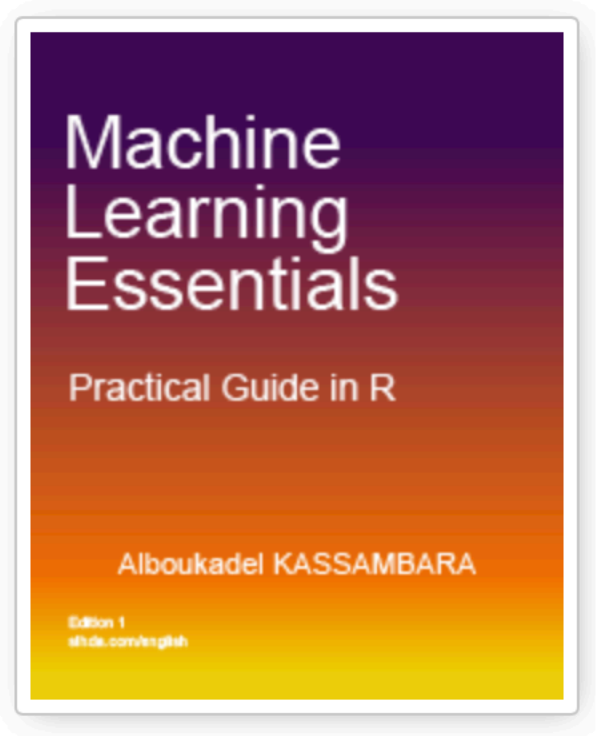
This practical session is based on tutorial from "Machine Learning Essentials: Practical Guide in R" book by A. Kassamara.



It will cover how to:

- Define the logistic regression equation and key terms such as log-odds and logit
- Perform logistic regression in R and interpret the results
- Make predictions on new test data and evaluate the model accuracy

Introduction:

We use Logistic regression to predict a class (or category) of items (e.g. individuals, cells) based on one or several predictor variables (x). It is used to model a binary outcome (y), which can have only two possible values: 0 or 1, yes or no, diseased or non-diseased, etc.
Logistic regression belongs to a family, named *Generalized Linear Model* (*GLM*), because it can e seen as an extension to the linear regression model. It also goes under names: *binary logistic regression*, *binomial logistic regression* and *logit model*.

Logistic regression does not return directly the class of observations. But it allows us to estimate the probability (p) of class membership. The probability will range between 0 and 1. You need to decide the threshold probability at which the category flips from one to the other. By default, this is set to p = 0.5, but it also can be set based on the analysis purpose.

Alternative formulation for Logistic function:

The standard logistic regression function, for predicting the outcome of an observation given a predictor variable (x), is an s-shaped curve defined as $p = 1/[1 + \exp(-y)]$, where:

$y = b0 + b1*x$,
exp() is the exponential and
p is the probability of event to occur (1) given x; so $p(x) = 1/[1 + \exp(-(b0 + b1*x))]$.

By a bit of manipulation, it can be demonstrated that $p/(1-p) = \exp(b0 + b1*x)$. By taking the logarithm of both sides, the formula becomes a linear combination of predictors:

$$\log[p/(1-p)] = b0 + b1*x.$$

When you have multiple predictor variables, the logistic function looks like:

$$\log[p/(1-p)] = b0 + b1*x1 + b2*x2 + \ldots + bn*xn$$

b0 and b1 are the regression beta coefficients. A positive b1 indicates that increasing x will be associated with increasing p. Conversely, a negative b1 indicates that increasing x will be associated with decreasing p.

The quantity $\log[p/(1-p)]$ is called the logarithm of the odds, also known as **logit function**.
The **odds** can be seen as the ratio of “successes” to “non-successes”.
Note that, the probability can be calculated from the odds as $p = Odds/(1 + Odds)$.

