Introduction to Machine Learning with R

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codecentric AG

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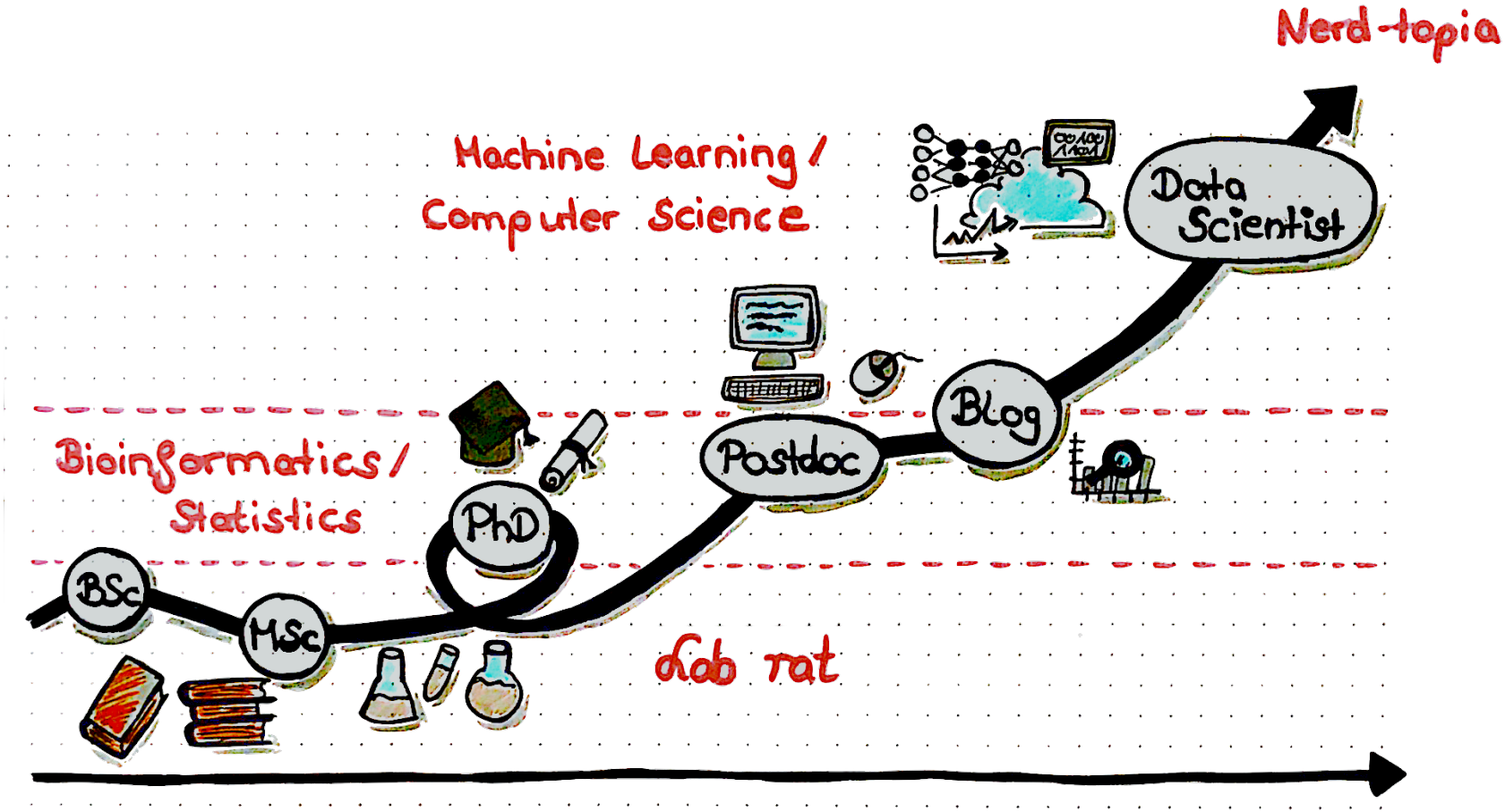
About me & this workshop

How I ended up here



About this workshop

Machine Learning with the caret package

- data prep
- missingness
- decision trees
- random forests
- gradient boosting
- feature selection
- hyperparameter tuning
- plotting

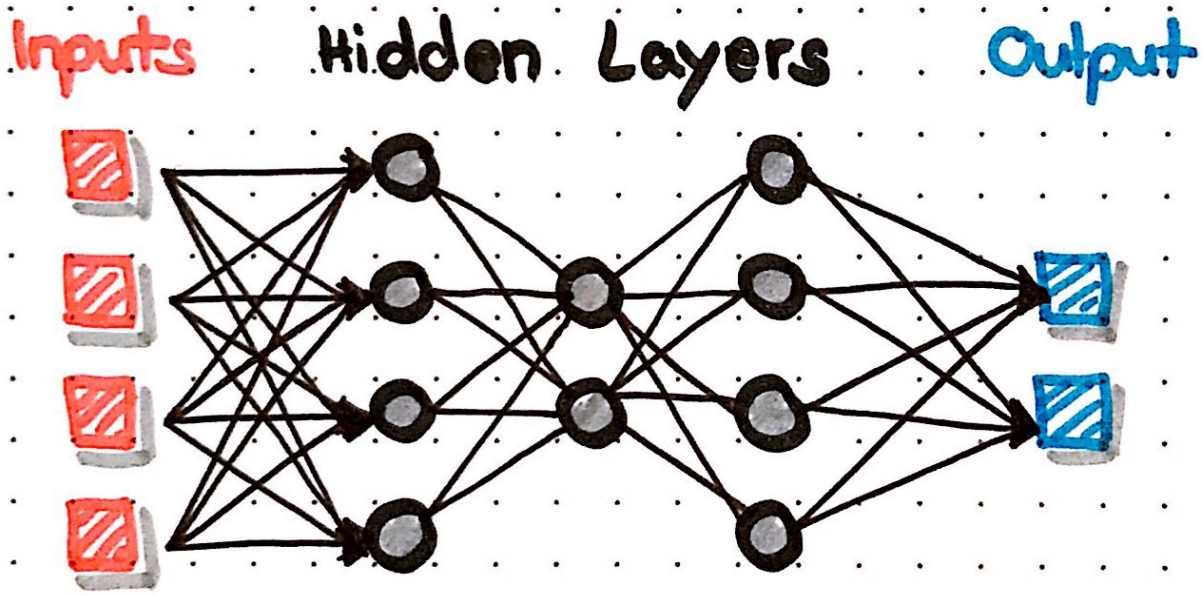
Machine Learning with the h2o package

- hyperparameter tuning

If there is still time...

Deep Dive into Neural Networks

- what are neural nets and what makes them special?
- how do neural nets learn?
- how to train neural nets with caret

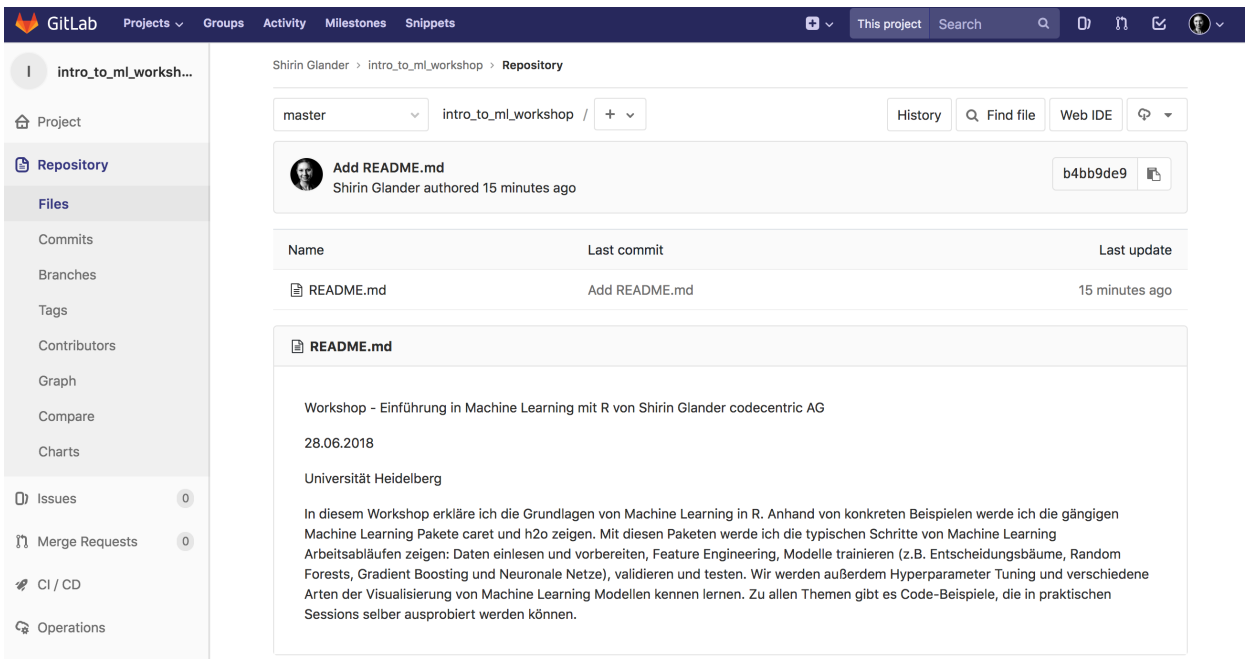


Workshop material

Scripts and code

https://gitlab.com/ShirinG/intro_to_ml_workshop

- Code-Through: intro_to_ml.html*
- Slides: slides/intro_to_ml_slides.pdf
- Datasets: datasets/



