  labs(title = "NN (4 neurons)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```



```
model <-x |> nnet::nnet(species ~ ., data = _, size = 10, trace = FALSE)
decisionplot(model, x, class_var  = "species",
  predict_type = c("class", "raw")) +
  labs(title = "NN (10 neurons)",
       x = "Bill length (mm)",
       y = "Bill depth (mm)",
       shape = "Species",
       fill = "Prediction")
```

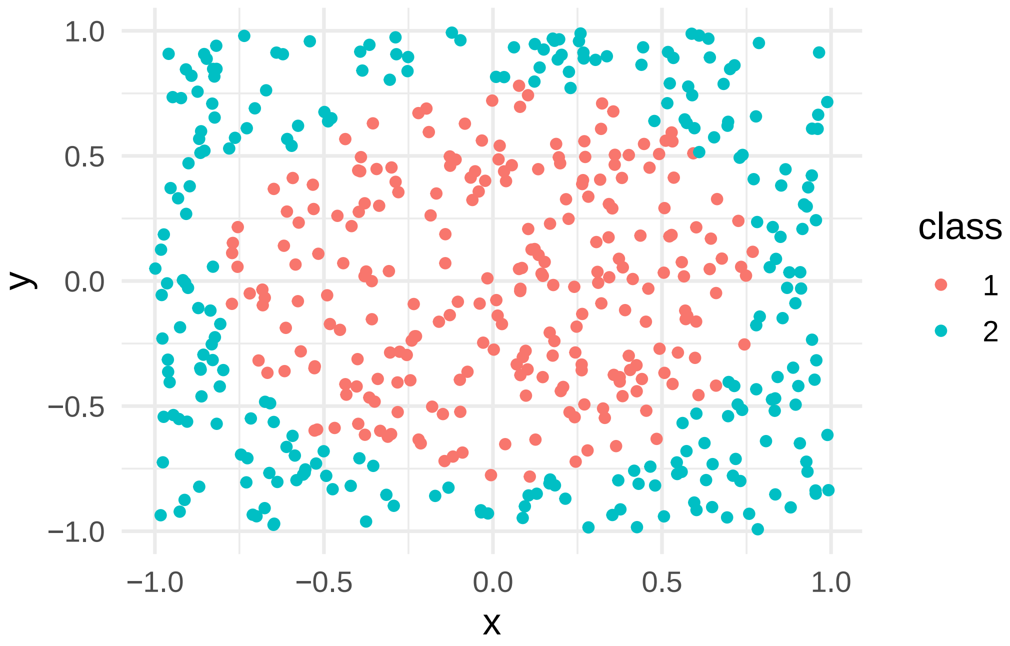


2.6.2 Circle Dataset

```r
set.seed(1000)

x <- mlbench::mlbench.circle(500)
###x <- mlbench::mlbench.cassini(500)
###x <- mlbench::mlbench.spirals(500, sd = .1)
###x <- mlbench::mlbench.smiley(500)
x <- cbind(as.data.frame(x$x), factor(x$classes))
colnames(x) <- c("x", "y", "class")
x <- as_tibble(x)
x
```

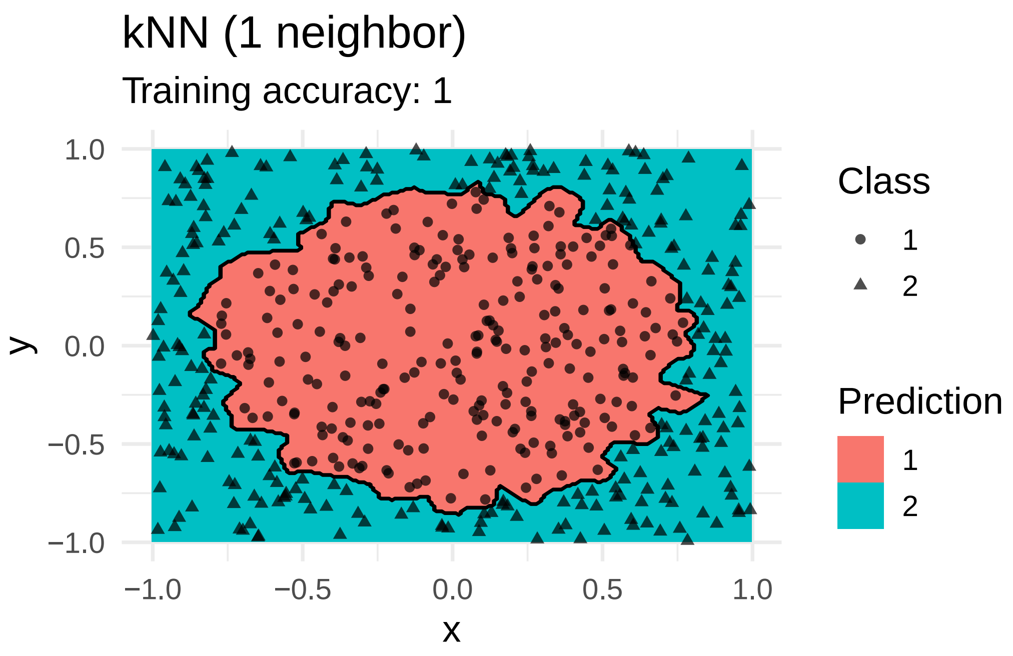
```
# A tibble: 500 x 3
        x       y class
    <dbl>   <dbl> <fct>
 1 -0.344   0.448  1
 2  0.518   0.915  2
 3 -0.772  -0.0913 1
 4  0.382   0.412  1
 5  0.0328  0.438  1
 6 -0.865  -0.354  2
 7  0.477   0.640  2
 8  0.167  -0.809  2
 9 -0.568  -0.281  1
10 -0.488   0.638  2
# i 490 more rows
```

```r
ggplot(x, aes(x = x, y = y, color = class)) +
  geom_point() +
  theme_minimal(base_size = 14)
```

