Iterative search and lineal regression

Gradient descent iterative method and lineal regression

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Chapter 1

Gradient descent

1.1 Gradient descent's algorithm

1.1.1 Introduction

Gradient descent is a general technique for minimizing differentiable functions through its slope. [1] It is used to find local minimums. The start point is crucial in the search.

The basic idea is to update the weights using the gradients until it is not possible to continuous minimizing the error.

1.1.2 Math

In order to understand the algorithm we are going to define:

Let $w(0) \in \mathbb{R}^d$ be an arbitrary initial point, $E : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$ a class C^1 function. The learning rate or step size $\eta \in \mathbb{R}^+$ is a experimental coefficient about how much are we going to follow the slope to obtain the new weight. Let $w(t) \in \mathbb{R}^d \quad t \in \mathbb{N}$ be the weight for t iteration which is defined as

$$w(t+1) = w(t) - \eta \nabla E_{in}(w(t))$$

Properties

- This algorithm gives local minimums.
- Convergence is not assured in a finite time, so it would be necessary some stop criteria.
- For a convex function it would be a unique global minimum.
- The convergence success (in time) depends on the learning rate, η.

1.1.3 Algorithm

The following code snippet implement the algorithm, where $w(0)$ is the $initial\_point$, E is the error, $\nabla E_{in}(w)$ is $gradient\_function$ and finally η is eta. The value $\eta = 0.1$ is a heuristic basic on purely practical observation [1].

In order to avoid an infinite search, our stop criteria are a limit in the number of iterations max_sitter and an error tolerance.

```
def gradient_descent(initial_point, loss_function,
                gradient_function,  eta, max_iter, target_error):
    '''
    initicial point: w_0
    E: error function
    gradient_function
    eta:  step size

    ### stop conditions ###
    max_iter
    target_error

    #### return ####
    (w,iterations)
    w: the coordenates that minimize E
    it: the numbers of iterations needed to obtain w

    '''

    iterations = 0
    error = E( initial_point[0], initial_point[1])
    w = initial_point

    while ( (iterations < max_iter) and(error > target_error)):

        w = w - eta * gradient_function(w[0], w[1])

        iterations += 1
        error = loss_function(w[0], w[1])


    return w, iterations
```

1.1.4 Problem 1

We want to solve the following problem:

Use gradient descent's algorithm to find a minimum for the function

$$E(u,v) = (u^3 e^{(v-2)} - 2 * v^2 e^{-u})^2.$$

Set $(u,v) = (1,1)$ as initial point and use learning rate $\eta = 0.1$.

Compute analytically the gradient of $E(u,v)$

$$\nabla E(u,v) = \left(\frac{\partial}{\partial u}(u^3 e^{(v-2)} - 2 * v^2 e^{-u})^2, \frac{\partial}{\partial v}(u^3 e^{(v-2)} - 2v^2 e^{-u})^2\right) =$$
$$= \left(2(u^3 e^{(v-2)} - 2 * v^2 e^{-u})(3u^2 e^{(v-2)} + 2v^2 e^{-u}), 2(u^3 e^{(v-2)} - 2 * v^2 e^{-u})(u^3 e^{(v-2)} - 4v e^{-u})\right)$$

Number of iterations and final coordinates.

Firstable we need to use 64-bits float, so we are going to use the data type $float64$ of numpy library [2].

The functions' declaration are:

```
  def dEu(u,v):
    '''
    Partial derivate of E with respect to the variable u
    '''
    return np.float64(
        2
        *( 3* u**2 * np.e**(v-2) + 2*v**2 * np.e**(-u) )
        *( u**3 * np.e**(v-2) - 2*v**2 * np.e**(-u))
    )

def dEv(u,v):
    '''
    Partial derivate of E with respect to the variable v
    '''
    return np.float64(
        2*
        ( u**3 * np.e**(v-2) - 2*v**2 * np.e**(-u) )
        *( u**3 * np.e**(v-2) - 4*v * np.e**(-u))
    )


def gradE(u,v):
    '''
        gradient of E
    '''
    return np.array([dEu(u,v), dEv(u,v)])
```

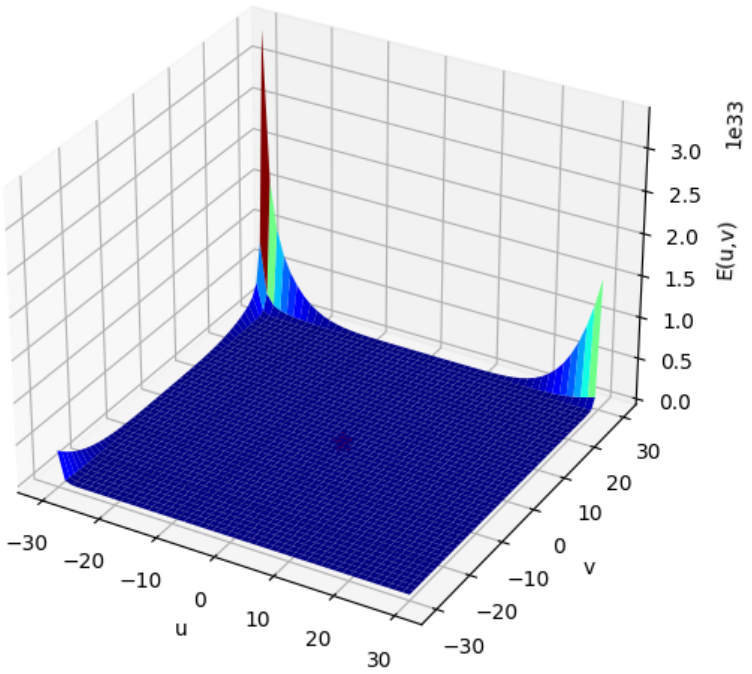
To obtain the number of iterations and the final coordinates, the only thing we need to do is to call *gradien_descent* function with the initial conditions:

```
eta = 0.01
max_iter = 10000000000
target_error = 1e-14
initial_point = np.array([1.0,1.0])
w, it = gradient_descent( initial_point,
                          E,
                          gradE,
                          eta,
                          max_iter,
                          target_error )
```

The result are:

- Numbers of iterations: 178.
- Final coordinates: $(1.162, 0.924)$.

A 3d graph with the result is



1.1.5 Problem 2

For function $f(x, y) = (x + 2)^2 + 2(y - 2)^2 + 2\sin(2\pi x)\sin(2\pi y)$

Use gradient descent to minimize f

The initial point is $(x_0 = -1, y_0 = 1)$, learning rate is $\eta = 0.01$ and the maximum number of iterations must be 50. Plot the result and repeat the experiment with $\eta = 0.1$.