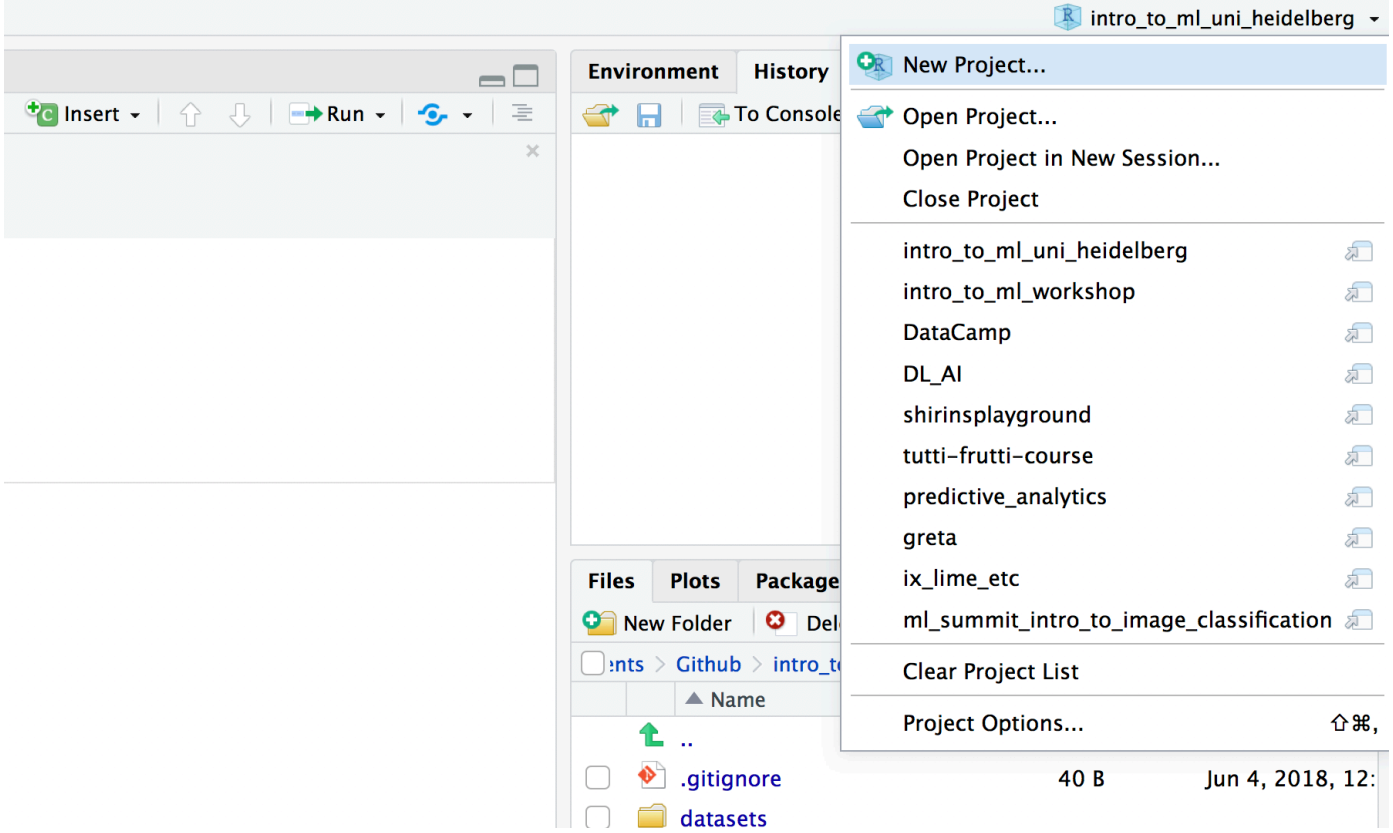
Why use R

- open-source, cross-platform
- established language (there are lots and lots of packages)
- high quality packages with proper documentation (CRAN)
- graphics capabilities - ggplot2!!!
- RStudio + R Markdown!!
- community support!

Getting started

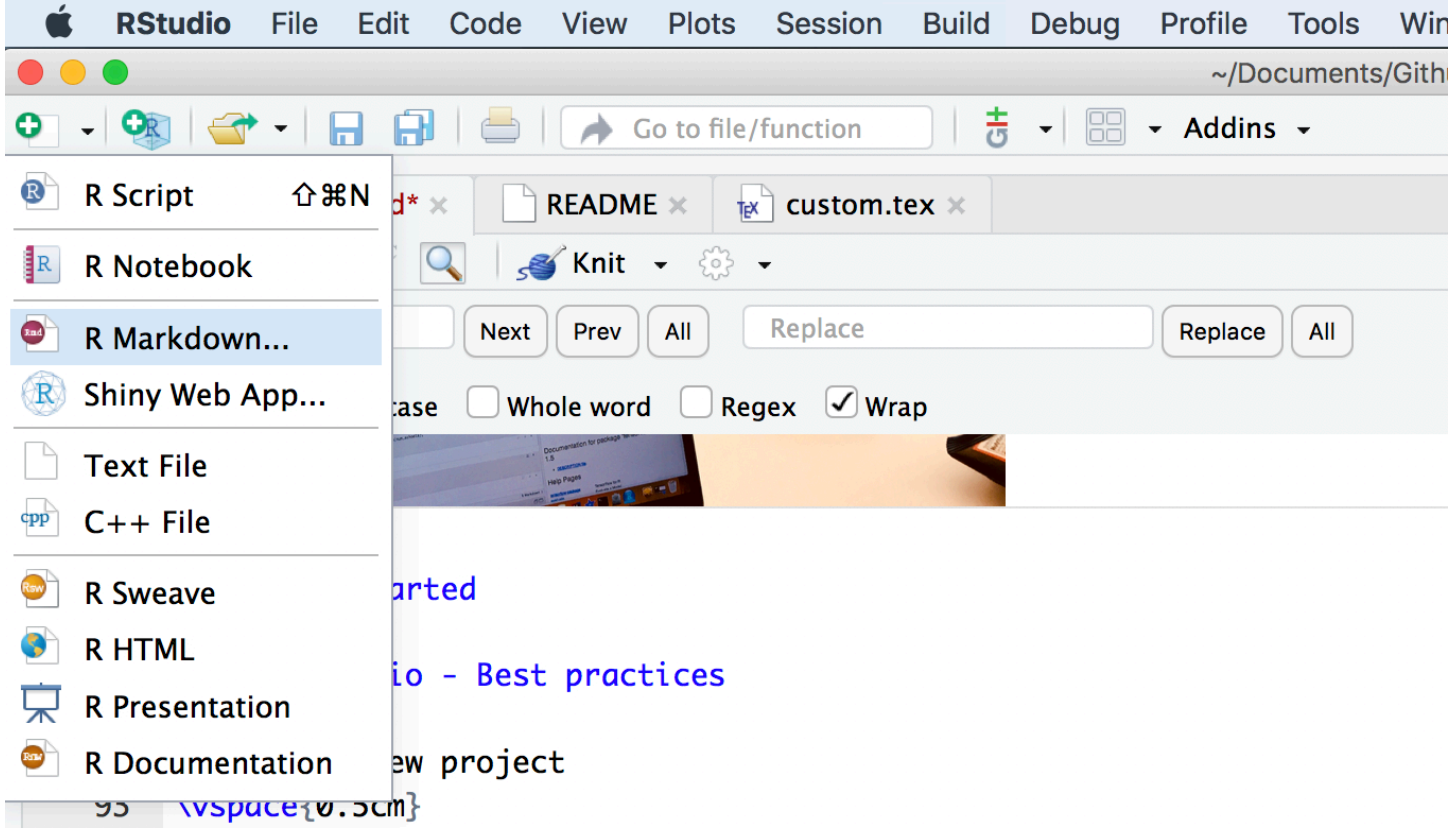
R + RStudio - Best practices

- Step 1) create a new project



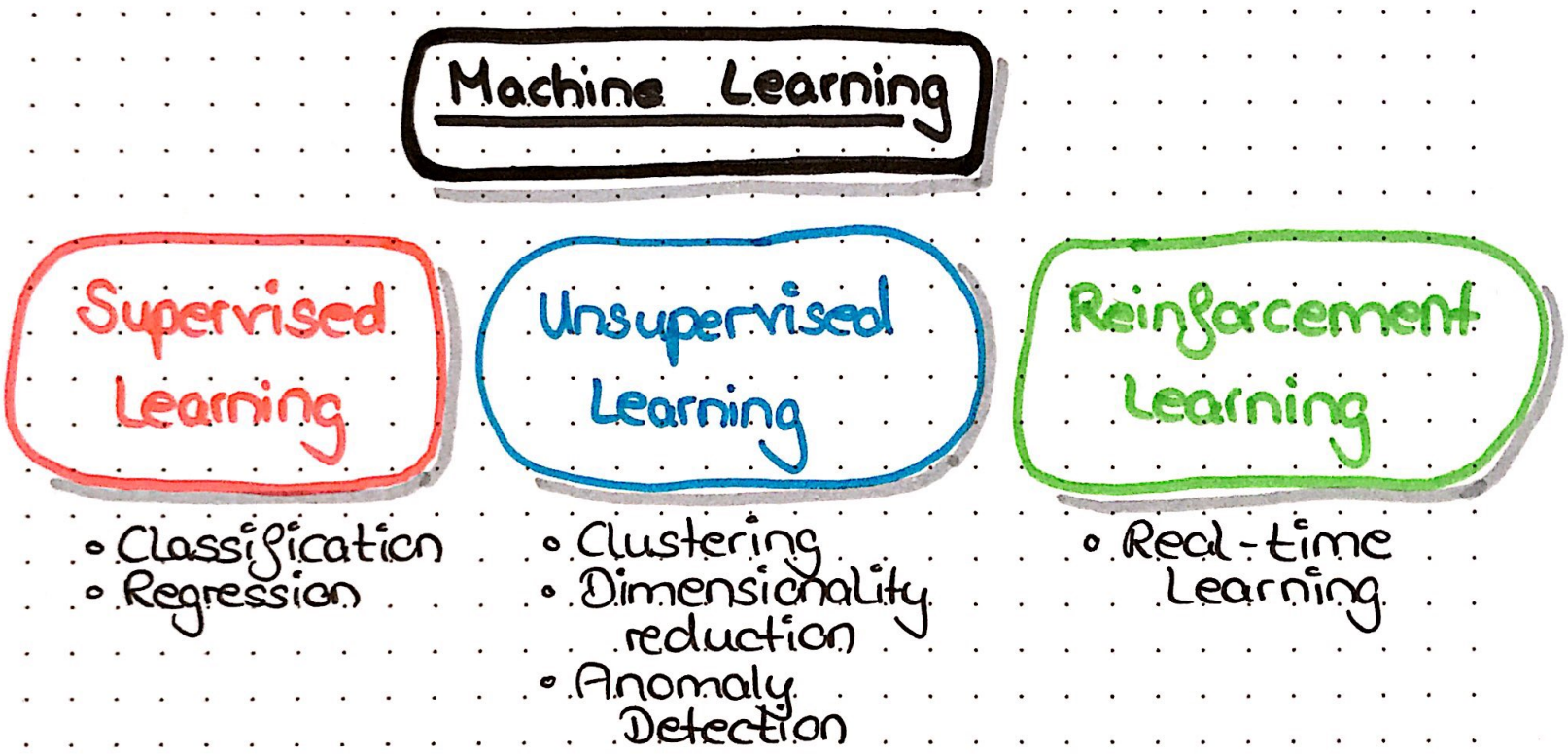
R + RStudio - Best practices

- Step 2) create a new R Markdown document



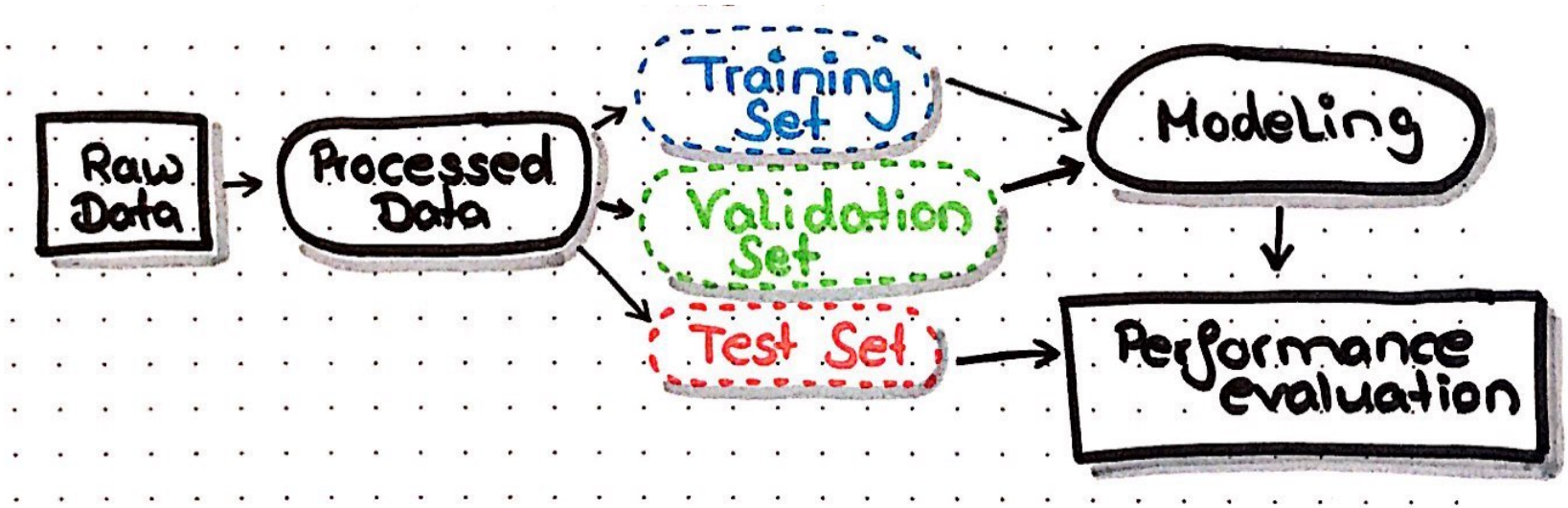
Machine Learning

Machine Learning (ML) overview



A general workflow

- Input data
- Data preprocessing
- Training, validation and test split
- Modeling
- Predictions and Evaluations



