Univariate-linear-regression

December 8, 2018

1 Use case

You receive a new weighing scale but notice it is not very accurate when comparing the displayed value to real known weights; you place 1 kg but it says you placed 2 kg, what can we do to calibrate it?

Suppose it is an industrial device whithout a calibration button but we have access to the "electronic weights" (i.e. the voltage measurements) sent by the firmware. Is there an option to use our own measures and calculus to calibrate it? The answer is yes because... the power is in the data.

In [1]:
```
from IPython.display import HTML
from IPython.display import display

# Taken from https://stackoverflow.com/questions/31517194/how-to-hide-one-specific-cell-
tag = HTML('''<script>
code_show=false;
function code_toggle() {
    if (!code_show){
        $('div.cell.code_cell.rendered.selected div.input').hide();
    } else {
        $('div.cell.code_cell.rendered.selected div.input').show();
    }
    code_show = !code_show
}
$( document ).ready(code_toggle);
</script>
<a href="javascript:code_toggle()">-</a>.''')
display(tag)

from IPython.display import Image
from IPython.core.display import HTML

Image(url= "https://raw.githubusercontent.com/GermanCM/univariate-linear-regression/work
```

```
<IPython.core.display.HTML object>
```

Out[1]:
```
<IPython.core.display.Image object>
```

So, what do we need to make the translation from "electronic weight" to "weight in kg"? Using items of known weight, we can place them over the balance and retrieve the voltage measure, so together with the known weight, we have the pairs electronic weight - mass weight.

A good approach could be finding the coefficients of a line which is as close as possible to our points, i.e. implementing a linear regression. But, are our points distributed approximately linearly? Let's check for it:

```
In [2]: import pandas as pd

        measures_raw_df = pd.read_csv('https://raw.githubusercontent.com/GermanCM/univariate-lin

In [3]: measures_raw_df.head(5)
```

Out[3]:

	electronic_weight	mass_weight
0	761	0.0
1	765	0.0
2	872	0.0
3	23567	27.0
4	23565	27.0

```
In [4]: measures_raw_df.describe()
```

Out[4]:

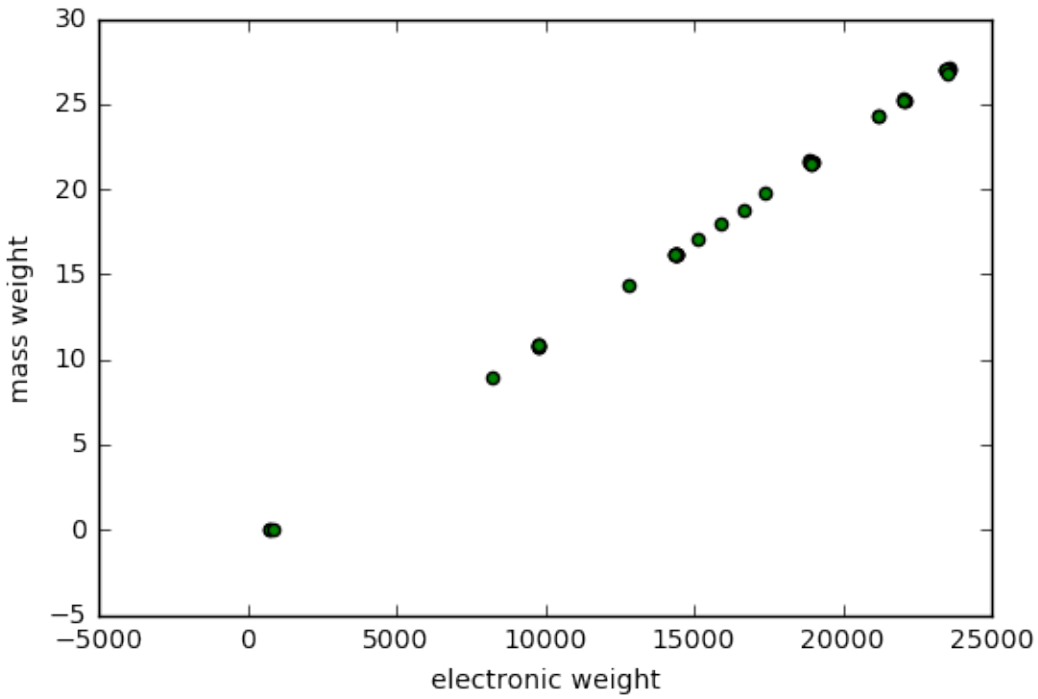
	electronic_weight	mass_weight
count	49.000000	49.000000
mean	16648.122449	18.881633
std	6248.144227	7.389736
min	761.000000	0.000000
25%	14354.000000	16.200000
50%	18888.000000	21.500000
75%	22054.000000	25.200000
max	23593.000000	27.100000

```
In [5]: import matplotlib as mpl
        import numpy as np
        import matplotlib.pyplot as plt

        mpl.rcParams['legend.fontsize'] = 40
        x = measures_raw_df['electronic_weight']
        y = measures_raw_df['mass_weight']
        plt.xlabel("electronic weight")
        plt.ylabel("mass weight")

        plt.scatter(x, y, c="g")

        plt.show()
```



