HW2 - Q1: Least Squares Regression (30 points)

Notes:

- Question (a) needs to be typewritten.
- Questions (b), (c), and (d) need to be programmed.
- Important:
  - Write all the steps of the solution.
  - Use proper LATEX formatting and notation for all mathematical equations, vectors, and matrices.
- For programming solution:
  - Properly add comments to your code.

A note about notation:

The notations in this homework are slightly different from the lecture notes. In lecture, we use notation for data as: (t_i, y_i) with regressor $\hat{y} = x^\top t$, x is a vector of unknown coefficients and solve $Ax = b$.
In this homework, the notation that we use for data is: (x_i, y_i) with regressor $\hat{y} = \beta^\top x$ and β is a vector of unknown coefficients to be solved.

(a) Consider a dataset with m datapoints: $(x_i, y_i), i = 1, \ldots, m$. Perform the multivariate calculus derivation of the least squares regression formula for an estimation function $\hat{y}(x) = ax^2 + bx + c$, where $a, b,$ and c are the scalar parameters. (6 points)

Your answer here:

We can write the function in matrix form:

$$Y = XB + E$$

where

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

$$X = \begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots \\ x_m^2 & x_m & 1 \end{bmatrix}$$

$$B = \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

$$E = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_m \end{bmatrix}$$

We have that

$$B = (X^T X)^{-1} X^T Y$$

The estimation function $\hat{y}(x) = ax^2 + bx + c$ can be seen as $\hat{y}(x) = ax_1 + bx_2 + c$. Therefore, we can denote the following:

$$S_{xx} = \sum_{i=1}^{m} x_i^2 - \frac{(\sum_{i=1}^{m} x_i)^2}{m}$$

$$S_{xy} = \sum_{i=1}^{m} x_i y_i - \frac{\sum_{i=1}^{m} y_i \sum_{i=1}^{m} x_i}{m}$$

$$S_{xx^2} = \sum_{i=1}^{m} x_i^3 - \frac{\sum_{i=1}^{m} x_i \sum_{i=1}^{m} x_i^2}{m}$$

$$S_{x^2y} = \sum_{i=1}^{m} x_i^2 y_i - \frac{\sum_{i=1}^{m} y_i \sum_{i=1}^{m} x_i^2}{m}$$

$$S_{x^2x^2} = \sum_{i=1}^{m} x_i^4 - \frac{(\sum_{i=1}^{m} x_i^2)^2}{m}$$

$$S_x = \frac{\sum_{i=1}^{m} x_i}{m}$$

$$S_{x^2} = \frac{\sum_{i=1}^{m} x_i^2}{m}$$

$$S_y = \frac{\sum_{i=1}^{m} y_i}{m}$$

The solutions to the unknown coefficients are:

$$a = \frac{S_{x^2y} S_{xx} - S_{xy} S_{xx^2}}{S_{xx} S_{x^2x^2} - (S_{xx^2})^2}$$

$$b = \frac{S_{xy} S_{x^2x^2} - S_{x^2y} S_{xx^2}}{S_{xx} S_{x^2x^2} - (S_{xx^2})^2}$$

$$c = S_y - bS_x - aS_{x^2}$$

Therefore, the coefficient matrix can be written as:

$$B = \begin{bmatrix} \frac{S_{x^2y} S_{xx} - S_{xy} S_{xx^2}}{S_{xx} S_{x^2x^2} - (S_{xx^2})^2} \\ \frac{S_{xy} S_{x^2x^2} - S_{x^2y} S_{xx^2}}{S_{xx} S_{x^2x^2} - (S_{xx^2})^2} \\ S_y - bS_x - aS_{x^2} \end{bmatrix}$$

(b) In this problem, we would like to use a linear regressor to fit the data, where $\hat{y}(x) = ax + b$ with a, b, x being scalars. Denote $\beta_{LS} = \begin{bmatrix} a \\ b \end{bmatrix}$ to contain the regressor coefficients, and recall that the linear algebraic formula for least squares gives $\beta_{LS} = (A^\top A)^{-1} A^\top y$ with $A^\dagger = (A^\top A)^{-1} A^\top$ known as the pseudo-inverse of A.

In this problem, we ask you to

#1. Use the function `np.linalg.pinv` to find the values of regressor coefficients β_{LS} and match it with your previous result. Note that the following piece of starter code generates a random least squares regression dataset with 500 data-points.