How to prepare your data for ML

Reading in data

Breast Cancer Wisconsin (Diagnostic) Dataset

```
library(tidyverse) # for tidy data analysis
bc_data <- readr::read_delim("../datasets/breast-cancer-wisconsin.data.txt",
                    delim = ",",
                    col_names = c("sample_code_number",
                     "clump_thickness",
                     "uniformity_of_cell_size",
                     "uniformity_of_cell_shape",
                     "marginal_adhesion",
                     "single_epithelial_cell_size",
                     "bare_nuclei",
                     "bland_chromatin",
                     "normal_nucleoli",
                     "mitosis",
                     "classes")) %>%
  mutate(bare_nuclei = as.numeric(bare_nuclei),
         classes = ifelse(classes == "2", "benign",
                          ifelse(classes == "4", "malignant", NA)))
```

Missingness

```
mice::md.pattern(bc_data, plot = FALSE)
```

```
##     sample_code_number clump_thickness uniformity_of_cell_size
## 683                  1               1                       1
## 16                   1               1                       1
##                      0               0                       0
##     uniformity_of_cell_shape marginal_adhesion single_epithelial_cell_size
## 683                        1                 1                          1
## 16                         1                 1                          1
##                            0                 0                          0
##     bland_chromatin normal_nucleoli mitosis classes bare_nuclei
## 683               1               1       1       1           1 0
## 16                1               1       1       1           0 1
##                   0               0       0       0          16 16
```

```
bc_data <- bc_data[complete.cases(bc_data), ] %>% .[, c(11, 2:10)]
```

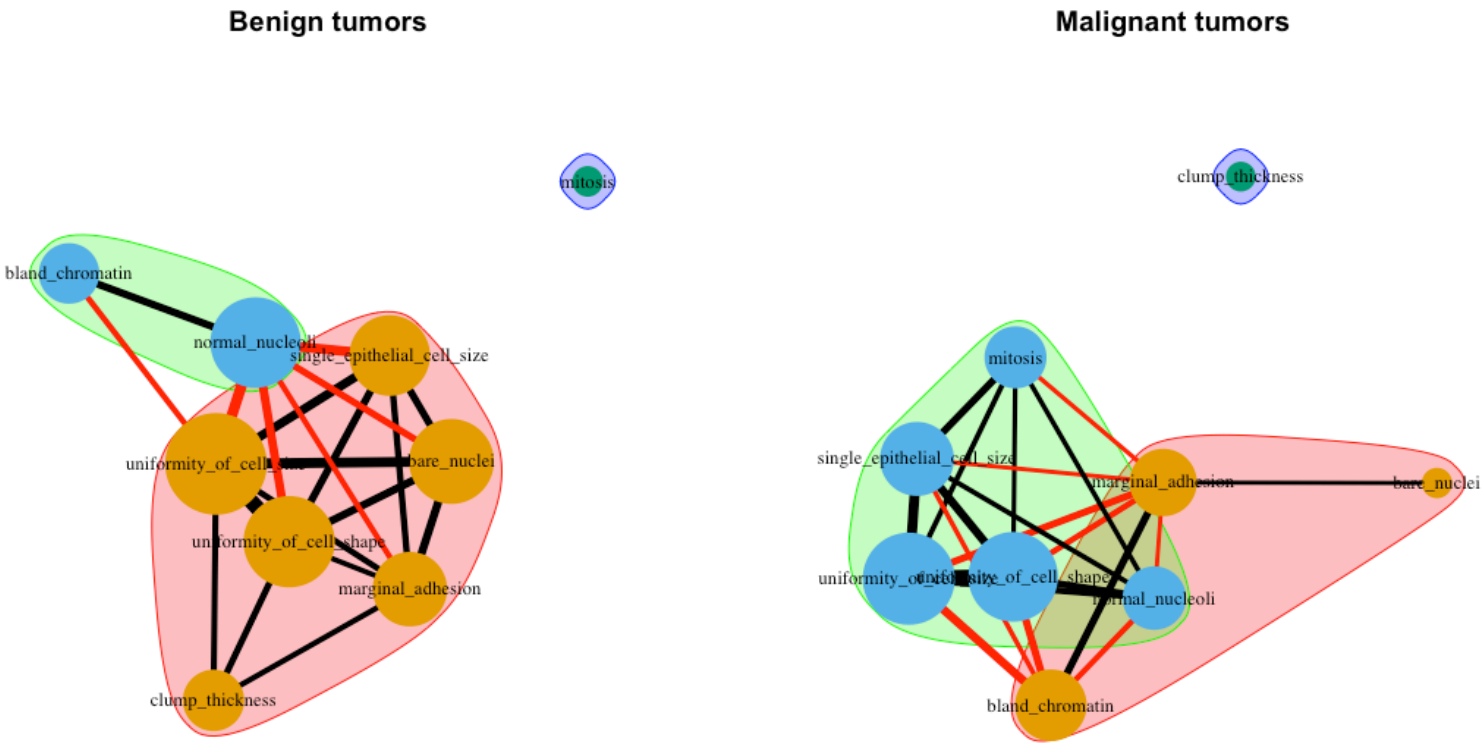
- or impute with the mice package

Response variable for classification

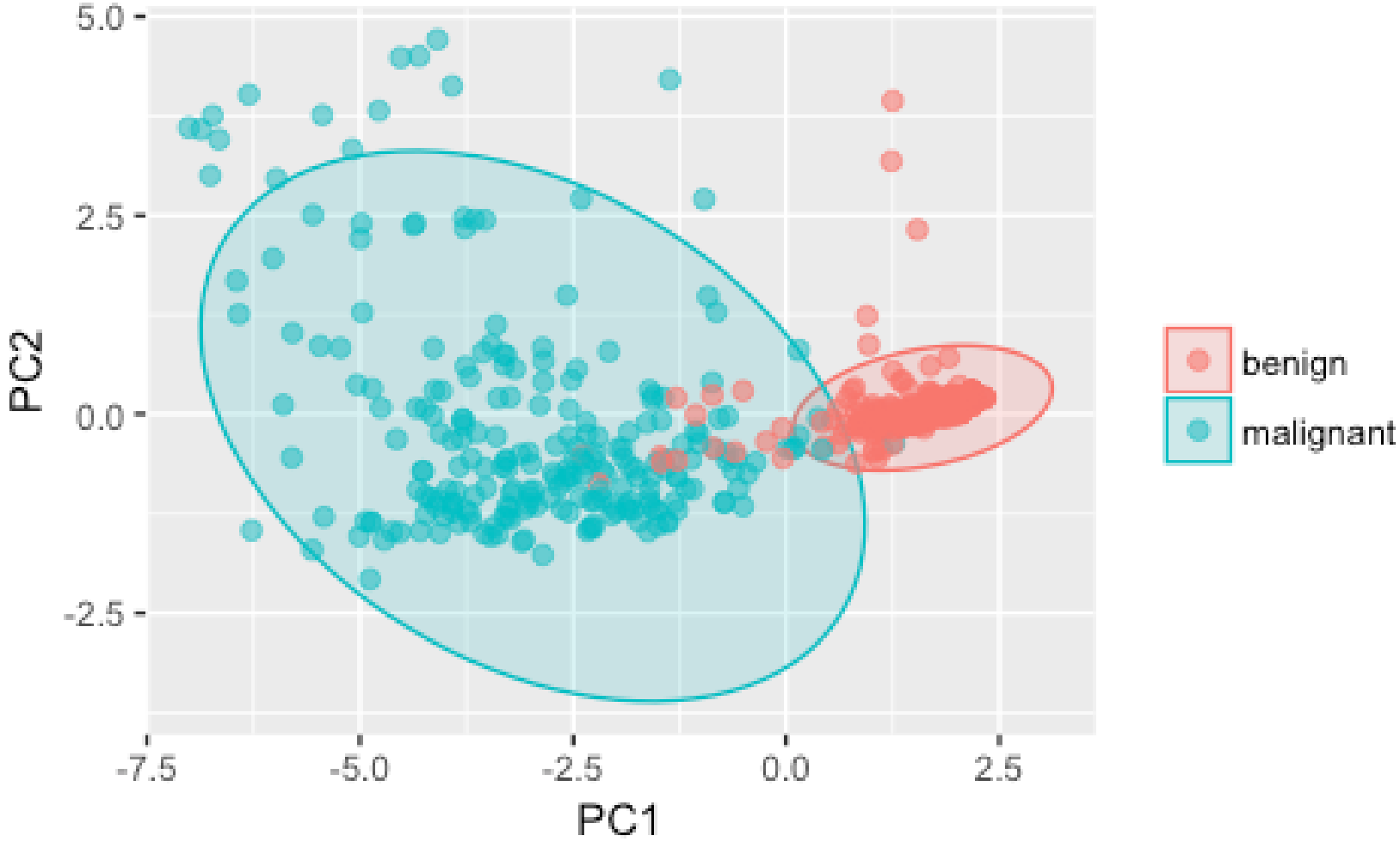
```
ggplot(bc_data, aes(x = classes, fill = classes)) + geom_bar()
```

- Consider balancing of response classes!!!

