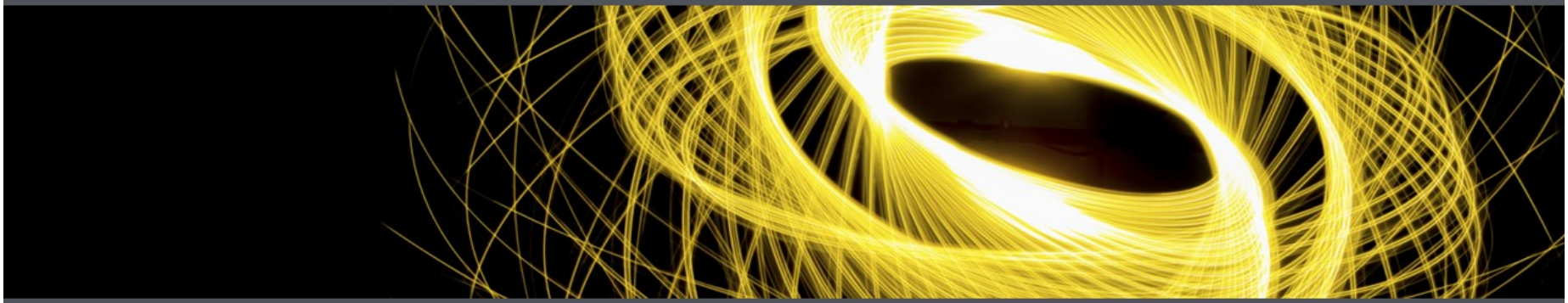
Department of Computer Science

University of Reading

CSMAD21 – Applied Data Science with Python



Regression

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Subjects Covered for Data Science

In previous lectures you have covered:

- NumPy
- Pandas
- Matplotlib
- Introduction to Data Science

In machine learning we will utilise all these skills to build statistical models

What is machine learning?

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- Fundamentally we build mathematical models to help understand data

- These models can be used in 2 ways:
  - **Descriptive**: It may be useful to know how feature *X* influences outcome *Y* so that we can understand how changes in *X* result in changes in *Y*

  - **Predictive:** want to learn the relationship between *X* and *Y* to be able to predict a value of *Y* for some known values of *X*.

Supervised Learning

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- Previously you have covered clustering, a method of unsupervised learning
- In supervised learning you have input variables (x) and an output variable (Y) and you use an algorithm to learn the mapping function from the input to the output.

$$Y = f(x)$$

- The goal is to approximate the mapping function so well that when you have new input data (x) that you can predict the output variables (Y) for that data.

Linear Regression

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- Described as linear equation that combines a specific set of input values (x) the solution to which is the predicted output (y)

=>Therefore both the input values (x) and the output value are continuous numeric values

- When there is a single input variable, the method is referred to as simple linear regression

Simple Linear Regression

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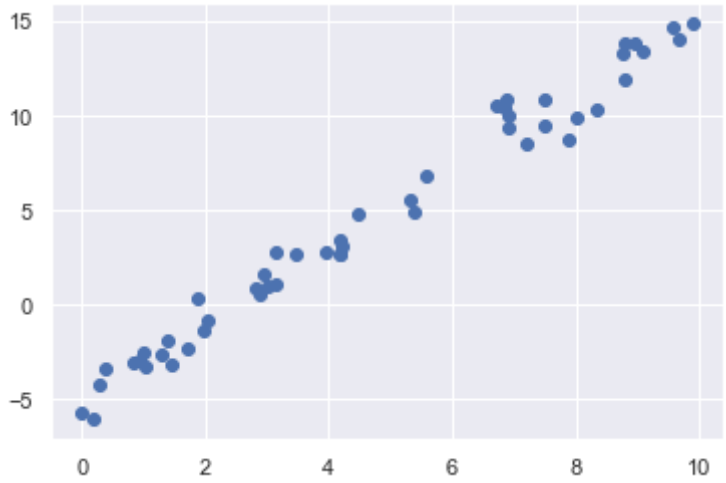
- The linear equation assigns one scale factor to each input value or column, called a coefficient and represented by the capital Greek letter Beta (B).
- One additional coefficient is also added, giving the line an additional degree of freedom (e.g. moving up and down on a two-dimensional plot) and is called the intercept.
- A simple regression problem (a single x and a single y), the form of the model would be:

$$y = B_0 + B_1 \mathrm{x}$$

More often than not you will be able to use the scikit learn API to implement linear regression

