Chapter 7 Linear Regression

7.1 Measures of association

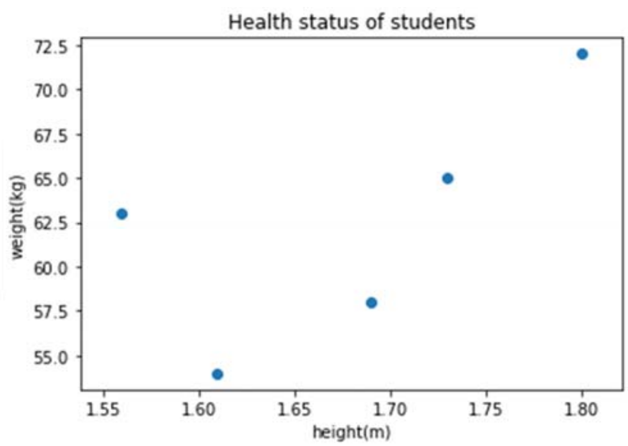
In statistics, **bivariate data** refers to a dataset with two variables. Each sample in this dataset contains values of both variables. A typical example is the health data we studied in a previous chapter. Each student is a sample with two variables height (m) and weight (kg).

```
import pandas as pd
df = pd.read_csv("health.csv")
x = df['height']
y = df['weight']
```

	sex	height	weight
0	M	1.73	65
1	F	1.61	54
2	M	1.80	72
3	F	1.56	63
4	F	1.69	58

To visualize the relationship between two variables from a bivariate data, we can draw a scatterplot. In a scatterplot, each data point represents a sample. The x-coordinate and y-coordinate represent the value of the two variables.

```
plt.scatter(x,y)
plt.title("Health status of students")
plt.xlabel("height(m)")
plt.ylabel("weight(kg)")
plt.show()
```



Here, we might want to study how the two variables are related to each other using measures of association. To have a rough idea, consider the example above. Do you think that weight and height are uncorrelated? Or do you believe a tall person should be heavier (positive correlation)? Or do you believe a tall person should be lighter (negative correlation)?

In descriptive statistics, we have introduced variance and standard deviation as measures of dispersion, meaning how far the values apart from the mean are. For the variables x and y, their variance and standard deviation are σ_x^2, σ_y^2 and σ_x, σ_y respectively. In order measure their association, we further introduce a measure called **population covariance**:

$$\sigma_{xy} = \frac{\sum\left(x^{(i)} - \bar{x}\right)\left(y^{(i)} - \bar{y}\right)}{N}$$

where $x^{(i)}, y^{(i)}$ are the values of variables x, y of the i-th sample, $\bar{x}, \bar{y}$ are the arithmetic means of the two variables, N is the population size.

This is to say, for each sample we evaluate product of difference between each variable with its mean. Notice that this can be positive or negative. The covariance is the average value of these products. Notice that the covariance is commutative, meaning that $\sigma_{xy} = \sigma_{yx}$. Also, the covariance of a variable with its own self results in the variance.

For **sample covariance**, we may simply replace N by $n - 1$ where n is the sample size. In pandas, we can use the function `cov()` to show the sample covariance between two variables, or to give a covariance table.

```
x.cov(y)
```

```
0.43849999999999995
```

```
df.cov()
```

	height	weight
height	0.00907	0.4385
weight	0.43850	47.3000

However, the value of covariance also depends on the scale of the variables. For example, if we use centimetre and pounds as the units for height and weight, the covariance will be difference. In order to study the association between two variables without considering scale and unit, we can standardize the covariance by the standard deviation of the two variables. This gives the **correlation coefficient**:

$$r_{xy} = \frac{\sigma_{xy}}{\sigma_x \sigma_y}$$

The complete formula is written as:

$$r_{xy} = \frac{\sum\left(x^{(i)} - \bar{x}\right)\left(y^{(i)} - \bar{y}\right)}{\sqrt{\sum(x^{(i)} - \bar{x})^2}\sqrt{\sum(y^{(i)} - \bar{y})^2}}$$

The result of correlation coefficient r_{xy} is a value between -1 and 1 inclusively. We can interpret the relationship between the two variables by the value of r_{xy}:

$r_{xy} = 0$ indicates no linear relationship, or in other words uncorrelated.