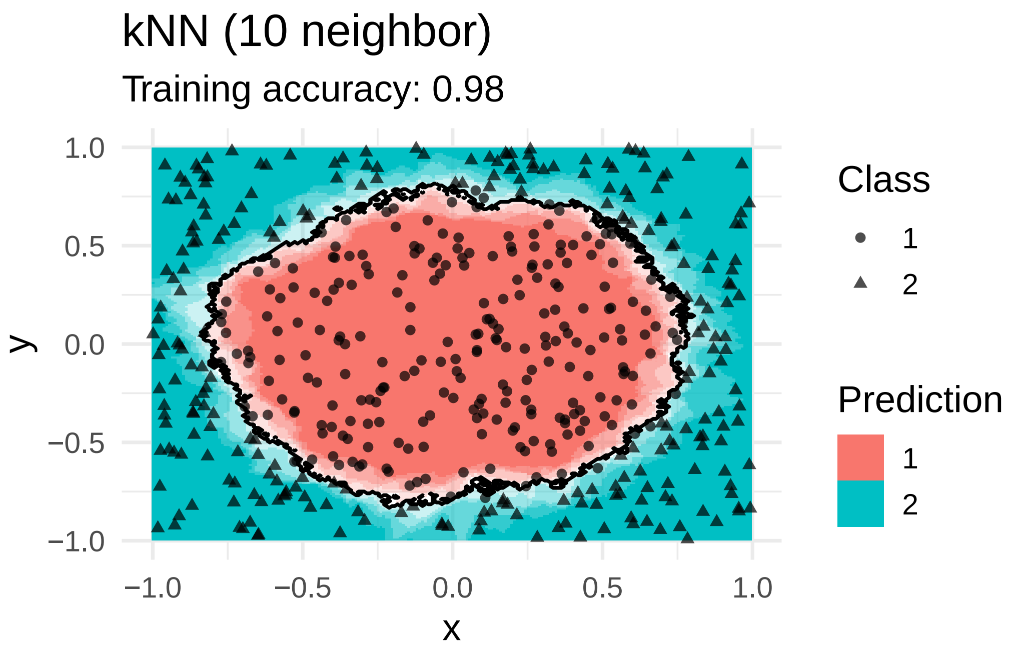


2.6.2.1 K-Nearest Neighbors Classifier

```r
model <- x |> caret::knn3(class ~ ., data = _, k = 1)
decisionplot(model, x, class_var = "class") +
  labs(title = "kNN (1 neighbor)",
       shape = "Class",
       fill = "Prediction")
```

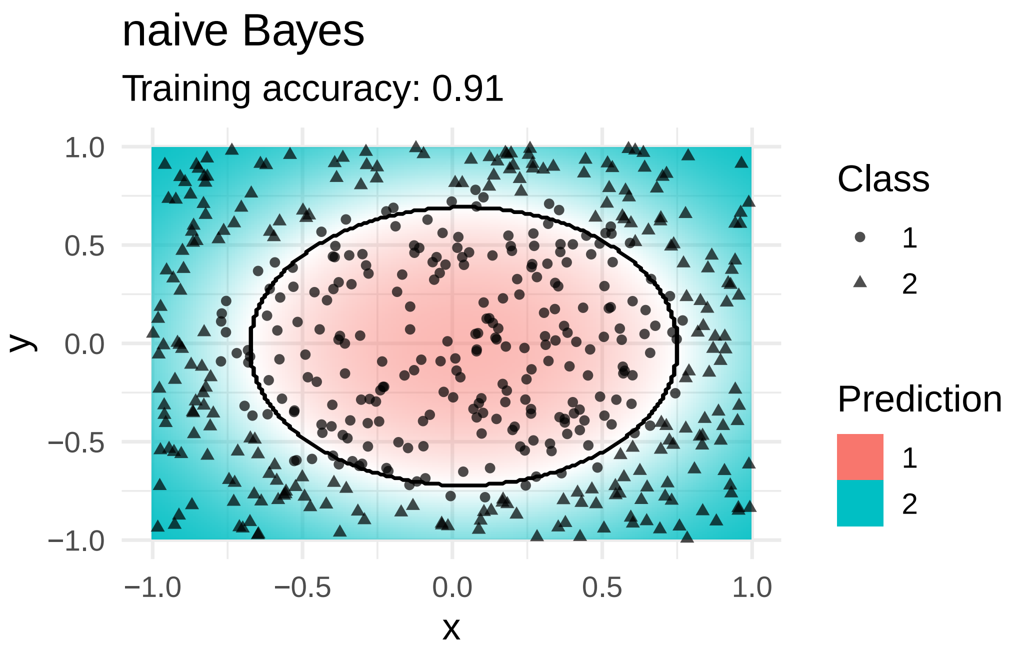


```
model <- x |> caret::knn3(class ~ ., data = _, k = 10)
decisionplot(model, x, class_var = "class") +
  labs(title = "kNN (10 neighbor)",
       shape = "Class",
       fill = "Prediction")
```