In [2]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn as sns; sns.set()
import numpy as np
import pandas as pd
```

In [3]:
```
rng = np.random.RandomState(1)
x = 10 * rng.rand(50)
y = 2 * x - 5 + rng.randn(50)
plt.scatter(x, y);
```

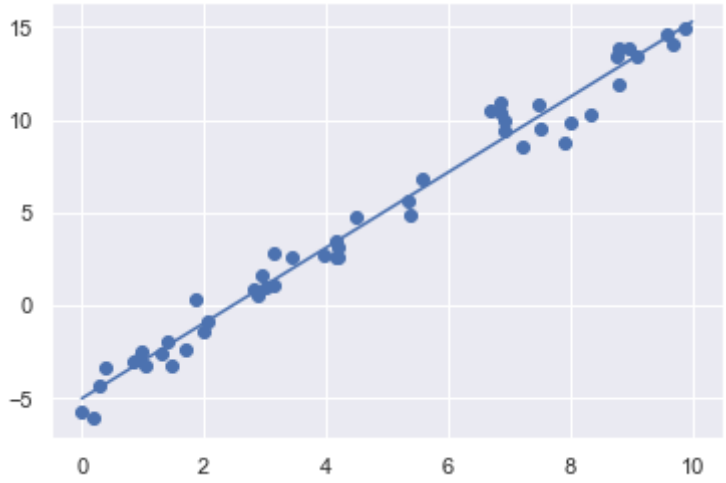


In [4]:
```
from sklearn.linear_model import LinearRegression
model = LinearRegression(fit_intercept=True)

model.fit(x[:, np.newaxis], y)

xfit = np.linspace(0, 10, 1000)
yfit = model.predict(xfit[:, np.newaxis])

plt.scatter(x, y)
plt.plot(xfit, yfit);
```



```
In [5]: print("Model slope:    ", model.coef_[0])
        print("Model intercept:", model.intercept_)
```