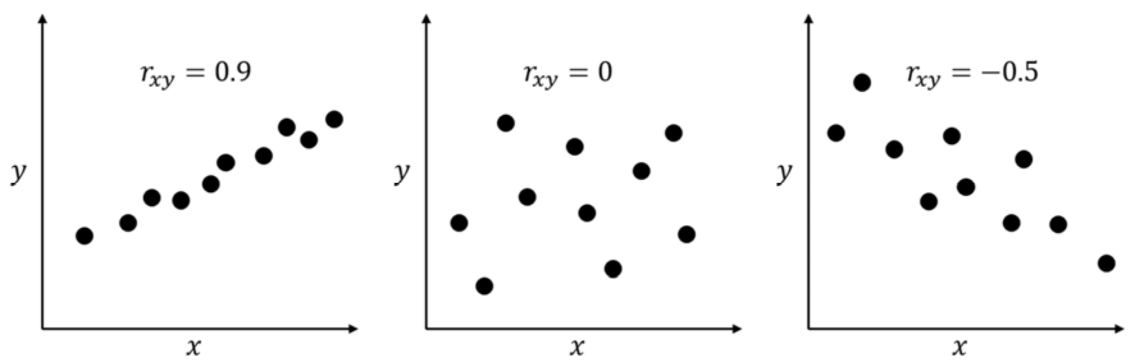
$r_{xy} = 1$ indicates a perfect positive linear relationship: as one variable increases in its values, the other variable also increases in its values through an exact linear rule.

$r_{xy} = -1$ indicates a perfect negative linear relationship: as one variable increases in its values, the other variable decreases in its values through an exact linear rule.

Other than these special cases, we can also distinguish the linear relationship between the variables as follows:

	weak	moderate	strong
positive	$0 < r_{xy} < 0.3$	$0.3 < r_{xy} < 0.7$	$0.7 < r_{xy} < 1$
negative	$-0.3 < r_{xy} < 0$	$-0.7 < r_{xy} < -0.3$	$-1 < r_{xy} < -0.7$

To illustrate this idea, compare the three figures below. In the left figure, we can easily draw a straight line with positive slope with the points lying close to it. In the right figure, we can also draw a line with negative slope, but the points are farther apart from it. However, for the middle figure we can hardly draw a linear relationship between the points.



We can evaluate the coefficient of correlation using pandas easily. Let's go back to the example of health data of five students. Read the csv file as a DataFrame first. We can then regard height and weight as the two variables. For convenience, we may assign the two columns as two Series `x` and `y`. We can evaluate the correlation coefficient by `corr()`. Notice that this operation is commutative meaning that `x.corr(y)` and `y.corr(x)` give the same result. The coefficient 0.669 indicates that height and weight are (moderate) positively correlated.

```
x.corr(y)
```

```
0.6694765721676758
```

```
df.corr()
```

	height	weight
height	1.000000	0.669477
weight	0.669477	1.000000

In case there are more than two variables in the dataset, it would be inconvenient to compare every pair of them. Instead, we might apply `corr()` to the whole DataFrame. This will give a table of correlation coefficient between each column pairwisely. Notice that non-numerical variables (e.g. sex) is ignored. The table is symmetry with the diagonal values equal to 1 since the correlation coefficient of a variable with itself must be 1.

