Libraries

```
library(tidyverse)
library(mlbench)
library(ggfortify)
library(GGally)
library(scagnostics)
library(mlr)
```

Dataset

Pima Indians Diabetes dataset from *mlbench* package.

```
data(PimaIndiansDiabetes)
PimaIndiansDiabetes %>%
  head()
##   pregnant glucose pressure triceps insulin mass pedigree age
diabetes
## 1        6     148       72      35       0 33.6    0.627  50
pos
## 2        1      85       66      29       0 26.6    0.351  31
neg
## 3        8     183       64       0       0 23.3    0.672  32
pos
## 4        1      89       66      23      94 28.1    0.167  21
neg
## 5        0     137       40      35     168 43.1    2.288  33
pos
## 6        5     116       74       0       0 25.6    0.201  30
neg
```

Colors

- set colorblind-friendly palettes

```
# The palette with grey:
cbp1 <- c("#999999", "#E69F00", "#56B4E9", "#009E73",
          "#F0E442", "#0072B2", "#D55E00", "#CC79A7")
ggplot <- function(...) ggplot2::ggplot(...) +
  scale_color_manual(values = cbp1) +
  scale_fill_manual(values = cbp1) + # note: needs to be overridden
when using continuous color scales
  theme_bw()
```

Visualizing Machine Learning models

Visualizing different steps of the machine learning pipeline can help us

- explore the data (EDA),
- understand the data (and identify potential problems),
- pre-process the data in a suitable way for optimal model performance,

- supervise the learning process,
- optimize modeling,
- interpret the model and
- compare and evaluate model predictions.

Visualization also greatly simplifies communication of our model and results to decision-makers or the public.

Exploratory Data Analysis

Exploratory Data Analysis (EDA) is the backbone of data analysis, including those that result in a machine learning model. EDA helps us to understand the data we are working with and put it into context, so that we are able to ask the right questions (or to put our questions into the right frame). It also helps us take appropriate measures for cleaning, normalization/transformation, dealing with missing values, feature preparation and engineering, etc. Particularly if our machine learning model is trained on a limited dataset (but not only then!), appropriate data preparation can vastly improve the machine learning process: models will often train faster and achieve higher accuracy.

An essential part of EDA is data visualization.

Typically, we want to start by exploring potential sources of errors in our data, like

- **wrong/useless data types** (sometimes data types are automatically set in a way that is not useful for our analysis, like *factors* versus *strings*, or wrong/strange entries in an otherwise numeric column will make it categorical)
- **missing values** (a collection of ways to visualize missingness can be found here),
- **outliers** (for example by plotting a box-plot of continuous variables)

Depending on the number of features/variables we have, it makes sense to look at them all individually and in correlation with each other. Depending on whether we have a categorical or continuous variable, we might be interested in properties that are shown by

- **histograms** (frequency distribution of binned continuous variables),
- **density distribution** (normalized distribution of continuous variables) or
- **bar-plots** (shows counts of categorical variables).

If our target variable is categorical, we will want to look at potential imbalances between the classes. Class imbalance will strongly affect the machine learning modeling process and will require us to consider up-/downsampling or similar techniques before we train a model.

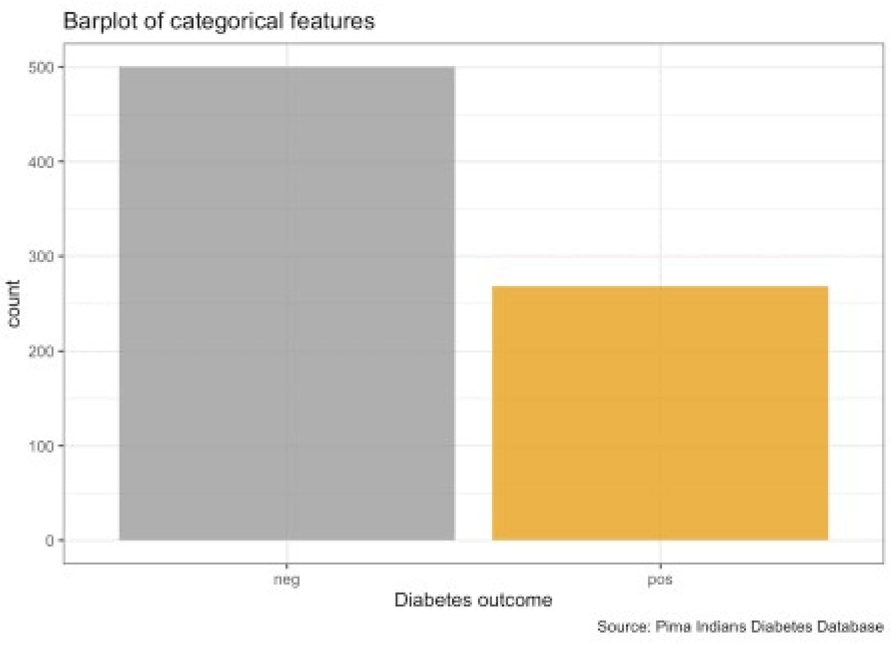
Correlation analysis can show us, for example

- how our **target/dependent variable correlates with the remaining features** (often, just by looking at the correlation, we can identify one ore more feature that will have a strong impact on predicting the target because they are strongly correlated) or
- whether some of the **independent variables/features correlate with each other** (**multicolinearity**; we might want to consider removing strongly correlated features, so that they won't contribute the "same" information multiple times to the model and thus lead to overfitting).

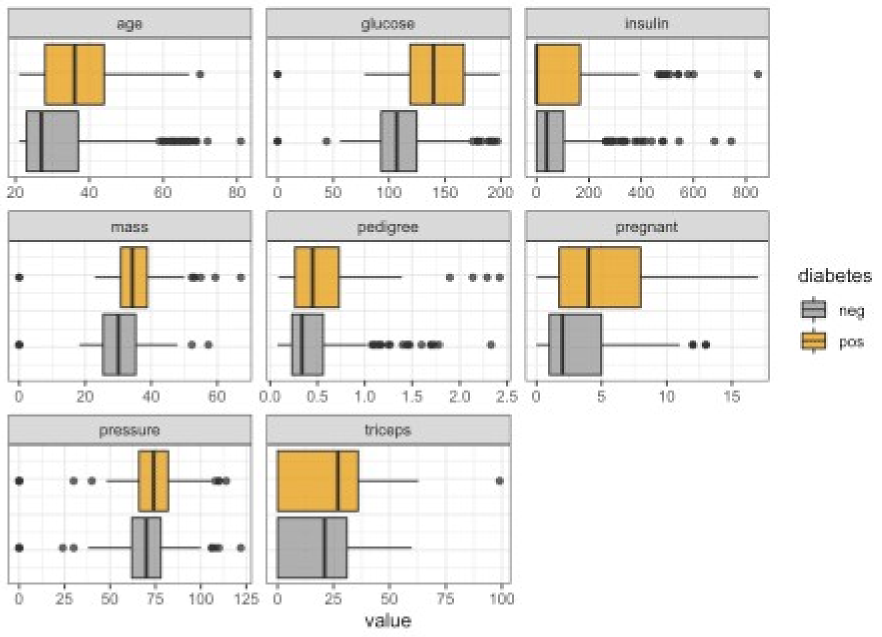
Additional methods can be used to visualize groups of related features. These methods are often especially useful if we have a large dataset with a large feature set (highly dimensional data). Some of these methods for visualizing groups of related features and/or for comparing multiple variables and visualizing their relationships are:

- **Dimensionality reduction**:
    - *Principal Component Analysis* (PCA, linear, shows as much variation in data as possible)
    - *Multidimensional scaling* (MDS, non-linear)
    - *Sammon mapping* (non-linear)
    - *T-Distributed Stochastic Neighbor Embedding* (t-SNE, non-linear)
    - *Uniform Manifold Approximation and Projection* (UMAP, non-linear, faster than T-SNE, often captures global variation better than T-SNE and PCA)
    - *Isometric Feature Mapping Ordination* (Isomap)
- Parallel coordinate plots
- scagnostics

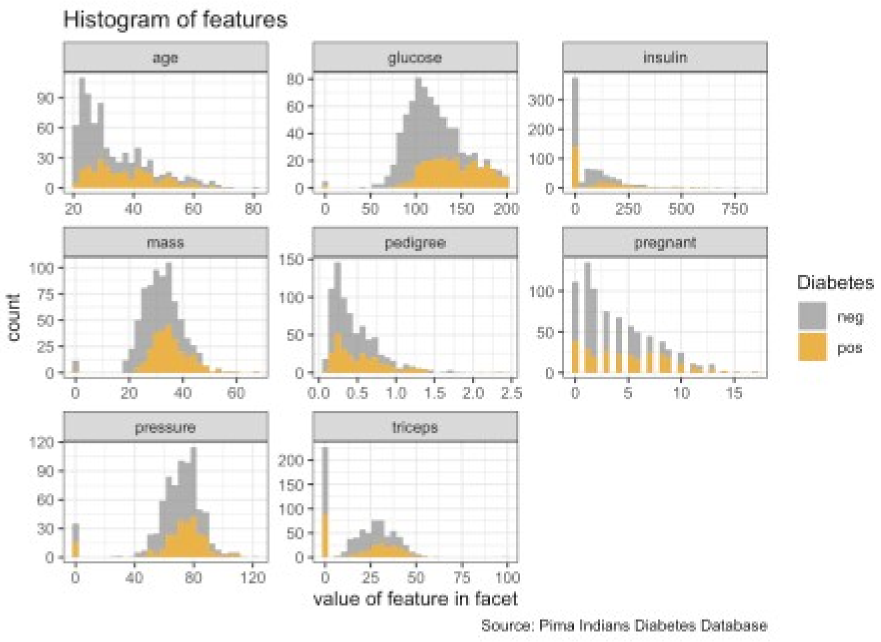
```
# in our dataset,
# continuous variables are
PimaIndiansDiabetes %>%
  dplyr::select(where(is.numeric)) %>%
  head()
##   pregnant glucose pressure triceps insulin mass pedigree age
## 1        6     148       72      35       0 33.6    0.627  50
## 2        1      85       66      29       0 26.6    0.351  31
## 3        8     183       64       0       0 23.3    0.672  32
## 4        1      89       66      23      94 28.1    0.167  21
## 5        0     137       40      35     168 43.1    2.288  33
## 6        5     116       74       0       0 25.6    0.201  30
# 'diabetes' is the only categorical variable is also our target or
dependent variable
PimaIndiansDiabetes %>%
  dplyr::select(!where(is.numeric)) %>%
  head()
##   diabetes
## 1      pos
## 2      neg
## 3      pos
## 4      neg
## 5      pos
## 6      neg
# bar plot of target
PimaIndiansDiabetes %>%
  ggplot(aes(x = diabetes, fill = diabetes)) +
    geom_bar(alpha = 0.8) +
    theme(legend.position = "none") +
    labs(x = "Diabetes outcome",
          y = "count",
        title = "Barplot of categorical features",
        caption = "Source: Pima Indians Diabetes Database")
```