Feature correlation graphs



Principal Component Analysis



Multidimensional Scaling

t-SNE dimensionality reduction

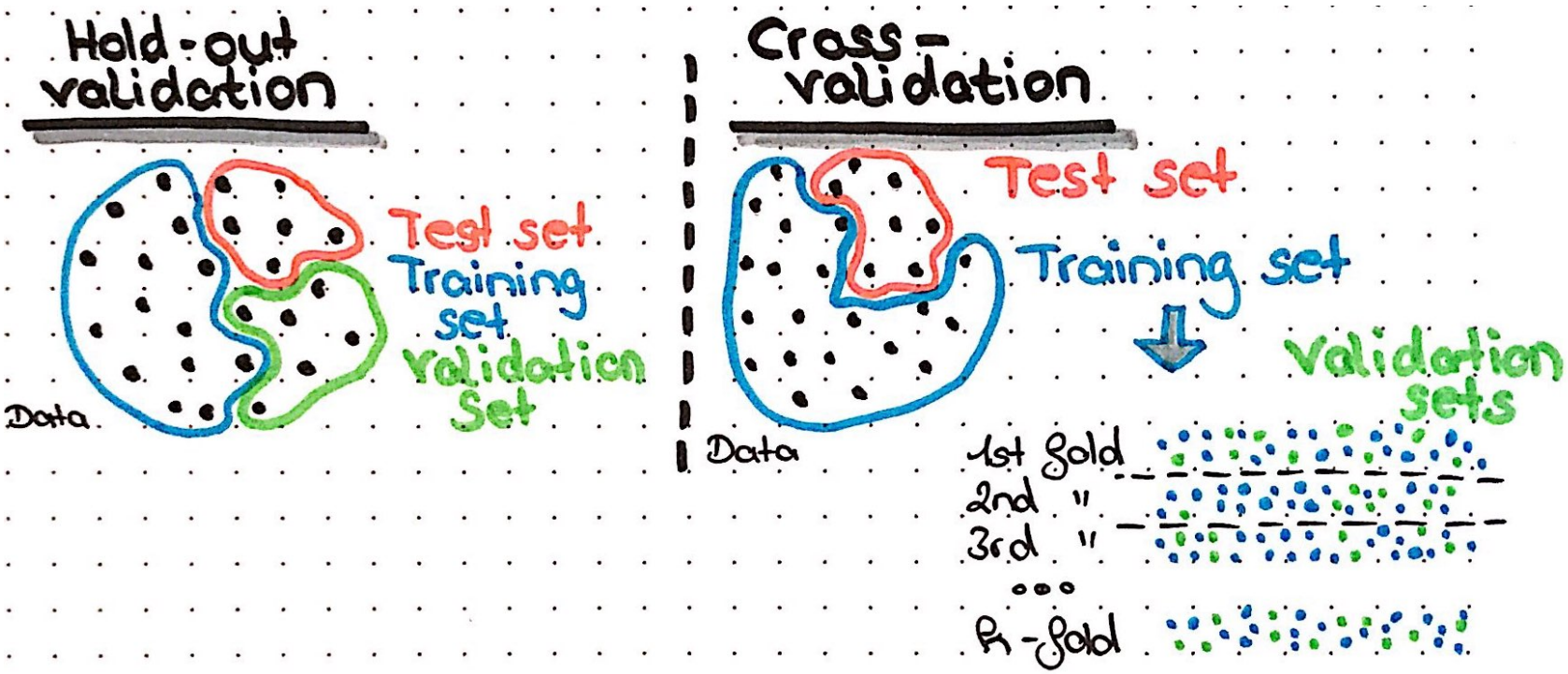
ML with caret

Training, validation & testing

- balance between generalization and specificity
- to prevent over-fitting!
- validation sets or cross-validation

Training, validation & testing

- balance between generalization and specificity
- to prevent over-fitting!
- validation sets or cross-validation



Training, validation and test data

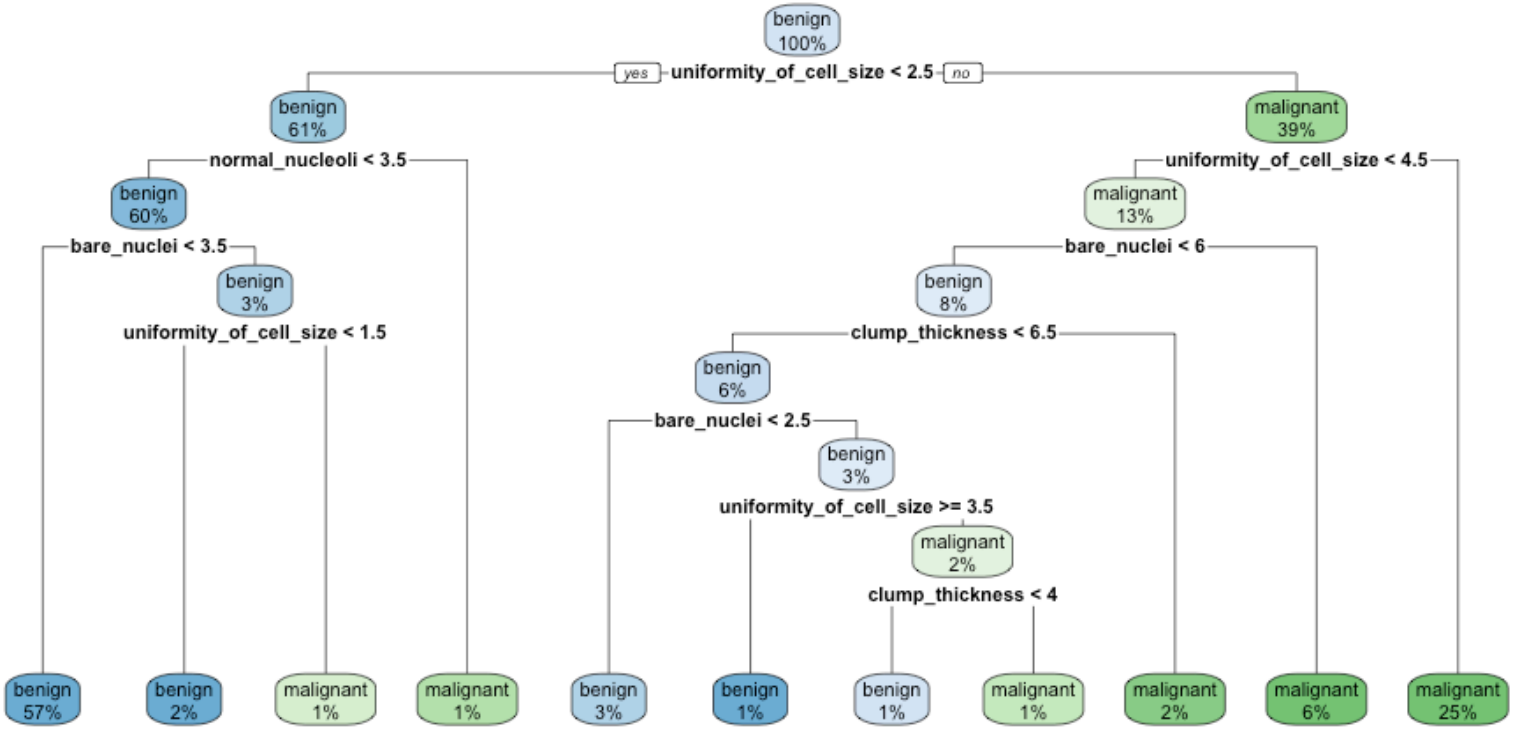
```
library(caret)
set.seed(42)
index <- createDataPartition(bc_data$classes, p = 0.7, list = FALSE)
train_data <- bc_data[index, ]
test_data  <- bc_data[-index, ]
```

- the main function in caret

```
?caret::train
```

This function sets up a grid of tuning parameters for a number of classification and regression routines, fits each model and calculates a resampling based performance measure.

Decision trees



Random Forests

```
set.seed(42)
model_rf <- caret::train(classes ~ .,
                         data = train_data,
                         method = "rf",
                         preProcess = c("scale", "center"),
                         trControl = trainControl(method = "repeatedcv",
                                                  number = 10,
                                                  repeats = 10,
                                                  savePredictions = TRUE,
                                                  verboseIter = FALSE))
```

```
model_rf$finalModel$confusion
```

```
##           benign malignant class.error
## benign       304         7  0.02250804
## malignant      5       163  0.02976190
```

Random Forests

```
model_rf
```

```
## Random Forest
##
## 479 samples
##   9 predictor
##   2 classes: 'benign', 'malignant'
##
## Pre-processing: scaled (9), centered (9)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 432, 431, 431, 431, 431, 431, ...
## Resampling results across tuning parameters:
##
##   mtry  Accuracy   Kappa
##   2     0.9776753  0.9513499
##   5     0.9757957  0.9469999
##   9     0.9714200  0.9370285
##
## Accuracy was used to select the optimal model using the largest value.
```

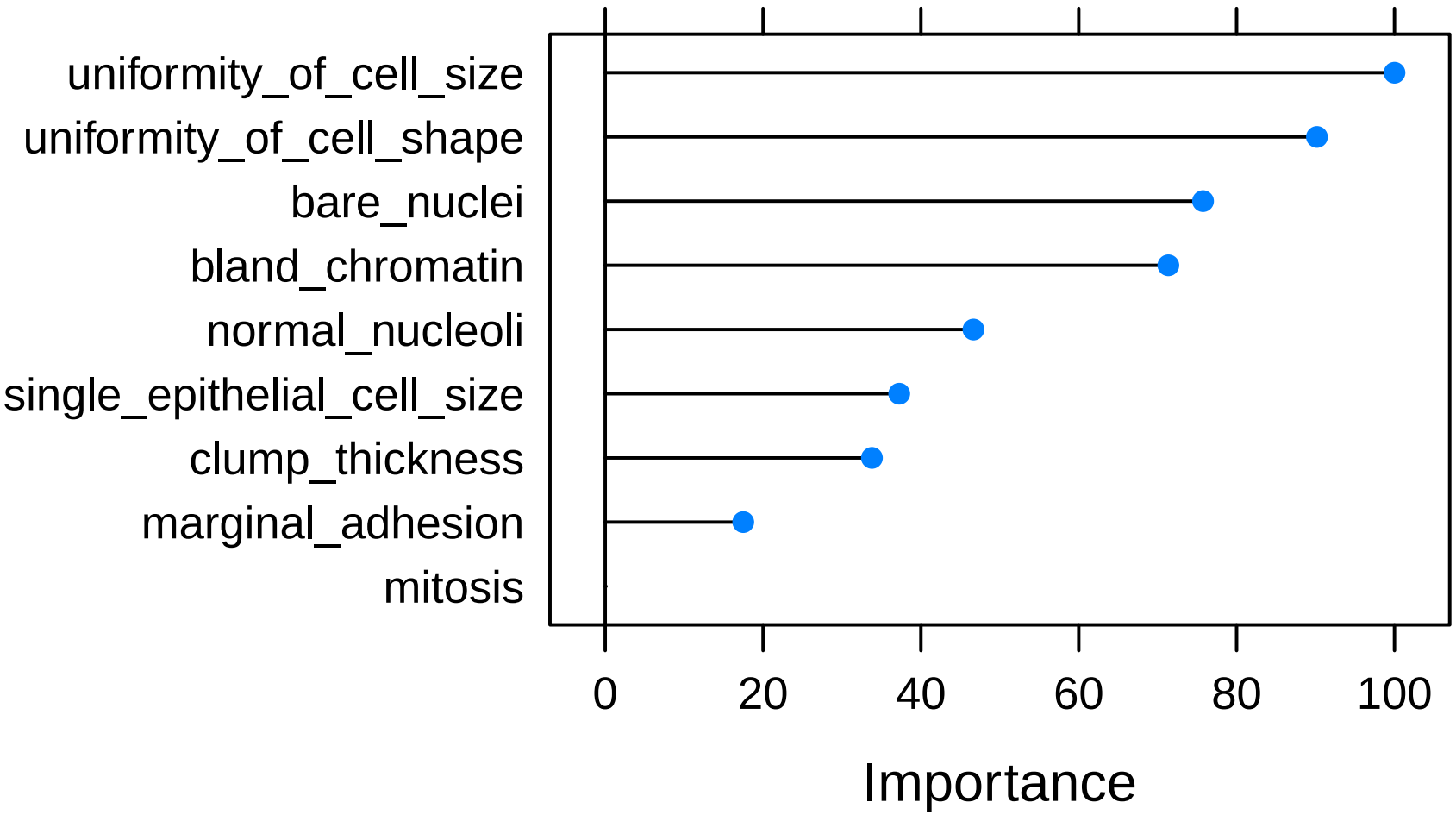
Balancing classes

- e.g. with downsampling

```
set.seed(42)
model_rf_down <- caret::train(classes ~ .,
                              data = train_data,
                              method = "rf",
                              preProcess = c("scale", "center"),
                              trControl = trainControl(method = "repeatedcv",
                                                       number = 10,
                                                       repeats = 10,
                                                       savePredictions = TRUE,
                                                       verboseIter = FALSE,
                                                       sampling = "down"))
```