```
Model slope:     2.0272088103606944
Model intercept: -4.9985770855532
```

What dictates a line of best fit?

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- ***Ordinary least squares*** aims to minimise the squared difference between the predicted values of *Y* based on *X* and the actual values of *Y* .
- If we have a mapping function that predicts the value of y based on the ith value of series x:

$$\hat{y}_i = \hat{B}_0 + \hat{B}_1 x_i$$

- Therefore the difference for the ith data point between the actual value and the prediction is:

$$e_i = (y_i - \hat{y}_i)^2$$

- Which means to get the sum of residual squares is:

$$RSS = e_1 + e_2 + \ldots + e_n \text{ or } \sum_{i=1}^{n} e_i$$

The Least Squares approach

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- The least squares approach modifies the B_0 and B_1 coefficients to minimise the RSS.

$$B_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$B_0 = \bar{y} - B_1 x$$

- The resulting model function then needs to be evaluated

An example of simple linear regression

Utilising skills learned with panda and seaborn a simple regression and visualisation can be made with very little code

In [6]:
```
#reading data
dataset = pd.read_csv('headbrain.csv')
print(dataset.shape)
dataset.head()
```

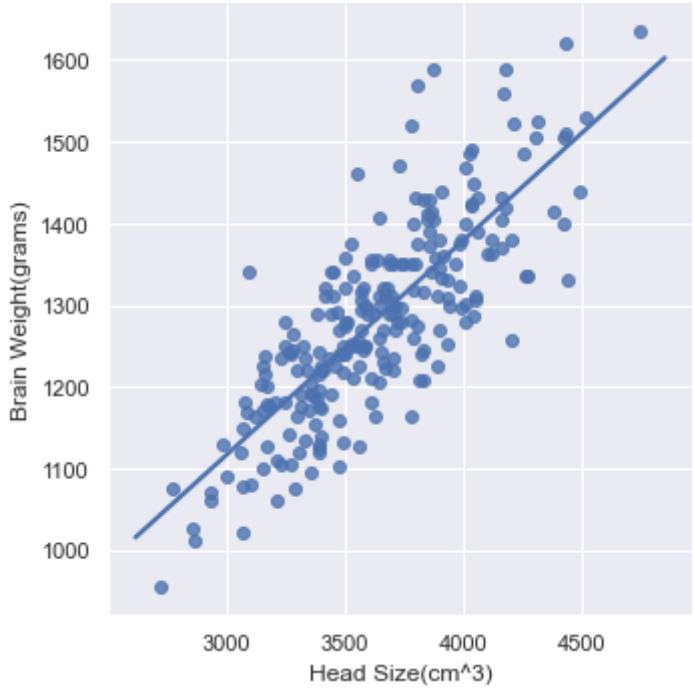
```
(237, 4)
```

Out[6]:

	Gender	Age Range	Head Size(cm^3)	Brain Weight(grams)
0	1	1	4512	1530
1	1	1	3738	1297
2	1	1	4261	1335
3	1	1	3777	1282
4	1	1	4177	1590

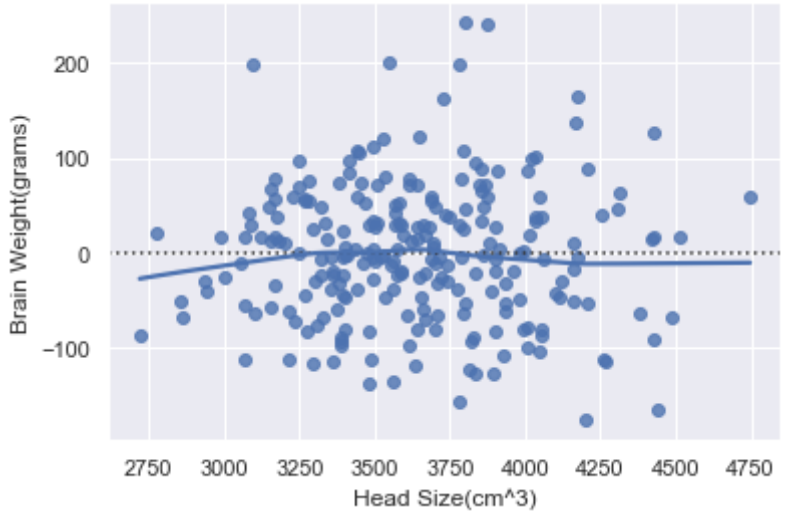
In [7]:
```
# Use integrated Seaborn function for single lenear regression
sns.lmplot(x='Head Size(cm^3)',y='Brain Weight(grams)',data=dataset,ci=None)
```

Out[7]: <seaborn.axisgrid.FacetGrid at 0x1a7d89a7888>



In [8]:
```
#Plot the residuals for the single linear regression fit
sns.residplot(x='Head Size(cm^3)',y='Brain Weight(grams)',data=dataset, lowess=True, color="b")
```

Out[8]: <matplotlib.axes._subplots.AxesSubplot at 0x1a7d88b37c8>

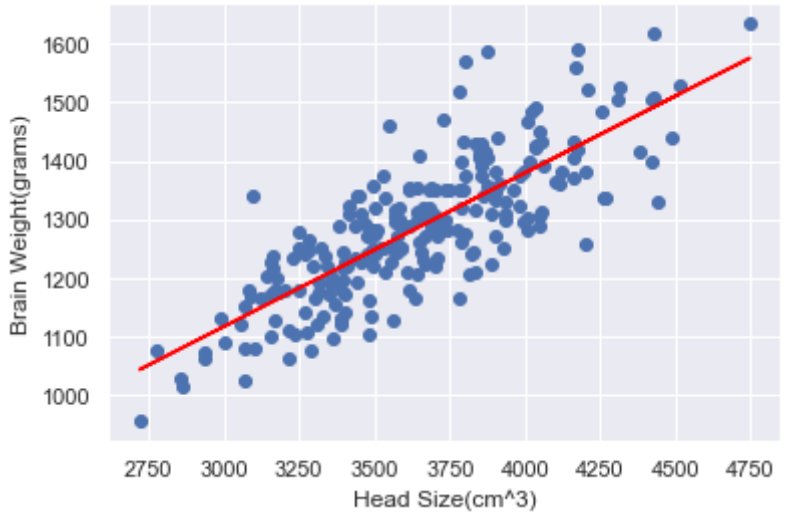


In [10]:
```
#Plot a regression model using scikit learn
X = dataset.iloc[:, 2].values.reshape(-1, 1)  # values converts it into a numpy array
Y = dataset.iloc[:, -1].values.reshape(-1, 1)  # -1 means that calculate the dimension of rows, but have 1 column
linear_regressor = LinearRegression()  # create object for the class
linear_regressor.fit(X, Y)  # perform linear regression
Y_pred = linear_regressor.predict(X)  # make predictions

