Logistic Regression

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Data and packages for these slides:

```
knitr::opts_chunk$set(echo = FALSE)
# required_packages = c("caret", "tree", "randomForest",
#                       "cowplot", "e1071")
# install.packages(required_packages)
suppressMessages(require(tidyverse))
suppressMessages(require(cowplot))
mice_df = read_csv("mice.csv")
```

```
## Parsed with column specification:
## cols(
##   Age = col_double(),
##   Sex = col_character(),
##   Condition = col_character(),
##   Mouse.Genotyping = col_character(),
##   ID = col_integer(),
##   Timepoint = col_character(),
##   Genotype = col_character(),
##   DaysOfEE = col_integer(),
##   DaysOfEE0 = col_integer()
## )
```

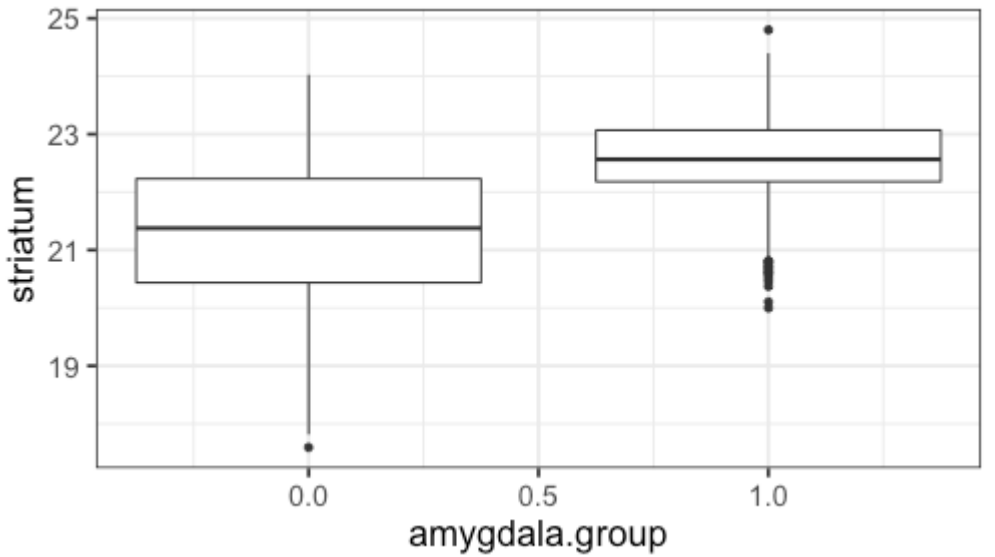
```
volume_df = read_csv("volumes.csv")
```

Logistic regression

Binary variables

Can we predict gender given striatum volume?

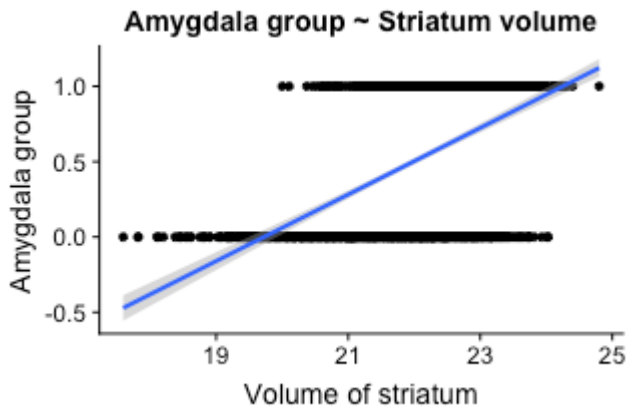
```
mice$amygdala.group = ifelse(mice$amygdala > 10, 1, 0)
ggplot(mice, aes(x=amygdala.group, y=striatum,
                 group=amygdala.group)) +
  geom_boxplot() +
  theme_bw(base_size=18)
```



Linear model for binary variables?