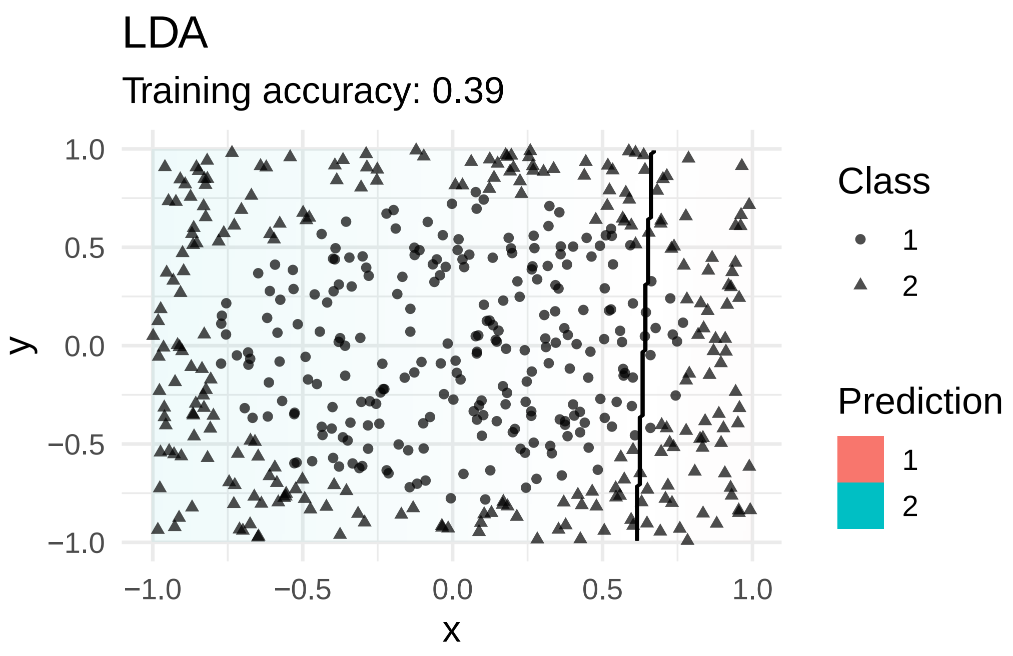
2.6.2.2 Naive Bayes Classifier

```
model <- x |> e1071::naiveBayes(class ~ ., data = _)
decisionplot(model, x, class_var = "class",
  predict_type = c("class", "raw")) +
  labs(title = "naive Bayes",
       shape = "Class",
       fill = "Prediction")
```



2.6.2.3 Linear Discriminant Analysis

```
model <- x |> MASS::lda(class ~ ., data = _)
decisionplot(model, x, class_var = "class") +
  labs(title = "LDA",
       shape = "Class",
       fill = "Prediction")
```

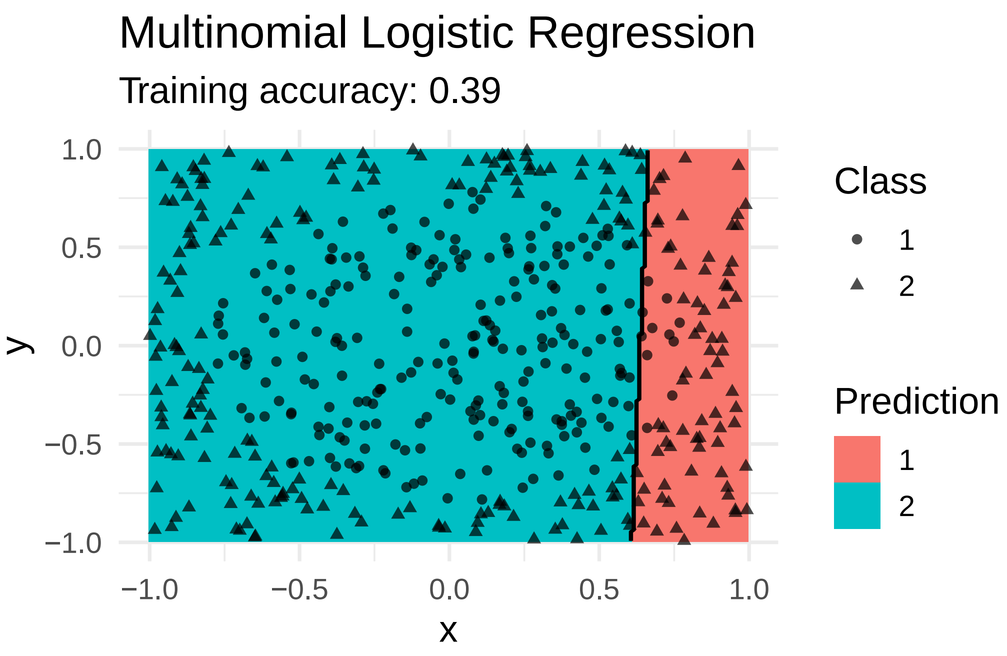


2.6.2.4 Logistic Regression (implemented in nnet)

```
model <- x |> nnet::multinom(class ~., data = _)
```

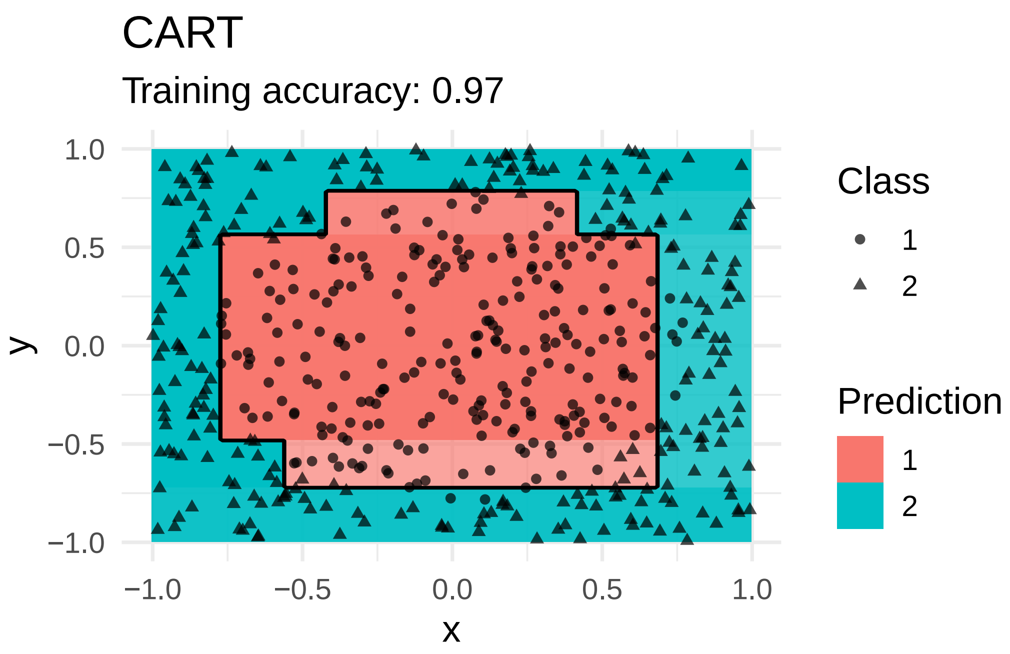
```
# weights:  4 (3 variable)
initial  value 346.573590
final  value 346.308371
converged
```

```
decisionplot(model, x, class_var = "class") +
  labs(title = "Multinomial Logistic Regression",
       shape = "Class",
       fill = "Prediction")
```