Firstly we are going to calculate partial derivatives and gradient of f.

$$\frac{\partial}{\partial x} f = 2(x+2) + 2\sin(2\pi y)\cos(2\pi x)2\pi = 2(x+2) + 4\pi\sin(2\pi y)\cos(2\pi x)$$

$$\frac{\partial}{\partial y} f = 2(y-2) + 4\pi\sin(2\pi x)\cos(2\pi y)$$

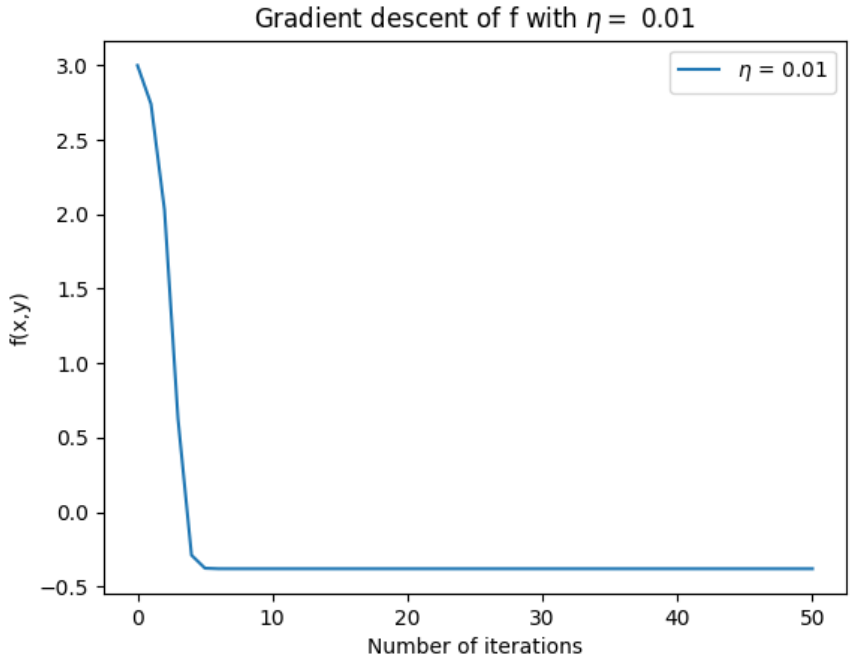
It is important to realise that $f(x, y) < 0$ for some values in $\mathbb{R}^3$ so the error target has been omitted in this algorithm.

Now the new algorithm is

```
def gradient_descent_trace(initial_point, loss_function,
  gradient_function,  eta, max_iter):
  '''
  initicial point: w_0
  loss_function: error function
  gradient_function
  eta:  step size

  ### stop conditions ###
  max_iter

  #### return ####
  (w,iterations)
  w: the coordenates that minimize loss_function
  it: the numbers of iterations needed to obtain w

  '''

  iterations = 0
  error = loss_function( initial_point[0], initial_point[1])
  w = [initial_point]

  while iterations < max_iter:

      new_w = w[-1] - eta * gradient_function(w[-1][0], w[-1][1])


      iterations += 1
```

```
        error = loss_function(new_w[0], new_w[1])
        w.append( new_w )

    return w, iterations
```

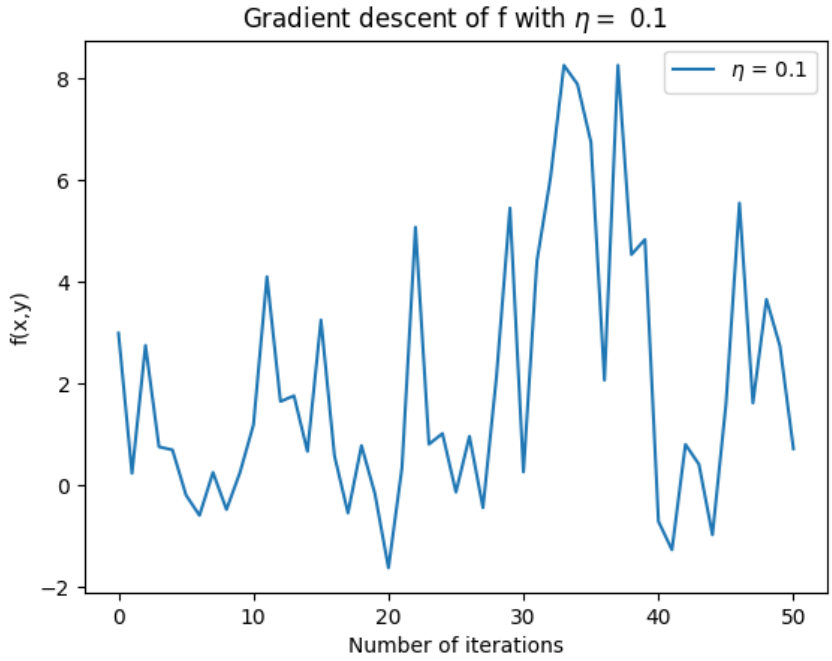
After 50 iterations for $\eta = 0.01$, the final coordinates are $(-1.269, 1.287)$ and their value is -0.381. The graph, which shows the relation between iterations and the function minimization is



As far as we have seen, before the 10^{th} iteration we are really close to the minimum and stay there without fluctuate.

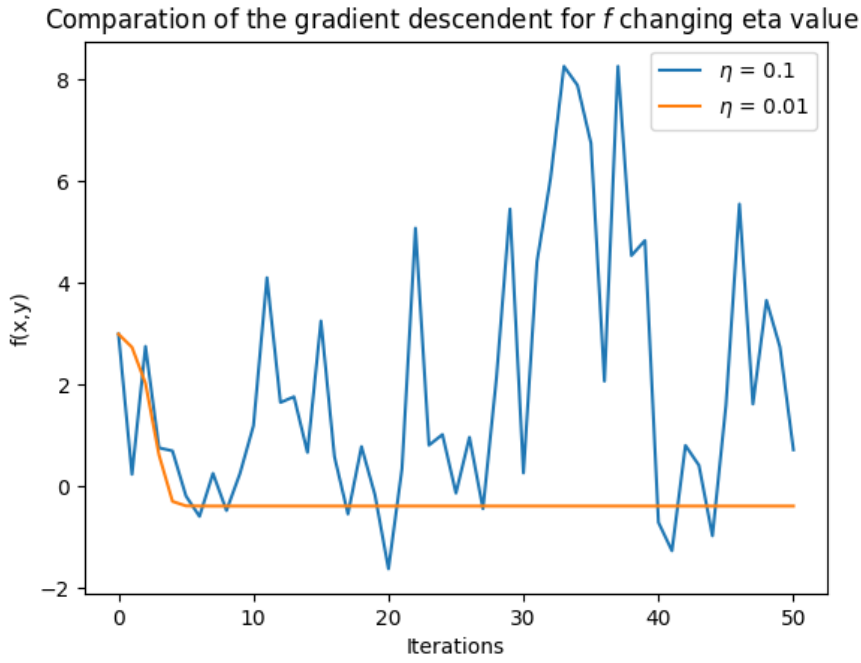
On the other hand, after 50 iterations for $\eta = 0.1$ the final coordinates are $(-2.939, 1.608)$ and their value is 0.724, so as we can see that this result is worse than the last one.