print('Coefficients: \n', linear_regressor.coef_)
print('Intercept: \n',linear_regressor.intercept_)
```

```
Coefficients:
 [[0.26342934]]
Intercept:
 [325.57342105]
```

In [11]:
```
# Plot outputs
plt.scatter(X, Y)
plt.plot(X, Y_pred, color='red')
plt.xlabel('Head Size(cm^3)')
plt.ylabel('Brain Weight(grams)')
plt.show()
```



Evaluating Simple Linear Regression

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- There are multiple evaluation measures of a regression model

- Root mean square error measures the absolute fit of the model to the data:

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{1}{n} (y_i - \hat{y}_i)^2}$$

- Whereas R^2 will measure the variability of Y using X or the predictive capacity of the model:

$$R^2 = 1 - \frac{RSS}{TSS}$$

Multiple Linear Regression

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- Single linear regression can be expanded out easily to fit multiple features at once:

$$y = B_0 + B_1 x_1 + B_2 x_2 + B_3 x_3 + \ \ldots + B_n x_n$$

- Where each feature (x) has a corresponding coefficient

- Geometrically, this is akin to fitting a plane to points in three dimensions, or fitting a hyper-plane to points in higher dimensions.

An example of multiple linear regression and use of Evaluation statistics

In this example we use multiple linear regression to build a model based on a real dataset. We use the data science methodology to build a fit and establish whether the model is an effective predictor of trends in the data

In [12]:
```
# Another way of getting datasets
from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, r2_score
diabetes = datasets.load_diabetes()
```

In [13]:
```
diabetes.data.shape
```

Out[13]:
```
(442, 10)
```

In [14]:
```
diabetes.target.shape
```

Out[14]:
```
(442,)
```

In [15]:
```
diabetes.feature_names
```

Out[15]:
```
['age', 'sex', 'bmi', 'bp', 's1', 's2', 's3', 's4', 's5', 's6']
```

In [16]:
```
X_train, X_test, y_train, y_test = train_test_split(diabetes.data, diabetes.target, test_size=0.2, random_state=42)
```

In [17]:
```
# 1. Set up the model
model = LinearRegression()
# 2. Use fit
model.fit(X_train, y_train)
# 3. Check the score
model.score(X_test, y_test)
```

Out[17]:
```
0.45260660216173787
```

In [18]:
```
y_pred = model.predict(X_test)
# The mean squared error
print('Mean squared error: %.2f'
      % mean_squared_error(y_test, y_pred))
# The root mean squared error
print('Root Mean squared error: %.2f'
      % np.sqrt(mean_squared_error(y_test, y_pred)))
# The coefficient of determination: 1 is perfect prediction
print('Coefficient of determination: %.2f'
      % r2_score(y_test, y_pred))
```