Required R packages for this practical:

- tidyverse for data manipulation and visualization
- caret for machine learning workflow
- mlench for data

Install them using install.packages() command

```r
library(tidyverse)
library(caret)
theme_set(theme_bw())
```

Preparing the data:

Logistic regression works for data that contain continuous and/or categorical predictor variables (x).

Performing the following steps might improve the accuracy of your model

- Remove potential outliers
- Make sure that the predictor variables are normally distributed. If not, you can use log, root, Box-Cox transformation.

- Remove highly correlated predictors to minimize overfitting. The presence of highly correlated predictors might lead to an unstable model solution.

Here, you will use the PimaIndiansDiabetes2 (available from mlbench package) for predicting the probability of being diabetes positive based on multiple clinical variables.
We'll randomly split the data into training set (80% for building a predictive model) and test set (20% for evaluating the model). Make sure to set seed for reproducibility.

```
# Load the data and remove NAs
data("PimaIndiansDiabetes2", package = "mlbench")
PimaIndiansDiabetes2 <- na.omit(PimaIndiansDiabetes2)
# Inspect the data
sample_n(PimaIndiansDiabetes2, 3)
# Split the data into training and test set
set.seed(123)
training.samples <- PimaIndiansDiabetes2$diabetes %>%
  createDataPartition(p = 0.8, list = FALSE)
train.data  <- PimaIndiansDiabetes2[training.samples, ]
test.data <- PimaIndiansDiabetes2[-training.samples, ]
```

Computing logistic regression:

The R function glm(), for generalized linear model, can be used to compute logistic regression. You need to specify the option family = binomial, which tells to R that we want to fit logistic regression.

```
# Fit the model
model <- glm( diabetes ~., data = train.data, family = binomial)
# Summarize the model
summary(model)
# Make predictions
probabilities <- model %>% predict(test.data, type = "response")
predicted.classes <- ifelse(probabilities > 0.5, "pos", "neg")
# Model accuracy
mean(predicted.classes == test.data$diabetes)
```

Simple logistic regression:

The simple logistic regression is used to predict the probability of class-membership based on a single predictor variable (x). The following R code builds a model to predict the probability of being diabetes-positive based only on plasma glucose concentration:

```
model <- glm( diabetes ~ glucose, data = train.data, family = binomial)
summary(model)$coef
```

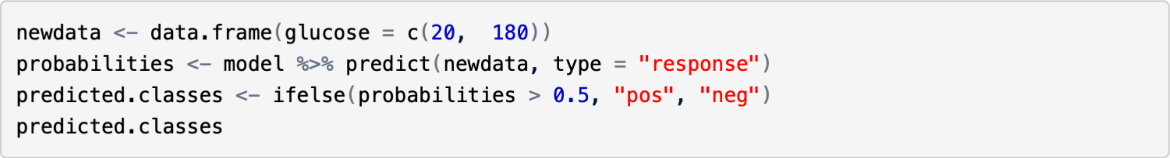
```
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -6.3267     0.7241   -8.74 2.39e-18
## glucose       0.0437     0.0054    8.09 6.01e-16
```

The output above shows the estimate of the regression beta coefficients and their significance levels. The intercept (b0) is -6.32 and the coefficient of glucose variable is 0.043. The logistic equation can be written as

p = exp(-6.32 + 0.043*glucose)/ [1 + exp(-6.32 + 0.043*glucose)].

Using this formula, for each new glucose plasma concentration value, you can predict the probability of individual(s) being diabetic (positive case).