In the following graph we can see the evolution fluctuation of the images iteration by iteration



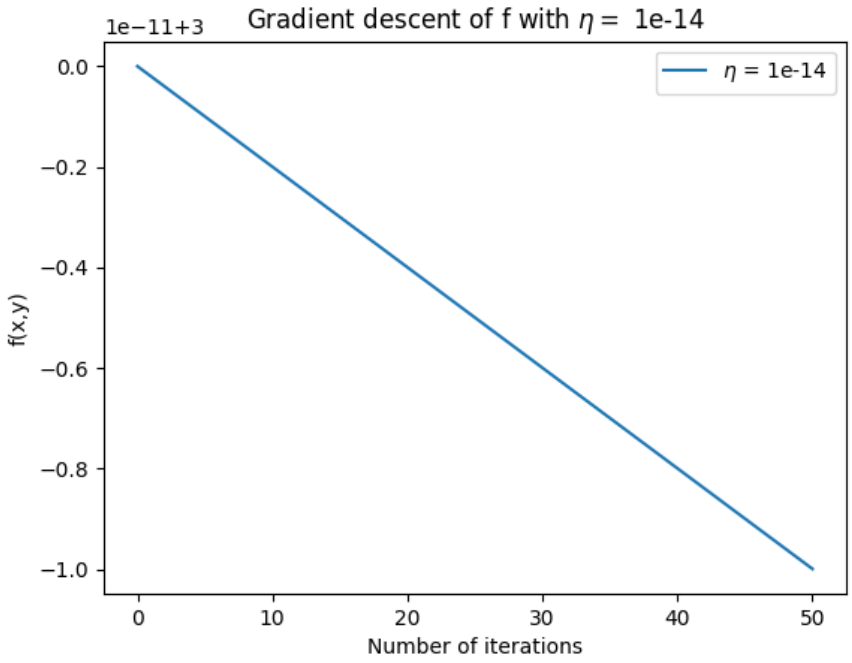
The reason for this irregularity is that the step size is too big, so it skips the minimum.

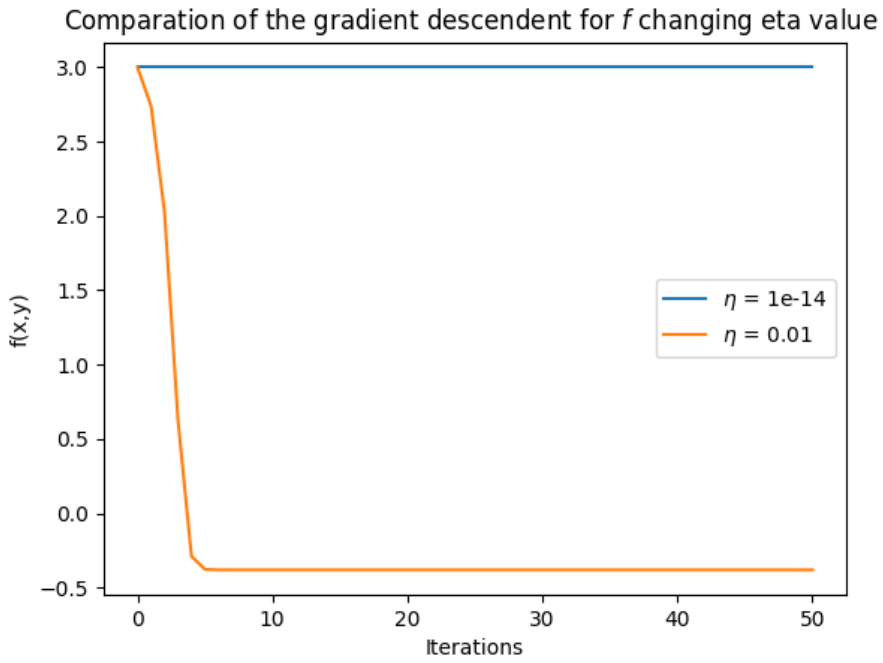
We can also compare the two experiment in the following graph.



Moreover, based on its mathematical proof, which use Taylor's series, we know that it should be small, but if it is too small the algorithm will never reach the minimum in time.

Let see a new example, now $\eta = 10^{-14}$, after 50 iteration the final coordinates are $(-1, 1)$ and the value is 3, so this new selection is even worse that the one with the bigger step size, although it goes without oscillate.





As a conclusion, a priory, it is difficult to select a step size value, each problem should have an appropriate one, and the selection must be empirical. Even though some heuristic [1] tell that $\eta = 0.01$ it is a good try.

Minimum value

Before running the algorithm is important to think about a good value for the learning rate η. Based on the last section, $\eta = 0.1$ is a good one.

After run the program the results are

Initial point	Final coordinates	Final value
(-0.5 -0.5)	(-0.793 -0.126)	9.125
(1 1)	(0.677 1.29)	6.437
(2.1 -2.1)	(0.149 -0.096)	12.491
(-3 3)	(-2.7315 2.713)	-0.381
(-2 2)	(-2. 2.)	0

This example gives the idea that the local minimums found depend on the start point w_0 and a priory, unless we know some properties of the function such as convexity or monotony we are not able to assure that the minimum found is global.

For a mathematical study we need differentiable functions, and a technique to find where their zeros are, so we need to solve their equations. Some time this is not possible and we use numeric methods.

1.1.6 Final conclusion about finding global functions' minimum by gradient descent

To sum up this first chapter, gradient descent algorithm is a technique to minimize differentiable functions. Dramatically depends on the initial point and the learning rate. Moreover, it does not give global a minimum unless the function is convex.