```
Mean squared error: 2900.17
Root Mean squared error: 53.85
Coefficient of determination: 0.45
```

In [19]:
```
model.coef_
```

Out[19]:
```
array([  37.90031426, -241.96624835,  542.42575342,  347.70830529,
       -931.46126093,  518.04405547,  163.40353476,  275.31003837,
        736.18909839,   48.67112488])
```

In [20]:
```
model.intercept_
```

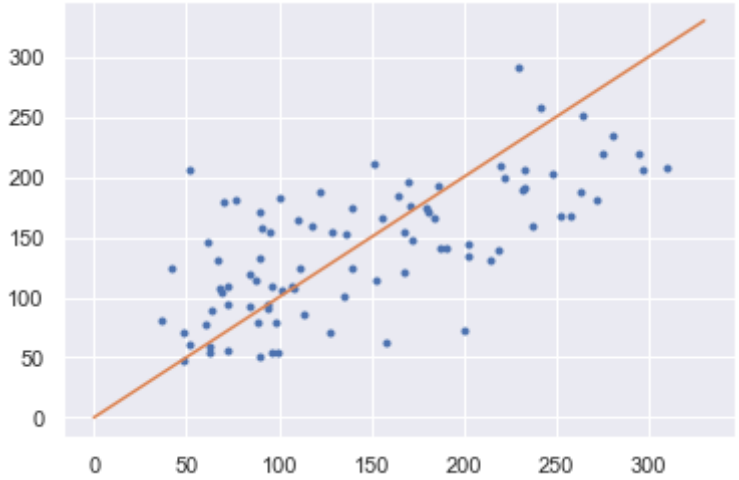
Out[20]:
```
151.3456553477407
```

In [21]:
```
model.predict(X_test)
```

Out[21]:
```
array([139.5483133 , 179.52030578, 134.04133298, 291.41193598,
       123.78723656,  92.17357677, 258.23409704, 181.33895238,
        90.22217862, 108.63143298,  94.13938654, 168.43379636,
        53.50669663, 206.63040068, 100.13238561, 130.66881649,
       219.53270758, 250.78291772, 196.36682356, 218.57497401,
       207.35002447,  88.48361667,  70.43428801, 188.95725301,
       154.88720039, 159.35957695, 188.31587948, 180.38835506,
        47.98988446, 108.97514644, 174.78080029,  86.36598906,
       132.95890535, 184.5410226 , 173.83298051, 190.35863287,
       124.41740796, 119.65426903, 147.95402494,  59.05311211,
        71.62636914, 107.68722902, 165.45544477, 155.00784964,
       171.04558668,  61.45763075,  71.66975626, 114.96330486,
        51.57808027, 167.57781958, 152.52505798,  62.95827693,
       103.49862017, 109.20495627, 175.63844013, 154.60247734,
        94.41476124, 210.74244148, 120.25601864,  77.61590087,
       187.93503183, 206.49543321, 140.63018684, 105.59463059,
       130.704246  , 202.18650868, 171.1330116 , 164.91246096,
       124.72637597, 144.81210187, 181.99631481, 199.41234515,
       234.21402489, 145.96053305,  79.86349114, 157.36828831,
       192.74737754, 208.8980067 , 158.58505486, 206.0226849 ,
       107.47978402, 140.93428553,  54.81856678,  55.92807758,
       115.00974554,  78.95886675,  81.55731377,  54.3774778 ,
       166.25477778])
```

In [22]:
```
#Multiple dimensional data is difficult to visualise
# plot prediction and actual data
y_pred = model.predict(X_test)
plt.plot(y_test, y_pred, '.')

# plot a line, a perfit predict would all fall on this line
x = np.linspace(0, 330, 100)
y = x
plt.plot(x, y)
plt.show()
```



Penalised Regression

- The introduction of multiple features to build a model on makes the model more flexible but can lead to model overfitting.

- Why?
  - **Multicollinearity:** The phenomemon that one (or more) of the independent variable(s) can be expressed as the linear combination of other independent variables.
  - When the number of independent variables is larger than the number of observations. When this happens, the OLS estimates are **not valid** because there are infinite solutions.

- **Regularization** is a process of introducing additional information in order to solve an ill-posed problem or to prevent overfitting the most common method is to add a constraint

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Ridge Regression

- The most common form of regularisation is ridge or L_2 regression
- This proceeds by penalising the sum of squares of the model coefficient as another term

$$P = \alpha \sum_{n=1}^{N} \theta_n^2$$

- Where from earlier: $e_i = (y_i - \hat{y}_i)^2$

$$\sum_{i=1}^{n} e_i + \alpha \sum_{j=1}^{P} \theta_j^2$$

- The additional parameter α controls how strict the penalty on the coefficient values is.

An example of penalised ridge regression

In [52]:
```
#Using an integrated sklearn dataset
from sklearn.linear_model import Ridge
from sklearn.preprocessing import StandardScaler
from sklearn.datasets import load_boston
```

In [53]:
```
boston = load_boston()
scaler = StandardScaler()
X = scaler.fit_transform(boston["data"])
Y = boston["target"]
names = boston["feature_names"]
```

In [54]:
```
X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=0.2, random_state=42)
```

In [66]:
```
# 1. Set up the model
ridge = Ridge(alpha=0.1)
# 2. Use fit
ridge.fit(X_train, y_train)
# 3. Check the score
ridge.score(X_test, y_test)
```

Out[66]:
```
0.6687275433090567
```

In [67]:
```
y_pred = ridge.predict(X_test)
# The mean squared error
print('Mean squared error: %.2f'
      % mean_squared_error(y_test, y_pred))
# The root mean squared error
print('Root Mean squared error: %.2f'
      % np.sqrt(mean_squared_error(y_test, y_pred)))
# The coefficient of determination: 1 is perfect prediction
print('Coefficient of determination: %.2f'
      % r2_score(y_test, y_pred))
```

