N-fold Cross-Validation

The **Leave-one-out Cross-Validation** method (or N-fold Cross-Validation) is a ressampling and data partitioning method which aims at estimating the prediction error of a model.

In the context of regressions models, the prediction error $\hat{\theta}_{pe}$ is defined as follows:

$$\hat{\theta}_{pe} = E[e_i^2] = E\Big[(y_i - \hat{y}_i)^2\Big] = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Then the **Root Mean Squared Error** (RMSE) is simply

$$RMSE = \sqrt{\hat{\theta}_{pe}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} e_i^2}$$

N-fold Cross-Validation algorithm

To implement the leave-one-out cross-validation method for regression models, the general procedure is the following:

For i in $1, ..., n$

1. Compute $\hat{y}_i^{(-i)}$ the predictions from the model fitted on all observations except for the i^{th} observation.

2. Compute the errors $e_i = y_i - \hat{y}_i^{(-i)}$

3. Compute the RMSE as $\sqrt{\frac{1}{n}\sum_{i=1}^{n} e_i^2}$

Working example

Example 1: We generate $n = 300$ artificial data points (x_i, y_i) from the following process:

$$x_i \sim N(5, 3)$$
$$y_i = x_i^2 + \epsilon_i \qquad \text{with } \epsilon_i \sim N(0, 8)$$

Suppose that we wish to fit the two following models:

$$\text{Model 1:} \qquad y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$
$$\text{Model 2:} \qquad y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i$$

We will use the Leave-one-out Cross-Validation method in R and Python to select the best model, that is the model with the lowest RMSE.

Code for scatterplots and fit in R

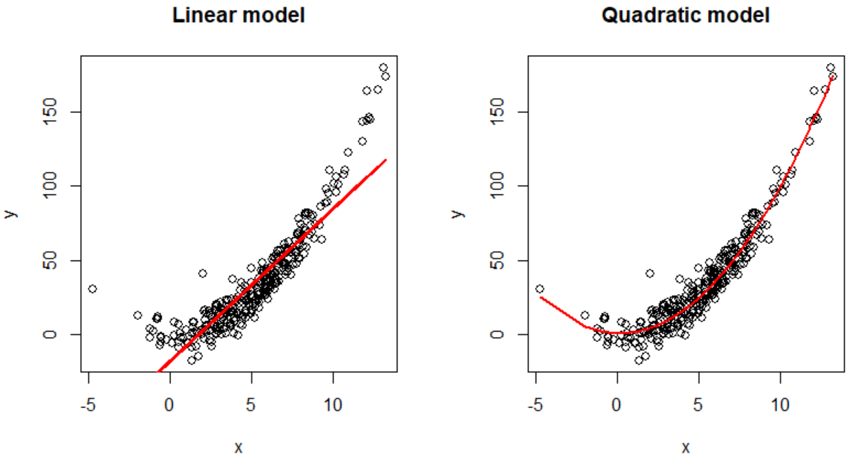
```r
# 1. generate artificial data
set.seed(2023)
n <- 300
x <- rnorm(n = n, mean = 5, sd = 3)
y <- x^2 + rnorm(n = n, mean = 0, sd = 8)
data = data.frame(x = x, y = y)

# 2. plot the models that we want to fit
par(mfrow = c(1,2), pty = "s")

model1 <- lm(y ~ x)
plot(x = x, y = y, main = 'Linear model', cex = 1.1, pch = 1, lwd = 1.2)
yhat1 <- model1$coef[1] + model1$coef[2] * x
lines(x, yhat1, lw = 2.5, col = 'red')

model2 <- lm(y ~ x + I(x^2))
plot(x = x, y = y, main = 'Quadratic model', cex = 1.1, pch = 1, lwd = 1.2)
yhat2 <- model2$coef[1] + model2$coef[2] * x  + model2$coef[3] * x^2
lines(x[order(x)], yhat2[order(x)], lw = 2.5, col = 'red')
```

Plots in R



Code for scatterplots and fit in Python

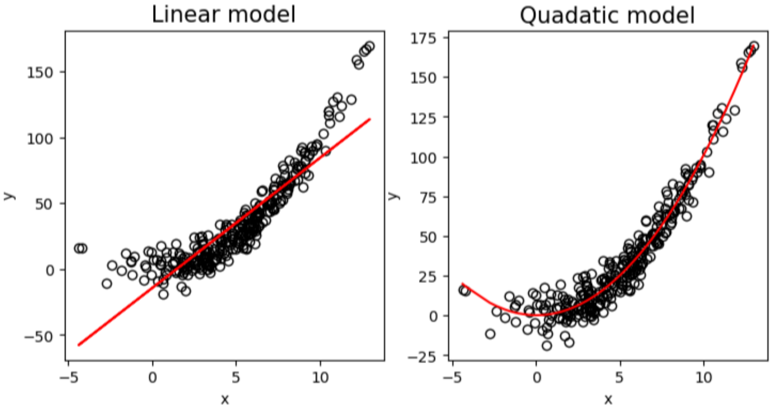
```python
# 1. generate artificial data
import numpy as np
np.random.seed(2023) ; n = 300
x = np.random.normal(loc = 5, scale = 3, size = n)
y = x**2 + np.random.normal(loc = 0, scale = 8, size = n)

# 2. plot the models that we want to fit
import matplotlib.pyplot as plt

plt.subplot(1, 2, 1)
plt.plot(x, y, 'o', fillstyle = 'none', color = 'black')
plt.title('Linear model', fontsize = 15)
plt.xlabel("x") ; plt.ylabel("y")
beta1, beta0 = np.polyfit(x, y, 1) ; yhat1 = beta0 + beta1*x
plt.plot(x, yhat1, color = 'red')

plt.subplot(1, 2, 2)
plt.plot(x, y, 'o', fillstyle = 'none', color = 'black')
plt.xlabel('x') ; plt.ylabel('y') ; plt.title('Quadatic model', fontsize = 15)
beta2, beta1, beta0 = np.polyfit(x, y, 2) ; yhat2 = beta0 + beta1*x + beta2*(x
    **2)
orders = np.argsort(x.ravel())
plt.plot(x[orders], yhat2[orders], color = 'red')
```