The computational cost of the function is $\mathcal{O}(Ni)$ where N is the size of the data set and i the maximum number of iterations.

Some useful examples of functions used in this algorithm are the mean quadratic error or the logistic functions are used as the functions to minimize the error.

Chapter 2

Linear Regression

2.1 Linear regression

2.1.1 Stochastic gradient descendent

Stochastic gradient descendent (SGD) is a sequential version of the gradient descent. Instead of considering the full batch gradient on all N training data points, we consider a stochastic version of the gradient. First, pick a training data point (x_n, y_n) uniformly random (hence the name 'stochastic') and consider only the error on that data point. [1]

The gradient of this single data point's error is used for the weight update in exactly the same that the gradient was used in batch gradient descent.

Another variants are the **mini-batch gradient descent** and the **batch gradient descendent**, the differences among them are the size of the batch: one for the pure stochastic gradient descendent, between 32 or 64 for the mini-batch variation and more than that for the batch gradient descendent.

2.1.2 Pseudo - inverse algorithm

Pseudo inverse algorithm also known as **linear regression algorithm** or **ordinary least squares**(OLS) is based on minimizing the squared error between the projection matrix $h(x) = w^T x$ and y, the target vector, where $x \in \mathbb{R}^{N \times (d+1)}$ is the feature matrix and $N \in \mathbb{N}$ the training data size.

$$E_{in}(w) = \frac{1}{N} \sum_{n=1} N(w^T x_n - y)^2 = \frac{1}{N} \|Xw - y\|^2$$

Where $\|.\|$ is the Euclidean norm of a vector.

Since $E_{in}(w)$ is differentiable we can use standard matrix calculus to find the w that minimizes E_{in} with respect to w is the zero vector:

$$\nabla E_{in}(w) = \frac{2}{N}(X^T X w - X^T y) = 0$$

Finally to get $\nabla E_{in}(w)$ to be 0, we should solve for w that satisfies

$$X^T X w = X y$$

If $X^T X$ is invertible, $w = X^\dagger y$ where $X^\dagger = (X^T X)^{-1}$ is the `pseudo-inverse` of X. The resulting w is the unique optimal solution that minimizes E_{in}. Otherwise a pseudo-inverse can still be defined, but the solution will not be unique.

In practice, $X^T X$ is invertible in most of the cases since N is often much bigger than $d + 1$, so there will likely be $d + 1$ linearly independent vector x_n.

2.1.3 Exercise 1

Estimate a linear regression model from the data provided by the feature vectors (Average intensity, Symmetry) using both the pseudo-inverse algorithm and the Stochastic Gradient Descent (SGD). The labels will be $\{-1, 1\}$, one for each feature vector of each number. Draw the solutions obtained together with the data used in the fitting. Assess the goodness of the result using E_{in} and E_{out} (for Eout calculate the predictions using the data from the test file).

Error

As we have said the error is the mean squared error:

$$E_{out}(h) = \mathbb{E}[(h(x) - y)^2]$$

$$E_{in}(w) = \frac{1}{N}\|Xw - y\|^2$$

A direct implementation is

```
def Error(x,y,w):
    '''quadratic error
    INPUT
    x: input data matrix
    y: target vector
    w:  vector to

    OUTPUT
    quadratic error >= 0
    '''
    error_times_n = np.linalg.norm(x.dot(w) - y.reshape(-1,1))**2

    return error_times_n/len(x)
```

For the euclidean norm we have used `np.linalg.norm` [3] numpy function.

The gradient computation is direct too:

$$\nabla E_{in}(w) = \frac{2}{N}(X^T X w - X^T y) = \frac{2}{N}(X^T(Xw - y))$$

```
def dError(x,y,w):
''' gradient
OUTPUT
column vector
  '''

  return (2/len(x)*(x.T.dot(x.dot(w) - y.reshape(-1,1))))
```

Interpretation of the mean squared error, E

The mean squared error function $E : \mathbb{R}^d \longrightarrow \mathbb{R}_0^+$ measures the average of the squared difference between the estimated values ant the actual value[4]. Hence, the nearer to zero, the better.

Pseudo-inverse algorithm

As we have described in pseudo inverse introduction, firstly we need to compute the pseudo-inverse. For that we have use `np.linalg.pinv` [5]function from numpy library.

```
def pseudoInverseMatrix ( X ):
  '''
  INPUT
  X: is a matrix (must be a np.array) to use transpose and dot method
  OUTPUT
  hat matrix
  '''

  '''
  #S =( X^TX ) ^{-1}
  simetric_inverse = np.linalg.inv( X.T.dot(X) )

  # S X^T = ( X^TX ) ^{-1} X^T
  return simetric_inverse.dot(X.T)
  '''
  return np.linalg.pinv(X)
```

Finally we have to compute $w = X^{\dagger} y$

```
def pseudoInverse(X, Y):
    '''
    INPUT
    X is the feature matrix
    Y is the target vector (y_1, ..., y_m)

    OUTPUT:
    w: weight vector
    '''
    X_pseudo_inverse = pseudoInverseMatrix ( X )
    Y_transposed = Y.reshape(-1, 1)

    w = X_pseudo_inverse.dot( Y_transposed)

    return w
```

Pseudo-inverse linear regression model

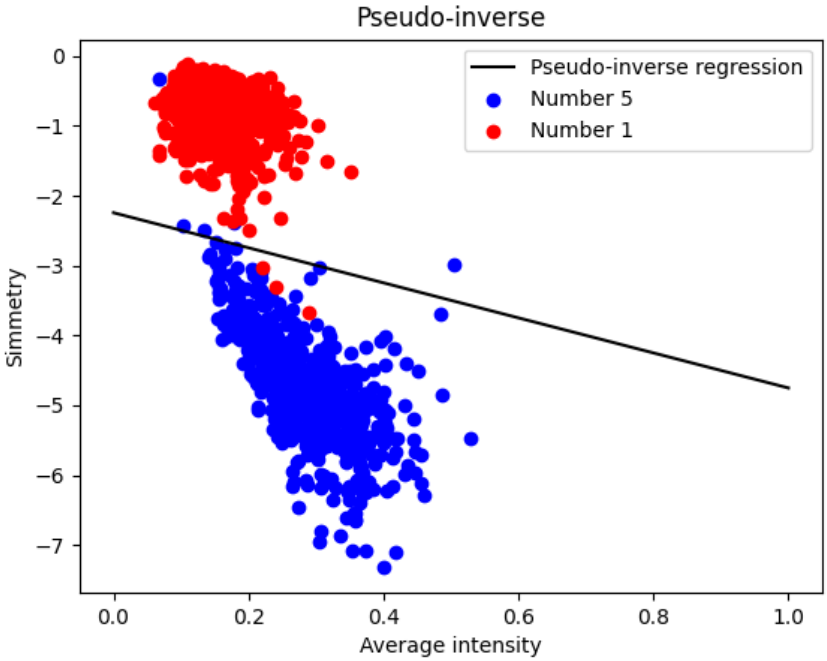
After execute the algorithm we obtain:

```
___ Goodness of the Pseudo-inverse fit ___

  Ein:   0.07918658628900395
  Eout:  0.1309538372005258

Evaluating output training data set
Input size:  1561
Bad negatives : 7
Bad positives : 3
Accuracy rate : 99.35938500960923 %

Evaluating output test data set
Input size:  424
Bad negatives : 1
Bad positives : 7
Accuracy rate : 98.11320754716981 %
```