```
Mean squared error: 24.29
Root Mean squared error: 4.93
Coefficient of determination: 0.67
```

In [68]:
```
ridge.coef_
```

Out[68]:
```
array([-0.97052404,  0.69960005,  0.27406007,  0.70692538, -1.9883985 ,
        3.11640735, -0.1772076 , -3.04214761,  2.27442714, -1.78483752,
       -1.97902616,  1.12626177, -3.62679724])
```

In [70]:
```
def ridge_alpha(alphas):
    '''
    Takes in a list of alphas. Outputs a dataframe containing the coefficients of lasso regressions from each alpha.
    '''
    # Create an empty data frame
    df = pd.DataFrame()

    # Create a column of feature names
    df['Feature Name'] = names

    # For each alpha value in the list of alpha values,
    for alpha in alphas:
        # Create a lasso regression with that alpha value,
        ridge = Ridge(alpha=alpha)

        # Fit the lasso regression
        ridge.fit(X_train, y_train)

        # Create a column name for that alpha value
        column_name = 'Alpha = %f' % alpha

        # Create a column of coefficient values
        df[column_name] = ridge.coef_

    # Return the datafram
    return df
```

In [71]:
```
ridge_alpha([1e-15, 1e-10, 1e-8, 1e-4, 1e-3,1e-2, 1, 5, 10, 20])
```

Out[71]:

	Feature Name	Alpha = 0.000000	Alpha = 0.000100	Alpha = 0.001000	Alpha = 0.010000	Alpha = 1.000000	Alpha = 5.000000	Alpha = 10.000000	Alpha = 20.000000
0	CRIM	-0.971494	-0.971493	-0.971485	-0.971397	-0.962034	-0.928802	-0.895069	-0.844167
1	ZN	0.701556	0.701554	0.701536	0.701359	0.682559	0.617167	0.553165	0.461981
2	INDUS	0.276752	0.276749	0.276725	0.276482	0.250716	0.163048	0.080063	-0.034186
3	CHAS	0.706532	0.706532	0.706535	0.706571	0.710338	0.723095	0.735054	0.751145
4	NOX	-1.991430	-1.991427	-1.991400	-1.991127	-1.961573	-1.851530	-1.731819	-1.537233
5	RM	3.115718	3.115719	3.115725	3.115788	3.122321	3.143227	3.159946	3.173161
6	AGE	-0.177060	-0.177060	-0.177062	-0.177075	-0.178459	-0.182664	-0.185753	-0.188060
7	DIS	-3.045771	-3.045767	-3.045734	-3.045408	-3.010025	-2.876908	-2.729280	-2.481511
8	RAD	2.282785	2.282776	2.282701	2.281946	2.201956	1.929837	1.672396	1.318493
9	TAX	-1.792605	-1.792597	-1.792527	-1.791825	-1.717846	-1.472739	-1.252253	-0.973654
10	PTRATIO	-1.979954	-1.979953	-1.979944	-1.979861	-1.970825	-1.937151	-1.900160	-1.838077
11	B	1.126499	1.126498	1.126496	1.126475	1.124140	1.114892	1.103629	1.081774
12	LSTAT	-3.628149	-3.628148	-3.628136	-3.628014	-3.614787	-3.564407	-3.506783	-3.403772

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Lasso Regression

- Another common method of regularisation is known as lasso or L_1 regularisation and instead involves penalising the sum of the absolute values of regression coefficients:

$$P = \alpha \sum_{n=1}^{N} |\theta_n|$$

- This results in different optimal parameter estimates for than the ridge regression penalty.

$$\sum_{i=1}^{n} e_i + \sum_{j=1}^{P} \alpha |\theta_n|$$

An example of penalised Lasso regression

In [27]:
```
#Using the same diabetes dataset
from sklearn.linear_model import Lasso
```

In [63]:
```
# 1. Set up the model
lasso = Lasso(alpha=0.1)
# 2. Use fit
lasso.fit(X_train, y_train)
# 3. Check the score
lasso.score(X_test, y_test)
```

Out[63]:
```
0.6497587169007897
```

In [64]:
```
y_pred = lasso.predict(X_test)
# The mean squared error
print('Mean squared error: %.2f'
      % mean_squared_error(y_test, y_pred))
# The root mean squared error
print('Root Mean squared error: %.2f'
      % np.sqrt(mean_squared_error(y_test, y_pred)))
# The coefficient of determination: 1 is perfect prediction
print('Coefficient of determination: %.2f'
      % r2_score(y_test, y_pred))
```