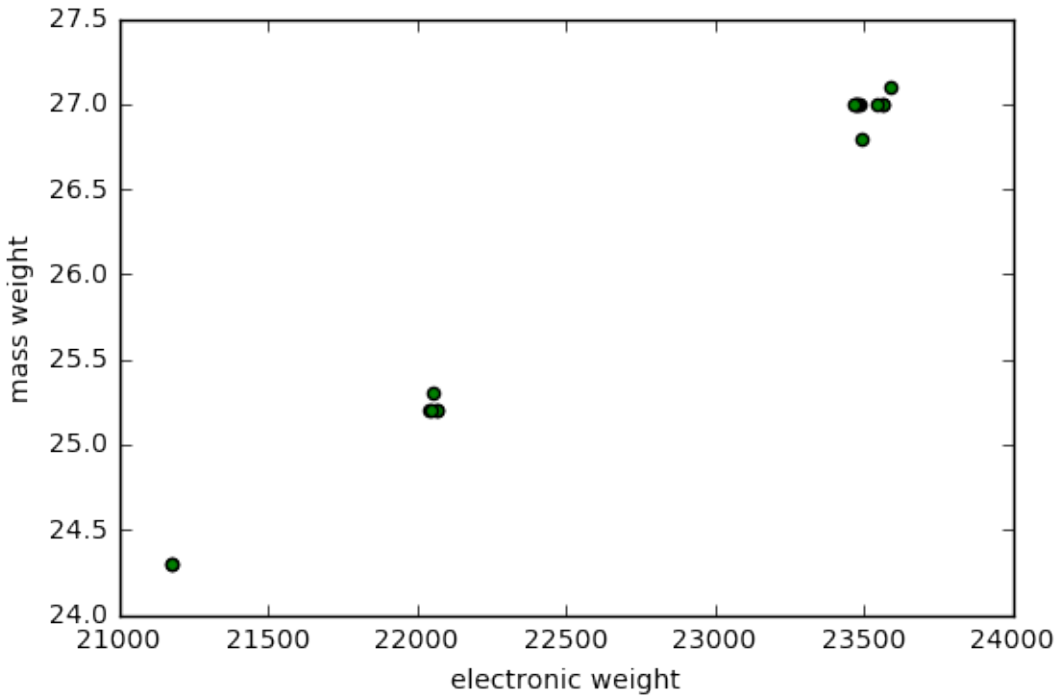
Voilà, it seems to be nearly a perfect line, so good that we could even find the desired linear regression coefficients with just 2 points? Let's zoom in:

```
In [6]: measures_raw_df_mini = measures_raw_df[measures_raw_df.electronic_weight>20000]

        mpl.rcParams['legend.fontsize'] = 40
        x = measures_raw_df_mini['electronic_weight']
        y = measures_raw_df_mini['mass_weight']
        plt.xlabel("electronic weight")
        plt.ylabel("mass weight")

        plt.scatter(x, y, c="g")

        plt.show()
```



So now it does not seem we could use 2 points to find a good fitting line right? Something to remember: never rely just on your first data visualization, or try at least to check your first assumptions with extra plots or some basic calculus.

So let's go on with our 49 points linear regression, and we will do it first from scratch based on the least squared errors (error = real_value - predicted_vale) using the famous gradient descent as the optimization algorithm.