To further illustrate the idea of correlation between different variables, we will study a famous example. In 1978, David Harrison Jr. and Daniel L. Rubinfeld published a paper called "Hedonic housing prices and the demand for clean air". To support their findings, they referred to the data for census tracts in the Boston Standard Metropolitan Statistical Area (SMSA) in 1970. This dataset is clean with lots of variables including the following:

1. CRIM - per capita crime rate by town
2. ZN - proportion of residential land zoned for lots over 25,000 sq.ft.
3. INDUS - proportion of non-retail business acres per town.
4. CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise)
5. NOX - nitric oxides concentration (parts per 10 million)
6. RM - average number of rooms per dwelling
7. AGE - proportion of owner-occupied units built prior to 1940
8. DIS - weighted distances to five Boston employment centres
9. RAD - index of accessibility to radial highways
10. TAX - full-value property-tax rate per $10,000
11. PTRATIO - pupil-teacher ratio by town
12. B - 1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
13. LSTAT - % lower status of the population
14. MEDV - Median value of owner-occupied homes in $1000's

This dataset has been store in "boston.csv". It contains 506 rows and 14 columns. We can first read it as a DataFrame.

```python
df = pd.read_csv("boston.csv")
```

```python
df.head()
```

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	B	LSTAT	MEDV
0	0.00632	18.0	2.31	0	0.538	6.575	65.2	4.0900	1	296	15.3	396.90	4.98	24.0
1	0.02731	0.0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	396.90	9.14	21.6
2	0.02729	0.0	7.07	0	0.469	7.185	61.1	4.9671	2	242	17.8	392.83	4.03	34.7
3	0.03237	0.0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
4	0.06905	0.0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	396.90	5.33	36.2

As this dataframe contains quite a number of variables, we can show correlations between each pair of variables in table form.

```python
df.corr()
```

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	B	LSTAT	MEDV
CRIM	1.000000	-0.200469	0.406583	-0.055892	0.420972	-0.219247	0.352734	-0.379670	0.625505	0.582764	0.289946	-0.385064	0.455621	-0.388305
ZN	-0.200469	1.000000	-0.533828	-0.042697	-0.516604	0.311991	-0.569537	0.664408	-0.311948	-0.314563	-0.391679	0.175520	-0.412995	0.360445
INDUS	0.406583	-0.533828	1.000000	0.062938	0.763651	-0.391676	0.644779	-0.708027	0.595129	0.720760	0.383248	-0.356977	0.603800	-0.483725
CHAS	-0.055892	-0.042697	0.062938	1.000000	0.091203	0.091251	0.086518	-0.099176	-0.007368	-0.035587	-0.121515	0.048788	-0.053929	0.175260
NOX	0.420972	-0.516604	0.763651	0.091203	1.000000	-0.302188	0.731470	-0.769230	0.611441	0.668023	0.188933	-0.380051	0.590879	-0.427321
RM	-0.219247	0.311991	-0.391676	0.091251	-0.302188	1.000000	-0.240265	0.205246	-0.209847	-0.292048	-0.355501	0.128069	-0.613808	0.695360
AGE	0.352734	-0.569537	0.644779	0.086518	0.731470	-0.240265	1.000000	-0.747881	0.456022	0.506456	0.261515	-0.273534	0.602339	-0.376955
DIS	-0.379670	0.664408	-0.708027	-0.099176	-0.769230	0.205246	-0.747881	1.000000	-0.494588	-0.534432	-0.232471	0.291512	-0.496996	0.249929
RAD	0.625505	-0.311948	0.595129	-0.007368	0.611441	-0.209847	0.456022	-0.494588	1.000000	0.910228	0.464741	-0.444413	0.488676	-0.381626
TAX	0.582764	-0.314563	0.720760	-0.035587	0.668023	-0.292048	0.506456	-0.534432	0.910228	1.000000	0.460853	-0.441808	0.543993	-0.468536
PTRATIO	0.289946	-0.391679	0.383248	-0.121515	0.188933	-0.355501	0.261515	-0.232471	0.464741	0.460853	1.000000	-0.177383	0.374044	-0.507787
B	-0.385064	0.175520	-0.356977	0.048788	-0.380051	0.128069	-0.273534	0.291512	-0.444413	-0.441808	-0.177383	1.000000	-0.366087	0.333461
LSTAT	0.455621	-0.412995	0.603800	-0.053929	0.590879	-0.613808	0.602339	-0.496996	0.488676	0.543993	0.374044	-0.366087	1.000000	-0.737663
MEDV	-0.388305	0.360445	-0.483725	0.175260	-0.427321	0.695360	-0.376955	0.249929	-0.381626	-0.468536	-0.507787	0.333461	-0.737663	1.000000