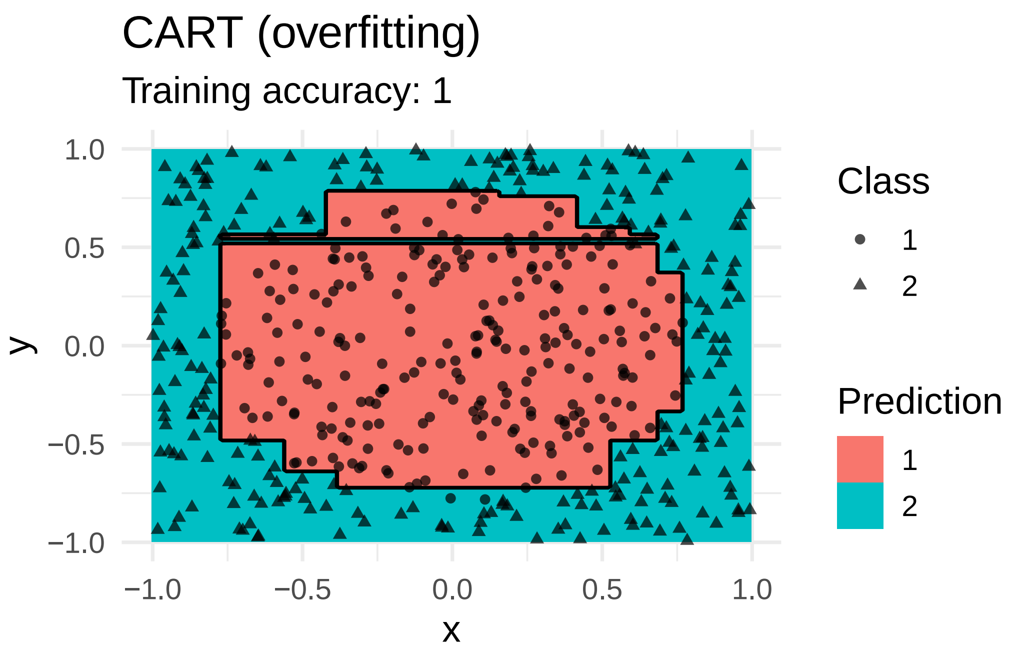


2.6.2.5 Decision Trees

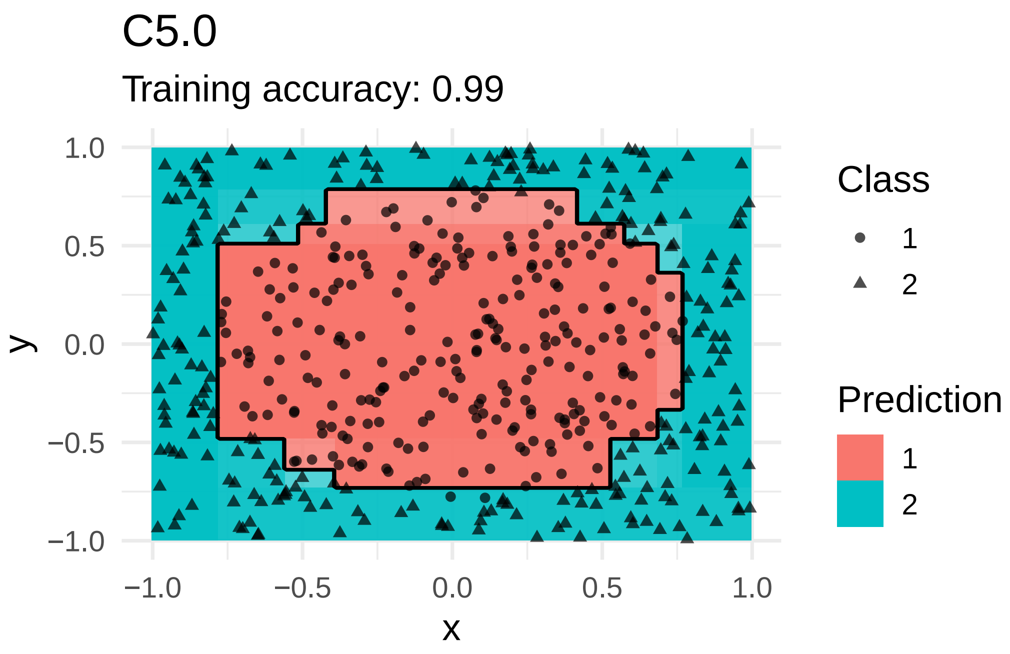
```r
model <- x |> rpart::rpart(class ~ ., data = _)
decisionplot(model, x, class_var = "class") +
  labs(title = "CART",
       shape = "Class",
       fill = "Prediction")
```