Steps: 1. write down the functions we will use for implementing linear regression 2. split our dataset into train and test sets 3. train our model 4. plot the evolution of the cost function along the training epochs 5. evaluate our model with some test data 6. conclusions based on our use case

```
In [7]: import math
        import numpy as np

        # get the overall cost of the model
        def compute_cost(X, y, coeff):
            '''
            inputs:
              * 'X': features matrix (independent variables)
              * 'y': target values (dependent variable)
              * 'coeff': regression coefficients
            output:
              * the mean squared error (MSE)
            '''
            squared_errors = np.power((predict_output(X, coeff) - y), 2)
```

```
    return np.sum(squared_errors) / (len(X))

# returns the dependent variable (y axis) value which the model assigns to a certain ind
def predict_output(feature_matrix, coefficients):
    '''
    inputs:
        * feature_matrix: two-dimensions array of the data points, where each columns is
        * coefficients: one-dimension array of estimated feature coefficients

    output:
        * one-dimension array of predictions
    '''
    predictions = np.dot(feature_matrix, coefficients)
    return predictions

# derivative of the cost function, the heart of the process which gradient descent will
def feature_derivative(errors, feature):
    N = len(feature)
    derivative = (2)*np.dot(errors, feature)
    return(derivative)

# gradient descent optimization algorithm (GD)
def gradient_descent_regression(H, y, initial_coefficients, alpha, max_iterations=10000)
    '''
    inputs:
        * H: two-dimensions array of data points, where each columns is a feature and a
        * y: one-dimension array with target values (dependent variable)
        * initial_coefficients: one-dimension array of initial coefficients (weights of
        * alpha: float value, it is the step size with which GD will "walk" towards the
        * max_iterations: int, tells the program when to terminate, based on the number

    output - one-dimensional array of estimated regression coefficients
    '''
    converged = False
    w = initial_coefficients
    iteration = 0
    cost=[]
    while iteration < max_iterations:
        pred = predict_output(H, w)
        residuals = pred-y
        gradient_sum_squares = 0
        for i in range(len(w)):
            partial = feature_derivative(residuals, H[:, i])
            gradient_sum_squares += partial**2
            w[i] = w[i] - alpha*partial
        iteration += 1
        cost.append(compute_cost(H, y, w))
    return w, cost
```

Brief resume of the process for finding the linear regression coefficients via the defined functions: 1.-initial coefficients are initialized to random numbers, or even zero in our case, inside the 'gradient_descent_regression' method 2.-predictions are made using the current coefficients, with the 'predict_output' method
3.-the gradient (first order derivate) of the residuals is made with the 'feature_derivative' method; this will let us update each weight (in our case the line slope and the intercept with the y-axis) via the gradient descent rule 4.-once the max_iterations number is reached, return the final coefficients and cost (computed with 'compute_cost')

You can find below the update weight rule in gradient descent; what it does is adding, to the current weight value (the 'theta' symbol), the derivative of the cost function with a minus sign (times an alpha step size). This way, it is updated in each epoch in the "direction" towards the cost function minimum. We will see it in more detail in another post.

In [8]:
```
display(tag)

        Image(url= "https://upload.wikimedia.org/wikipedia/commons/6/68/Gradient_descent.jpg", w
```

```
<IPython.core.display.HTML object>
```

Out[8]:
```
<IPython.core.display.Image object>
```

We won't use in this case any early stopping value if a certain tolerance is reached in the cost function; we will only use the max_iterations value instead, which is far enough for our purpose.

1.0.1 Train-test split

We will use the 'train_test_split' package from scikit-learn to split our data into training and test sets:

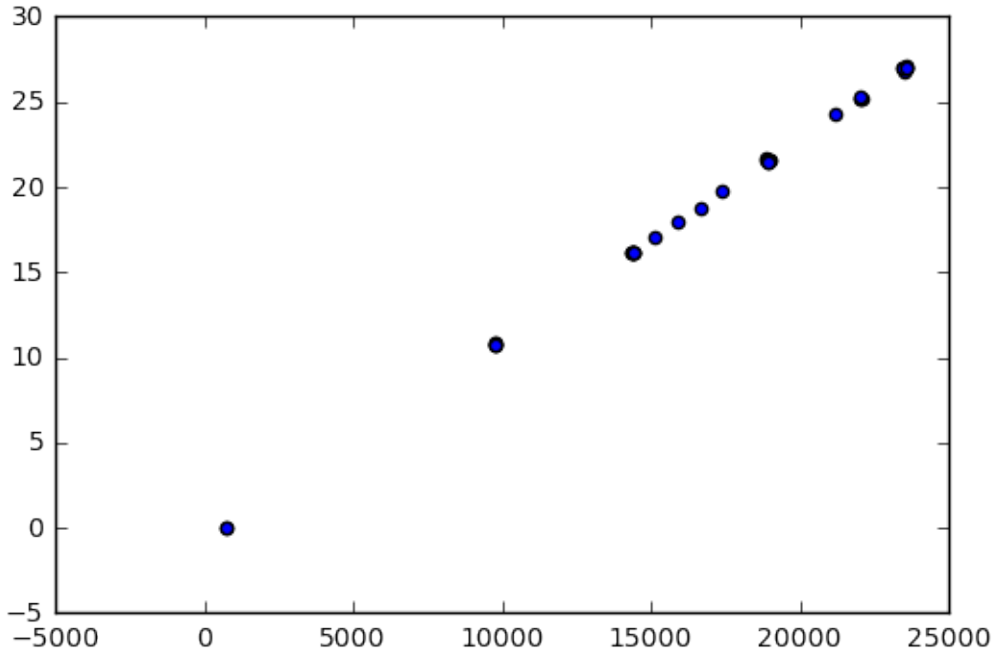
In [9]:
```
from sklearn.model_selection import train_test_split

        n = len(measures_raw_df)
        H = measures_raw_df

        X_train, X_test, y_train, y_test = train_test_split(H['electronic_weight'], H['mass_weig
```

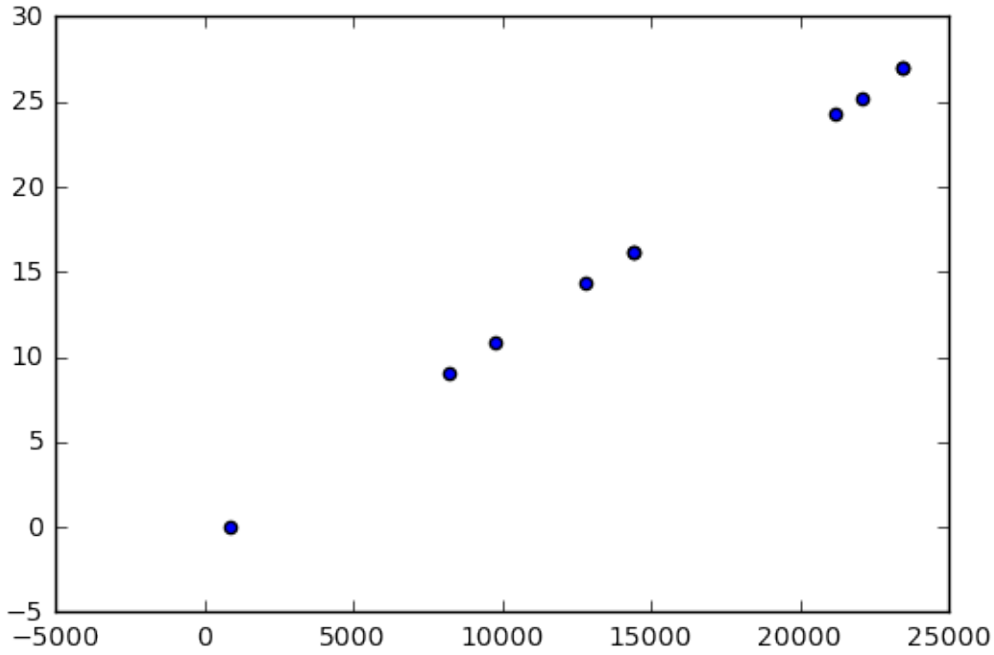
In [10]:
```
# Train set
         plt.scatter(X_train, y_train)

         plt.show()
```