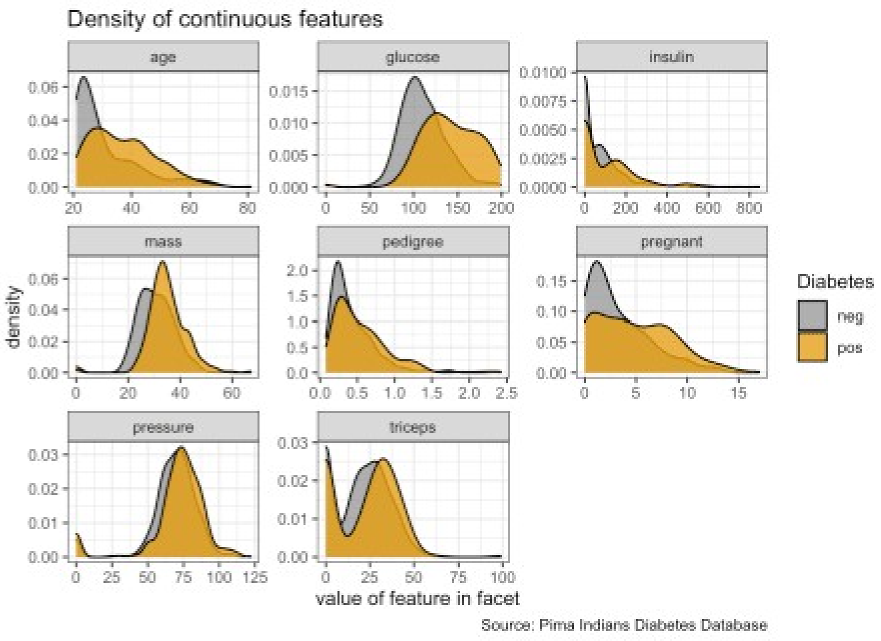
```
# boxplot of continuous features
PimaIndiansDiabetes %>%
  gather("key", "value", pregnant:age) %>%
  ggplot(aes(x = value, fill = diabetes)) +
    facet_wrap(vars(key), ncol = 3, scales = "free") +
    geom_boxplot(alpha = 0.8) +
    theme(axis.text.y = element_blank(),
          axis.ticks.y = element_blank())
```



```
# histogram of features
PimaIndiansDiabetes %>%
  gather("key", "value", pregnant:age) %>%
  ggplot(aes(x = value, fill = diabetes)) +
    facet_wrap(vars(key), ncol = 3, scales = "free") +
    geom_histogram(alpha = 0.8) +
    labs(x = "value of feature in facet",
         y = "count",
         fill = "Diabetes",
        title = "Histogram of features",
        caption = "Source: Pima Indians Diabetes Database")
```



```
# density plot of of features
PimaIndiansDiabetes %>%
  gather("key", "value", pregnant:age) %>%
  ggplot(aes(x = value, fill = diabetes)) +
    facet_wrap(vars(key), ncol = 3, scales = "free") +
    geom_density(alpha = 0.8) +
    labs(x = "value of feature in facet",
          y = "density",
          fill = "Diabetes",
         title = "Density of continuous features",
         caption = "Source: Pima Indians Diabetes Database")
```

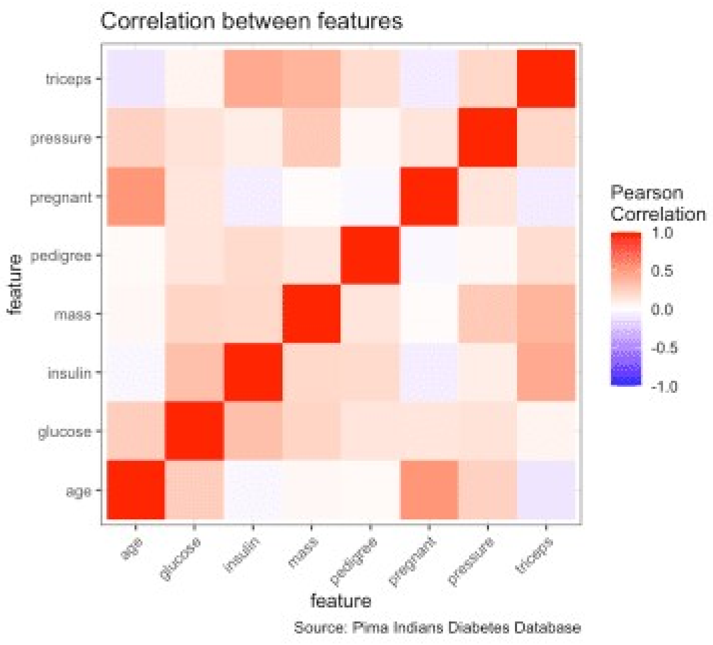


```
# correlation plot of features
mat <- PimaIndiansDiabetes %>%
  dplyr::select(where(is.numeric))

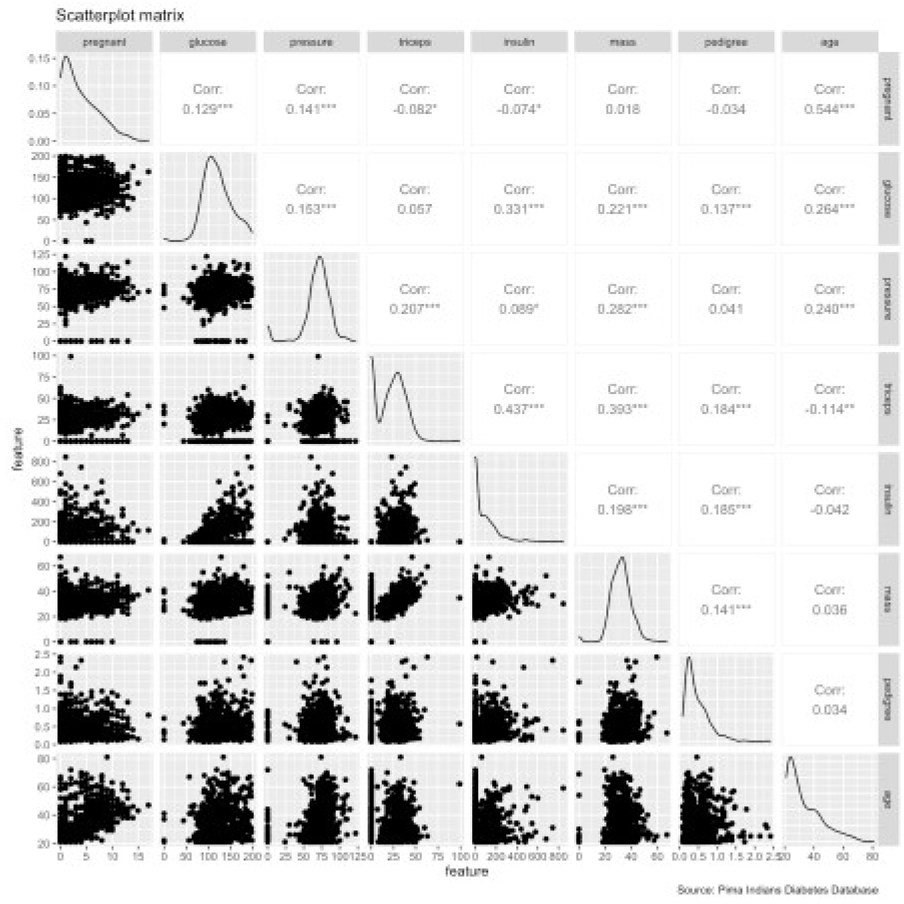
cormat <- round(cor(mat), 2)

cormat <- cormat %>%
  as_data_frame() %>%
  mutate(x = colnames(mat)) %>%
  gather(key = "y", value = "value", pregnant:age)

cormat %>%
    remove_missing() %>%
    arrange(x, y) %>%
    ggplot(aes(x = x, y = y, fill = value)) +
    geom_tile() +
    scale_fill_gradient2(low = "blue", high = "red", mid = "white",
     midpoint = 0, limit = c(-1,1), space = "Lab",
     name = "Pearson\nCorrelation") +
    theme(axis.text.x = element_text(angle = 45, vjust = 1, hjust = 1))
+
    coord_fixed() +
    labs(x = "feature",
         y = "feature",
        title = "Correlation between features",
        caption = "Source: Pima Indians Diabetes Database")
```



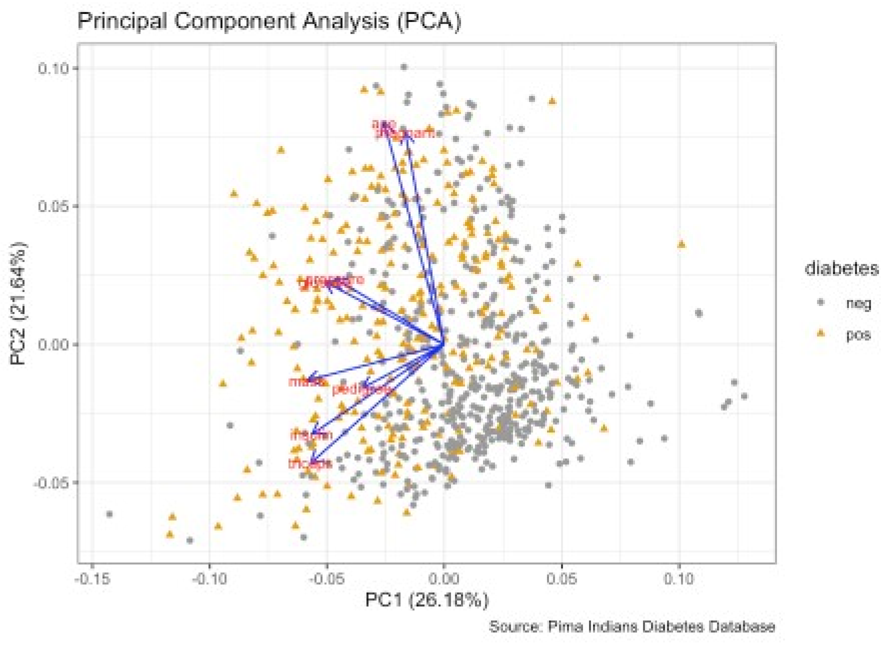
```
# scatterplot matrix
ggpairs(PimaIndiansDiabetes,
        columns = c(1:8),
        alpha = 0.7) +
    labs(x = "feature",
         y = "feature",
        title = "Scatterplot matrix",
        caption = "Source: Pima Indians Diabetes Database")
```