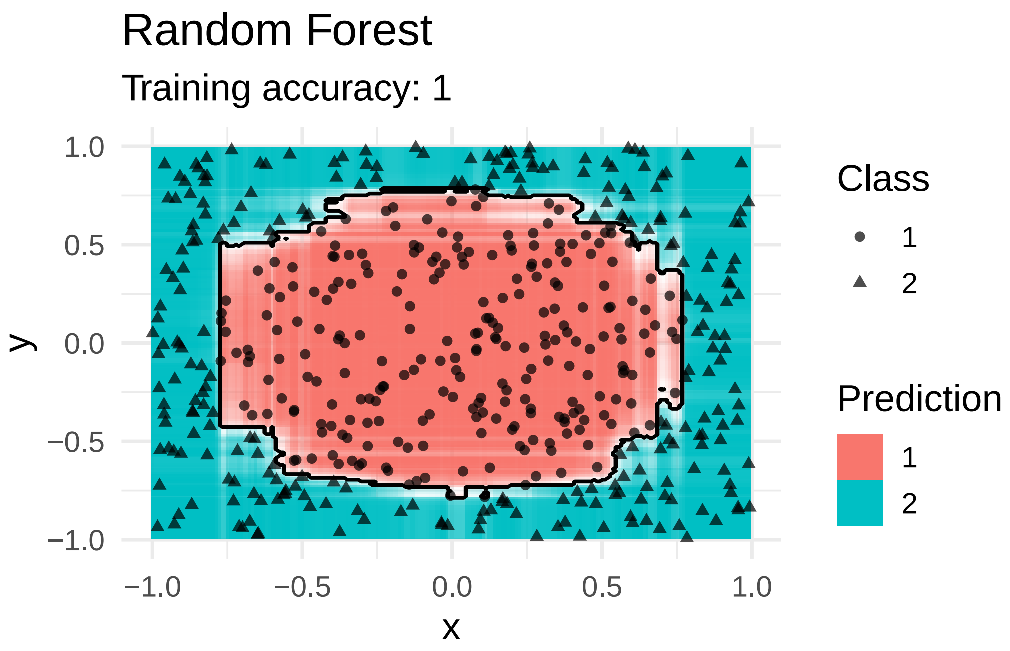
```
model <- x |> rpart::rpart(class ~ ., data = _,
  control = rpart.control(cp = 0.001, minsplit = 1))
decisionplot(model, x, class_var = "class") +
  labs(title = "CART (overfitting)",
       shape = "Class",
       fill = "Prediction")
```



```
model <- x |> C50::C5.0(class ~ ., data = _)
decisionplot(model, x, class_var = "class") +
  labs(title = "C5.0",
       shape = "Class",
       fill = "Prediction")
```



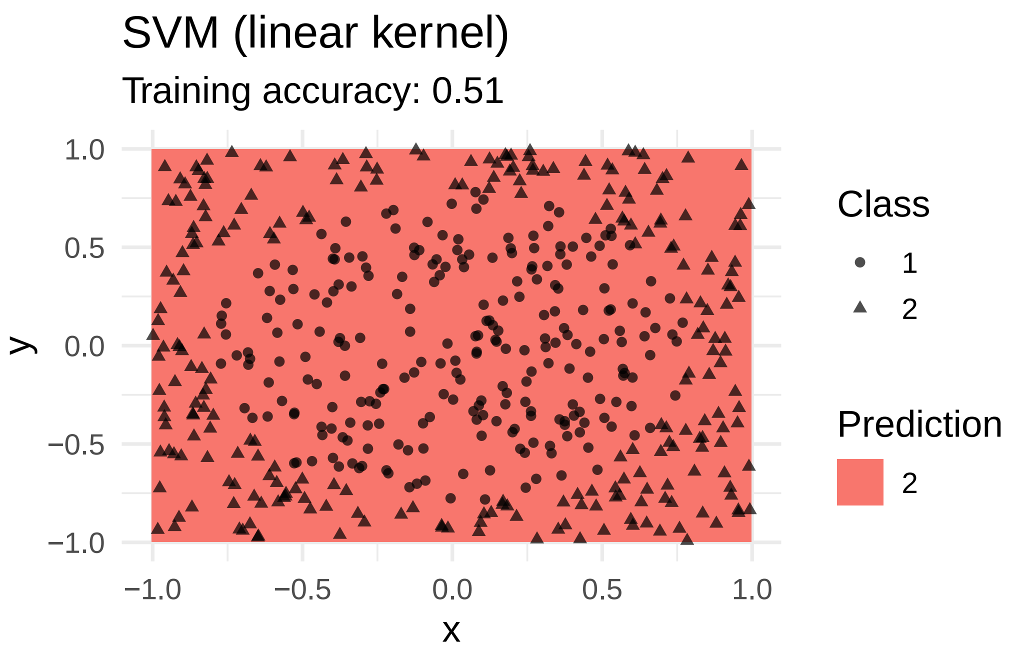
```r
library(randomForest)
model <- x |> randomForest(class ~ ., data = _)
decisionplot(model, x, class_var = "class") +
  labs(title = "Random Forest",
       shape = "Class",
       fill = "Prediction")
```