In [11]:
```
# Test set
plt.scatter(X_test, y_test)

plt.show()
```



```
In [12]: def normalize_features(df):
             """
             Normalize the features in the data set.

             Returns the normalized values, mean and standard deviation fo each feature
             """
             mu = df.mean()
             sigma = df.std()

             if (sigma == 0).any():
                 raise Exception("One or more features had the same value for all samples, and t
                                 "not be normalized. Please do not include features with only a
                                 "in your model.")
             df_normalized = (df - df.mean()) / df.std()

             return df_normalized, mu, sigma

         def find_r2_score(labels_test, predicted_outputs):
             from sklearn.metrics import r2_score
             corr_coeff = r2_score(labels_test, predicted_outputs)
             print('the value of r2 is: ', corr_coeff)
```

Another function to use in our implementation of the linear regression via GD from scratch is the normalization of the features; again, it is not the goal of this post to go into details for this, but scaling is necessary for this implementation, and we will use the standardization to rescale our values to the range 0-1.

Now that we have all our functions and our dataset split into train and test groups, let's train our model.

Model training

```
In [13]: display(tag)

         from IPython.display import Image
         Image(url="https://tenor.com/view/workout-rhino-unicorn-goals-body-sizes-gif-4905556.gi
```

```
<IPython.core.display.HTML object>
```

```
Out[13]: <IPython.core.display.Image object>
```

```
In [14]: feature_train_matrix = np.zeros(len(X_train)*2)
         feature_train_matrix.shape = (len(X_train), 2)
         feature_train_matrix[:,0] = 1
         feature_train_matrix[:,1] = X_train

         feature_train_matrix, train_mu, train_sigma = normalize_features(feature_train_matrix)
```

```
        initial_coefficients = np.zeros(len(feature_train_matrix[0]))

        coef, cost = gradient_descent_regression(feature_train_matrix, y_train, initial_coeffic
                                                 max_iterations=10000)

        print('first weight: {}'.format(coef[0]))
        print('second weight: {}'.format(coef[1]))
        print('cost: {}'.format(cost[-1]))
```

```
first weight: -10.32256050647614
second weight: 11.191002738125563
cost: 0.006022601073742206
```

So in our simple case for linear regression, what we expect is to obtain a couple of values, the first weight is the intercept with the y-axis, and the second weight is actually the slope of our line, according to:

```
In [15]: display(tag)

         Image(url= "https://raw.githubusercontent.com/GermanCM/univariate-linear-regression/wor
```

```
<IPython.core.display.HTML object>
```

```
Out[15]: <IPython.core.display.Image object>
```

Take into account that those values will work for scaled data, i.e., applying the same standardization operation (we'll see it in a bit when predicting unseen data). As we can also see, our model returns a final squared mean error 0.006