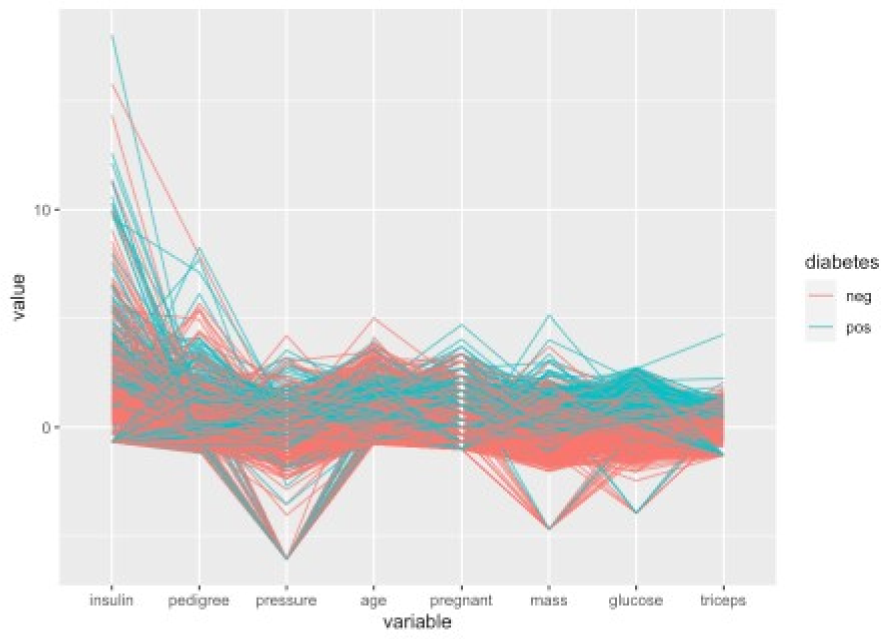
```
# PCA
prep <- PimaIndiansDiabetes %>%
  dplyr::select(where(is.numeric))

pca <- prep %>%
  prcomp(scale. = TRUE)

autoplot(pca,
                data = PimaIndiansDiabetes,
                colour = 'diabetes',
                shape = 'diabetes',
                loadings = TRUE,
                loadings.colour = 'blue',
                loadings.label = TRUE,
                loadings.label.size = 3) +
      scale_color_manual(values = cbp1) +
  scale_fill_manual(values = cbp1) +
  theme_bw() +
    labs(title = "Principal Component Analysis (PCA)",
        caption = "Source: Pima Indians Diabetes Database")
```



```
# MDS
d <- dist(prep) # euclidean distances between the rows
fit <- cmdscale(d,eig=TRUE, k=2) # k is the number of dim
fit$points %>%
  head()
##          [,1]       [,2]
## 1 -75.71465 -35.950783
## 2 -82.35827  28.908213
## 3 -74.63064 -67.906496
## 4  11.07742  34.898486
## 5  89.74379  -2.746937
## 6 -80.97792  -3.946887
# Sammon mapping
library(MASS)
sam <- sammon(dist(prep))
## Initial stress        : 0.03033
## stress after   0 iters: 0.03033
sam$points %>%
  head()
##          [,1]       [,2]
## 1 -75.71465 -35.950783
## 2 -82.35827  28.908213
## 3 -74.63064 -67.906496
## 4  11.07742  34.898486
## 5  89.74379  -2.746937
## 6 -80.97792  -3.946887
# parallel coordinate plots
ggparcoord(data = PimaIndiansDiabetes,
           columns = c(1:8),
           groupColumn = 9,
           scale = "robust",
           order = "skewness",
           alpha = 0.7)
```



```
# scagnostics
scagnostics_dataset <- scagnostics(PimaIndiansDiabetes)

# scagnostics grid
scagnostics_grid_dataset <- scagnosticsGrid(scagnostics_dataset)

# outliers
scagnostics_o_dataset <- scagnosticsOutliers(scagnostics_dataset)
scagnostics_o_dataset[scagnostics_o_dataset]
## pregnant * age
##           TRUE
outlier <- scagnostics_grid_dataset[scagnostics_o_dataset,]

# scagnostics exemplars
scagnostics_ex_dataset <- scagnosticsExemplars(scagnostics_dataset)
scagnostics_ex_dataset[scagnostics_ex_dataset]
## pregnant * triceps         mass * age triceps * diabetes
##               TRUE               TRUE               TRUE
exemplars <- scagnostics_grid_dataset[scagnostics_ex_dataset,]
```

Training a machine learning model

(using `mlr` package)

- create training and test set

```
set.seed(1000)

train_index <- sample(1:nrow(PimaIndiansDiabetes), 0.8 *
nrow(PimaIndiansDiabetes))
test_index <- setdiff(1:nrow(PimaIndiansDiabetes), train_index)

train <- PimaIndiansDiabetes[train_index,]
test <- PimaIndiansDiabetes[test_index,]
```

```
list( train = summary(train), test = summary(test) )
## $train
##     pregnant         glucose         pressure         triceps
##  Min.   : 0.000   Min.   :  0.0   Min.   :  0.00   Min.   : 0.00
##  1st Qu.: 1.000   1st Qu.:100.0   1st Qu.: 64.00   1st Qu.: 0.00
##  Median : 3.000   Median :119.0   Median : 72.00   Median :23.00
##  Mean   : 3.894   Mean   :123.1   Mean   : 68.89   Mean   :20.66
##  3rd Qu.: 6.000   3rd Qu.:143.0   3rd Qu.: 80.00   3rd Qu.:32.75
##  Max.   :17.000   Max.   :199.0   Max.   :114.00   Max.   :99.00
##     insulin            mass          pedigree           age
diabetes
##  Min.   :  0.00   Min.   : 0.00   Min.   :0.0780   Min.   :21.00
neg:386
##  1st Qu.:  0.00   1st Qu.:27.10   1st Qu.:0.2442   1st Qu.:24.00
pos:228
##  Median : 36.50   Median :32.00   Median :0.3780   Median :29.00
##  Mean   : 81.65   Mean   :31.92   Mean   :0.4742   Mean   :33.42
##  3rd Qu.:131.50   3rd Qu.:36.38   3rd Qu.:0.6355   3rd Qu.:41.00
##  Max.   :846.00   Max.   :59.40   Max.   :2.4200   Max.   :81.00
##
## $test
##     pregnant         glucose         pressure         triceps
##  Min.   : 0.000   Min.   :  0.0   Min.   :  0.00   Min.   : 0.00
##  1st Qu.: 1.000   1st Qu.: 93.0   1st Qu.: 62.00   1st Qu.: 0.00
##  Median : 2.000   Median :108.0   Median : 72.00   Median :23.00
##  Mean   : 3.649   Mean   :112.3   Mean   : 69.96   Mean   :20.03
##  3rd Qu.: 6.000   3rd Qu.:133.8   3rd Qu.: 79.50   3rd Qu.:32.00
##  Max.   :14.000   Max.   :197.0   Max.   :122.00   Max.   :56.00
##     insulin           mass          pedigree           age
diabetes
##  Min.   :  0.0   Min.   : 0.00   Min.   :0.0850   Min.   :21.00
neg:114
##  1st Qu.:  0.0   1st Qu.:27.80   1st Qu.:0.2395   1st Qu.:23.25
pos: 40
##  Median : 20.5   Median :32.40   Median :0.3380   Median :29.00
##  Mean   : 72.4   Mean   :32.29   Mean   :0.4627   Mean   :32.54
##  3rd Qu.:100.0   3rd Qu.:36.88   3rd Qu.:0.6008   3rd Qu.:39.75
##  Max.   :744.0   Max.   :67.10   Max.   :2.3290   Max.   :67.00
```

- create classification task and learner

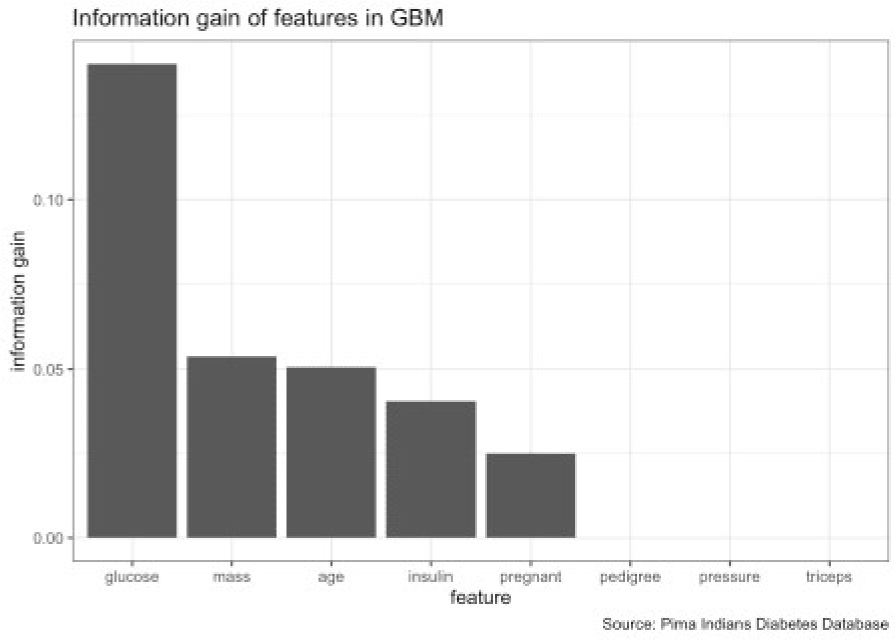
```
listLearners() %>%
  head()
##                 class                               name  short.name
## 1         classif.ada                       ada Boosting         ada
## 2  classif.adaboostm1                    ada Boosting M1  adaboostm1
## 3 classif.bartMachine Bayesian Additive Regression Trees bartmachine
## 4    classif.binomial                Binomial Regression    binomial
## 5    classif.boosting                    Adabag Boosting      adabag
## 6         classif.bst                  Gradient Boosting         bst
##       package
## 1    ada,rpart
## 2        RWeka
## 3  bartMachine
## 4        stats
## 5 adabag,rpart
## 6    bst,rpart
##
note
## 1
`xval` has been set to `0` by default for speed.
## 2
NAs are directly passed to WEKA with `na.action = na.pass`.
## 3
`use_missing_data` has been set to `TRUE` by default to allow missing
data support.
## 4  Delegates to `glm` with freely choosable binomial link function
via learner parameter `link`. We set 'model' to FALSE by default to
save memory.
## 5
`xval` has been set to `0` by default for speed.
## 6 Renamed parameter `learner` to `Learner` due to nameclash with
`setHyperPars`. Default changes: `Learner = "ls"`, `xval = 0`, and
`maxdepth = 1`.
##      type installed numerics factors ordered missings weights  prob
oneclass
## 1 classif     FALSE     TRUE    TRUE   FALSE    FALSE   FALSE  TRUE
FALSE
## 2 classif      TRUE     TRUE    TRUE   FALSE    FALSE   FALSE  TRUE
FALSE
## 3 classif     FALSE     TRUE    TRUE   FALSE     TRUE   FALSE  TRUE
FALSE
## 4 classif      TRUE     TRUE    TRUE   FALSE    FALSE    TRUE  TRUE
FALSE
## 5 classif     FALSE     TRUE    TRUE   FALSE     TRUE   FALSE  TRUE
FALSE
## 6 classif     FALSE     TRUE   FALSE   FALSE    FALSE   FALSE FALSE
FALSE
##   twoclass multiclass class.weights featimp oobpreds functionals
## 1     TRUE      FALSE         FALSE   FALSE    FALSE       FALSE
## 2     TRUE       TRUE         FALSE   FALSE    FALSE       FALSE
## 3     TRUE      FALSE         FALSE   FALSE    FALSE       FALSE
## 4     TRUE      FALSE         FALSE   FALSE    FALSE       FALSE
## 5     TRUE       TRUE         FALSE    TRUE    FALSE       FALSE
## 6     TRUE      FALSE         FALSE   FALSE    FALSE       FALSE
##   single.functional    se lcens rcens icens
## 1             FALSE FALSE FALSE FALSE FALSE
## 2             FALSE FALSE FALSE FALSE FALSE
## 3             FALSE FALSE FALSE FALSE FALSE
## 4             FALSE FALSE FALSE FALSE FALSE
## 5             FALSE FALSE FALSE FALSE FALSE
## 6             FALSE FALSE FALSE FALSE FALSE
(dt_task <- makeClassifTask(data = train, target = "diabetes"))
## Supervised task: train
## Type: classif
## Target: diabetes
## Observations: 614
## Features:
##    numerics     factors     ordered functionals
##           8           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 2
## neg pos
## 386 228
## Positive class: neg
(dt_prob <- makeLearner('classif.gbm', predict.type = "prob"))
## Learner classif.gbm from package gbm
## Type: classif
## Name: Gradient Boosting Machine; Short name: gbm
## Class: classif.gbm
## Properties: twoclass,multiclass,missings,
numerics,factors,prob,weights,featimp
## Predict-Type: prob
## Hyperparameters: keep.data=FALSE
```