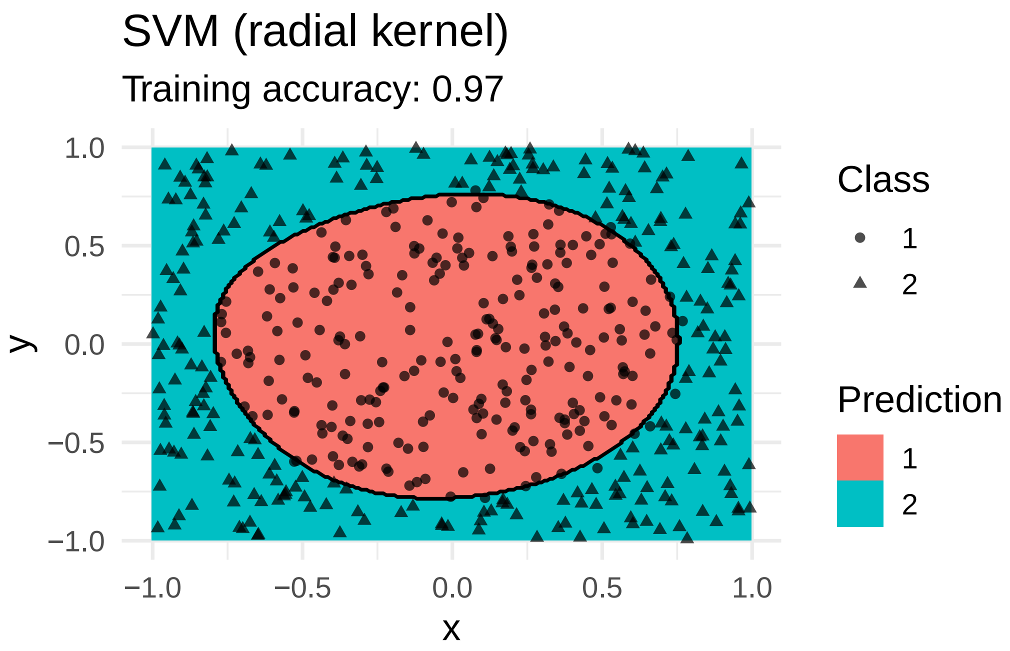
2.6.2.6 SVM

```r
model <- x |> e1071::svm(class ~ ., data = _, kernel = "linear")
decisionplot(model, x, class_var = "class") +
  labs(title = "SVM (linear kernel)",
       shape = "Class",
       fill = "Prediction")
```

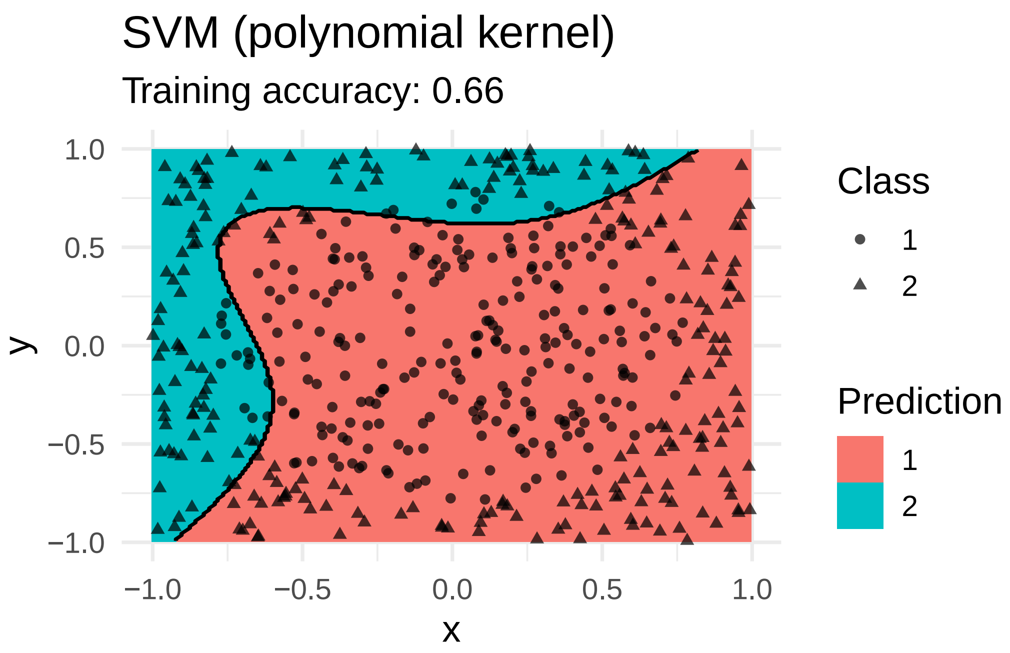
```
Warning: Computation failed in `stat_contour()`
Caused by error in `if (zero_range(range)) ...`:
! missing value where TRUE/FALSE needed
```



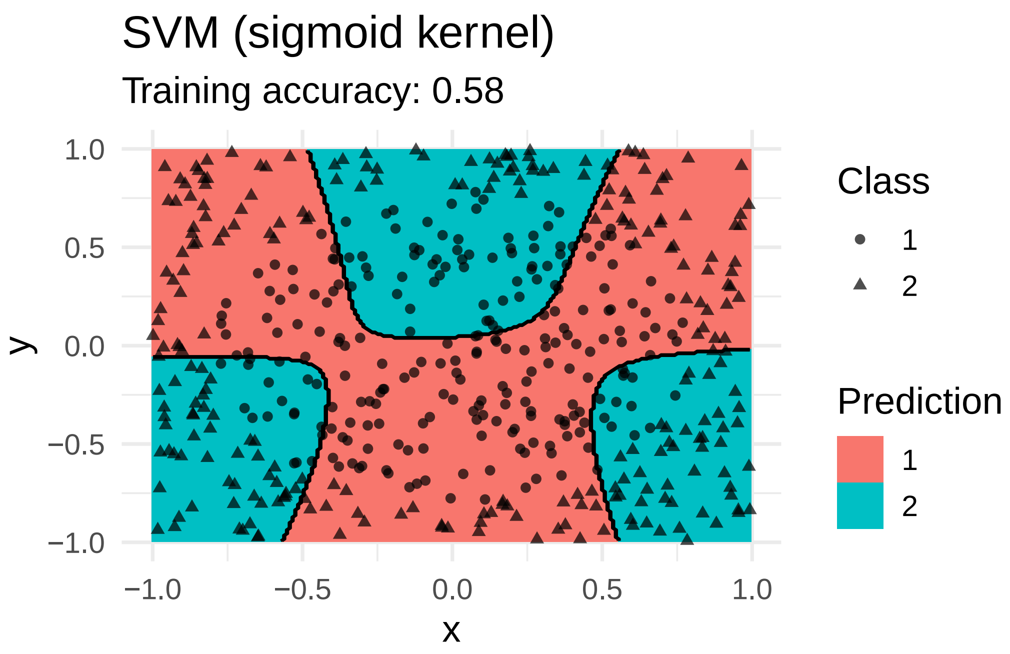
```
model <- x |> e1071::svm(class ~ ., data = _, kernel = "radial")
decisionplot(model, x, class_var = "class") +
  labs(title = "SVM (radial kernel)",
       shape = "Class",
       fill = "Prediction")
```



```r
model <- x |> e1071::svm(class ~ ., data = _, kernel = "polynomial")
decisionplot(model, x, class_var = "class") +
  labs(title = "SVM (polynomial kernel)",
       shape = "Class",
       fill = "Prediction")
```