- If the independent variable is binary, can we fit the linear model?

```
ggplot(mice, aes(x=striatum, y=amygdala.group)) +
  geom_point() + xlab("Volume of striatum") +
  ylab("Amygdala group") +
  geom_smooth(method="lm") +
  ggtitle("Amygdala group ~ Striatum volume")
```



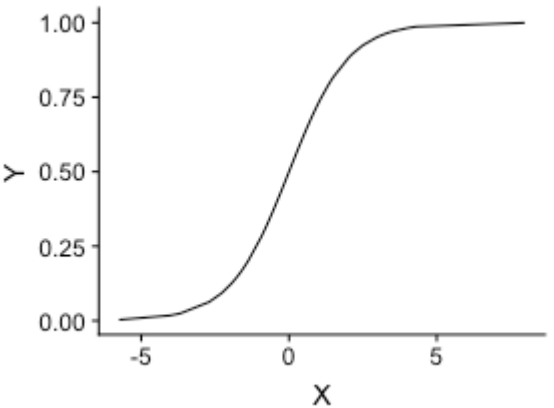
Why we can't use linear model for classification?

- Suppose we want to predict seizure, stroke, or overdose given some measurements from patients
- If we model them as 1, 2, and 3 respectively, we are assuming order
- Even in case of binary variables, our estimates may exceed range of [0, 1], making the interpretation unnecessarily hard
- Any other reasons that contradict assumptions of the linear model?

Logistic function

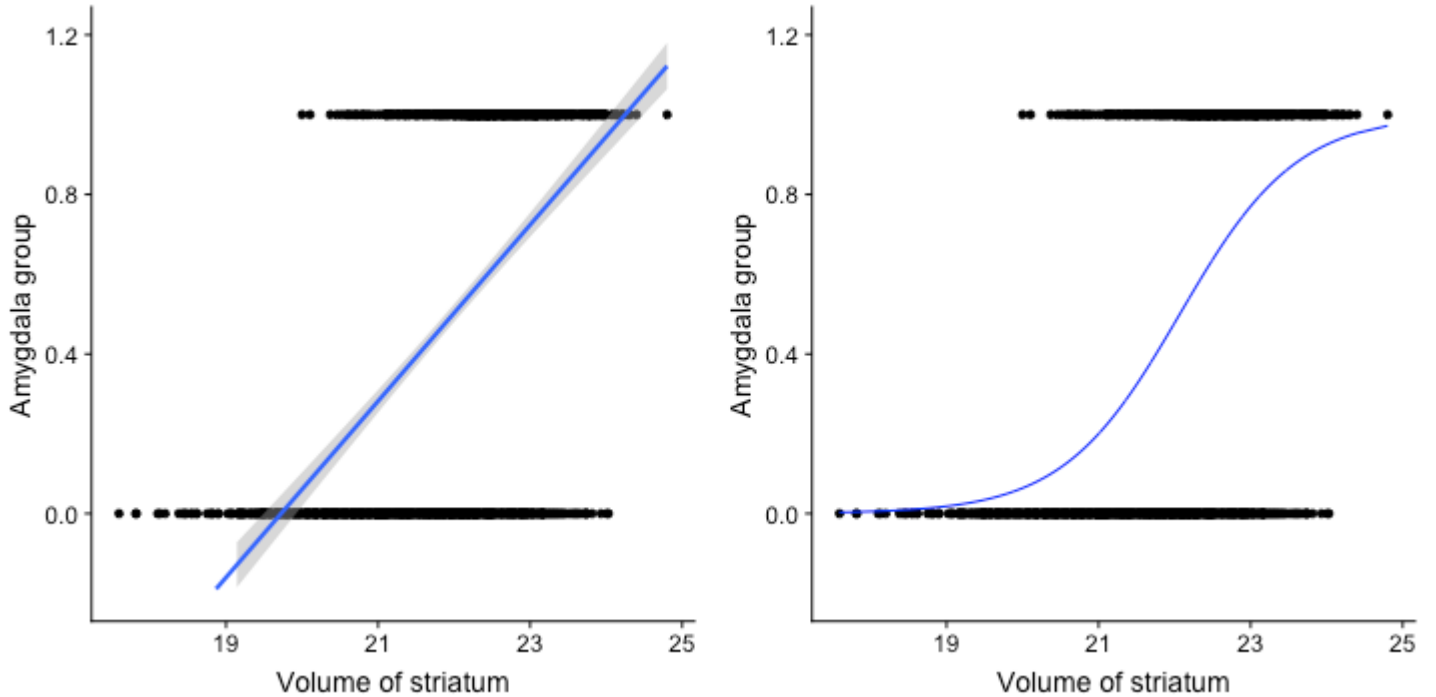
- $\frac{L}{1+e^{-k*(x-\sigma_0)}}$

```
logistic_function = function(input, curve_max=1,
                             curve_steepness=1, sig_mid=0){
  output = curve_max /
    (1 + exp(-curve_steepness * (input - sig_mid)))
}
input_vals = rnorm(50, sd=3)
out_df = data.frame(
  X=input_vals, Y=logistic_function(input_vals))
ggplot(out_df, aes(x=X, y=Y)) + geom_line()
```