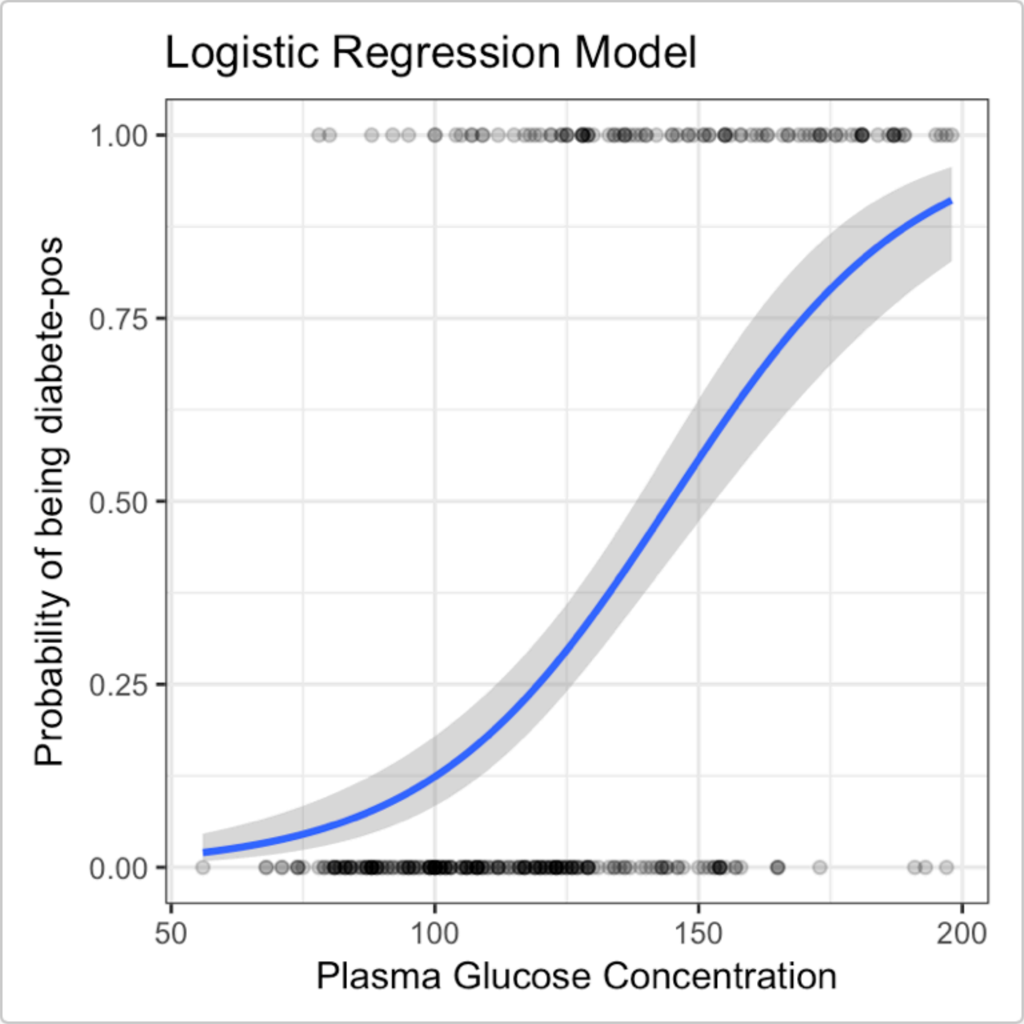
Predictions can be easily made using predict()function. Use the option *type = "response"* to directly obtain probabilities



```
newdata <- data.frame(glucose = c(20,  180))
probabilities <- model %>% predict(newdata, type = "response")
predicted.classes <- ifelse(probabilities > 0.5, "pos", "neg")
predicted.classes
```

The logistic function gives an s-shaped probability curve illustrated as follow:

```
train.data %>%
  mutate(prob = ifelse(diabetes == "pos", 1, 0)) %>%
  ggplot(aes(glucose, prob)) +
  geom_point(alpha = 0.2) +
  geom_smooth(method = "glm", method.args = list(family = "binomial")) +
  labs(
    title = "Logistic Regression Model",
    x = "Plasma Glucose Concentration",
    y = "Probability of being diabete-pos"
    )
```



Multiple predictors:

We can predict the probability of class-membership based on multiple predictor variables, this can be done as follows:

```
model <- glm( diabetes ~ glucose + mass + pregnant,
                data = train.data, family = binomial)
summary(model)$coef
```

To include all available predictor variables within this dataset use ~.:

```
model <- glm( diabetes ~., data = train.data, family = binomial)
summary(model)$coef
```

```
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept) -9.50372    1.31719  -7.215 5.39e-13
## pregnant     0.04571    0.06218   0.735 4.62e-01
## glucose      0.04230    0.00657   6.439 1.20e-10
## pressure    -0.00700    0.01291  -0.542 5.87e-01
## triceps      0.01858    0.01861   0.998 3.18e-01
## insulin     -0.00159    0.00139  -1.144 2.52e-01
## mass         0.04502    0.02887   1.559 1.19e-01
## pedigree     0.96845    0.46020   2.104 3.53e-02
## age          0.04256    0.02158   1.972 4.86e-02
```

Above output shows beta coefficient estimates and their significance levels. In columns are:

- Estimate: the intercept (b0) and all beta coefficient estimates associated with each predictor variable
- Std.Error: the standard error of the coefficient estimates. This represents the accuracy of the coefficients. The larger the standard error, the less confident we are about the estimate.
- z value: the z-statistic, which is the coefficient estimate (column 2) divided by the standard error of the estimate (column 3)
- Pr(>|z|): The p-value corresponding to the z-statistic. The smaller the p-value, the more significant the estimate is.

Note that, the function coef() can be used to extract only the coefficients.

Interpretation:

It can be seen that only 5 out of the 8 predictors are significantly associated to the outcome. These include: pregnant, glucose, pressure, mass and pedigree.

The coefficient estimate of the variable glucose is b = 0.045, which is positive. This means that an increase in glucose is associated with increase in the probability of being diabetic (positive). However the coefficient for the variable pressure is b = -0.007, which is negative. This means that an increase in blood pressure will be associated with a decreased probability of being diabetic (positive).
An important concept to understand, for interpreting the logistic beta coefficients, is the **odds ratio**. An odds ratio measures the association between a predictor variable (x) and the outcome variable (y). It represents the ratio of the odds that an event will occur (event = 1) given the presence of the predictor x (x = 1), compared to the odds of the event occurring in the absence of that predictor (x = 0).
For a given predictor (say x1 = glucose), the associated beta coefficient (b1) in the logistic regression function corresponds to the log of the odds ratio for that predictor.

If the odds ratio is 2, then the odds that the event occurs (event = 1) are two times higher when the predictor x is present (x = 1) versus x is absent (x = 0).
For example, the regression coefficient for glucose is 0.042. This indicate that one unit increase in the glucose concentration will increase the odds of being diabetes-positive by exp(0.042) 1.04 times.

From the logistic regression results, it can be noticed that some variables - triceps, insulin and age - are not statistically significant. Keeping them in the model may contribute to overfitting. Therefore, they can be eliminated. This can be done automatically using statistical techniques, including **stepwise regression** and **penalized regression** methods. This methods are described in other sections of this book. Briefly, they consist of selecting an optimal model with a reduced set of variables, without compromising the model curacy.
Here, as we have a small number of predictors (n = 9), we can select manually the most significant:

```
model <- glm( diabetes ~ pregnant + glucose + pressure + mass + pedigree,
                data = train.data, family = binomial)
```

Making predictions:

We'll make predictions using the test data in order to evaluate the performance of our logistic regression model.