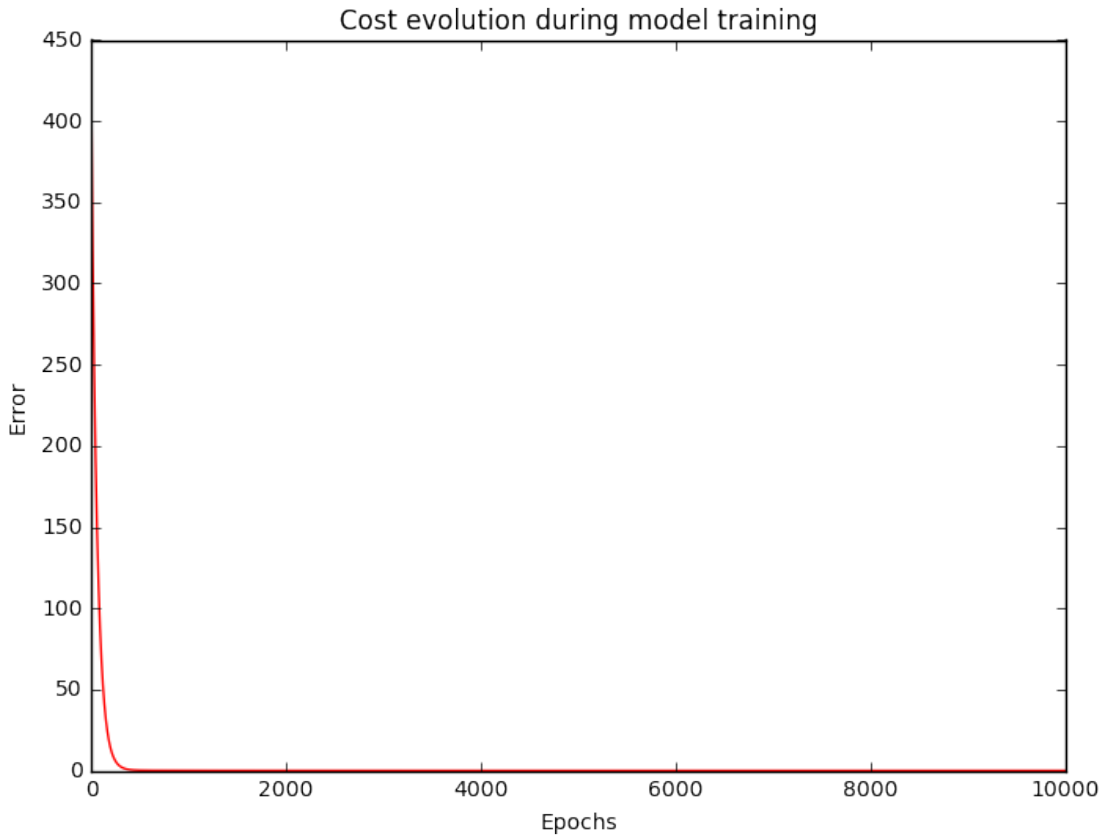
Nevertheless, we are interested in the root means squared error, which is in the same units as our features:

```
In [16]: train_mse = compute_cost(feature_train_matrix, y_train, coef)
         np.around(np.sqrt(train_mse), decimals=3)
```

```
Out[16]: 0.078
```

1.0.2 Plot of the cost evolution along the training process:

```
In [17]: fig, ax = plt.subplots(figsize=(8,6))
         ax.plot(np.arange(len(cost)), cost, 'r')
         ax.set_xlabel('Epochs')
         ax.set_ylabel('Error')
         ax.set_title('Cost evolution during model training')
         plt.show()
```



1.0.3 Model evaluation:

So now let's apply our model to unseen data from the test dataset:

```
In [18]: n = len(X_test)
         feature_test_matrix = np.zeros(n*2)
         feature_test_matrix.shape = (n, 2)
         feature_test_matrix[:,0] = 1
         feature_test_matrix[:,1] = X_test

         # We use the same mean and std obtained for the train set:
         feature_test_matrix = (feature_test_matrix - train_mu) / train_sigma

         #calculamos mse en test set:
         test_mse = compute_cost(feature_test_matrix, y_test, coef)
         np.sqrt(test_mse)

Out[18]: 0.10634757043674785
```

The RMSE (root mean squared error) on unseen data seems quite ok, so let's predict on some values of the test set:

```
In [19]: def normalize_and_predict(feature_values):
             X = [feature_values]
             H = pd.DataFrame({'X': X})

             # for a single point:
             n = 1
             feature_to_predict = np.zeros(n*2)
             feature_to_predict.shape = (n, 2)
             feature_to_predict[:,0] = 1
             feature_to_predict[:,1] = H['X']

             #normalize test feature with the same values as in the training set:
             feature_to_predict = (feature_to_predict - train_mu) / train_sigma

             return predict_output(feature_to_predict, coef)

         print(normalize_and_predict(8241))
```

```
[ 8.95052887]
```

It looks quite nice for the single value x = 8241 to get the prediction 8.95 compared to the expected 9.0; we actually expected that good result in average, since we obtained a RMSE = 0.1.