#2. Further match your results by directly solving the problem using the builtin numpy function: `np.linalg.lstsq`

In [1]:
```
### !!! DO NOT EDIT !!!
# starter code to generate a random least squares regression dataset with 500 points
import numpy as np
from scipy import optimize
import matplotlib.pyplot as plt
from sklearn import datasets

# generate x and y
X, y =  datasets.make_regression(n_samples=500, n_features=1, n_informative=1, n_targets=1, 
print('Shape of X is:', X.shape)
print('Shape of y is:', y.shape)
```

```
Shape of X is: (500, 1)
Shape of y is: (500,)
```

In [2]:
```
#######
# !!! YOUR CODE HERE !!!

#1

# Normal NumPy matrix operations
def normal_equation(X, Y):
    X = np.insert(X.T, 0, 1, axis=0)
    X_cross = np.dot(np.linalg.inv(np.dot(X, X.T)), X)
    beta = np.dot(X_cross, y)
    return beta
beta1 = normal_equation(X, y)
print("Normal NumPy matrix operations gives us: ", beta1)
```

```
Normal NumPy matrix operations gives us:  [ 9.02058667 63.18605572]
```

In [45]:
```
# Using function np.linalg.pinv
def pinv_fit(X, y):
    X = np.insert(X.T, 0, 1, axis=0)
    X_cross = np.dot(np.linalg.pinv(np.dot(X, X.T)), X)
    beta = np.dot(X_cross, y)
    return beta
beta2 = pinv_fit(X, y)
print("Using function np.linalg.pinv gives us: ", beta2)
```

```
Using function np.linalg.pinv gives us:  [ 9.02058667 63.18605572]
```

We can see that the two operations gives us the same results

In [48]:
```
#2

#Using function np.linalg.lstsq
A = np.column_stack([np.ones(len(X), float), X])
beta3 = np.linalg.lstsq(A, y, rcond=None)[0]
print("Using function np.linalg.lstsq gives us: ", beta3)
```

```
Using function np.linalg.lstsq gives us:  [ 9.02058667 63.18605572]
```

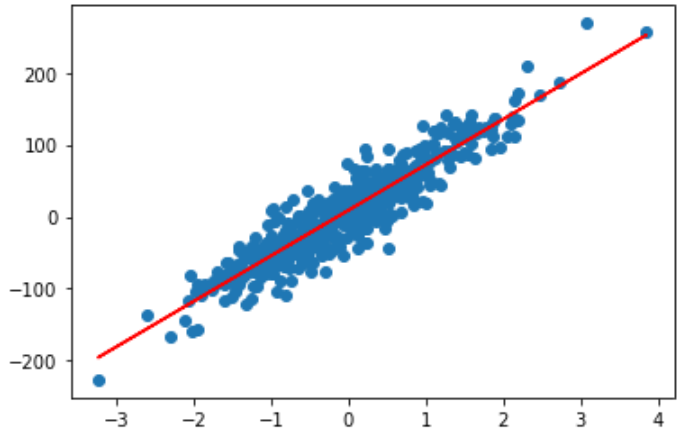
We can see that using function np.linalg.lstsq also gives us the same results.

In [5]:
```
# Generate predictions
def predict(X_test, beta):
    X_test = np.insert(X_test.T, 0, 1, axis=0)
    predictions = np.dot(beta, X_test)
    return predictions
predictions = predict(X, beta1)

# plot data and predictions
plt.scatter(X, y)
plt.plot(X, predictions, color='red')

#######
```

Out[5]: [<matplotlib.lines.Line2D at 0x1b5db509a00>]



(c) In this problem, we ask you to

#1. Write a function `my_func_fit (X,y)`, where `X` and `y` are column vectors of the same size containing experimental data. The function should return the values for α and β which are the scalar parameters of the estimation function $\hat{y}(x) = \alpha x^{\beta}$.

#2. Test your code on the generated sample dataset and report the coefficients. The given piece of starter code generates a logarithmic dataset.

#3. Plot a graph between X vs y, and overlay it with the linear regression line. (8 points)

Linear regression for non-linear estimation function:

In [3]:
```
### !!! DO NOT EDIT !!!
# starter code to generate a random exponential dataset
X = np.linspace(1, 10, 101)
y = 2*(X**(0.3)) + 0.3*np.random.random(len(X))
print('Shape of X is:', X.shape)
print('Shape of y is:', y.shape)
```

```
Shape of X is: (101,)
Shape of y is: (101,)
```

In [4]:
```
#######
# !!! YOUR CODE HERE !!!
```

We can model the data using model:

$$log(y) = log(\alpha) + \beta log(x)$$

This can be seen as a simple linear regression, and the code is similar to the previous question.