The procedure is the following:

1. Predict the class membership probabilities of observations based on predictor variables
2. Assign the observations to the class with highest probability score (i.e above 0.5)

The R function predict() can be used to predict the probability of being diabetes-positive, given the predictor values:

```
probabilities <- model %>% predict(test.data, type = "response")
head(probabilities)
```

```
##     21     25     28     29     32     36
## 0.3914 0.6706 0.0501 0.5735 0.6444 0.1494
```

Which classes do these probabilities refer to? In our example, the output is the probability that the diabetes test will be positive. We know that these values correspond to the probability of the test to be positive, rather than negative, because the contrasts() function indicates that R has created a dummy variable with a 1 for "pos" and "0" for neg. The probabilities always refer to the class dummy-coded as "1".
Check the dummy coding:

```
contrasts(test.data$diabetes)
```

```
##     pos
## neg   0
## pos   1
```

How to predict a class for different individuals? R code can categorize individuals into two groups based on their predicted probabilities (p) of being diabetes-positive. Individuals, with p above 0.5, are considered as diabetes-positive:

```r
predicted.classes <- ifelse(probabilities > 0.5, "pos", "neg")
head(predicted.classes)
```

```
##    21    25    28    29    32    36
## "neg" "pos" "neg" "pos" "pos" "neg"
```

Assessing model accuracy:

The model accuracy can be measured as the proportion of observations that have been correctly classified. Inversely, the classification error is defined as the proportion of observations that have been misclassified.

Proportion of correctly classified observations:

```r
mean(predicted.classes == test.data$diabetes)
```

```
## [1] 0.756
```

The classification prediction accuracy is about 76%, which is not bad. The misclassification error rate is 24%.
There are alternative metrics for evaluating the performance of a classification model (see Chapter on classification-model-evaluation).

Further notes:

Here we have described how logistic regression works in R. Additionally, we demonstrated how to make predictions and to assess the model accuracy. Logistic regression model output is very easy to interpret compared to other classification methods. Additionally, because of its simplicity it is less prone to overfitting than flexible methods such as decision trees.

Note that, many concepts for linear regression hold true for the logistic regression modelling. For example, you need to perform some diagnostics to make sure that the assumptions made by the model are met for your data.

Furthermore, you need to measure how good the model is in predicting the outcome of new test data observations. Here, we described how to compute the raw classification accuracy, other important performance metric exists (see Chapter on classification-model-evaluation).

In a situation, where you have many predictors you can select, without compromising the prediction accuracy, a minimal list of predictor variables that contribute the most to the model using stepwise regression (see Chapter on stepwise-logistic-regression) and lasso regression techniques (see Chapter on penalized-logistic-regression).

Additionally, you can add interaction terms in the model, or include spline terms.

The same problems concerning confounding (a confounder is a variable that influences both the dependent variable and independent variable, causing a spurious association

) and correlated variables apply to logistic regression (see Chapter on confounding-variables and multicollinearity).

You can also fit *generalized additive models* (see Chapter on polynomial-and-spline-regression), when linearity of the predictor (x) cannot be assumed. This can be done using the mgcv package:

```
library("mgcv")
# Fit the model
gam.model <- gam(diabetes ~ s(glucose) + mass + pregnant,
                 data = train.data, family = "binomial")
# Summarize model
summary(gam.model )
# Make predictions
probabilities <- gam.model %>% predict(test.data, type = "response")
predicted.classes <- ifelse(probabilities> 0.5, "pos", "neg")
# Model Accuracy
mean(predicted.classes == test.data$diabetes)
```

Logistic regression is limited to only two-class classification problems. There is an extension, for multiclass classification problem (see Chapter multinomial-logistic-regression). Note that, *Linear Discriminant Analysis* (see Chapter on discriminant-analysis) can handle multiclass tasks.

Further references:

- Bruce, Peter, and Andrew Bruce. 2017. *Practical Statistics for Data Scientists*. O'Reilly Media.
- James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani. 2014. *An Introduction to Statistical Learning: With Applications in R*. Springer Publishing Company, Incorporated.

Optional, more "advanced stuff":

To better understand how logistic regression and gradient descent work you can study this implementation code "Understanding Logistic Regression from Scratch" available via GitHub: https://github.com/JunWorks/Logistic-Regression-from-scratch-in-R