Feature Importance

```
importance <- varImp(model_rf, scale = TRUE)
plot(importance)
```



Predictions on test data

```
confusionMatrix(predict(model_rf, test_data), as.factor(test_data$classes))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  benign malignant
##   benign       128         4
##   malignant      5        67
##
##                Accuracy : 0.9559
##                  95% CI : (0.9179, 0.9796)
##     No Information Rate : 0.652
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9031
##  Mcnemar's Test P-Value : 1
##
##             Sensitivity : 0.9624
##             Specificity : 0.9437
```

Extreme gradient boosting trees

- available models in caret: https://topepo.github.io/caret

```
set.seed(42)
model_xgb <- caret::train(classes ~ .,
                          data = train_data,
                          method = "xgbTree",
                          preProcess = c("scale", "center"),
                          trControl = trainControl(method = "repeatedcv",
                                                   number = 10,
                                                   repeats = 10,
                                                   savePredictions = TRUE,
                                                   verboseIter = FALSE))
```

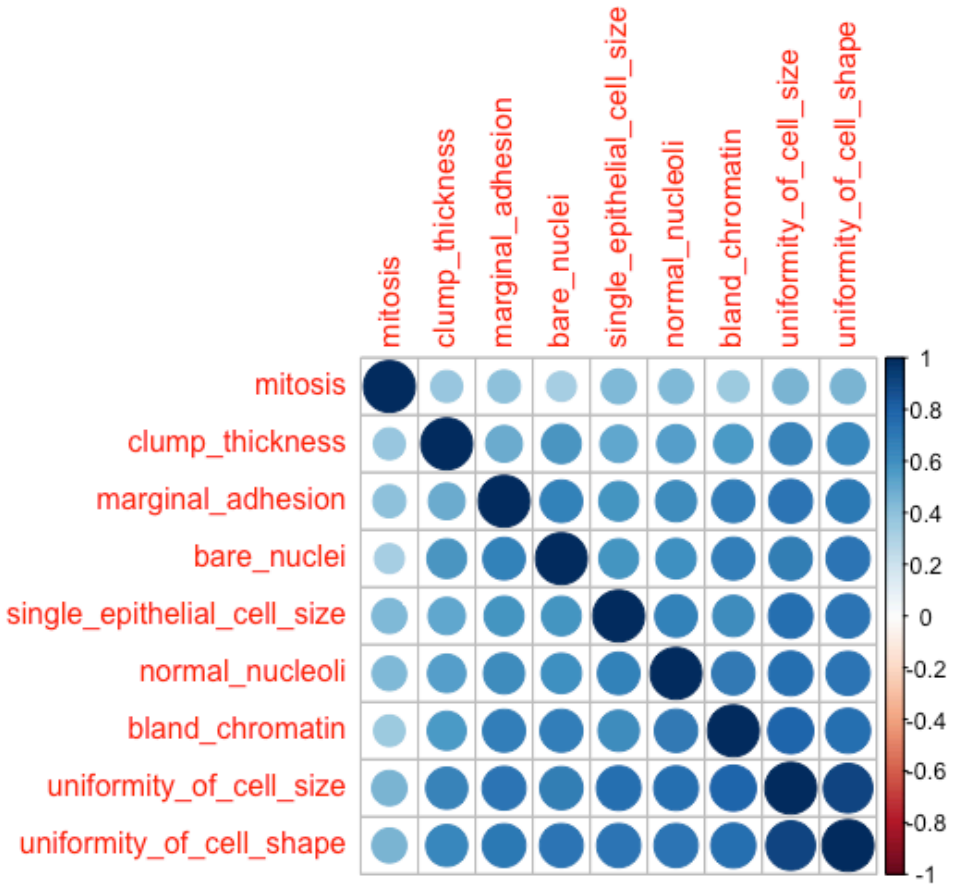
Extreme gradient boosting trees

```
model_xgb
```

```
## eXtreme Gradient Boosting
##
## 479 samples
##   9 predictor
##   2 classes: 'benign', 'malignant'
##
## Pre-processing: scaled (9), centered (9)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 432, 431, 431, 431, 431, 431, ...
## Resampling results across tuning parameters:
##
##   eta  max_depth  colsample_bytree  subsample  nrounds  Accuracy
##   0.3  1          0.6               0.50        50      0.9567788
##   0.3  1          0.6               0.50       100      0.9544912
##   0.3  1          0.6               0.50       150      0.9513572
##   0.3  1          0.6               0.75        50      0.9576164
##   0.3  1          0.6               0.75       100      0.9536448
```

Feature Selection

- correlation
- Recursive Feature elimination (RFE)
- Genetic Algorithm (GA)



Hyperparameter tuning with caret

- Cartesian Grid

```
grid <- expand.grid(mtry = c(1:10))
train(..., tuneGrid = grid)
```

- Random Search

```
trainControl(..., tuneGrid = grid, search = "random")
```

ML with h2o

ML with h2o

```
library(h2o)
h2o.init(nthreads = -1)
```

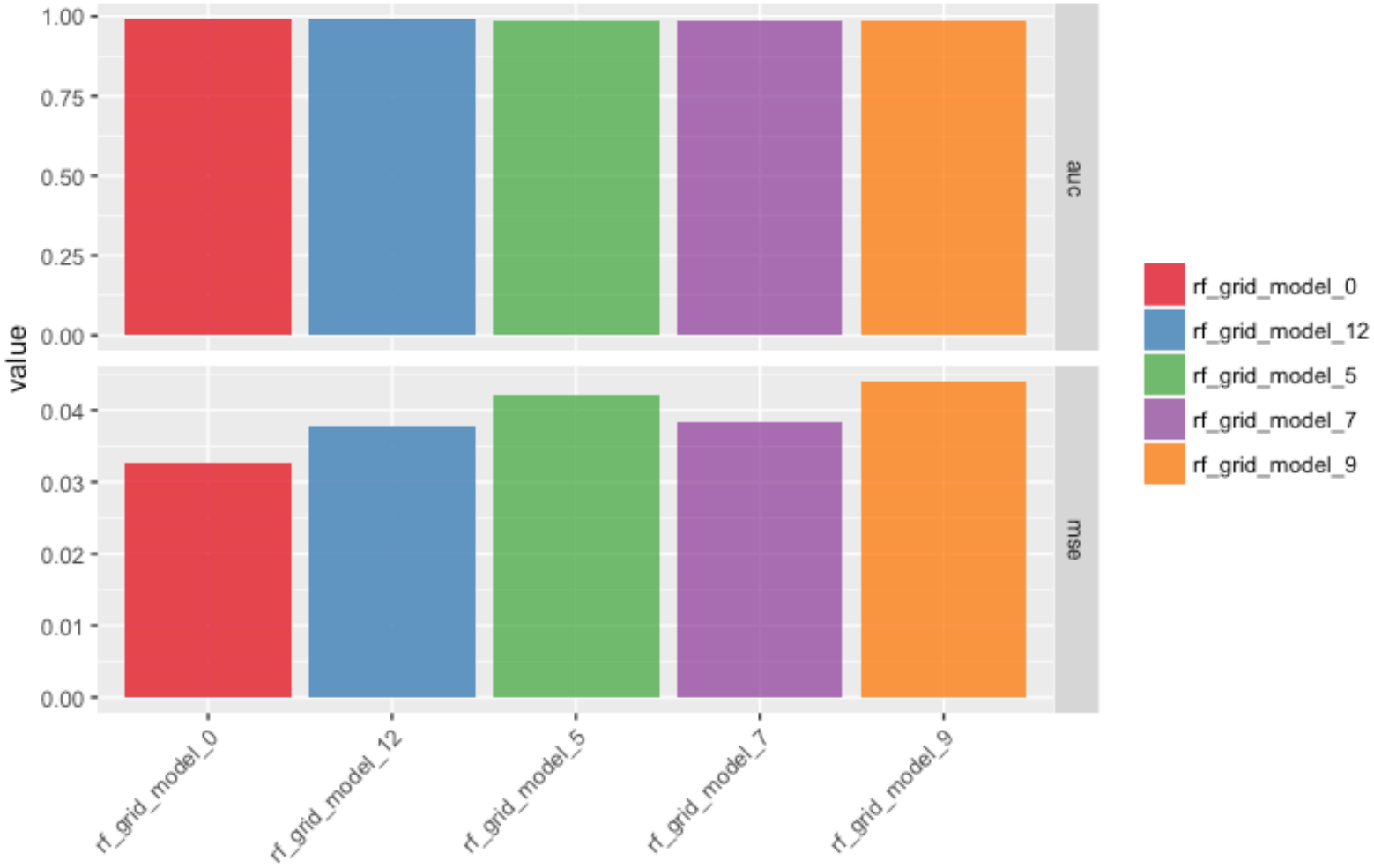
```
##  Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         13 minutes 18 seconds
##     H2O cluster timezone:       Europe/Berlin
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.20.0.2
##     H2O cluster version age:    6 days
##     H2O cluster name:           H2O_started_from_R_shiringlander_jrj894
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   3.13 GB
##     H2O cluster total cores:    8
##     H2O cluster allowed cores:  8
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
```

Grid search with h2o

```
hyper_params <- list(
                ntrees = c(25, 50, 75, 100),
                max_depth = c(10, 20, 30),
                min_rows = c(1, 3, 5)
                )

search_criteria <- list(
                  strategy = "RandomDiscrete",
                  max_models = 50,
                  max_runtime_secs = 360,
                  stopping_rounds = 5,
                  stopping_metric = "AUC",
                  stopping_tolerance = 0.0005,
                  seed = 42
                  )
```