Feature Selection

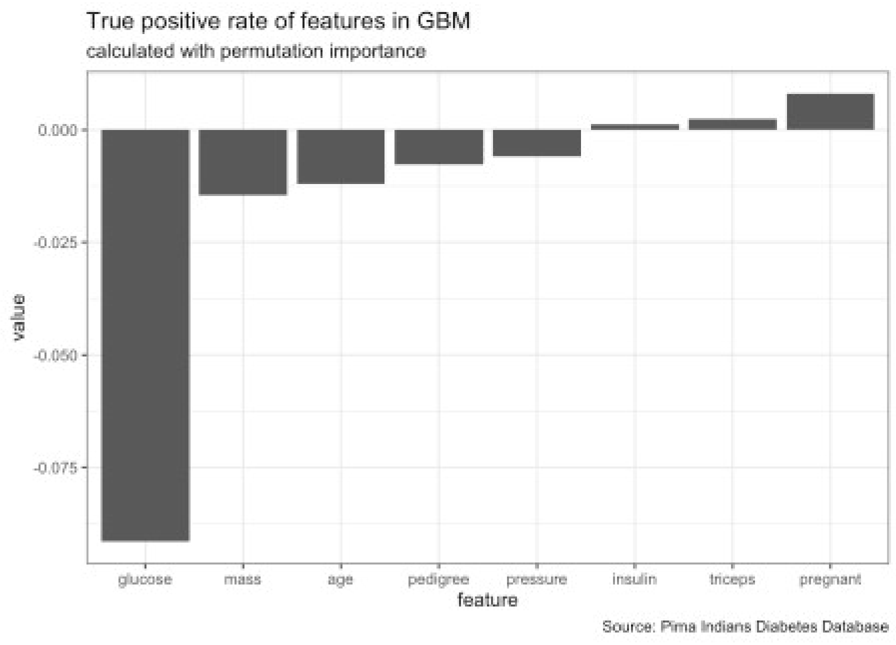
```
library(FSelector)

listFilterMethods() %>%
  head()
##                           id   package
desc
## 1                 anova.test           ANOVA Test for binary and
multiclass ...
## 2                        auc           AUC filter for binary
classification ...
## 3                   carscore      care
CAR scores
## 4      FSelector_chi.squared FSelector Chi-squared statistic of
independence...
## 5       FSelector_gain.ratio FSelector Chi-squared statistic of
independence...
## 6 FSelector_information.gain FSelector Entropy-based information
gain betwee...
listFilterEnsembleMethods() %>%
  head()
##         id
## 1  E-Borda
## 2    E-max
## 3   E-mean
## 4 E-median
## 5    E-min
```

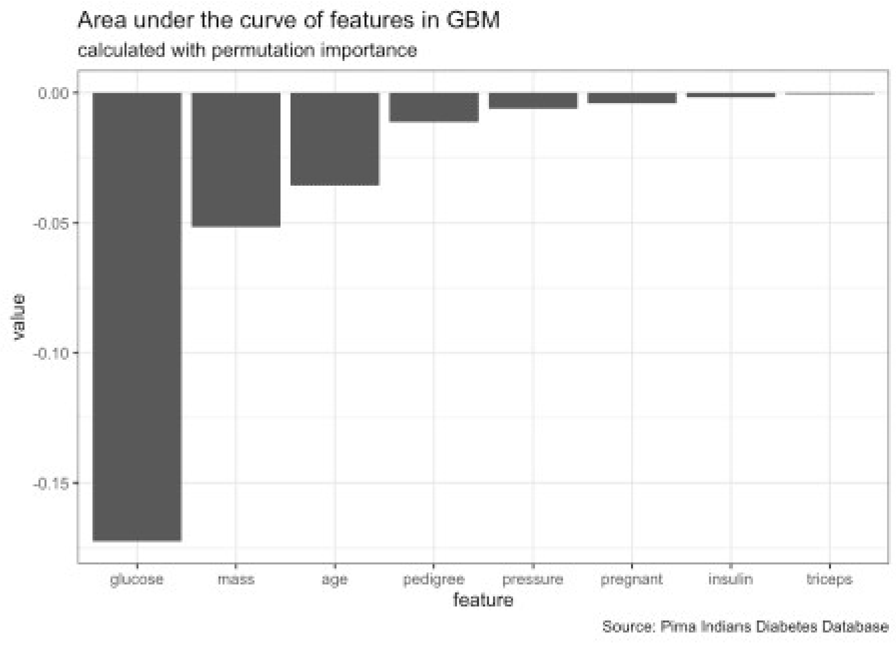
```
##
desc
## 1                  Borda ensemble filter. Takes the sum across all
base filter methods for each feature.
## 2 Maximum ensemble filter. Takes the best maximum value across all
base filter methods for each feature.
## 3                  Mean ensemble filter. Takes the mean across all
base filter methods for each feature.
## 4              Median ensemble filter. Takes the median across all
base filter methods for each feature.
## 5 Minimum ensemble filter. Takes the best minimum value across all
base filter methods for each feature.
generateFilterValuesData(dt_task, method =
"FSelector_information.gain") %>%
  plotFilterValues() +
  theme_bw() +
    labs(x = "feature",
         y = "information gain",
         title = "Information gain of features in GBM",
         caption = "Source: Pima Indians Diabetes Database")
```



```
feat_imp_tpr <- generateFeatureImportanceData(task = dt_task,
                              learner = dt_prob,
                              measure = tpr,
                              interaction = FALSE)
## Distribution not specified, assuming bernoulli ...
feat_imp_tpr$res %>%
  gather() %>%
  ggplot(aes(x = reorder(key, value), y = value)) +
    geom_bar(stat = "identity") +
    labs(x = "feature",
         title = "True positive rate of features in GBM",
         subtitle = "calculated with permutation importance",
         caption = "Source: Pima Indians Diabetes Database")
```



```
feat_imp_auc <- generateFeatureImportanceData(task = dt_task,
                              learner = dt_prob,
                              measure = auc,
                              interaction = FALSE)
## Distribution not specified, assuming bernoulli ...
feat_imp_auc$res %>%
  gather() %>%
  ggplot(aes(x = reorder(key, value), y = value)) +
    geom_bar(stat = "identity") +
    labs(x = "feature",
         title = "Area under the curve of features in GBM",
         subtitle = "calculated with permutation importance",
         caption = "Source: Pima Indians Diabetes Database")
```



```
set.seed(1000)
train <- dplyr::select(train, -pedigree, -pressure, -triceps)
test <- dplyr::select(test, -pedigree, -pressure, -triceps)
```

```
list(train = summary(train), test = summary(test))
## $train
##     pregnant         glucose         insulin           mass
##  Min.   : 0.000   Min.   :  0.0   Min.   :  0.00   Min.   : 0.00
##  1st Qu.: 1.000   1st Qu.:100.0   1st Qu.:  0.00   1st Qu.:27.10
##  Median : 3.000   Median :119.0   Median : 36.50   Median :32.00
##  Mean   : 3.894   Mean   :123.1   Mean   : 81.65   Mean   :31.92
##  3rd Qu.: 6.000   3rd Qu.:143.0   3rd Qu.:131.50   3rd Qu.:36.38
##  Max.   :17.000   Max.   :199.0   Max.   :846.00   Max.   :59.40
##       age        diabetes
##  Min.   :21.00   neg:386
##  1st Qu.:24.00   pos:228
##  Median :29.00
##  Mean   :33.42
##  3rd Qu.:41.00
##  Max.   :81.00
##
## $test
##     pregnant         glucose         insulin          mass
##  Min.   : 0.000   Min.   :  0.0   Min.   :  0.0   Min.   : 0.00
##  1st Qu.: 1.000   1st Qu.: 93.0   1st Qu.:  0.0   1st Qu.:27.80
##  Median : 2.000   Median :108.0   Median : 20.5   Median :32.40
##  Mean   : 3.649   Mean   :112.3   Mean   : 72.4   Mean   :32.29
##  3rd Qu.: 6.000   3rd Qu.:133.8   3rd Qu.:100.0   3rd Qu.:36.88
##  Max.   :14.000   Max.   :197.0   Max.   :744.0   Max.   :67.10
##       age        diabetes
##  Min.   :21.00   neg:114
##  1st Qu.:23.25   pos: 40
##  Median :29.00
##  Mean   :32.54
##  3rd Qu.:39.75
##  Max.   :67.00
(dt_task <- makeClassifTask(data = train, target = "diabetes"))
## Supervised task: train
## Type: classif
## Target: diabetes
## Observations: 614
## Features:
##    numerics     factors     ordered functionals
##           5           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 2
## neg pos
## 386 228
## Positive class: neg
```