Which means that the w computed by our pseudo-inverse algorithm we the training data set has a $E_{in}(w) = 0.079$ and with the test data $E_{out}(w) = 0.131$, for our experiment it is a good fit, because it is close enough to zero. In addition, if we evaluate the data classification, from 1561 training data it only misclassify 10, whereof 7 was truly positives. The accuracy rate ($\frac{\text{good classified data}}{\text{data set size}}$) is 99.358%, which continues being really good.

Initially, we could think that it classifies the positives values better, but if we analyse the output from test data set, there are more negatives values misclassified, so we cannot establish any relation. Moreover here the accuracy rate is 98.113%

Finally, a graphic representation for the solutions is



Something really import about this method is that it would be better o equal than the gradient descent, therefore in the next experiment we are going to compare the results which it.

How have we plotted the regression line.

Firstable, to draw a line we need two points.

Therefore we use the sign um to classify the numbers, we are going to find two points in $\mathbb{R}^2$ that their estimation is zero, which means that they are in the middle of classification (the regression line).

The obtained weight vector $w^T = (w_1, w_2, w_3)^T$, means that for a point $(x, y) \in \mathbb{R}^2$ its estimation is $h(x, y) = (1, x, y)w = w_1 + w_2x + w_3y$.

To calculate the two points we are going to equal $h(x, y) = 0$ and from the infinities solution we can calculate:

if $x = 0$ then $y = \frac{-w_1}{w_3}$, and if $x = 1$ then $y = \frac{-w_1-w_2}{w_3}$.

The related code is

```
# regression line
# x= 0
```

```
    symmetry_for_cero_intensity = -w[0]/w[2]

    #  x = 1, 0 = w0 + w1 * w2 * x2
    # then y = (-w0 - w1) /w2
    symmetry_for_one_intensity= (-w[0] - w[1])/w[2]

    # plotting order
    plt.plot([0, 1],
             [symmetry_for_cero_intensity,symmetry_for_one_intensity],
             'k-',
             label=(title+ ' regression'))
```

Stochastic gradient descendent

Based on the description of the algorithm, we have done two implementations:

This one is strictly based on the classroom's slides, however depending on the `batch_size` the exact number of iterations will be

$$\texttt{max\_iter} \times \lfloor \frac{\texttt{(len(y))}}{\texttt{batch\_size}} \rfloor$$

```
def sgd(x,y, eta = 0.01, max_iter = 1000, batch_size = 32, error=10**(-10)):
        '''
        Stochastic gradient descent
        INPUT
        x: data set
        y: target vector
        eta: learning rate
        max_iter

        OUTPUT
        w: weight vector
        '''

        #initialize data
        w = np.zeros((x.shape[1], 1), np.float64)
        n_iterations = 0

        len_x = len(x)
        x_index = np.arange( len_x )
        batch_start = 0
        w_error = Error(x,y,w)

        while n_iterations < max_iter and w_error > error :
```

```
            #shuffle and split the same into a sequence of mini-batches
            np.random.shuffle(x_index)
            for batch_start in range(0,  len_x, batch_size):
                    iter_index = x_index[ batch_start : batch_start + batch_size]


                    w = w - eta* dError(x[iter_index, :], y[iter_index], w)

            n_iterations += 1
            w_error = Error(x,y,w)


    return w
```

In order to control exactly the numbers of iterations apart from exercise 1, we are going to use this

```
def sgd_exact_number_iter(x,y, eta = 0.01,
max_iter = 1000, batch_size = 32, error = 10**(-10)):
'''
Stochastic gradient descent
INPUT
x: data set
y: target vector
eta: learning rate
max_iter
OUTPUT
w: weight vector
'''
#initialize data
w = np.zeros((x.shape[1], 1), np.float64)

n_iterations = 0
batch_start = 0
len_x = len(x)

x_index = np.arange( len_x )
w_error = Error(x,y,w)

while n_iterations < max_iter and w_error > error:
        #shuffle and split the same into a sequence of mini-batches
        if batch_start == 0:
                x_index = np.random.permutation(x_index)
```

```
            iter_index = x_index[ batch_start : batch_start + batch_size]

            w = w - eta* dError(x[iter_index, :], y[iter_index], w)

            n_iterations += 1

            batch_start += batch_size
            if batch_start >= len_x: # if end, restart
                    batch_start = 0

            w_error = Error(x,y,w)


    return w
```

Due to the fact that this is a stochastic method and the gradient descendent do not reduce the error in every step, there are other variations, for example we can save and return only the w found which has the less error.

```
 def sgd_save_w(x,y, eta = 0.01, max_iter = 1000,
                            batch_size = 32, error = 10**(-10)):
'''
Stochastic gradient descent
INPUT
x: data set
y: target vector
eta: learning rate
max_iter
OUTPUT
w: weight vector
'''
#initialize data
w = np.zeros((x.shape[1], 1), np.float64)

n_iterations = 0
batch_start = 0
len_x = len(x)

x_index = np.arange( len_x )
w_error = Error(x,y,w)

#IMPROVEMENT
best_error = w_error
best_w = w
```

```
while n_iterations < max_iter and w_error > error:
        #shuffle and split the same into a sequence of mini-batches
        if batch_start == 0:
                x_index = np.random.permutation(x_index)
        iter_index = x_index[ batch_start : batch_start + batch_size]

        w = w - eta* dError(x[iter_index, :], y[iter_index], w)

        n_iterations += 1

        batch_start += batch_size
        if batch_start >= len_x: # if end, restart
                batch_start = 0

        w_error = Error(x,y,w)

        # IMPROVEMENT
        if w_error < best_error:
                best_w = w
                best_error = w_error


return best_w
```

This algorithm is interesting because it return the best w found and has (in order) the same computational cost.