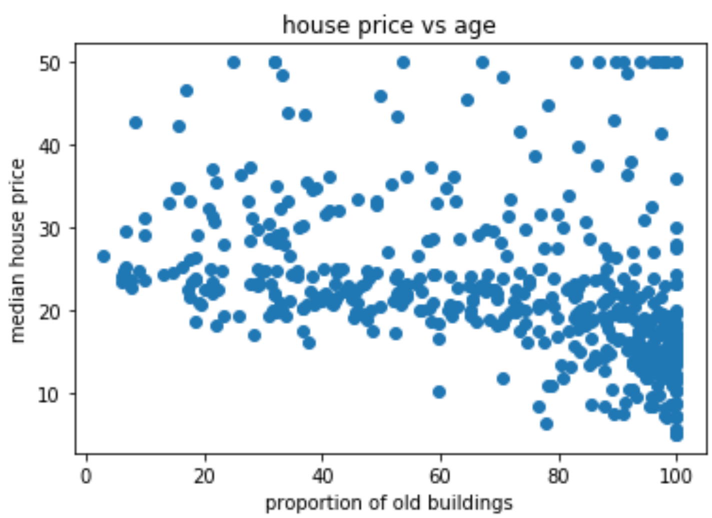
In particular, we would like to study how is the target variable median house price (MEDV) being correlated to two factors average room number (RM) and proportional of old buildings (AGE). First we can extract these columns from the DataFrame as three Series.

```python
x1 = df['RM']
x2 = df['AGE']
x3 = df['MEDV']
```

To visualize the data, make a scatter plot for each pair of variables. We can see that the house price is positively correlated to the average room number, meaning that in general more rooms result in higher price. However, it is negatively correlated to the proportional of old buildings, meaning that for more old buildings in the district the house price is more likely to be lower.

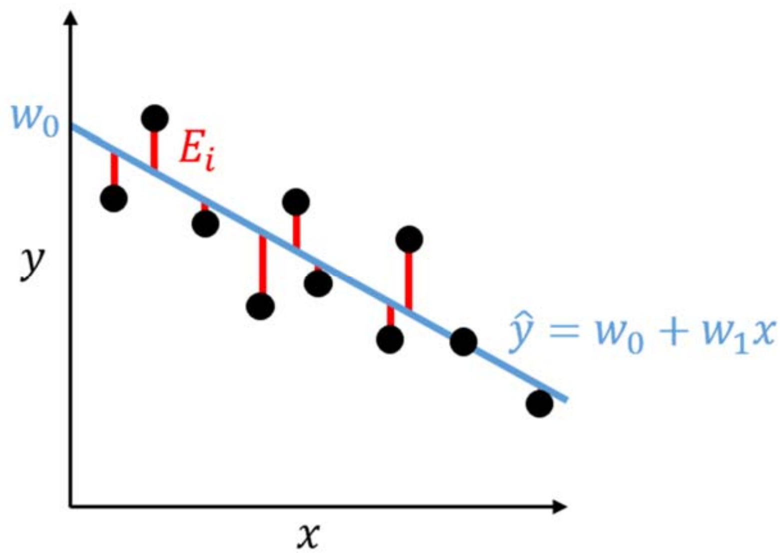
```
plt.scatter(x1,x3)
plt.title("house price vs room number")
plt.xlabel("average room number")
plt.ylabel("median house price")
plt.show()
```


```
plt.scatter(x2,x3)
plt.title("house price vs age")
plt.xlabel("proportion of old buildings")
plt.ylabel("median house price")
plt.show()
```



7.2 Introduction to linear regression

In the previous section, we have introduced the correlation coefficient for measuring the association between two variables. The value of this coefficient suggests whether it is a linear relationship between the two variables. To further analyze the association and make reasonable prediction, we can use a statistical technique called **linear regression**. For simplicity, we are looking for a straight line that best fit the data set of two variables. Recall the figure in the previous section. We can draw a straight line graphically to fit the points. In general, we need to know how to find the equation of such line, and how to evaluate the performance of the line fitting the points.