Hyperparameter Optimization

```
getParamSet("classif.gbm")
```

```
##                           Type len       Def
## distribution      discrete   - bernoulli
## n.trees            integer   -       100
## cv.folds           integer   -         0
## interaction.depth  integer   -         1
## n.minobsinnode     integer   -        10
## shrinkage          numeric   -       0.1
## bag.fraction       numeric   -       0.5
## train.fraction     numeric   -         1
## keep.data          logical   -      TRUE
## verbose            logical   -     FALSE
## n.cores            integer   -         1
##                                                         Constr Req
Tunable Trafo
## distribution      gaussian,bernoulli,huberized,adaboost...   -
TRUE     -
## n.trees                                              1 to Inf   -
TRUE     -
## cv.folds                                          -Inf to Inf   -
TRUE     -
## interaction.depth                                    1 to Inf   -
TRUE     -
## n.minobsinnode                                       1 to Inf   -
TRUE     -
## shrinkage                                            0 to Inf   -
TRUE     -
## bag.fraction                                           0 to 1   -
TRUE     -
## train.fraction                                         0 to 1   -
TRUE     -
## keep.data                                                   -   -
FALSE     -
## verbose                                                     -   -
FALSE     -
## n.cores                                           -Inf to Inf   -
FALSE     -
dt_param <- makeParamSet(
  makeIntegerParam("n.trees", lower = 20, upper = 150),
  makeNumericParam("shrinkage", lower = 0.01, upper = 0.1))

ctrl = makeTuneControlGrid()

rdesc = makeResampleDesc("CV",
                         iters = 3L,
                         stratify = TRUE)
set.seed(1000)
(dt_tuneparam <- tuneParams(learner = dt_prob,
                             resampling = rdesc,
                             measures = list(tpr,auc, fnr, mmce, tnr,
setAggregation(tpr, test.sd)),
                             par.set = dt_param,
                             control = ctrl,
                                task = dt_task,
                                show.info = FALSE))
## Distribution not specified, assuming bernoulli ...
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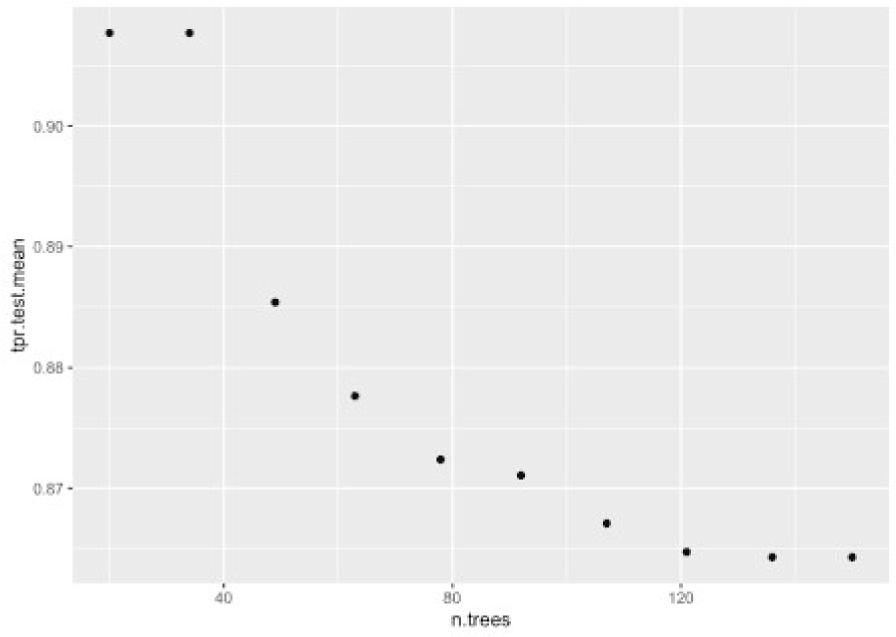
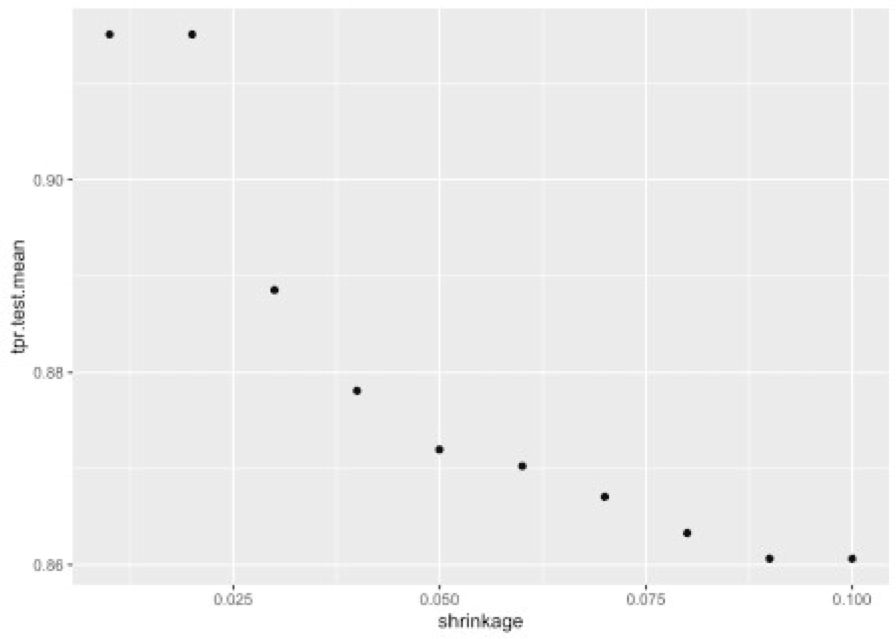
## Tune result:
## Op. pars: n.trees=20; shrinkage=0.02
## tpr.test.mean=1.0000000,auc.test.mean=0.7878691,fnr.test.
mean=0.0000000,mmce.test.mean=0.3713375,tnr.test.mean=0.
0000000,tpr.test.sd=0.0000000
data = generateHyperParsEffectData(dt_tuneparam,
                                   partial.dep = TRUE)

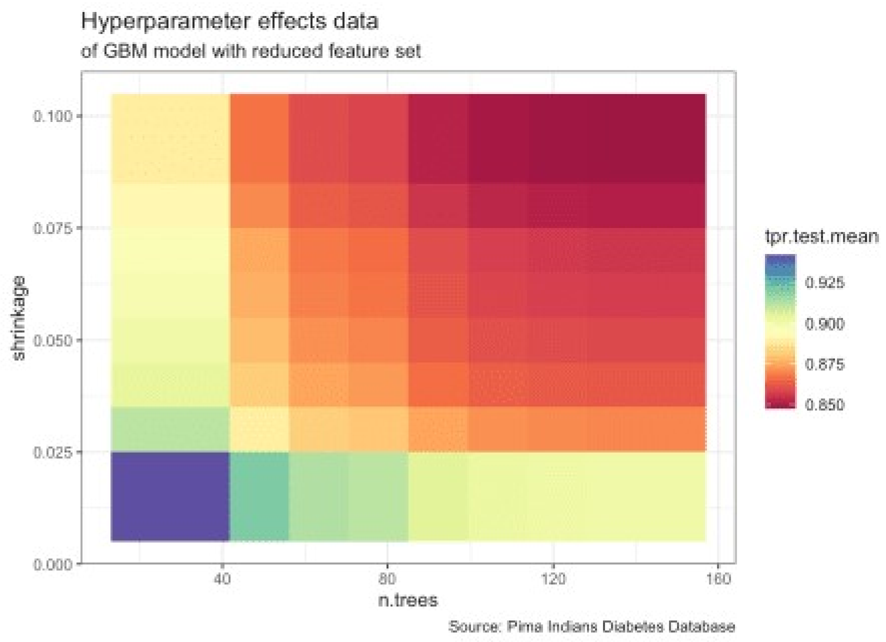
plotHyperParsEffect(data, x = "n.trees", y = "tpr.test.mean",
partial.dep.learn = makeLearner("regr.gbm"))
```



```
plotHyperParsEffect(data, x = "shrinkage", y = "tpr.test.mean",
partial.dep.learn = makeLearner("regr.gbm"))
```



```
plotHyperParsEffect(data,
                    x = "n.trees",
                    y = "shrinkage",
                    z = "tpr.test.mean",
                    plot.type = "heatmap",
                    partial.dep.learn = makeLearner("regr.gbm")) +
  theme_bw() +
    labs(title = "Hyperparameter effects data",
         subtitle = "of GBM model with reduced feature set",
         caption = "Source: Pima Indians Diabetes Database")
```



```
list( `Optimal HyperParameters` = dt_tuneparam$x,
      `Optimal Metrics` = dt_tuneparam$y )
## $`Optimal HyperParameters`
## $`Optimal HyperParameters`$n.trees
## [1] 20
##
## $`Optimal HyperParameters`$shrinkage
## [1] 0.02
##
##
## $`Optimal Metrics`
##  tpr.test.mean  auc.test.mean  fnr.test.mean mmce.test.mean
tnr.test.mean
##      1.0000000      0.7878691      0.0000000      0.3713375
0.0000000
##      tpr.test.sd
##      0.0000000
gbm_final <- setHyperPars(dt_prob, par.vals = dt_tuneparam$x)

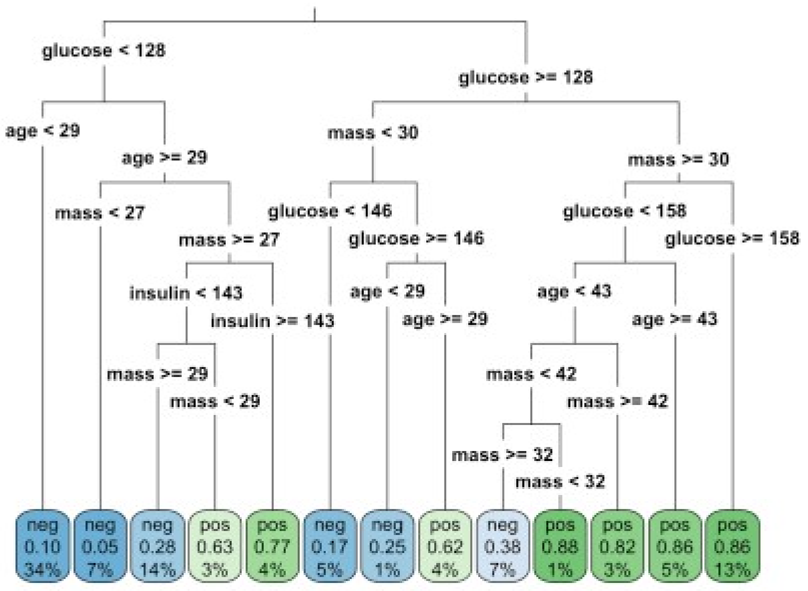
set.seed(1000)
gbm_final_train <- train(learner = gbm_final, task = dt_task)
## Distribution not specified, assuming bernoulli ...
getLearnerModel(gbm_final_train)
## gbm::gbm(formula = f, data = d, n.trees = 20L, shrinkage = 0.02,
##     keep.data = FALSE)
## A gradient boosted model with bernoulli loss function.
## 20 iterations were performed.
## There were 5 predictors of which 3 had non-zero influence.
```

Decision Trees

- Recursive Partitioning (`rpart` & `rpart.plot`)

```
library(rpart)
library(rpart.plot)
```

```
rpart_tree <- rpart(diabetes ~ .,
                    data = train,
                    method = "class")
rpart.plot(rpart_tree,
           roundint=FALSE,
           type = 3,
           clip.right.labs = FALSE)
```

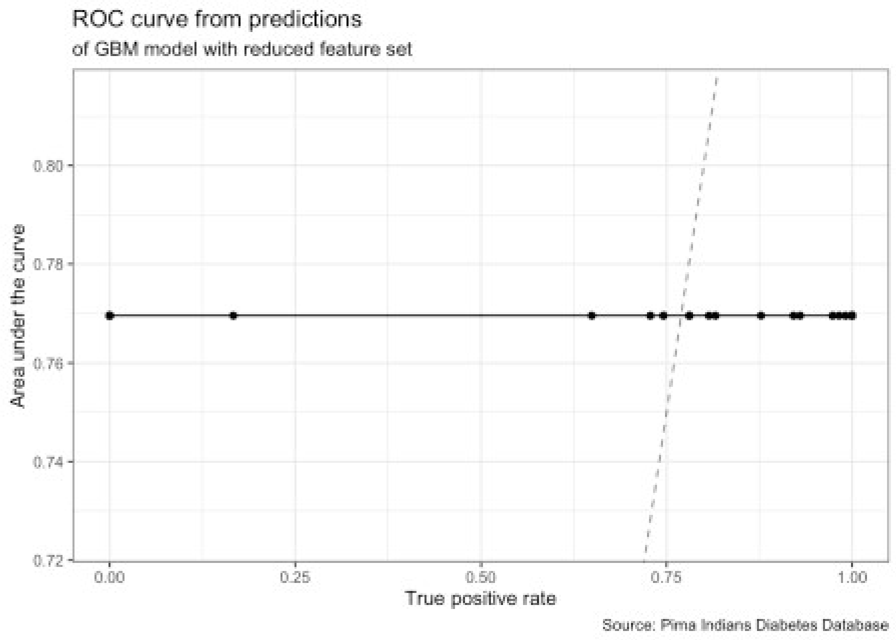


```
rpart.rules(rpart_tree, roundint = FALSE)
##  diabetes
##      0.05 when glucose <  128        & mass <  27        & age >= 29
##      0.10 when glucose <  128                            & age <  29
##      0.17 when glucose is 128 to 146 & mass <  30
##      0.25 when glucose >=        146 & mass <  30        & age <  29
##      0.28 when glucose <  128        & mass >=       29 & age >= 29
& insulin <  143
##      0.38 when glucose is 128 to 158 & mass is 32 to 42 & age <  43
##      0.62 when glucose >=        146 & mass <  30        & age >= 29
##      0.63 when glucose <  128        & mass is 27 to 29 & age >= 29
& insulin <  143
##      0.77 when glucose <  128        & mass >=       27 & age >= 29
& insulin >= 143
##      0.82 when glucose is 128 to 158 & mass >=       42 & age <  43
##      0.86 when glucose is 128 to 158 & mass >=       30 & age >= 43
##      0.86 when glucose >=        158 & mass >=       30
##      0.88 when glucose is 128 to 158 & mass is 30 to 32 & age <  43
```