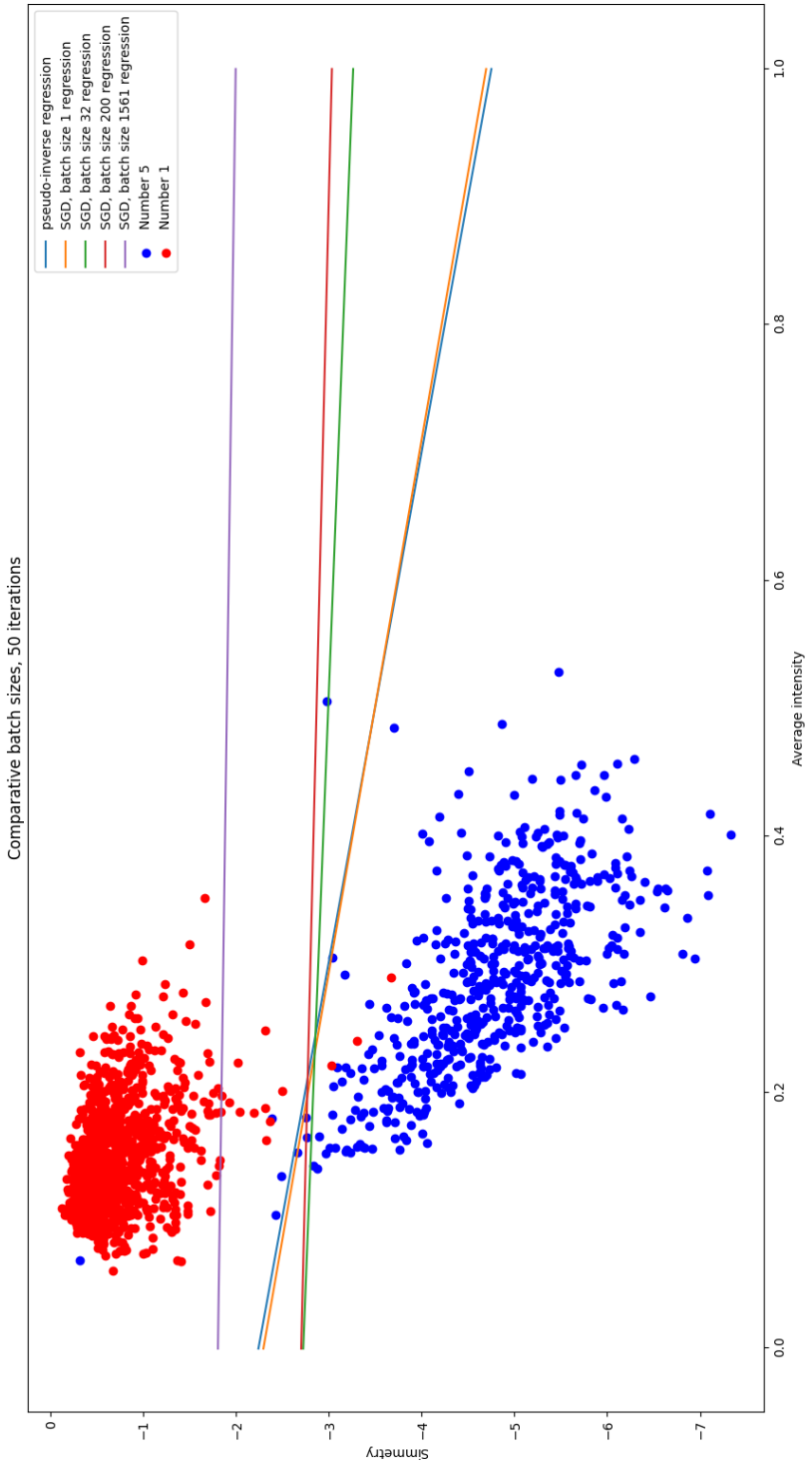
Initial point Another consideration is that as we know, it is really important the chosen of the initial point in gradient descendent. However, due to the fact that we are working with the mean quadratic error, we know that only exists one global minimum, so here the relevance of the initial point is to reduce iterations. Therefore we theoretically do not have more information, we have chosen the $w_0 = 0 \in \mathbb{R}^d$.

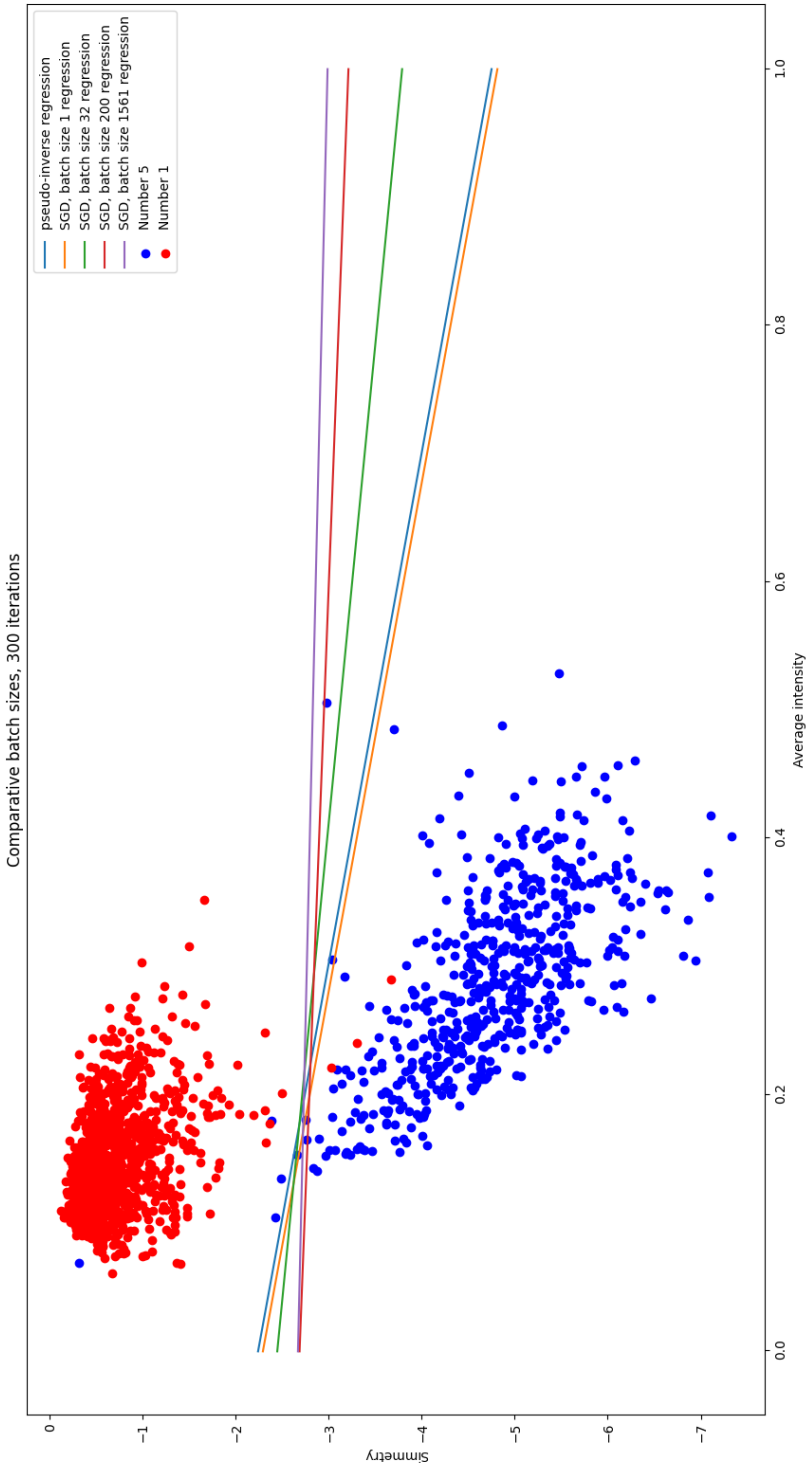
The experiment result We are going to execute the `sgd` algorithm (one iteration is one step) with $\eta = 0.01$ batch sizes $1, 32, 200$ and `len(y)` and the numbers of steps 50 and 300.