Linear model for binary variables?

```
## Warning: Removed 14 rows containing missing values (geom_smooth).
```



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- In linear regression, we used least squared to minimize mean squared error
- In logistic regression, we use **maximum likelihood**
- $l(\beta_0, \beta) = \Pi_{i:y_i=1} p(x_i) \Pi_{i\prime:y_{i\prime}=0} (1 - p(x_{i\prime})) \rightarrow$ Likelihood function

K-nearest neighbours

- Example of a non-parametric, simple, and powerful machine learning method

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*Let's implement it in R!

K-NN algorithm

- Split data to training and test

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```
split_ratio = 0.8
idx_train = sample(1:nrow(mice),
                   size=floor(nrow(mice) * split_ratio))
train_df = mice[idx_train, ]
test_df = mice[-idx_train, ]
```

- Predict amygdala size given volume of striatum and midbrain

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- Finding nearest neighbours

```
get_neighbours = function(test_data, train_df, K=5){
  print(test_data)
  merged_df = rbind(test_data, train_df)
  dist_df = as.matrix(dist(merged_df))
  distances = as.numeric(dist_df[1, ])
  idx_out = order(distances, decreasing=FALSE)[2:(K + 1)]
  return(idx_out)
}
```

K-NN prediction

```
predictive_features = c("striatum", "midbrain")
response = "amygdala.group"
test_df$Posterior = NA
for(i in 1:nrow(test_df)){
   idx_neighbours = get_neighbours(
     test_df[i, predictive_features],
     train_df[, predictive_features])
   labels = unlist(train_df[idx_neighbours, response])
   prob = mean(labels)
   test_df$Posterior[i] = prob
}
```

```
## # A tibble: 1 x 2
##   striatum midbrain
##      <dbl>    <dbl>
## 1     22.0     13.8
## # A tibble: 1 x 2
##   striatum midbrain
##      <dbl>    <dbl>
## 1     22.3     14.0
## # A tibble: 1 x 2
##   striatum midbrain
```

Calculating threshold-based metrics