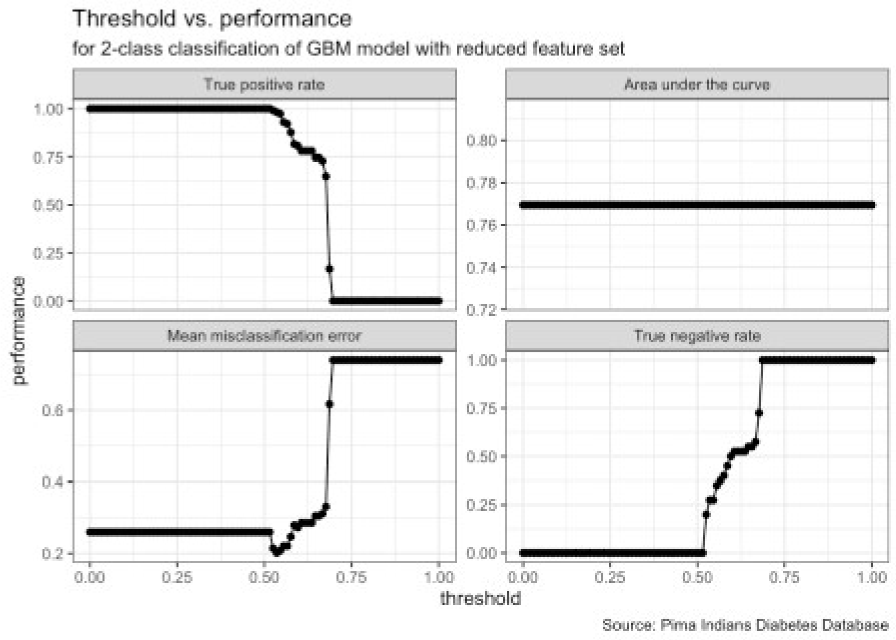
Prediction

```
set.seed(1000)
(gbm_final_predict <- predict(gbm_final_train, newdata = test))
## Prediction: 154 observations
## predict.type: prob
## threshold: neg=0.50,pos=0.50
## time: 0.00
##    truth  prob.pos  prob.neg response
## 12   pos 0.4807717 0.5192283      neg
## 18   pos 0.3229851 0.6770149      neg
## 19   neg 0.3229851 0.6770149      neg
## 20   pos 0.3300235 0.6699765      neg
## 34   neg 0.3091184 0.6908816      neg
## 38   pos 0.3229851 0.6770149      neg
## ... (#rows: 154, #cols: 4)
gbm_final_predict %>% calculateROCMeasures()
##      predicted
## true  neg       pos
##   neg 114       0        tpr: 1   fnr: 0
##   pos 40        0        fpr: 1   tnr: 0
##       ppv: 0.74 for: NaN lrp: 1   acc: 0.74
##       fdr: 0.26 npv: NaN lrm: NaN dor: NaN
##
##
## Abbreviations:
## tpr - True positive rate (Sensitivity, Recall)
## fpr - False positive rate (Fall-out)
## fnr - False negative rate (Miss rate)
## tnr - True negative rate (Specificity)
## ppv - Positive predictive value (Precision)
## for - False omission rate
## lrp - Positive likelihood ratio (LR+)
## fdr - False discovery rate
## npv - Negative predictive value
## acc - Accuracy
## lrm - Negative likelihood ratio (LR-)
## dor - Diagnostic odds ratio
model_performance <- performance(gbm_final_predict,
                                 measures = list(tpr, auc, mmce, acc,
tnr)) %>%
  as.data.frame(row.names = c("True Positive Rate","Area Under Curve",
"Mean Misclassification Error","Accuracy","True Negative Rate"))

model_performance
##                                      .
## True Positive Rate           1.0000000
## Area Under Curve             0.7695175
## Mean Misclassification Error 0.2597403
## Accuracy                     0.7402597
## True Negative Rate           0.0000000
gbm_final_threshold <- generateThreshVsPerfData(gbm_final_predict,
                                                measures = list(tpr,
auc, mmce, tnr))
gbm_final_threshold %>%
   plotROCCurves() +
   geom_point() +
    theme_bw() +
    labs(title = "ROC curve from predictions",
         subtitle = "of GBM model with reduced feature set",
         caption = "Source: Pima Indians Diabetes Database")
```



```
gbm_final_threshold %>%
   plotThreshVsPerf() +
   geom_point() +
    theme_bw() +
    labs(title = "Threshold vs. performance",
         subtitle = "for 2-class classification of GBM model with
reduced feature set",
         caption = "Source: Pima Indians Diabetes Database")
```



```
gbm_final_threshold$data %>%
  head()
##   tpr       auc      mmce tnr  threshold
## 1   1 0.7695175 0.2597403   0 0.00000000
## 2   1 0.7695175 0.2597403   0 0.01010101
## 3   1 0.7695175 0.2597403   0 0.02020202
## 4   1 0.7695175 0.2597403   0 0.03030303
## 5   1 0.7695175 0.2597403   0 0.04040404
## 6   1 0.7695175 0.2597403   0 0.05050505
gbm_final_thr <- gbm_final_predict %>%
  setThreshold(0.59595960)

(dt_performance <- gbm_final_thr %>% performance(measures = list(tpr,
auc, mmce, tnr)) )
##       tpr       auc      mmce       tnr
## 0.8070175 0.7695175 0.2727273 0.5000000
(dt_cm <- gbm_final_thr %>% calculateROCMeasures() )
##      predicted
## true  neg       pos
##   neg 92        22        tpr: 0.81 fnr: 0.19
##   pos 20        20        fpr: 0.5  tnr: 0.5
##       ppv: 0.82 for: 0.52 lrp: 1.61 acc: 0.73
##       fdr: 0.18 npv: 0.48 lrm: 0.39 dor: 4.18
##
##
## Abbreviations:
## tpr - True positive rate (Sensitivity, Recall)
## fpr - False positive rate (Fall-out)
## fnr - False negative rate (Miss rate)
## tnr - True negative rate (Specificity)
## ppv - Positive predictive value (Precision)
## for - False omission rate
## lrp - Positive likelihood ratio (LR+)
## fdr - False discovery rate
## npv - Negative predictive value
## acc - Accuracy
## lrm - Negative likelihood ratio (LR-)
## dor - Diagnostic odds ratio
performance_threshold <- performance(gbm_final_thr, measures =
list(tpr, auc, mmce, acc, tnr)) %>%
  as.data.frame(row.names = c("True Positive Rate", "Area Under Curve",
"Mean Misclassification Error", "Accuracy", "True Negative Rate"))

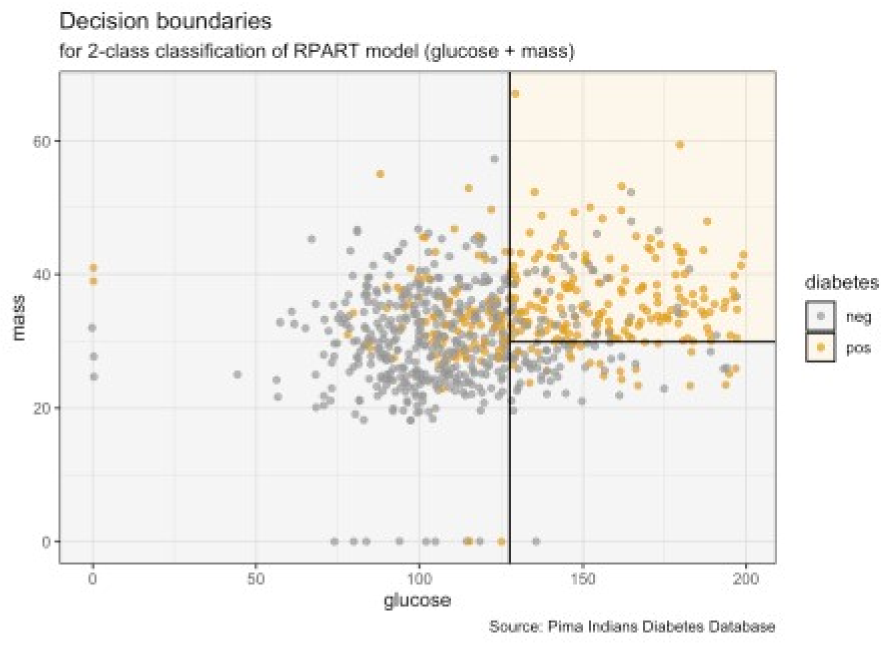
performance_threshold
##                                      .
## True Positive Rate           0.8070175
## Area Under Curve             0.7695175
## Mean Misclassification Error 0.2727273
## Accuracy                     0.7272727
## True Negative Rate           0.5000000
```

Decision Boundaries

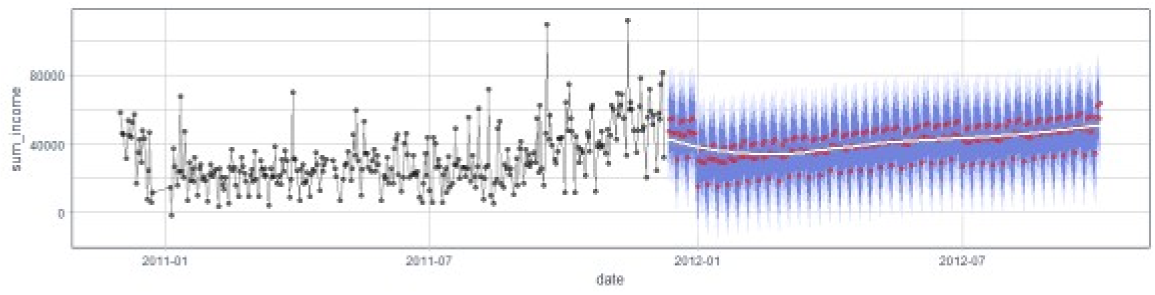
```
#remotes::install_github("grantmcdermott/parttree")
library(parsnip)
library(parttree)
set.seed(123) ## For consistent jitter
```

```
## Build our tree using parsnip (but with rpart as the model engine)
ti_tree =
  decision_tree() %>%
  set_engine("rpart") %>%
  set_mode("classification") %>%
  fit(diabetes ~ glucose + mass, data = PimaIndiansDiabetes)

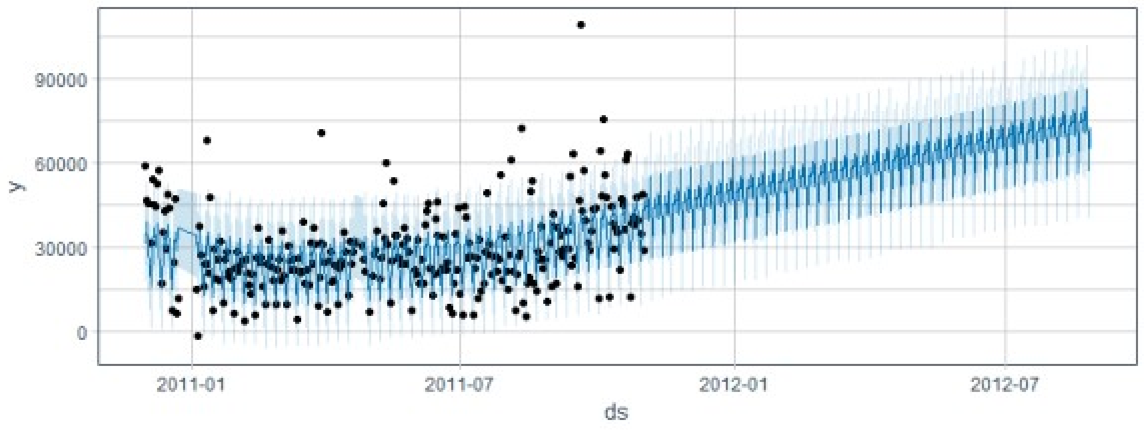
## Plot the data and model partitions
PimaIndiansDiabetes %>%
  ggplot(aes(x = glucose, y = mass)) +
  geom_jitter(aes(col = diabetes), alpha = 0.7) +
  geom_parttree(data = ti_tree, aes(fill = diabetes), alpha = 0.1) +
  theme_bw() +
    labs(title = "Decision boundaries",
         subtitle = "for 2-class classification of RPART model (glucose
+ mass)",
         caption = "Source: Pima Indians Diabetes Database")
```