Batch size	Iterations	E_{in}	E_{out}	Training accuracy rate (%)	Test accuracy rate (%)
1	50	0.0798	0.131	99.423	98.349
32	50	0.081	0.133	99.295	98.113
200	50	0.082	0.135	99.424	98.113
1561	50	0.404	0.428	99.167	95.28

As we can see, as bigger is the batch size the worse is the error. Something really interesting is that we are minimizing based on the quadratic error, but it does not mean we are minimizing the accuracy error (there is a correlation but not a coincidence. A good example of that is if we compare bath size 200's with bath size 32. As we increase the numbers of iterations the general error decrease (see 300 steps).

Another interesting observation is that for batch 1: 200 iterations is worst than 50, this is because we are oscillating over the solution. The algorithm which save the best w, `sgd_save_w` would solve this problem.


Comparative batch sizes, 50 iterations
pseudo-inverse regression
SGD, batch size 1 regression
SGD, batch size 32 regression
SGD, batch size 200 regression
SGD, batch size 1561 regression
Number 5
Number 1
Average intensity
Simmetry
0.0
0.2
0.4
0.6
0.8
1.0
0
−1
−2
−3
−4
−5
−6
−7


Comparative batch sizes, 300 iterations
pseudo-inverse regression
SGD, batch size 1 regression
SGD, batch size 32 regression
SGD, batch size 200 regression
SGD, batch size 1561 regression
Number 5
Number 1
Symmetry
Average intensity
0
−1
−2
−3
−4
−5
−6
−7
0.0
0.2
0.4
0.6
0.8
1.0

50 steps

```
___ Goodness of the Stochastic Gradient Descendt (SGD) fit ___


SGD, batch size 1
Ein:  0.07981803904587495
Eout:  0.13188855705205335

Evaluating output training data set
For w^T = [[-1.15690746 -1.20909308 -0.50379833]]
Input size:  1561
Bad negatives : 6
Bad positives : 3
Accuracy rate : 99.4234465086483 %

Evaluating output test data set
For w^T = [[-1.15690746 -1.20909308 -0.50379833]]
Input size:  424
Bad negatives : 0
Bad positives : 7
Accuracy rate : 98.34905660377359 %

--- End of a section, press any enter to continue ---


SGD, batch size 32
Ein:  0.08183880846320654
Eout:  0.13300563169544255

Evaluating output training data set
For w^T = [[-1.23840622 -0.24445313 -0.45432575]]
Input size:  1561
Bad negatives : 8
Bad positives : 3
Accuracy rate : 99.29532351057014 %

Evaluating output test data set
For w^T = [[-1.23840622 -0.24445313 -0.45432575]]
Input size:  424
Bad negatives : 1
Bad positives : 7
Accuracy rate : 98.11320754716981 %
```

```
--- End of a section, press any enter to continue ---


SGD, batch size 200
Ein:  0.0824097083428238
Eout:  0.13514678139988967

Evaluating output training data set
For w^T = [[-1.21138905 -0.14846307 -0.44806566]]
Input size:  1561
Bad negatives : 6
Bad positives : 3
Accuracy rate : 99.4234465086483 %

Evaluating output test data set
For w^T = [[-1.21138905 -0.14846307 -0.44806566]]
Input size:  424
Bad negatives : 1
Bad positives : 7
Accuracy rate : 98.11320754716981 %

--- End of a section, press any enter to continue ---


SGD, batch size 1561
Ein:  0.40484272492435486
Eout:  0.42805781278130317

Evaluating output training data set
For w^T = [[-0.42953442 -0.04548081 -0.23773542]]
Input size:  1561
Bad negatives : 1
Bad positives : 12
Accuracy rate : 99.16720051249199 %

Evaluating output test data set
For w^T = [[-0.42953442 -0.04548081 -0.23773542]]
Input size:  424
Bad negatives : 0
Bad positives : 20
Accuracy rate : 95.28301886792453 %

--- End of a section, press any enter to continue ---
```