We define $\hat{y}$ as the predicted value, which is a linear function x given by:

$$\hat{y} = w_0 + w_1 x$$

where the weights w_0, w_1 represents the y-intercept and slope of the line. For the i-th sample, we define the error E_i as the difference between the predicted value $\hat{y}^{(i)}$ and the actual value $y^{(i)}$. Our target is to find the weights with the least **sum of square error** (SSE). In other words, try to minimize:

$$SSE = \sum_{i=1}^{n} E_i^2 = \sum_{i=1}^{n} \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

In case the target variable y is correlated to several variable, we can express the predicted value as the following expression giving a plane or hyperplane rather than a line.

$$\hat{y} = w_0 + w_1 x_1 + \cdots + w_m x_m$$

In such situation, we need to use a multiple regression model.

7.3 Building a linear regression model

In scikit-learn, there is a linear regression model using the least square error method. We will revisit the Boston house price example to illustrate the techniques of such model. As we have found from the previous session, the average number of rooms (RM) has the highest positive correlation with the house price (MEDV). To create a simple regression model, we regard RM as one column in X and MEDV as y, extract the related columns from the DataFrame. Notice that X is a DataFrame which might contain one or more than one columns. For a simple linear regression model, we are only using one variable. On the other hand, y is a Series which is the only target variable to be predicted.

```
import pandas as pd
df = pd.read_csv('boston.csv')
X = df[['RM']]
y = df['MEDV']
```

Create a linear regression model by `LinearRegression` in scikit-learn, then use the fit method to train the model using the variable X and target y.

```
from sklearn.linear_model import LinearRegression
slr = LinearRegression()
slr.fit(X, y)
```

After evaluation, the slope w_1 and the y-intercept w_0 can be found by `coef_` and `intercept_` under the object. Notice that `coef_` is an array of numbers as there can be more than one variables $w_1. w_2, w_3, \ldots$ in a multiple regression model.

```
slr.intercept_
```

```
-34.670620776438554
```

```
slr.coef_
```

```
array([9.10210898])
```

Therefore we have $w_0 \approx -34.67, w_1 \approx 9.1$. The regression line is given by:

$$\hat{y} = -34.67 + 9.1x$$

$y = mx + c$

where $\hat{y}$ is the predicted median house price and x is the average number of rooms.

$y = c + mx$

With this regression model, we can evaluate all the predict values $\hat{y}^{(i)}$ directly using `predict()`:

```
y_pred = slr.predict(X)
```

One may also make prediction of a single value. For example, the expected price (in $1000) of a house with 5 rooms is given by:

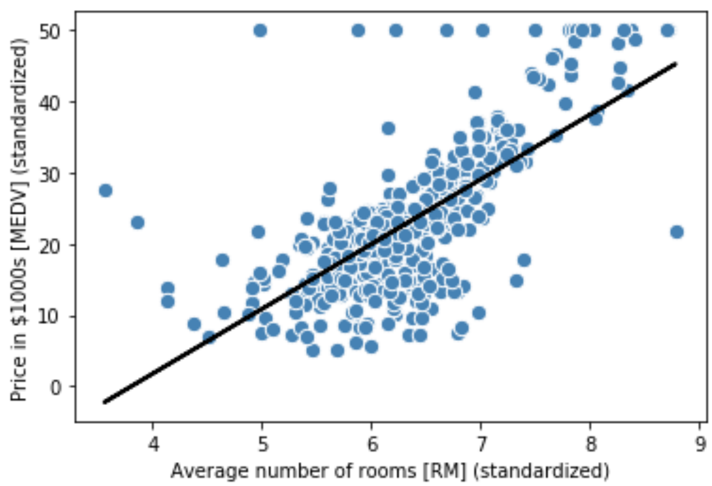
predict

```
slr.predict([[5]])
```

```
array([10.83992413])
```