```
suppressMessages(require(caret))
suppressMessages(require(e1071))
confMat = confusionMatrix(
  factor(test_df$Posterior > 0.5), factor(test_df$amygdala.group == 1
print(as.data.frame(confMat$byClass))
```

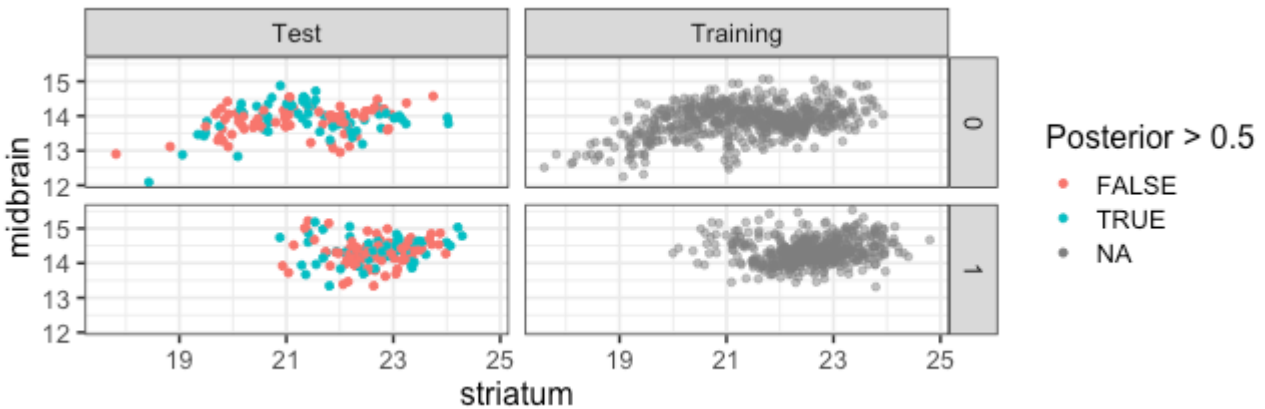
```
##                      confMat$byClass
## Sensitivity                0.5338346
## Specificity                0.3767123
## Pos Pred Value             0.4382716
## Neg Pred Value             0.4700855
## Precision                  0.4382716
## Recall                     0.5338346
## F1                         0.4813559
## Prevalence                 0.4767025
## Detection Rate             0.2544803
## Detection Prevalence       0.5806452
## Balanced Accuracy          0.4552735
```

```
print(paste("Accuracy =", signif(confMat$overall["Accuracy"], 3)))
```

```
## [1] "Accuracy = 0.452"
```

Plotting performance

```
train_df$Posterior = NA
train_df$Dataset = "Training"
test_df$Dataset = "Test"
merged_df = rbind(train_df, test_df)
ggplot(merged_df) +
  aes(x=striatum, y=midbrain, colour=Posterior > 0.5) +
  geom_point(alpha=0.5) +
  geom_point(data=test_df, aes(colour=Posterior > 0.5)) +
  theme_bw(base_size=16) +
  facet_grid(factor(amygdala.group)~Dataset)
```



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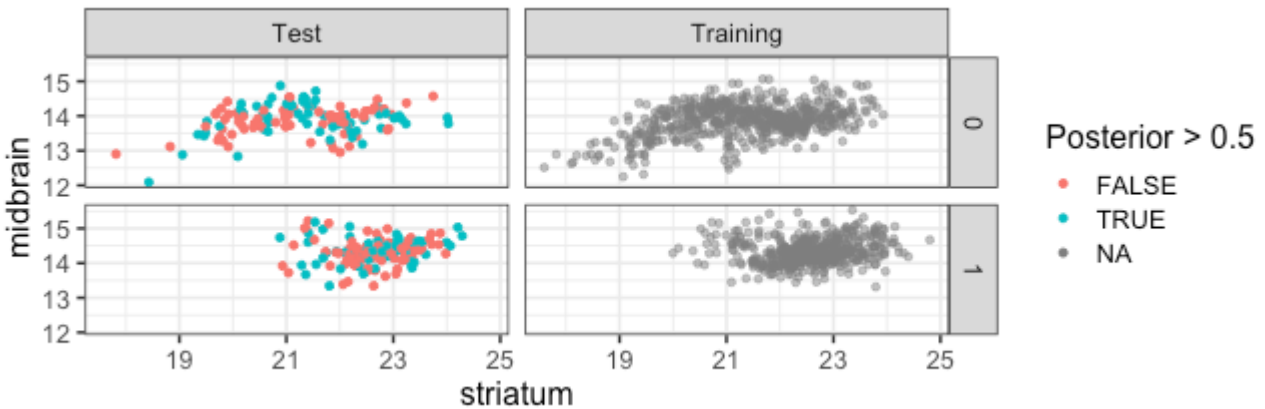

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- Random forests can regress or classify, and they are made of hundreds of trees
- Each tree uses some of data (samples) and some of the features
- We identify which feature can classify (or regress) the outcome better
- We split the data at the point which classifies training data best, and repeat the last step on each split until all data points are grouped
- We build hundreds of trees based on training data. When it comes to new data, we use the majority vote to decide on the response for output variable

Classification tree