Time-series



https://shiring.github.io/forecasting/2017/06/09/retail_forcasting_part2



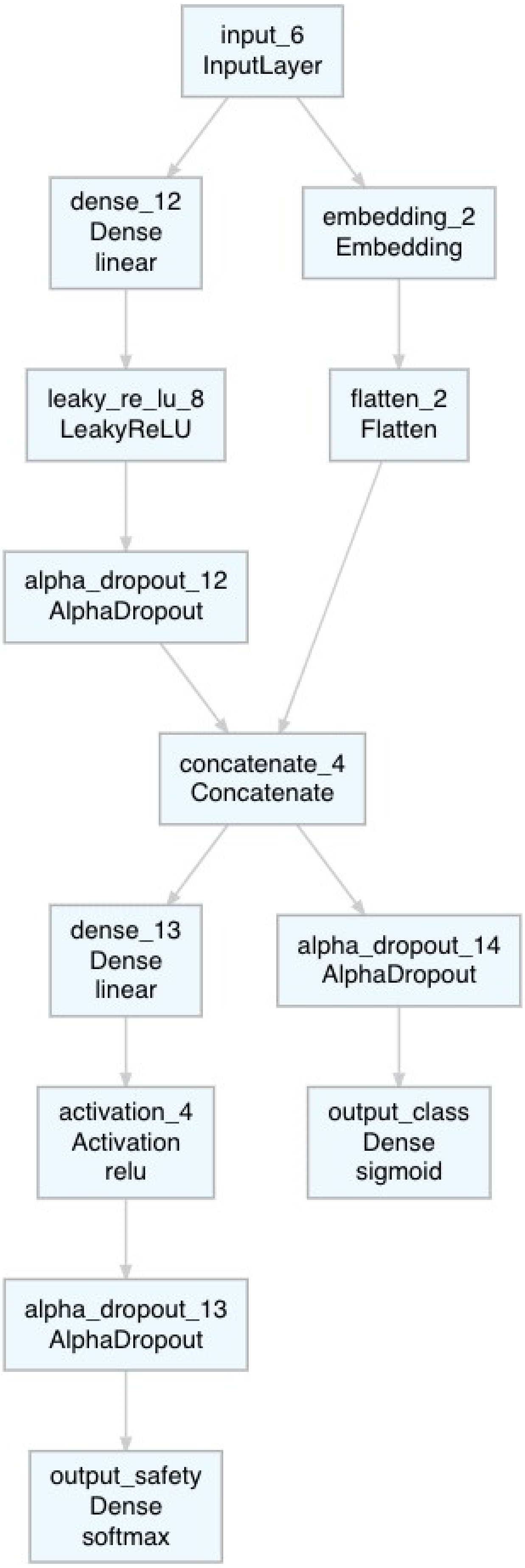
https://shiring.github.io/forecasting/2017/06/13/retail_forcasting_part3

Artificial Neural Networks (ANNs)

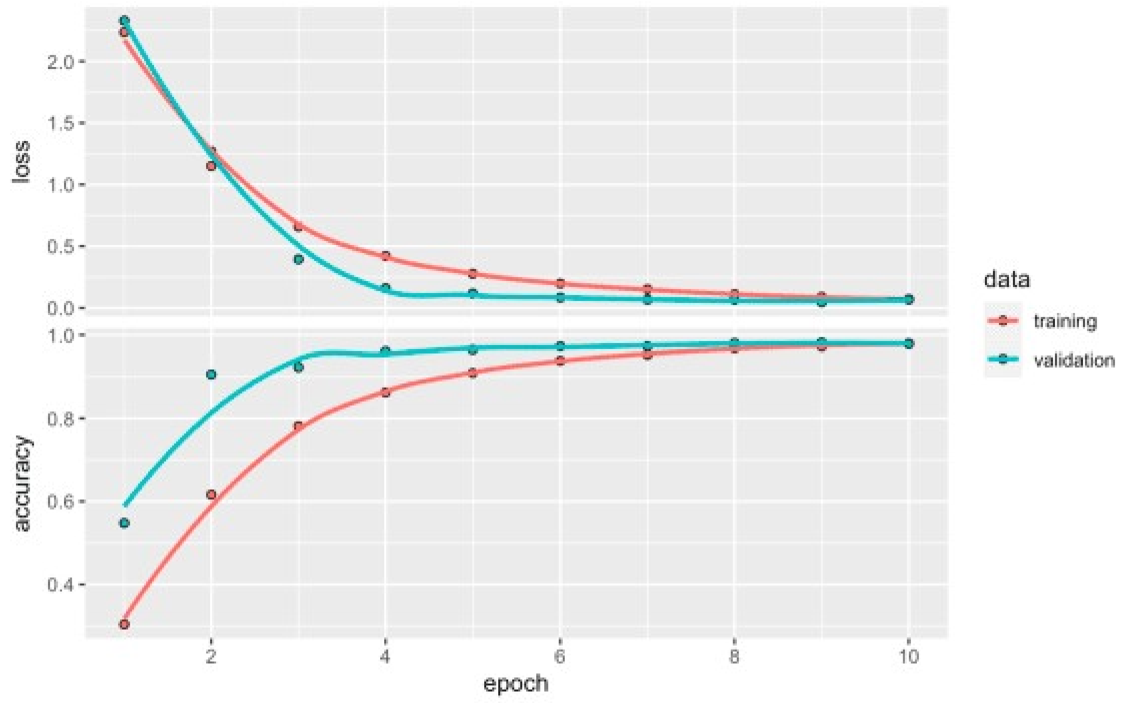
- playground.tensorflow.org
- Deep Learning with R

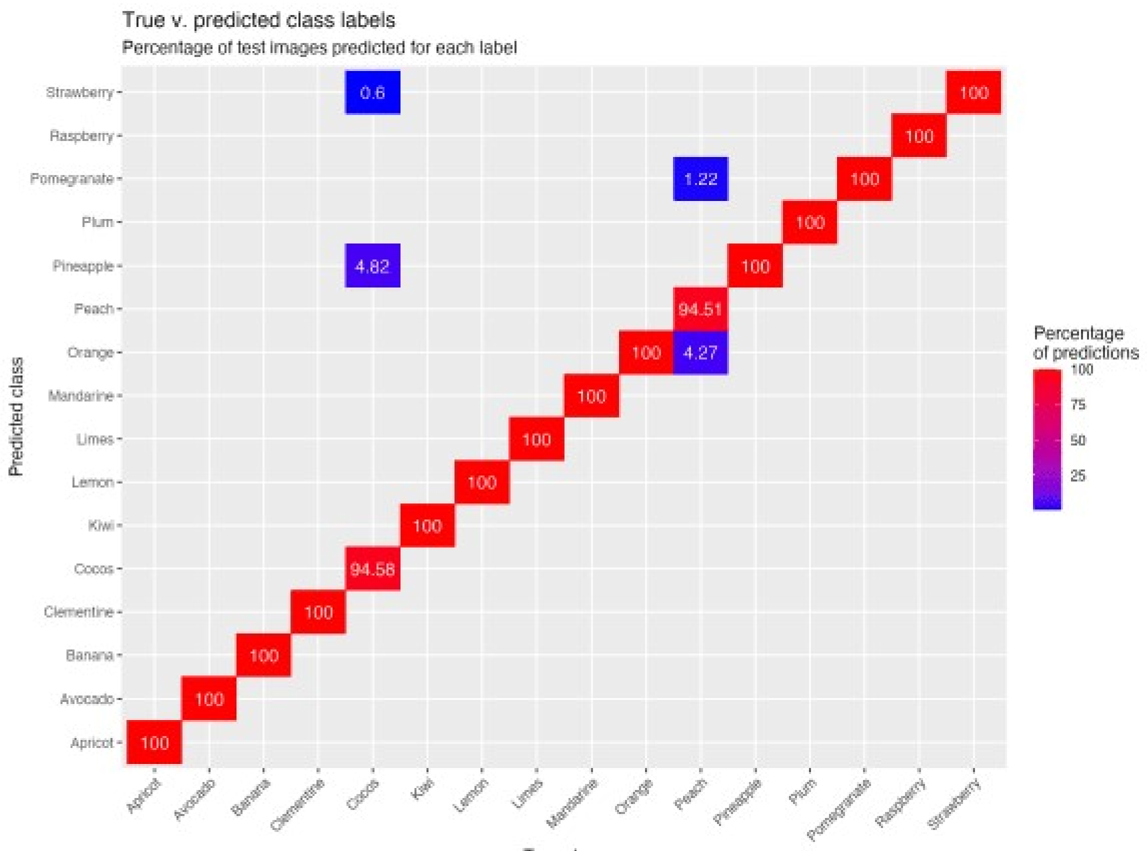
1. Visualizing what convnets learn
2. Deep Dreaming
3. Neural style transfer

- Li et al, Visualizing the Loss Landscape of Neural Nets, 2018
- Understanding Neural Networks Through Deep Visualization, Jason Yosinski, Jeff Clune, Anh Nguyen, Thomas Fuchs, and Hod Lipson
- Visualizing Data using the Embedding Projector in TensorBoard
- Visualizing and Understanding Convolutional Networks, Zeiler & Fergus, 2013
- The Building Blocks of Interpretability, Olah, Satyanarayan, Johnson, Carter, Schubert, Ye, Mordvintsev
- Google Creative Lab
- Play with Generative Adversarial Networks (GANs) in your browser
- Visual Analysis for Recurrent Neural Networks
- Whose dream is this? When and how to use the Keras Functional API

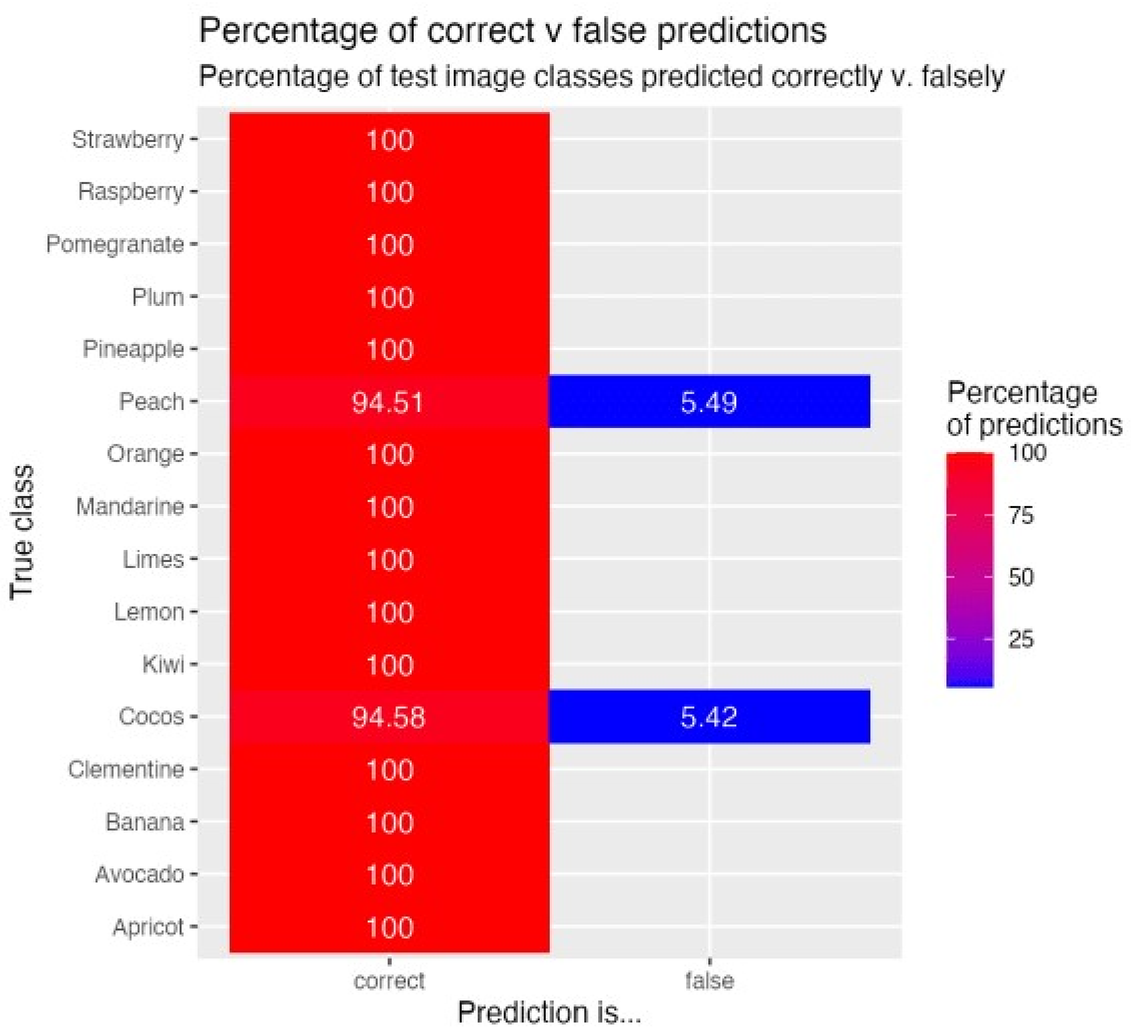


- Deep Learning with Keras and TensorFlow & Update with TF 2.0: Image classification with Keras and TensorFlow





For every class of test images, this figure shows the percentage of images with predicted labels for each possible label.
E.g.: 100% of test images in the class 'Apricot' were predicted correctly. Of test images from the class 'Cocos'
only 94.58% were predicted correctly, while 0.6% of these images were predicted to show a Strawberry and 4.82% a Pineapple.