In [8]:
```
import math
import numpy as np

# function for modeling the data
def my_func_fit(X, y):
    A = np.vstack([np.log(X), np.ones(len(X))]).T
    beta, log_alpha = np.linalg.lstsq(A, np.log(y), rcond = None)[0]
    alpha = np.exp(log_alpha)
    return alpha, beta
alpha, beta = my_func_fit(X, y)

print("The coefficients: ",(alpha, beta))
```

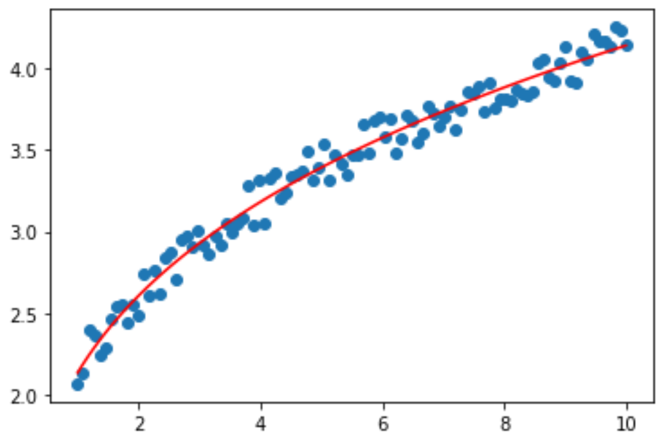
```
The coefficients:  (2.1383591787044627, 0.2864299526632125)
```

In [9]:
```
# Generate predictions
def predict(X_test, alpha, beta):
    return alpha*(X_test**beta)
predictions = predict(X, alpha, beta)

# plot data and predictions
plt.scatter(X, y)
plt.plot(X, predictions, color='red')

#######
```

Out[9]:
```
[<matplotlib.lines.Line2D at 0x1fb0c412f70>]
```



(d) In this problem, we ask you to

#1. Write a function `my_lin_regression(f, X, y)`, where `f` is a list containing function objects to basis functions that are pre-defined, and `X` and `y` are arrays containing noisy data. Assume that `X` and `y` are the same size, i.e, $X^{(i)} \in \mathbb{R}, y^{(i)} \in \mathbb{R}$. Return an array `beta` which represent the coefficients of the

solved problem. I.e. we are solving the β which contains the coefficients in the regressor $\hat{y}(x) = \beta_1 \cdot f_1(x) + \beta_2 \cdot f_2(x) + \cdots + \beta_n \cdot f_n(x)$ with f_i being basis functions.

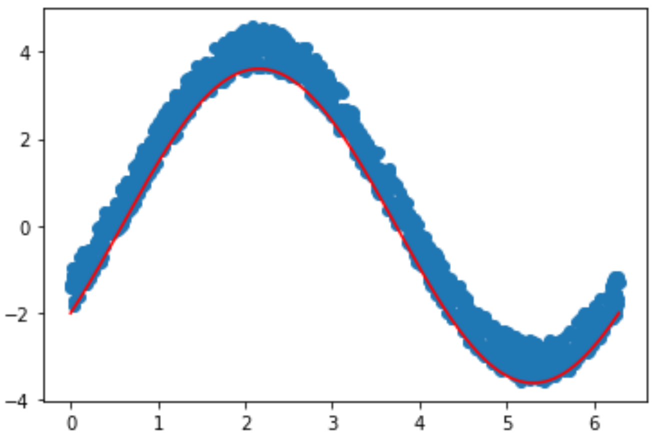
#2. Also write a function `regression_plot(f,X,y,beta)` which plots a graph between `X` and `y`, and overlays it with the regression line. A few test scenarios are given to validate your code. (10 points)

In [178]:
```
#######
# !!! YOUR CODE HERE !!!
import numpy as np
def my_lin_regression(f, X, y):
    A = np.ones(len(X))
    for i in f:
        A = np.vstack([A, i(X)])
    A = A[1:]
    A_cross = np.dot(np.linalg.pinv(np.dot(A, A.T)), A)
    betas = np.dot(A_cross, y)
    return betas

def regression_plot(f,X,y,beta):
    plt.scatter(X, y)
    predictions = np.zeros(len(X))
    for i in range(len(f)):
        predictions += beta[i]*f[i](X)
    plt.plot(X, predictions, color='red')
    return
#######
```

In [182]:
```
### !!! DO NOT EDIT !!!
### Test-1
X = np.linspace(0, 2*np.pi, 1000)
y = 3*np.sin(X) - 2*np.cos(X) + np.random.random(len(X))
f = [np.sin, np.cos] # f1 = sin, f2 = cos

beta = my_lin_regression(f, X, y)
regression_plot(f,X,y,beta)
```



In [180]:
```
### !!! DO NOT EDIT !!!
### Test-2
X = np.linspace(0, 1, 1000)
y = 2*np.exp(0.5*X) + 0.25*np.random.random(len(X))
f = [np.exp] # f1 = exp

beta = my_lin_regression(f, X, y)
regression_plot(f,X,y,beta)
```