To visualize the data and also the regression, show the line graph and scatter plot:

```
import matplotlib.pyplot as plt
plt.scatter(X, y, c='steelblue', edgecolor='white', s=70)
plt.plot(X, slr.predict(X), color='black', lw=2)
plt.xlabel('Average number of rooms [RM] (standardized)')
plt.ylabel('Price in $1000s [MEDV] (standardized)')
plt.show()
```



7.4 Performance of linear regression model

In the previous section, we have introduced how to fit a regression model on training data. However, just as training a classification model, it is crucial to test the model on data that it hasn't seen during training to obtain a more unbiased estimate of its generalization performance. We will use scikit-learn to split the dataset into train data and test data, and compare their performance.

With train_test_split we can split both X and y into train data and test data:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.3, random_state=0)
```

The linear regression model is then trained with only the train data:

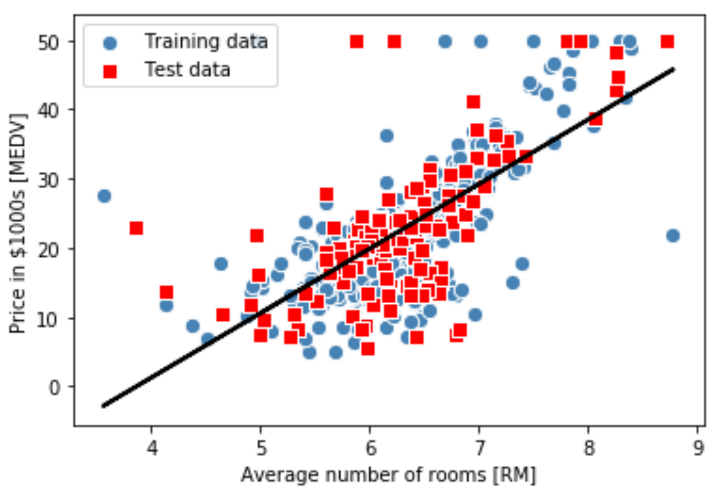
```
from sklearn.linear_model import LinearRegression
slr2 = LinearRegression()
slr2.fit(X_train, y_train)
```

After the model is trained, apply it to X_train and X_test separately to make prediction:

```
y_train_pred = slr2.predict(X_train)
y_test_pred = slr2.predict(X_test)
```

To compare, create scatter plot of the train data and test data with different styles, and also the line graph of the regression model on the same figure.

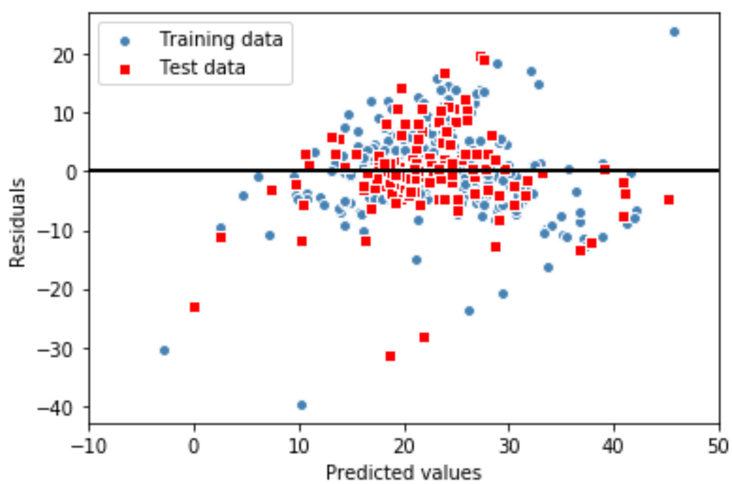
```
plt.scatter(X_train, y_train, c='steelblue', marker='o',
            edgecolor='white', s=70, label='Training data')
plt.scatter(X_test, y_test, c='red', marker='s',
            edgecolor='white', s=70, label='Test data')
plt.plot(X_train, y_train_pred, color='black', lw=2)
plt.legend(loc='upper left')
plt.xlabel('Average number of rooms [RM]')
plt.ylabel('Price in $1000s [MEDV]')
plt.show()
```



The figure, however, is not very effective in visualizing the performance of the model. Moreover, if it is a multiple regression model with variables $x_1, x_2, x_3, \ldots$ it would be impossible to visualize it on a 2D figure.

To visualize the performance of a regression model, we can use **residual plot**. The **residual** of a point refers to the difference between its actual and predicted values, i.e. $\hat{y}^{(i)} - y^{(i)}$. It is also referred as **error** of the prediction at a point. Notice that the residual can be positive or negative, mean that the model over-estimate or under-estimate the actual value. The case of zero residual means the prediction about this point is exact. Residual plot refers to the scatter plot of the residuals against predicted values. Despite the number of variables in X, the residual plot is always a 2D visualization.