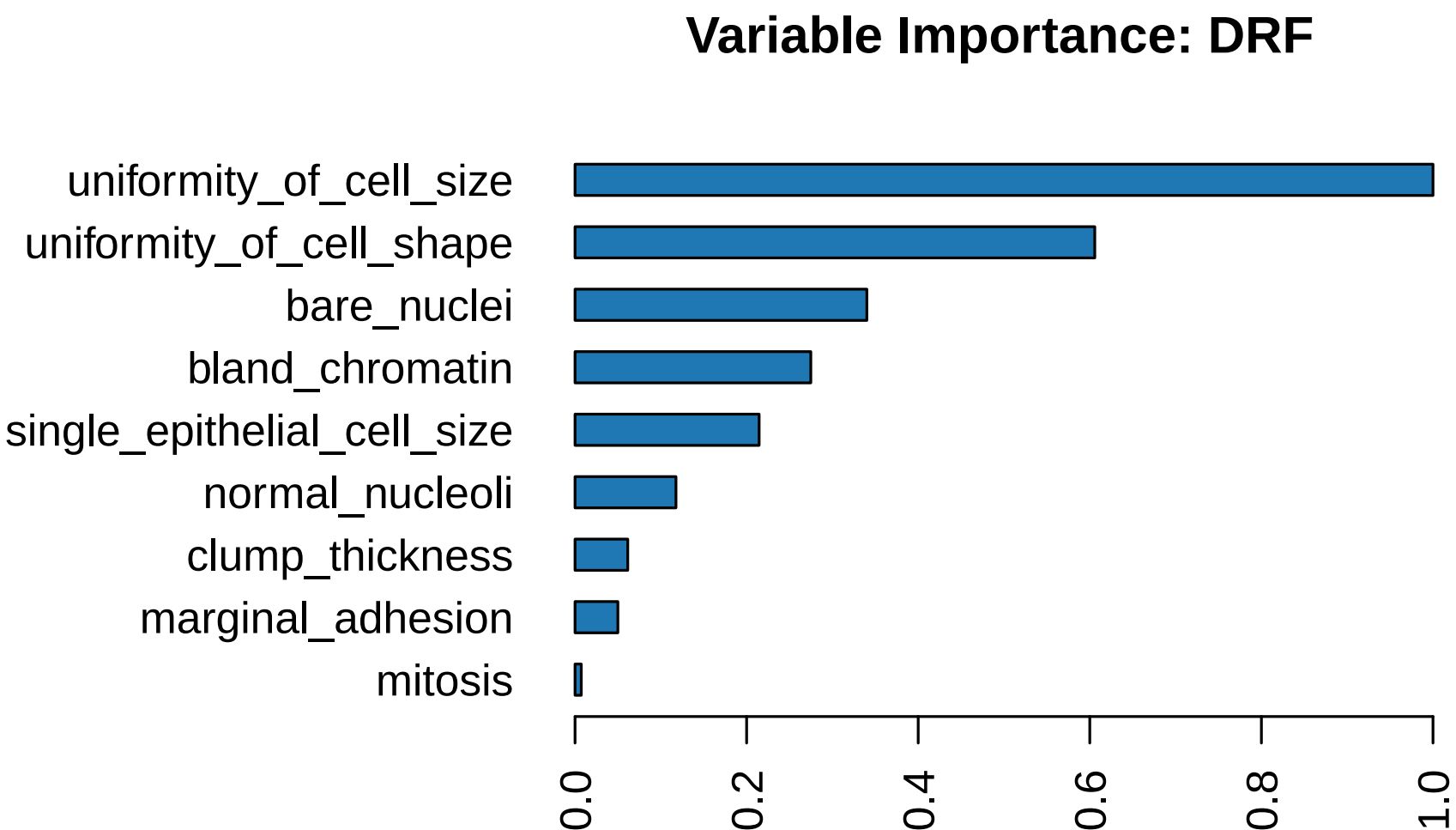
Grid search with h2o



Evaluate model performance

- Variable importance

```
h2o.varimp_plot(rf_model)
```



Evaluate model performance

```
h2o.mean_per_class_error(rf_model, train = TRUE, valid = TRUE, xval = TRUE)
```

```
##      train      valid       xval
## 0.02196246 0.02343750 0.02515735
```

```
h2o.confusionMatrix(rf_model, valid = TRUE)
```

```
## Confusion Matrix (vertical: actual; across: predicted)  for max f1 @ threshold = 0.5333333
##           benign malignant    Error    Rate
## benign        61         3 0.046875   =3/64
## malignant      0        38 0.000000   =0/38
## Totals        61        41 0.029412  =3/102
```

Evaluate model performance

```
perf <- h2o.performance(rf_model, test)

h2o.logloss(perf)
```

```
## [1] 0.1072519
```

```
h2o.mse(perf)
```

```
## [1] 0.03258482
```