Plots in Python



N-fold Cross-Validation in R

```r
# 3. Cross-Validation
# fit the models on leave-one-out samples

pred.cv.mod1 <- pred.cv.mod2 <- numeric(n)

for(i in 1:n) {

  # quadratic model
  mod1 = lm(y ~ x, subset = -i)
  pred.cv.mod1[i] = predict(mod1, data[i,])

  # quadratic model
  mod2 = lm(y ~ x + I(x^2), subset = -i)
  pred.cv.mod2[i] = predict(mod2, data[i,])

}
```

N-fold Cross-Validation in Python

```python
# 3. Cross-Validation
# fit the models on leave-one-out samples

import pandas as pd

data = pd.DataFrame({'x': x, 'y': y})
xn = data['x'].values.reshape(-1,1); yn = data['y'].values.reshape(-1,1)

from sklearn.preprocessing import PolynomialFeatures
from sklearn.model_selection import LeaveOneOut, cross_val_score

loocv = LeaveOneOut()

# linear model
mod1 = PolynomialFeatures(degree = 1, include_bias = False).fit_transform(xn)
mod11 = LinearRegression().fit(mod1, yn)
scoresmod1 = cross_val_score(mod11, mod1, yn,
                         scoring = 'neg_mean_squared_error',
                         cv = loocv)
# quadratic model
mod2 = PolynomialFeatures(degree = 2, include_bias = False).fit_transform(xn)
mod22 = LinearRegression().fit(mod2, yn)
scoresmod2 = cross_val_score(mod22,  mod2, yn,
                         scoring = 'neg_mean_squared_error',
                         cv = loocv)
```

Conclusion from R and Python outputs

In R:

```r
MSE1 = (1/n) * sum((y - pred.cv.mod1)^2) # theta_hat_pe
MSE2 = (1/n) * sum((y - pred.cv.mod2)^2) # theta_hat_pe

# Root Mean Squared Error (RMSE)
sqrt(c(MSE1, MSE2))
# [1] 15.68599  7.99332
```

In Python

```python
# Root Mean Squared Error (RMSE)
import statistics
import math

RMSE1 = math.sqrt(statistics.mean(abs(scoresmod1)))
RMSE2 = math.sqrt(statistics.mean(abs(scoresmod2)))
[RMSE1, RMSE2]
# [16.169293289892607, 7.873829105930071]
```

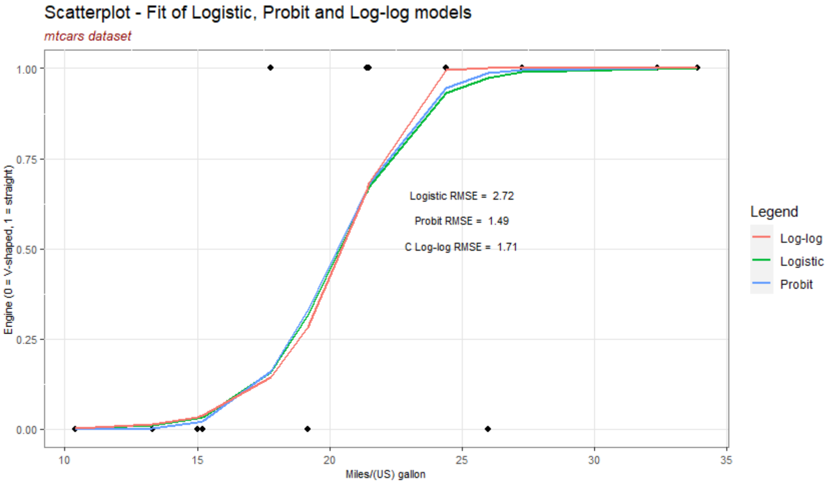
The second model (Quadratic) has the lowest RMSE and thus is prefered (to the Linear) in both cases. It was expected since the fit as described by the red line or curve on the graphs decribe the generated data more accurately.

Real world example

Example 2: We use the dataset mtcars and split it into a training set, containing about 60% of observations and a testing set containing the remaining 40%. We try to predict the variable 'vs', corresponding to the type of engine with the variable 'mpg' or miles per gallon using Logistic, Probit and Complementary Log-Log models, well suited for binary regression. Here are the first lines of the dataset. We only use R and find that the Probit model is the best among the three.

```
head(mtcars)
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

Scatterplot and fit after LOOCV in R



Further reading and code

Rizzo, M.L. (2019). Statistical Computing with R, Second Edition (2nd ed.). Chapman and Hall/CRC. https://doi.org/10.1201/9780429192760

The R Project for Statistical Computing:
https://www.r-project.org/

Python:
https://www.python.org/

Accessing R and Python code:
https://github.com/JRigh/LOOCV-Cross-validation-for-regression