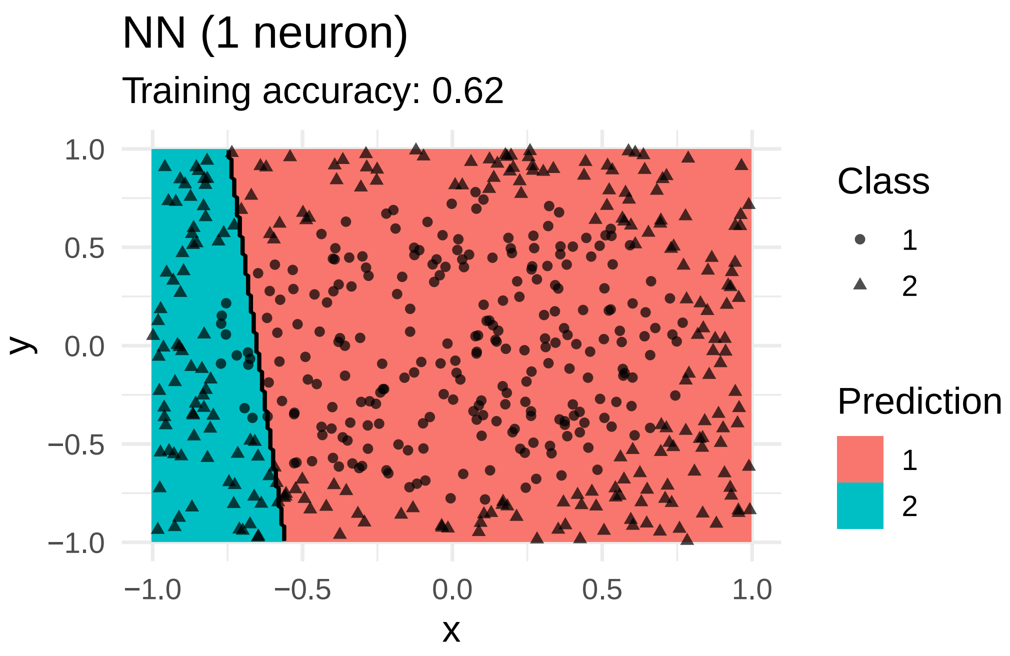


```r
model <- x |> e1071::svm(class ~ ., data = _, kernel = "sigmoid")
decisionplot(model, x, class_var = "class") +
  labs(title = "SVM (sigmoid kernel)",
       shape = "Class",
       fill = "Prediction")
```