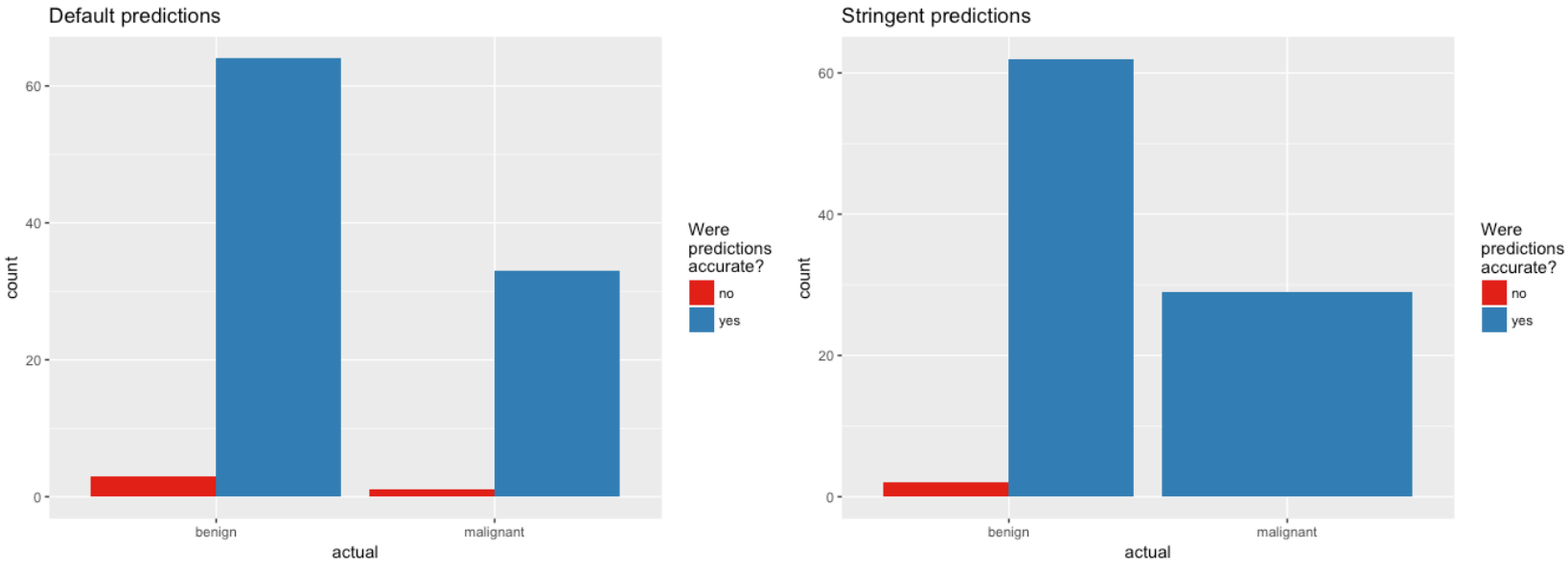
```
h2o.auc(perf)
```

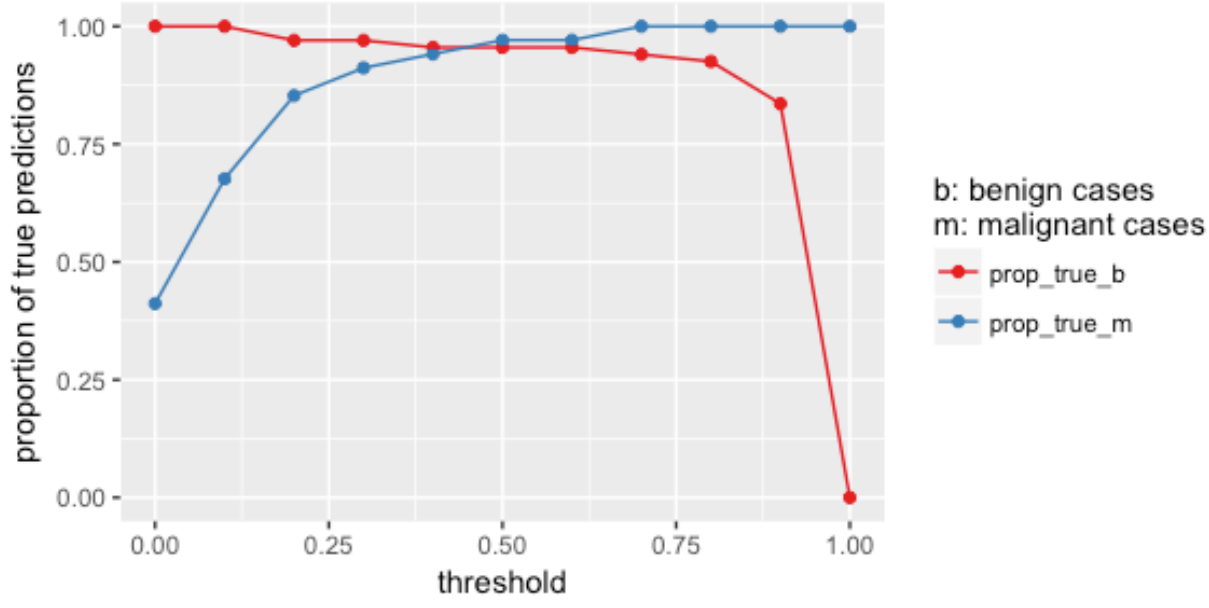
```
## [1] 0.9916594
```

Evaluate model performance

```
plot(perf)
```

Evaluate model performance

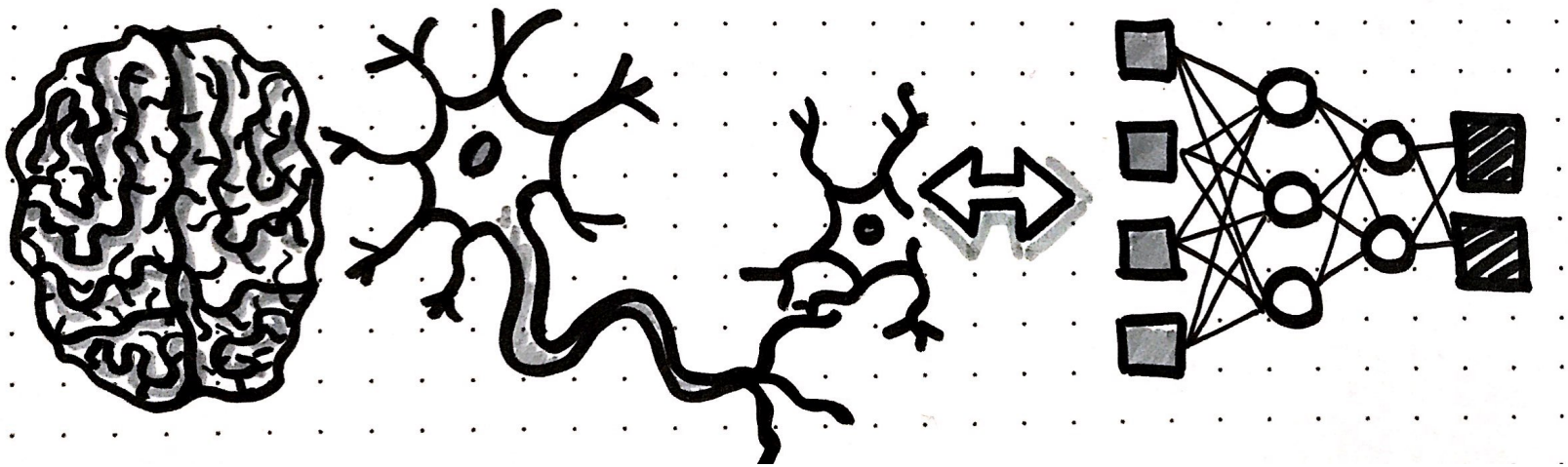




Deep Dive into Neural Networks

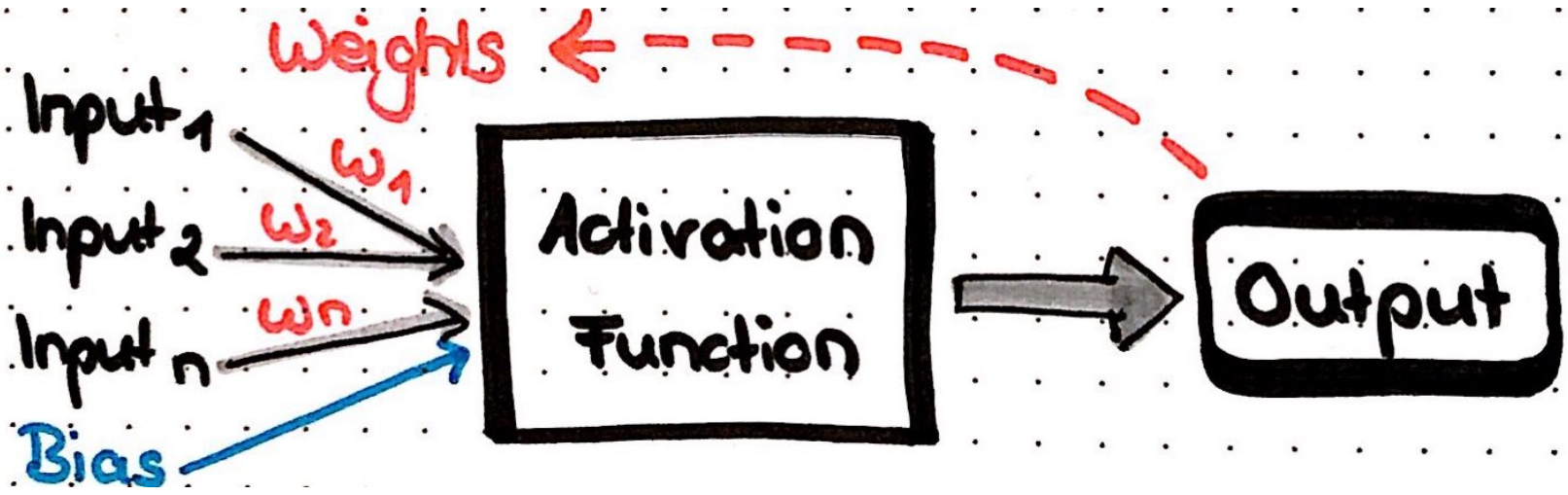
Introduction to Neural Networks (NN)

- machine learning framework
- attempts to mimic the learning pattern of the brain (biological neural networks)
- Artificial Neural Networks = ANNs



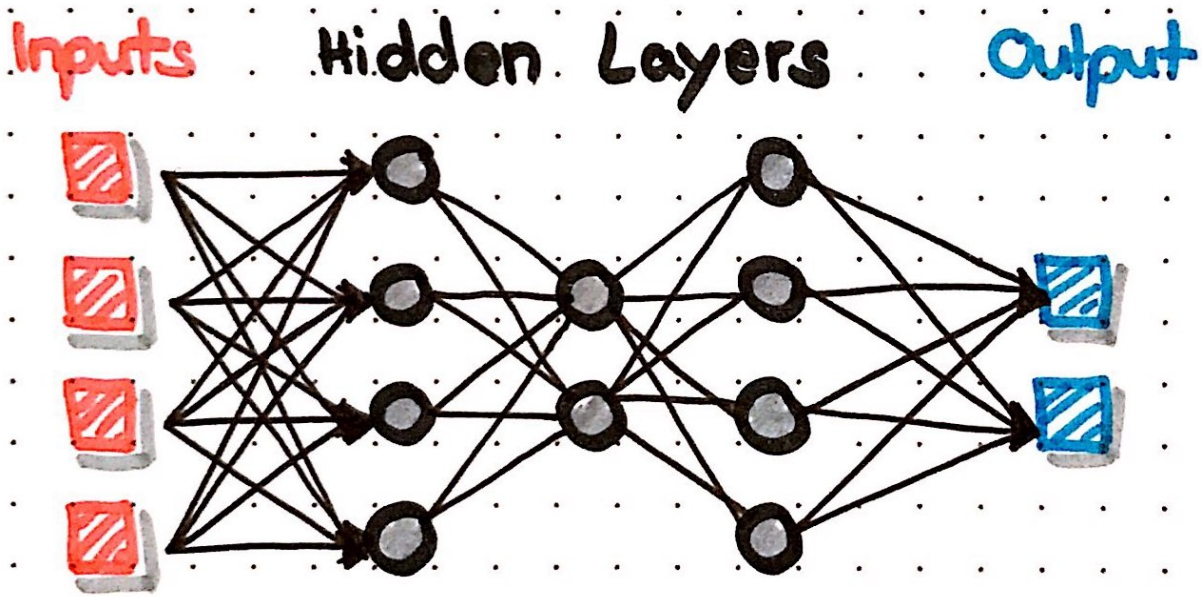
Perceptrons

- Input (multiplied by weight)
- Bias
- Activation function
- Output



Multi-Layer Perceptrons (MLP)

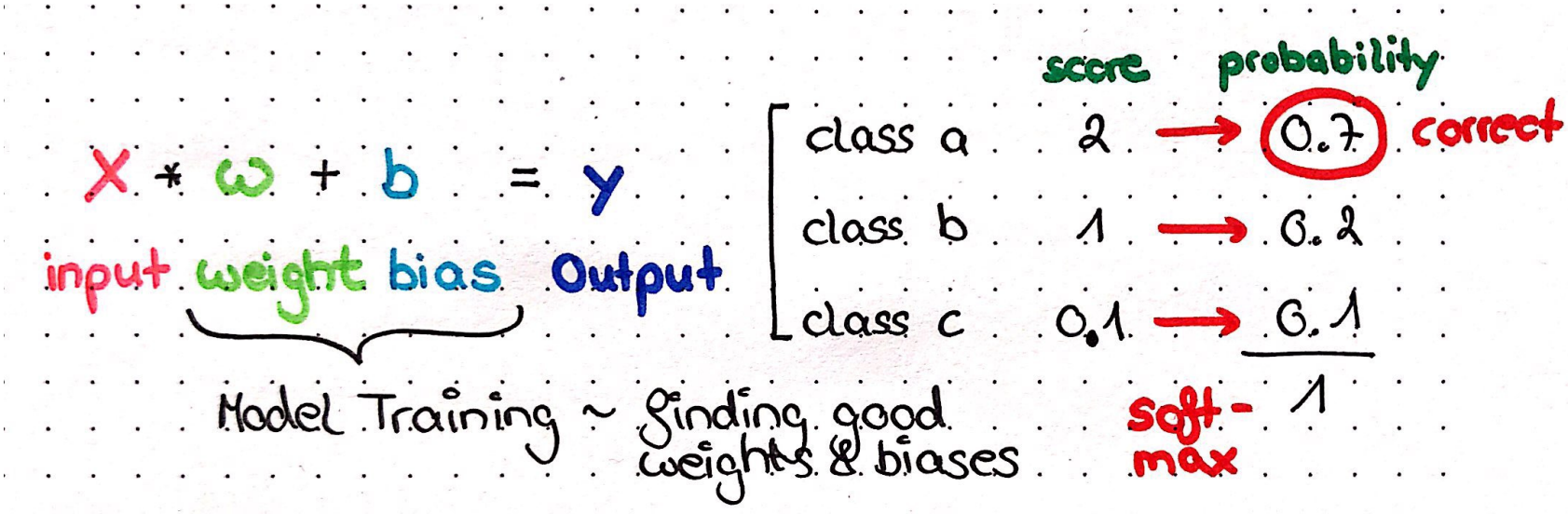
- multiple layers of perceptrons
- input
- output
- hidden layers



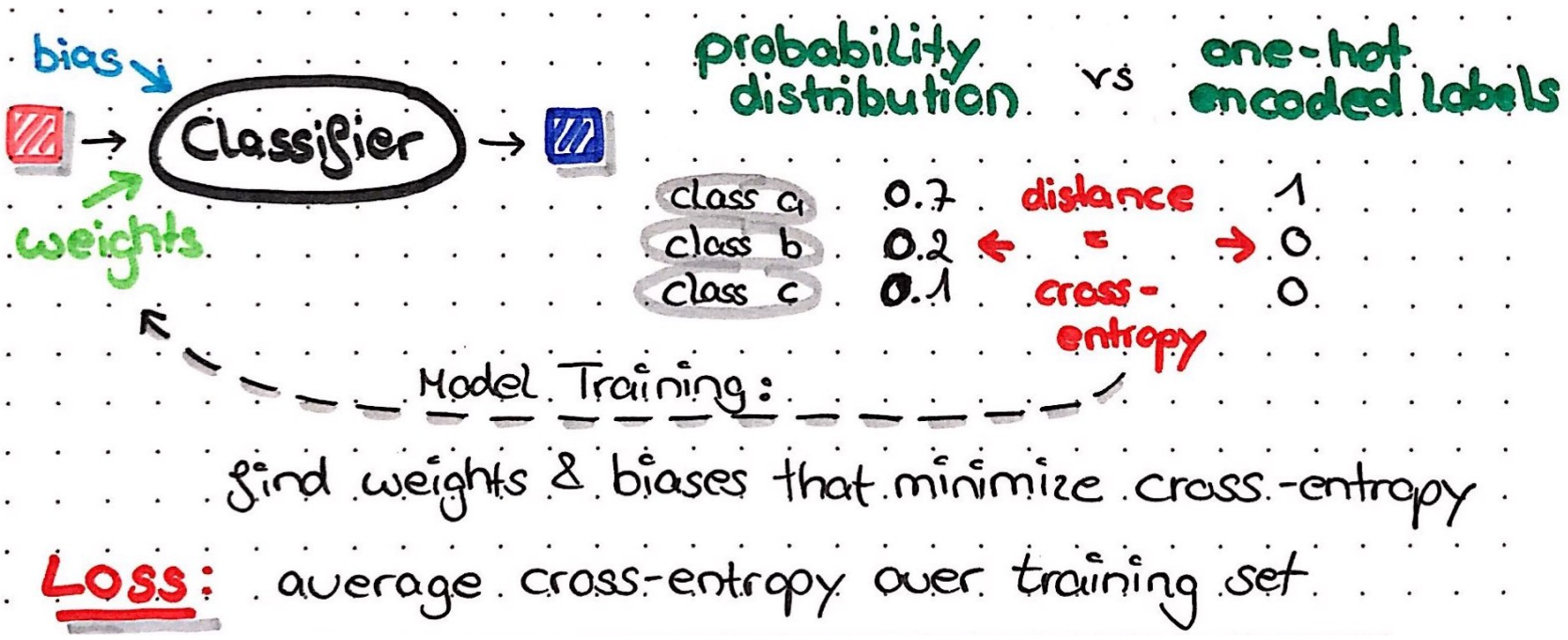
How do Neural Nets learn?