For every class of test images, this figure shows the percentage of images with correctly and falsely predicted labels. E.g.: 100% of test images in the class 'Apricot' were predicted correctly. Of test images from the class 'Cocos' only 94.58% were predicted correctly, while 5.42% were predicted falsely.

- Visualize the effectiveness of different learning rates & Setting the learning rate of your neural network.

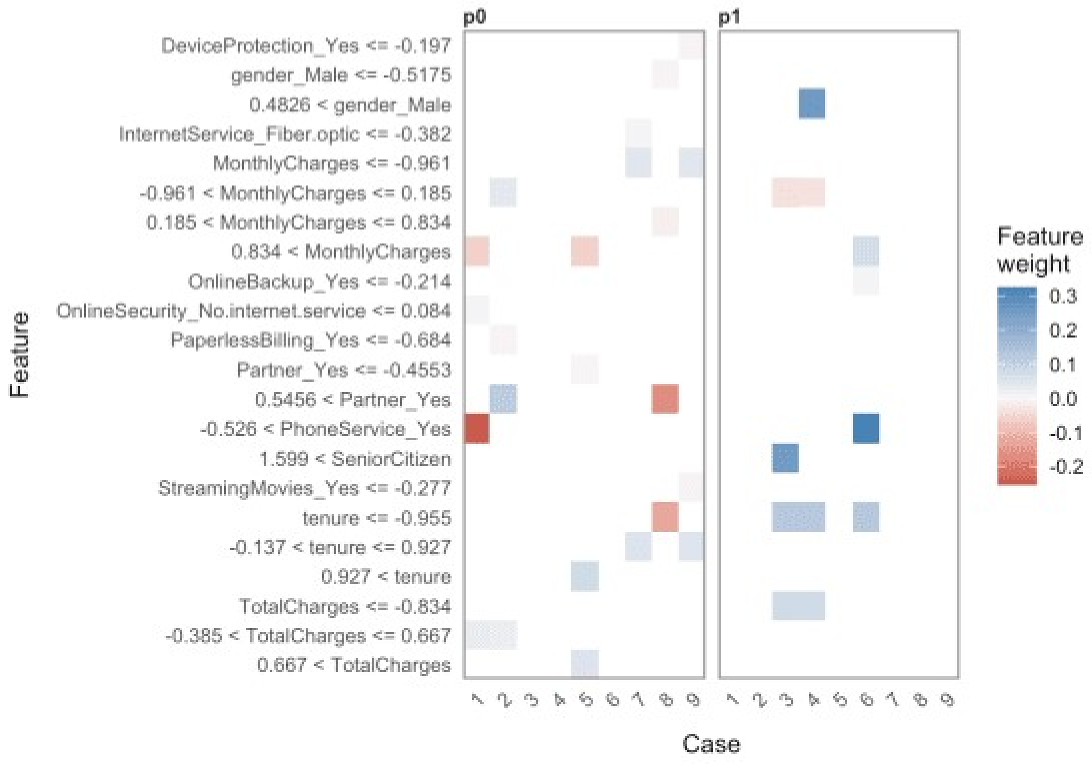
Graphical representation of a model in TensorBoard

https://www.tensorflow.org/tensorboard

Word Embeddings

- The Unreasonable Effectiveness of Recurrent Neural Networks, Karpathy, 2015
- Seq2Seq-Vis: Visual Debugging Tool for Sequenceto- Sequence Models, Strobelt, 2018
- Google's Multilingual Neural Machine Translation System: Enabling Zero-Shot Translation

Explainable AI



https://shirinsplayground.netlify.app/2021/03/update_customer_churn/

- Interpretable Machine Learning, A Guide for Making Black Box Models Explainable. Christoph Molnar
- Equality of Opportunity in Supervised Learning

```
# session info
devtools::session_info()
## ─ Session info ──────────────────────────────
──────────────────────────────────
##  setting  value
##  version  R version 4.0.4 (2021-02-15)
##  os       macOS Big Sur 10.16
##  system   x86_64, darwin17.0
##  ui       X11
##  language (EN)
##  collate  en_US.UTF-8
##  ctype    en_US.UTF-8
##  tz       Europe/Berlin
##  date     2021-04-27
##
## ─ Packages ──────────────────────────────
─────────────────────────────────────
##  package      * version    date       lib
##  assertthat     0.2.1      2019-03-21 [2]
##  backports      1.2.1      2020-12-09 [2]
##  BBmisc         1.11       2017-03-10 [2]
##  blogdown       1.2        2021-03-04 [2]
##  bookdown       0.21       2020-10-13 [2]
## broom          0.7.5    2021-02-19 [2]
## bslib          0.2.4    2021-01-25 [2]
## cachem         1.0.4    2021-02-13 [2]
## callr          3.5.1    2020-10-13 [2]
## cellranger     1.1.0    2016-07-27 [2]
## checkmate      2.0.0    2020-02-06 [2]
## cli            2.3.1    2021-02-23 [2]
## colorspace     2.0-0    2020-11-11 [2]
## crayon         1.4.1    2021-02-08 [2]
## data.table     1.14.0   2021-02-21 [2]
## DBI            1.1.1    2021-01-15 [2]
## dbplyr         2.1.0    2021-02-03 [2]
## desc           1.3.0    2021-03-05 [2]
## devtools       2.3.2    2020-09-18 [2]
## digest         0.6.27   2020-10-24 [2]
## dplyr        * 1.0.5    2021-03-05 [2]
## ellipsis       0.3.1    2020-05-15 [2]
## entropy        1.2.1    2014-11-14 [1]
## evaluate       0.14     2019-05-28 [2]
## fansi          0.4.2    2021-01-15 [2]
## farver         2.1.0    2021-02-28 [2]
## fastmap        1.1.0    2021-01-25 [2]
## fastmatch      1.1-0    2017-01-28 [2]
## forcats      * 0.5.1    2021-01-27 [2]
## fs             1.5.0    2020-07-31 [2]
## FSelector    * 0.33     2021-02-16 [1]
## gbm            2.1.8    2020-07-15 [2]
## generics       0.1.0    2020-10-31 [2]
## GGally       * 2.1.1    2021-03-08 [1]
## ggfortify    * 0.4.11   2020-10-02 [2]
## ggplot2      * 3.3.3    2020-12-30 [2]
## glue           1.4.2    2020-08-27 [2]
## gridExtra      2.3      2017-09-09 [2]
## gtable         0.3.0    2019-03-25 [2]
## haven          2.3.1    2020-06-01 [2]
## highr          0.8      2019-03-20 [2]
## hms            1.0.0    2021-01-13 [2]
## htmltools      0.5.1.1  2021-01-22 [2]
## httr           1.4.2    2020-07-20 [2]
## jquerylib      0.1.3    2020-12-17 [2]
## jsonlite       1.7.2    2020-12-09 [2]
## knitr          1.31     2021-01-27 [2]
## labeling       0.4.2    2020-10-20 [2]
## lattice        0.20-41  2020-04-02 [2]
## lifecycle      1.0.0    2021-02-15 [2]
## lubridate      1.7.10   2021-02-26 [2]
## magrittr       2.0.1    2020-11-17 [2]
## MASS         * 7.3-53.1 2021-02-12 [2]
## Matrix         1.3-2    2021-01-06 [2]
## memoise        2.0.0    2021-01-26 [2]
## mlbench      * 2.1-3    2021-01-29 [1]
## mlr          * 2.19.0   2021-02-22 [2]
##  mmpf         * 0.0.5      2018-10-24 [2]
##  modelr         0.1.8      2020-05-19 [2]
##  munsell        0.5.0      2018-06-12 [2]
##  parallelMap    1.5.0      2020-03-26 [2]
##  ParamHelpers * 1.14       2020-03-24 [2]
##  parsnip      * 0.1.5      2021-01-19 [2]
##  parttree     * 0.0.1.9000 2021-03-14 [1]
##  pillar         1.5.1      2021-03-05 [2]
##  pkgbuild       1.2.0      2020-12-15 [2]
##  pkgconfig      2.0.3      2019-09-22 [2]
##  pkgload        1.2.0      2021-02-23 [2]
##  plyr           1.8.6      2020-03-03 [2]
##  prettyunits    1.1.1      2020-01-24 [2]
##  processx       3.4.5      2020-11-30 [2]
##  ps             1.6.0      2021-02-28 [2]
##  purrr        * 0.3.4      2020-04-17 [2]
##  R6             2.5.0      2020-10-28 [2]
##  randomForest   4.6-14     2018-03-25 [2]
##  RColorBrewer   1.1-2      2014-12-07 [2]
##  Rcpp           1.0.6      2021-01-15 [2]
##  readr        * 1.4.0      2020-10-05 [2]
##  readxl         1.3.1      2019-03-13 [1]
##  remotes        2.2.0      2020-07-21 [2]
##  reprex         1.0.0      2021-01-27 [2]
##  reshape        0.8.8      2018-10-23 [1]
##  rJava        * 0.9-13     2020-07-06 [2]
##  rlang          0.4.10     2020-12-30 [2]
##  rmarkdown      2.7        2021-02-19 [2]
##  rpart        * 4.1-15     2019-04-12 [2]
##  rpart.plot   * 3.0.9      2020-09-17 [1]
##  rprojroot      2.0.2      2020-11-15 [2]
##  rstudioapi     0.13       2020-11-12 [2]
##  rvest          1.0.0      2021-03-09 [2]
##  RWeka          0.4-43     2020-08-23 [1]
##  RWekajars      3.9.3-2    2019-10-19 [1]
##  sass           0.3.1      2021-01-24 [2]
##  scagnostics  * 0.2-4.1    2018-04-04 [1]
##  scales         1.1.1      2020-05-11 [2]
##  sessioninfo    1.1.1      2018-11-05 [2]
##  stringi        1.5.3      2020-09-09 [2]
##  stringr      * 1.4.0      2019-02-10 [2]
##  survival       3.2-7      2020-09-28 [2]
##  testthat       3.0.2      2021-02-14 [2]
##  tibble       * 3.1.0      2021-02-25 [2]
##  tidyr        * 1.1.3      2021-03-03 [2]
##  tidyselect     1.1.0      2020-05-11 [2]
##  tidyverse    * 1.3.0      2019-11-21 [2]
##  usethis        2.0.1      2021-02-10 [2]
##  utf8           1.2.1      2021-03-12 [2]
##  vctrs          0.3.6      2020-12-17 [2]
##  withr          2.4.1      2021-01-26 [2]
##  xfun           0.22       2021-03-11 [2]
##  XML              3.99-0.5   2020-07-23 [2]
##  xml2             1.3.2      2020-04-23 [2]
##  yaml             2.2.1      2020-02-01 [2]
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##  Github (grantmcdermott/parttree@9d25d2c)
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## [2] /Library/Frameworks/R.framework/Versions/4.0/Resources/library
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