```
plt.scatter(y_train_pred,  y_train_pred - y_train,
            c='steelblue', marker='o', edgecolor='white',
            label='Training data')
plt.scatter(y_test_pred,  y_test_pred - y_test,
            c='red', marker='s', edgecolor='white',
            label='Test data')
plt.xlabel('Predicted values')
plt.ylabel('Residuals')
plt.legend(loc='upper left')
plt.hlines(y=0, xmin=-10, xmax=50, color='black', lw=2)
plt.xlim([-10, 50])
plt.show()
```



In the case of a perfect prediction, the residuals would be exactly zero, which we will probably never encounter in realistic and practical applications. However, for a good regression model, we would expect the errors to be randomly distributed and the residuals to be randomly scattered around the centreline. If we see patterns in a residual plot, it means that our model is unable to capture some explanatory information, which has leaked into the residuals.

Another useful quantitative measure of a model's performance is the **mean squared error (MSE)** which is simply the averaged value of the SSE. The MSE is useful for comparing different regression models or for tuning their parameters via grid search and cross-validation, as it normalizes the SSE by the sample size:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(\hat{y}^{(i)} - y^{(i)}\right)^2$$

Compute MSE of the train and test predictions in our example:

```
from sklearn.metrics import mean_squared_error
```

```
mean_squared_error(y_train, y_train_pred)
```

```
42.15765086312225
```

```
mean_squared_error(y_test, y_test_pred)
```

```
47.03304747975518
```

We can see the MSE on the training dataset is significantly larger than the MSE on the test dataset. This indicates our model is overfitting the training data. However, please be aware that the MSE is unbounded in contrast to the classification accuracy, for example. In other words, the interpretation of the MSE depends on the dataset and feature scaling. For example, if the house prices were presented as multiples of 1,000 (with the K suffix), the same model would yield a lower MSE compared to a model that worked with unscaled features.

Thus, it may sometimes be more useful to report the **coefficient of determination** (R^2), which can be understood as a standardized version of the MSE, for better interpretability of the model's performance. Or, in other words, R^2 is the fraction of response variance that is captured by the model. The mathematical expression is as follows:

$$R^2 = 1 - \frac{SSE}{SST} = 1 - \frac{\frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}{\frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - \bar{y}\right)^2} = 1 - \frac{MSE}{Var(y)}$$

Notice that R^2 is a value in between 0 to 1. If the error is smaller, value of R^2 become bigger. In case of perfect fit, all the errors are 0 resulting $R^2 = 1$.

To computer R^2 using scikit-learn:

```
from sklearn.metrics import r2_score
```

```
r2_score(y_train, y_train_pred)
```

```
0.5026497630040827
```

```
r2_score(y_test, y_test_pred)
```

```
0.43514364832115193
```

We can see that the value of R^2 of the train data is higher than that of the test data. This suggests our regression model gives less error for the train data.