```
Mean squared error: 25.68
Root Mean squared error: 5.07
Coefficient of determination: 0.65
```

In [65]:
```
lasso.coef_
```

Out[65]:
```
array([-0.70055192,  0.25661452, -0.        ,  0.6885726 , -1.55739022,
        3.24310432, -0.        , -2.26125359,  0.66703856, -0.33847362,
       -1.84590977,  1.02848143, -3.62100991])
```

In [73]:
```
def lasso_alpha(alphas):
    '''
    Takes in a list of alphas. Outputs a dataframe containing the coefficients of lasso regressions from each alpha.
    '''
    # Create an empty data frame
    df = pd.DataFrame()

    # Create a column of feature names
    df['Feature Name'] = names

    # For each alpha value in the list of alpha values,
    for alpha in alphas:
        # Create a lasso regression with that alpha value,
        lasso = Lasso(alpha=alpha)

        # Fit the lasso regression
        lasso.fit(X_train, y_train)

        # Create a column name for that alpha value
        column_name = 'Alpha = %f' % alpha

        # Create a column of coefficient values
        df[column_name] = lasso.coef_

    # Return the datafram
    return df
```

In [74]:
```
lasso_alpha([1e-15, 1e-10, 1e-8, 1e-4, 1e-3,1e-2, 1, 5, 10, 20])
```