```
require(tree)
```

```
## Loading required package: tree
```

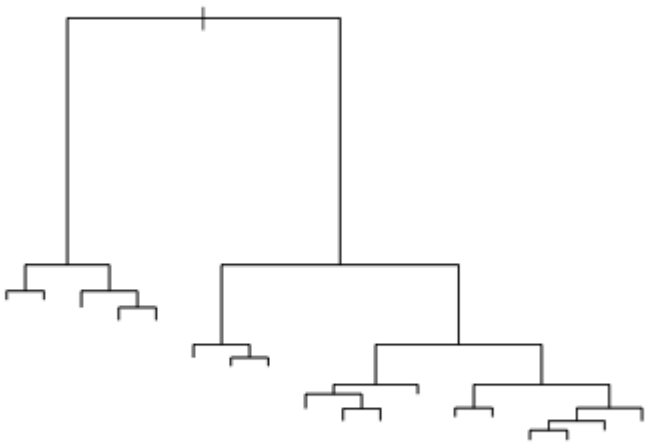
```
volume_df = read.csv("volumes.csv")
volume_df = volume_df[, !colnames(volume_df) %in% c("ID", "Timepoint'
volume_df$amygdala.group = ifelse(volume_df$amygdala > 10, 1, 0)
train_df = volume_df[idx_train, ]
test_df = volume_df[-idx_train, ]
tree_model = tree(factor(amygdala.group) ~.-amygdala, train_df)
summary(tree_model)
```

```
##
## Classification tree:
## tree(formula = factor(amygdala.group) ~ . - amygdala, data = train_df)
## Variables actually used in tree construction:
##  [1] "hippocampus"
##  [2] "Posteromedial.cortical.amygdaloid.area"
##  [3] "optic.tract"
##  [4] "pons"
##  [5] "Secondary.visual.cortex..mediolateral.area"
##  [6] "Secondary.visual.cortex..lateral.area"
```

```
pred_tree = predict(tree_model, test_df, type="class")
confMat = confusionMatrix(pred_tree, factor(test_df$amygdala.group))
acc_tree = signif(confMat$overall["Accuracy"], 3)
print(paste("Accuracy =", acc_tree))
```

```
## [1] "Accuracy = 0.839"
```

```
plot(tree_model)
```



Fitting a random forest

```
suppressMessages(require(randomForest))
rf_model = randomForest(factor(amygdala.group) ~.-amygdala,
                        data=train_df, ntree=100, importance=TRUE)
pred_rf = predict(rf_model, newdata=test_df)
confMat = confusionMatrix(pred_rf, factor(test_df$amygdala.group))
acc_rf = signif(confMat$overall["Accuracy"], 3)
print(paste("Accuracy RF =", acc_rf, "and tree =", acc_tree))
```

```
## [1] "Accuracy RF = 0.892 and tree = 0.839"
```

Feature importance by random forest

- Mean decrease Gini is the sum of Gini impurity of a feature across all trees.

Feature importance by random forest

- Mean decrease Gini is the sum of Gini impurity of a feature across all trees.
- Gini impurity is a measure of how often a randomly chosen element from the set would be incorrectly labeled

```
imp_df = as.data.frame(importance(rf_model))
imp_df$Feature = rownames(imp_df)
imp_df = imp_df[order(imp_df$MeanDecreaseGini, decreasing=TRUE)[1:10]
imp_df$Feature = factor(
  imp_df$Feature,
  levels=imp_df$Feature[order(imp_df$MeanDecreaseGini)])
```

```
ggplot(imp_df) +
  aes(x=Feature, y=MeanDecreaseGini) +
  geom_bar(stat="identity", fill="purple") +
  coord_flip()
```