Let's find the predictions for each value in our test dataframe and compare it with the expected values:

```
In [20]: test_df = pd.DataFrame({'x': X_test, 'y': y_test})
         test_df
```

```
Out[20]:         x     y
         7   22068  25.2
         43   8241   9.0
         42   9752  10.9
         25  21180  24.3
         14  14393  16.2
         2     872   0.0
         23  23471  27.0
         30  12813  14.4
         17  14403  16.2
         46  23471  27.0
```

```
In [21]: preds_reg_from_scratch = [float(np.around(normalize_and_predict(ft), decimals=4)) for f
         preds_reg_from_scratch
```

```
Out[21]: [25.2811,
          8.9505,
          10.7351,
          24.2324,
          16.2165,
```

```
 0.2472,
 26.9382,
 14.3504,
 16.2283,
 26.9382]
```

In [22]:
```
test_df['preds_reg_from_scratch'] = preds_reg_from_scratch
test_df
```

Out[22]:

	x	y	preds_reg_from_scratch
7	22068	25.2	25.2811
43	8241	9.0	8.9505
42	9752	10.9	10.7351
25	21180	24.3	24.2324
14	14393	16.2	16.2165
2	872	0.0	0.2472
23	23471	27.0	26.9382
30	12813	14.4	14.3504
17	14403	16.2	16.2283
46	23471	27.0	26.9382

In [23]:
```
display(tag)

Image(url= "https://raw.githubusercontent.com/GermanCM/univariate-linear-regression/wor
```

```
<IPython.core.display.HTML object>
```

Out[23]:
```
<IPython.core.display.Image object>
```

1.0.4 Linear regression with scikit-learn

So after implementing our linear regressor from scratch understanding all the steps (which is quite useful to get the key ideas behind machine learning algorithms), let's see how to implement it and serialize it with scikit-learn much faster:

In [24]:
```
from sklearn import linear_model

linear_reg = linear_model.LinearRegression()
linear_reg.fit(X_train.values.reshape((len(X_train),1)), y_train.values.reshape((len(X_
```

Out[24]:
```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1, normalize=False)
```

Notice with this option we do not need to explicitely normalize our data points, already carried out by scikit; let's see how good the predictions are using the same test dataframe as before:

In [25]:
```
linear_reg.predict(8241)
```

Out[25]:
```
array([[ 8.95084297]])
```

```
In [26]: preds_reg_scikit = [float(np.around(linear_reg.predict(ft), decimals=4)) for ft in test
         preds_reg_scikit

Out[26]: [25.2811,
          8.9508,
          10.7354,
          24.2323,
          16.2166,
          0.2478,
          26.9381,
          14.3506,
          16.2284,
          26.9381]

In [27]: test_df['preds_reg_scikit'] = preds_reg_scikit
         test_df

Out[27]:        x     y  preds_reg_from_scratch  preds_reg_scikit
         7   22068  25.2                 25.2811           25.2811
         43   8241   9.0                  8.9505            8.9508
         42   9752  10.9                 10.7351           10.7354
         25  21180  24.3                 24.2324           24.2323
         14  14393  16.2                 16.2165           16.2166
         2     872   0.0                  0.2472            0.2478
         23  23471  27.0                 26.9382           26.9381
         30  12813  14.4                 14.3504           14.3506
         17  14403  16.2                 16.2283           16.2284
         46  23471  27.0                 26.9382           26.9381
```

And we can see the predictions with the scikit-learn model are basically the same, just a very little difference usually in the 4th floating point. Good to see that we can reproduce scikit results with our implementation from scratch :-)

One more question we might ask ourselves is, ok nice results but is it useful for my real life use case? Well it depends on your real use case; if the mean (could also be the median) difference between the prediction and the real value is below the uncertainty that you are willing to accept, then it is a good result. In my case, I needed to be able to detect a change of at least one third of kilogram, so these results are very good.

Another question it might arise (and this is the last one for now in this post) is: what happens if we make more measurements for larger weights on the weighing scale? Does it keep being so linear that we can apply the same algorithm? I'll show it in another post.

1.0.5 Summary of our use case

- Weighing scale not calibrated; electronic weight (i.e. voltages) data retrieved from its firmware
- Dataset built with the pair of values 'electronic weight - known weight in kilograms'
- Univariate linear regression from scratch to find the equation to translate electronic weight into real mass weight

- Comparison with scikit-learn results
- Validation of results in the frame of our real use case

1.0.6 Next steps

- Will our points follow the same linearity for higher weights?
- Can we still use the same process to cover these new data?

We will see in a next post :)

Interesting sources: https://github.com/llSourcell/Intro_to_the_Math_of_intelligence
http://charlesfranzen.com/posts/multiple-regression-in-python-gradient-descent/
https://www.johnwittenauer.net/machine-learning-exercises-in-python-part-1/