Classfication with supervised learning - Softmax

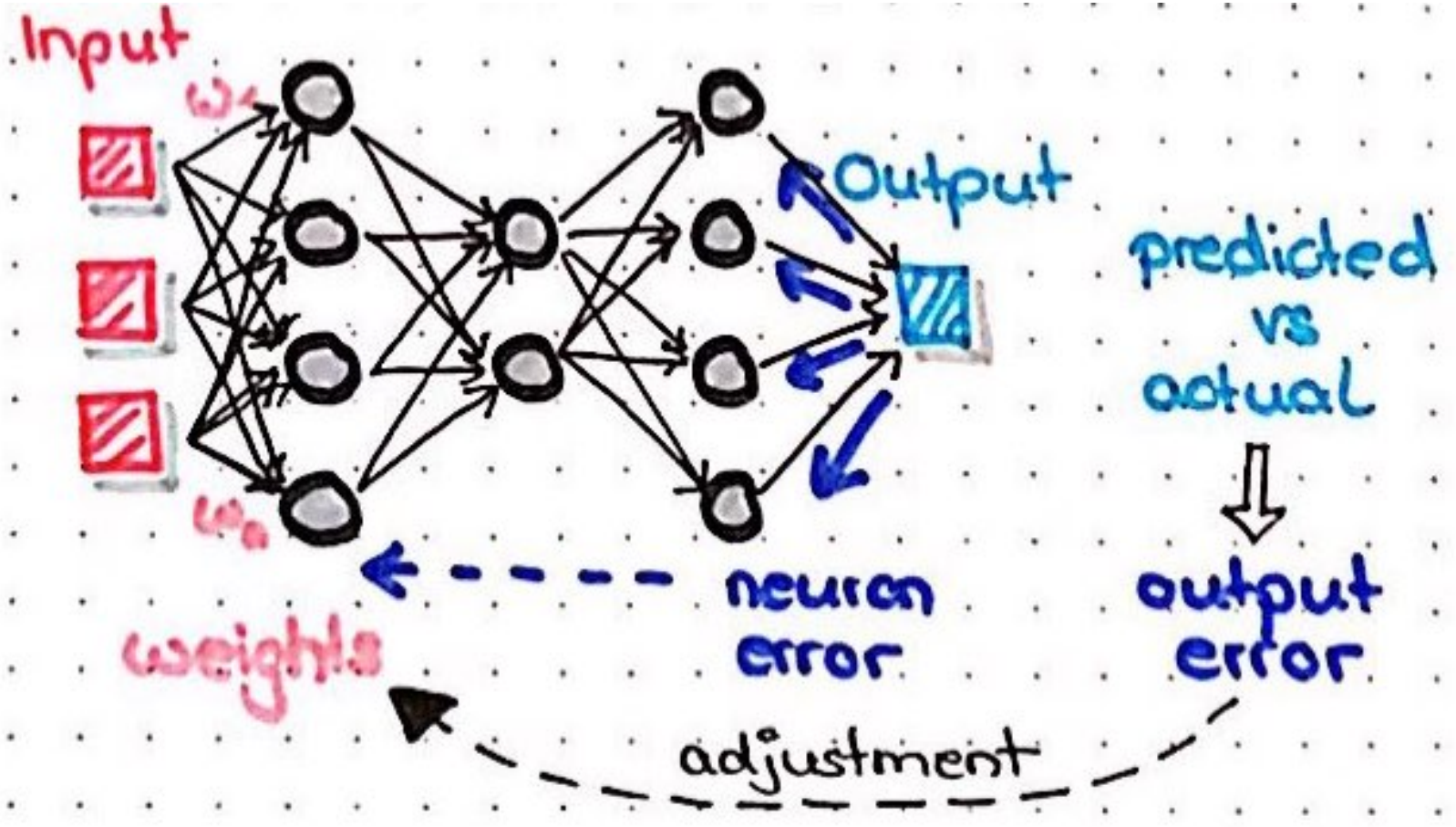
- input = features
- weights
- biases
- output = classes



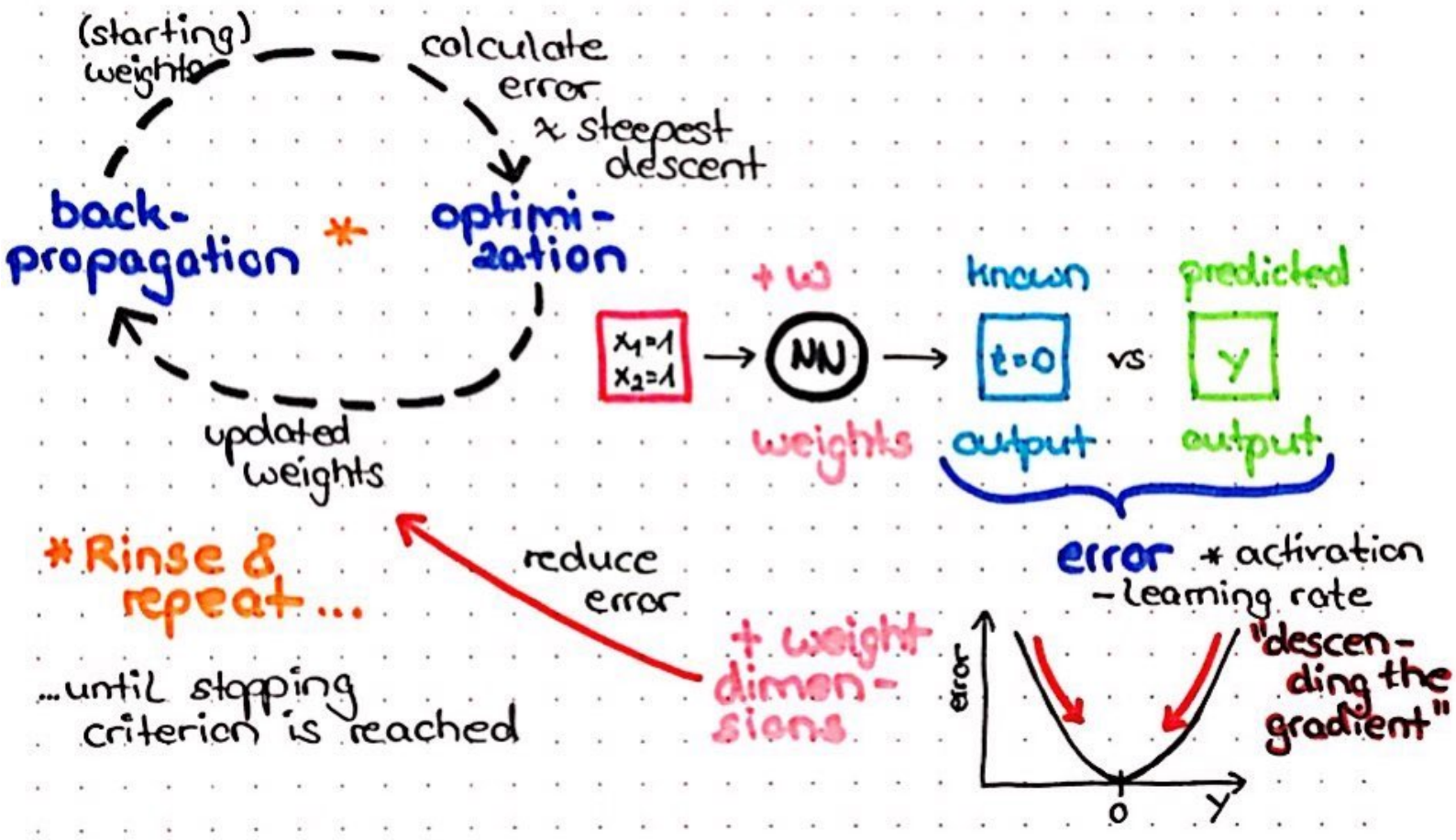
Cross-entropy



Backpropagation



Gradient Descent Optimization



Training neural nets in R

Features & data preprocessing

```
library(ISLR)
```

```
print(head(College))
```

	Private	Apps	Accept	Enroll	Top10perc	Top25perc	F.Undergrad	P.Undergrad	Outstate	Room.Board	Books	Personal	PhD	Terminal	S.F.Ratio	perc.alumni	Expend	Grad.Rate
Abilene Christian University	Yes	1660.00	1232.00	721.00	23.00	52.00	2885.00	537.00	7440.00	3300.00	450.00	2200.00	70.00	78.00	18.10	12.00	7041.00	60.00
Adelphi University	Yes	2186.00	1924.00	512.00	16.00	29.00	2683.00	1227.00	12280.00	6450.00	750.00	1500.00	29.00	30.00	12.20	16.00	10527.00	56.00
Adrian College	Yes	1428.00	1097.00	336.00	22.00	50.00	1036.00	99.00	11250.00	3750.00	400.00	1165.00	53.00	66.00	12.90	30.00	8735.00	54.00
Agnes Scott College	Yes	417.00	349.00	137.00	60.00	89.00	510.00	63.00	12960.00	5450.00	450.00	875.00	92.00	97.00	7.70	37.00	19016.00	59.00
Alaska Pacific University	Yes	193.00	146.00	55.00	16.00	44.00	249.00	869.00	7560.00	4120.00	800.00	1500.00	76.00	72.00	11.90	2.00	10922.00	15.00
Albertson College	Yes	587.00	479.00	158.00	38.00	62.00	678.00	41.00	13500.00	3335.00	500.00	675.00	67.00	73.00	9.40	11.00	9727.00	55.00

```
# Create vector of column max and min values
maxs <- apply(College[, 2:18], 2, max)
mins <- apply(College[, 2:18], 2, min)

# Use scale() and convert the resulting matrix to a data frame
scaled.data <- as.data.frame(scale(College[,2:18],
                                   center = mins,
                                   scale = maxs - mins))
```

Train and test split

```
# Convert column Private from Yes/No to 1/0
Private = as.numeric(College$Private)-1
data = cbind(Private,scaled.data)

library(caret)
set.seed(42)

# Create split
idx <- createDataPartition(data$Private, p = .75, list = FALSE)
train <- data[idx, ]
test  <- data[-idx, ]
```

Modeling

```
# 10 x 10 repeated CV
fitControl <- trainControl(method = "repeatedcv",
                           number = 5,
                           repeats = 3)
```

```
nn <- train(factor(Private) ~ .,
            data = train,
            method = "nnet",
            trControl = fitControl,
            verbose= FALSE)
```

```
## # weights:  20
## initial  value 309.585951
## iter  10 value 86.596132
## iter  20 value 67.277050
## iter  30 value 61.130402
## iter  40 value 59.828879
## iter  50 value 59.689365
## iter  60 value 59.548075
```

Predictions and Evaluations

```
# Compute predictions on test set
predicted.nn.values <- predict(nn, test[2:18])

# print results
print(head(predicted.nn.values, 3))
```

```
## [1] 1 1 1
## Levels: 0 1
```

```
table(test$Private, predicted.nn.values)
```

```
##     predicted.nn.values
##       0   1
##   0  47   3
##   1   4 140
```

Thank you!

... and stay in contact

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