```
C:\Users\micha\Anaconda3\lib\site-packages\sklearn\linear_model\coordinate_descent.py:475: ConvergenceWarning: Objectiv
e did not converge. You might want to increase the number of iterations. Duality gap: 277.3236445999537, tolerance: 3.5
09685514851485
  positive)
```

Out[74]:

	Feature Name	Alpha = 0.000000	Alpha = 0.000100	Alpha = 0.001000	Alpha = 0.010000	Alpha = 1.000000	Alpha = 5.000000	Alpha = 10.000000	Alpha = 20.000000
0	CRIM	-0.971494	-0.971228	-0.968845	-0.945019	-0.047615	-0.000000	-0.0	-0.0
1	ZN	0.701556	0.701049	0.696498	0.651064	0.000000	0.000000	0.0	0.0
2	INDUS	0.276752	0.275844	0.267644	0.186036	-0.000000	-0.000000	-0.0	-0.0
3	CHAS	0.706532	0.706548	0.706694	0.708092	0.051141	0.000000	0.0	0.0
4	NOX	-1.991430	-1.990821	-1.985364	-1.930494	-0.000000	-0.000000	-0.0	-0.0
5	RM	3.115718	3.115783	3.116360	3.122050	3.065898	0.861183	0.0	0.0
6	AGE	-0.177060	-0.176831	-0.174767	-0.153989	-0.000000	-0.000000	-0.0	-0.0
7	DIS	-3.045771	-3.045080	-3.038895	-2.976730	-0.000000	0.000000	0.0	0.0
8	RAD	2.282785	2.280938	2.264323	2.098768	-0.000000	-0.000000	-0.0	-0.0
9	TAX	-1.792604	-1.790754	-1.774082	-1.608121	-0.000000	-0.000000	-0.0	-0.0
10	PTRATIO	-1.979953	-1.979780	-1.978217	-1.962598	-1.210801	-0.000000	-0.0	-0.0
11	B	1.126499	1.126379	1.125303	1.114591	0.444365	0.000000	0.0	0.0
12	LSTAT	-3.628149	-3.628120	-3.627845	-3.625330	-3.353957	-1.314498	-0.0	-0.0

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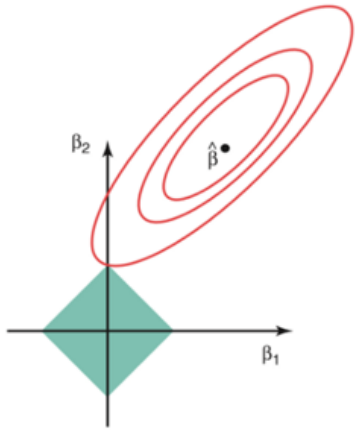
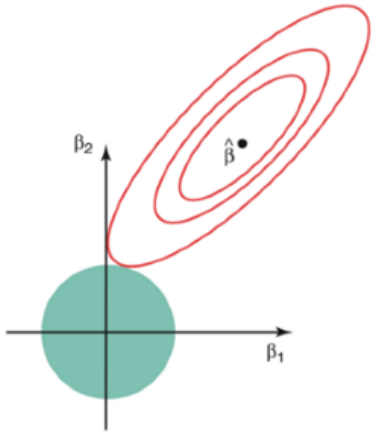
How does regularisation work?

- In 2D feature space:
  - The plots show the constraint regions for the 2 regularisation functions
  - Whereas the ellipses show the OLS function for linear regression



Lasso Regression

- Both methods determine coefficients by finding the first point where the elliptical contours hit the region of constraints



Ridge Regression

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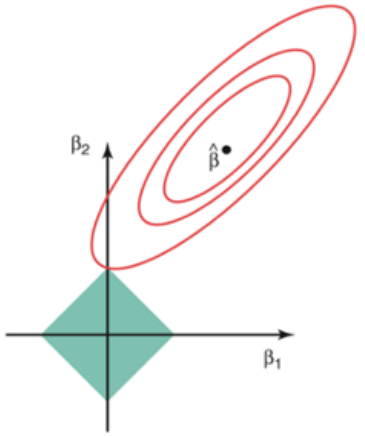
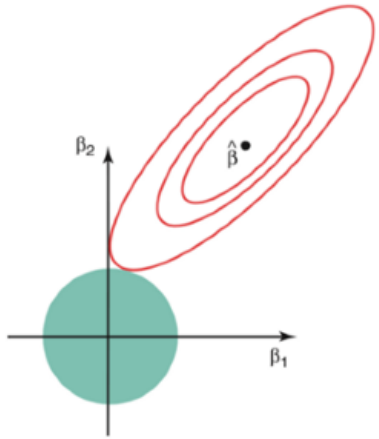
Ridge vs Lasso

- The diamond (Lasso) has corners on the axes, unlike the disk, and whenever the elliptical region hits such a point, the resulting feature coefficient is zero



Lasso Regression

- For higher dimensional feature space there can be many solutions on the axis with Lasso regression and thus we get only the important features selected in the model



Ridge Regression

Regression in SciKit Learn

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- scikit-learn features various other regression methods that could be classed as statistical or machine learning approaches:
- Variations of penalised regression Elastic Nets
- Lasso Least Angle
- Regression (LassoLARS),
- Orthogonal Matching
- Pursuit (OMP)
- These approaches all apply penalties to learn regression coefficients.

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Summary

- In this lecture we have covered:
  - Supervised learning using linear regression
  - Simple and multiple linear regression
  - Ordinary least squares loss function for regression fitting
  - R^2 and RMSE evaluation metrics for regression models
  - Penalised Regression using regularisation
  - Ridge and Lasso regularised regression