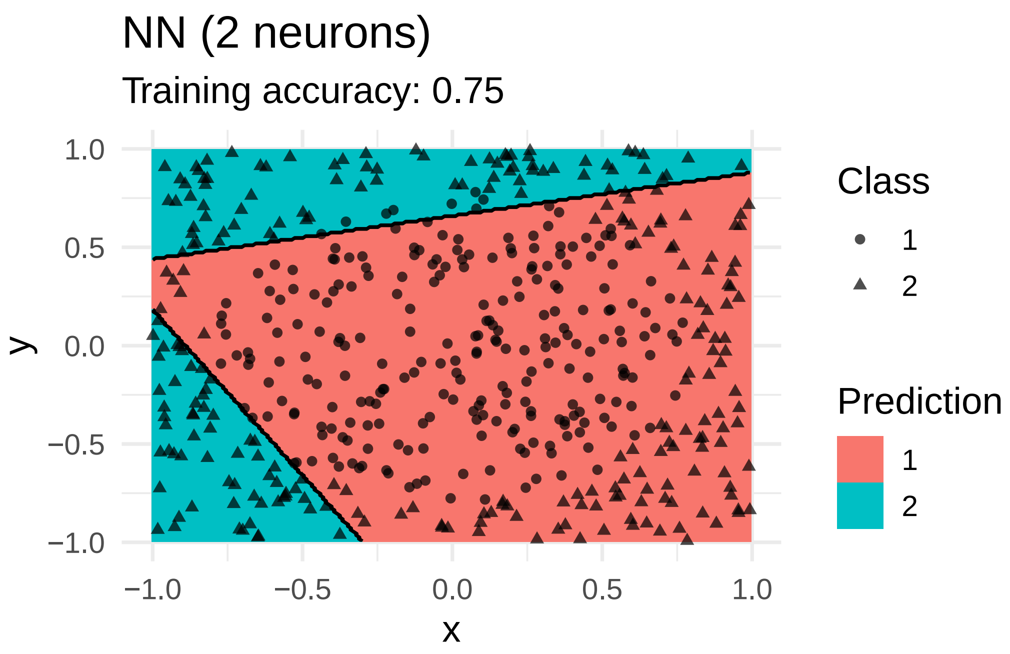


2.6.2.7 Single Layer Feed-forward Neural Networks

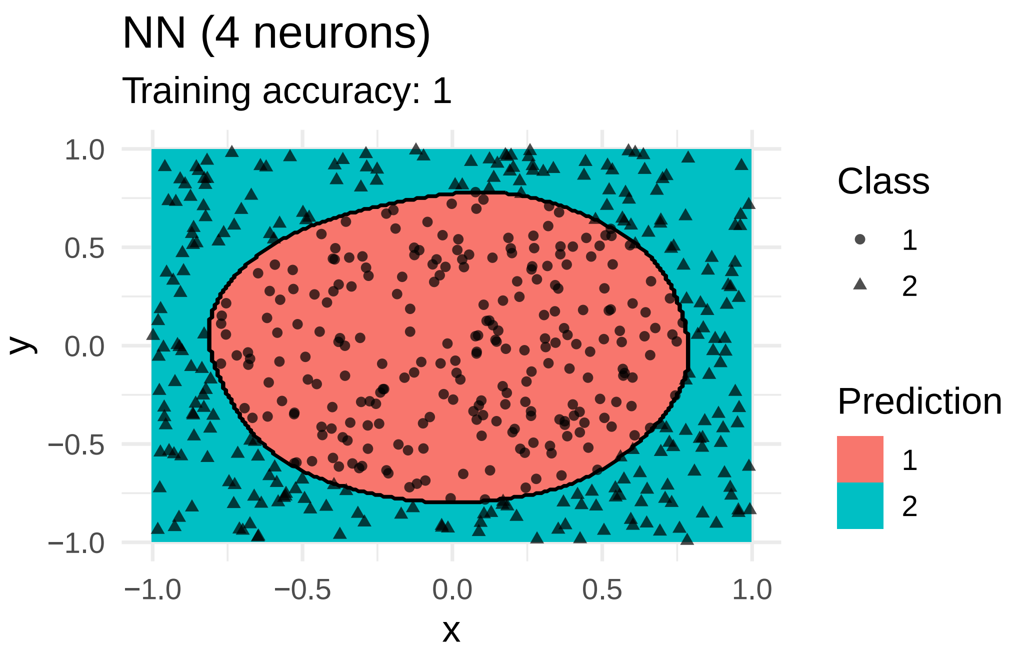
```
model <-x |> nnet::nnet(class ~ ., data = _, size = 1, trace = FALSE)
decisionplot(model, x, class_var = "class",
  predict_type = c("class")) +
  labs(title = "NN (1 neuron)",
       shape = "Class",
       fill = "Prediction")
```



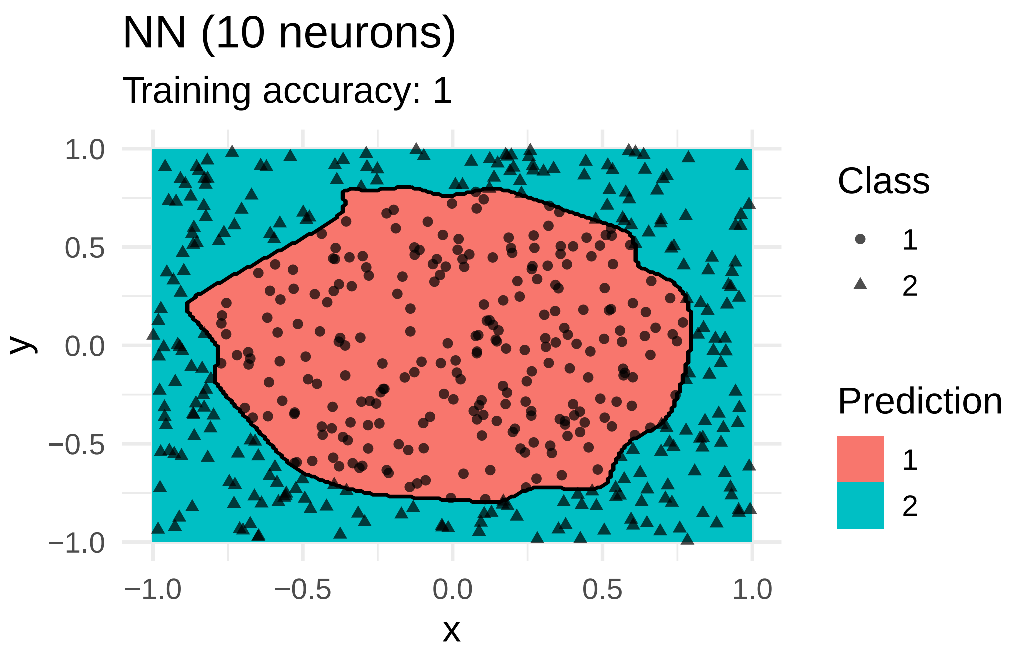
```
model <-x |> nnet::nnet(class ~ ., data = _, size = 2, trace = FALSE)
decisionplot(model, x, class_var = "class",
  predict_type = c("class")) +
  labs(title = "NN (2 neurons)",
       shape = "Class",
       fill = "Prediction")
```



```
model <-x |> nnet::nnet(class ~ ., data = _, size = 4, trace = FALSE)
decisionplot(model, x, class_var = "class",
  predict_type = c("class")) +
  labs(title = "NN (4 neurons)",
       shape = "Class",
       fill = "Prediction")
```



```
model <-x |> nnet::nnet(class ~ ., data = _, size = 10, trace = FALSE)
decisionplot(model, x, class_var = "class",
  predict_type = c("class")) +
  labs(title = "NN (10 neurons)",
       shape = "Class",
       fill = "Prediction")
```



2.7 More Information on Classification with R

- Package caret: http://topepo.github.io/caret/index.html
- Tidymodels (machine learning with tidyverse): https://www.tidymodels.org/
- R taskview on machine learning: http://cran.r-project.org/web/views/MachineLearnin g.html{r}