300 steps

```
SGD, batch size 1
Ein:  0.07991429824341009
Eout:  0.13043428762931666

Evaluating output training data set
For w^T = [[-1.14204678 -1.25437994 -0.4976879 ]]
Input size:  1561
Bad negatives : 7
Bad positives : 3
Accuracy rate : 99.35938500960923 %

Evaluating output test data set
For w^T = [[-1.14204678 -1.25437994 -0.4976879 ]]
Input size:  424
Bad negatives : 0
Bad positives : 7
Accuracy rate : 98.34905660377359 %

--- End of a section, press any enter to continue ---

SGD, batch size 32
Ein:  0.08063407701065878
Eout:  0.13581316178349648

Evaluating output training data set
For w^T = [[-1.18587205 -0.6497891  -0.48419008]]
Input size:  1561
Bad negatives : 5
Bad positives : 3
Accuracy rate : 99.48750800768738 %

Evaluating output test data set
For w^T = [[-1.18587205 -0.6497891  -0.48419008]]
Input size:  424
Bad negatives : 0
Bad positives : 7
Accuracy rate : 98.34905660377359 %

--- End of a section, press any enter to continue ---
```

```
SGD, batch size 200
Ein:  0.08138110980377243
Eout:  0.1344240103546277

Evaluating output training data set
For w^T = [[-1.23721465 -0.24176584 -0.46011533]]
Input size:  1561
Bad negatives : 7
Bad positives : 3
Accuracy rate : 99.35938500960923 %

Evaluating output test data set
For w^T = [[-1.23721465 -0.24176584 -0.46011533]]
Input size:  424
Bad negatives : 1
Bad positives : 7
Accuracy rate : 98.11320754716981 %

--- End of a section, press any enter to continue ---


SGD, batch size 1561
Ein:  0.085568968925448
Eout:  0.13713701679830562

Evaluating output training data set
For w^T = [[-1.15962485 -0.13812568 -0.43405538]]
Input size:  1561
Bad negatives : 5
Bad positives : 3
Accuracy rate : 99.48750800768738 %

Evaluating output test data set
For w^T = [[-1.15962485 -0.13812568 -0.43405538]]
Input size:  424
Bad negatives : 0
Bad positives : 7
Accuracy rate : 98.34905660377359 %

--- End of a section, press any enter to continue ---
```

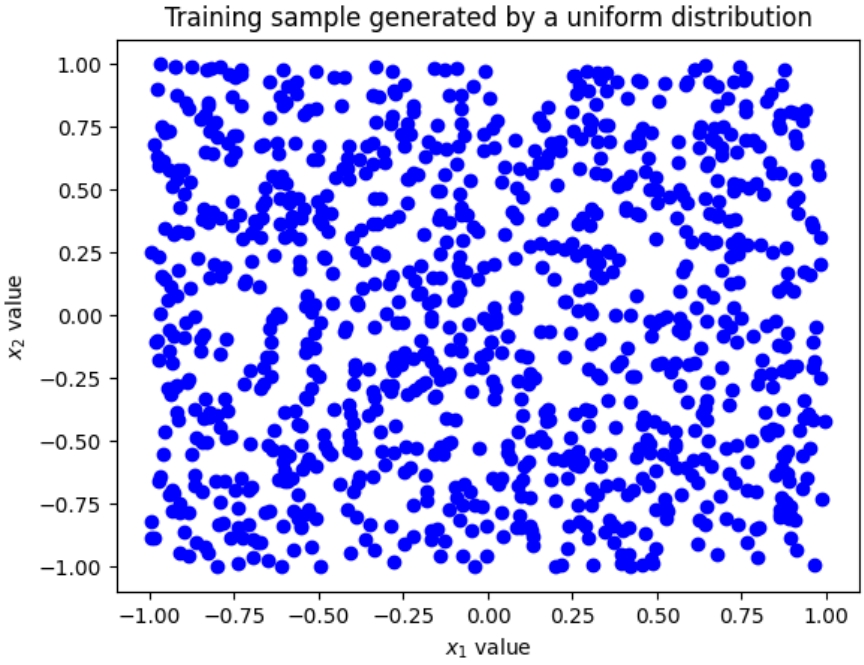
2.2 Experiment

2.2.1 a) Generate a training sample

We are going to use a uniform generation:

```
def simula_unif(N, d, size):
        ''' generate a trining sample of N  points
in the square [-size,size]x[-size,size]
'''
        return np.random.uniform(-size,size,(N,d))
```

After fixed random seed to 1.
The final 2D map is



2.2.2 b) Labels, noise and map

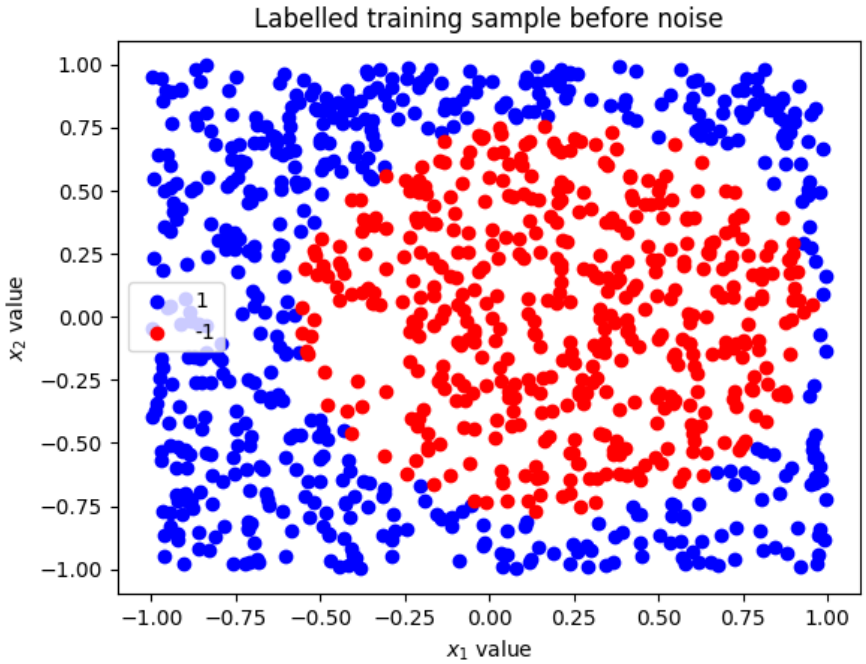
b) Let's consider the function $f(x_1, x_2) = sign((x_1 - 0.2)^2 + x_2^2 - 0.6)$ that we will use to assign a label to each point of the previous sample. We introduce noise on the labels, randomly changing the sign of 10 % of them. Draw the obtained labels map.

Before plotting, It is important to have in mind that a circumference with radius r and center $(c_1, c_2) \in \mathbb{R}^2$ are the points $(x_1, x_2) \in \mathbb{R}^2$ that verify

$$(x_1 - c_1)^2 + (x_2 - c_2)^2 = r^2$$

Therefore looking at f it is easy to think that we are going to see a circle of radius $\sqrt{0.6}$ and center $(0.2, 0)$.

The plotting is

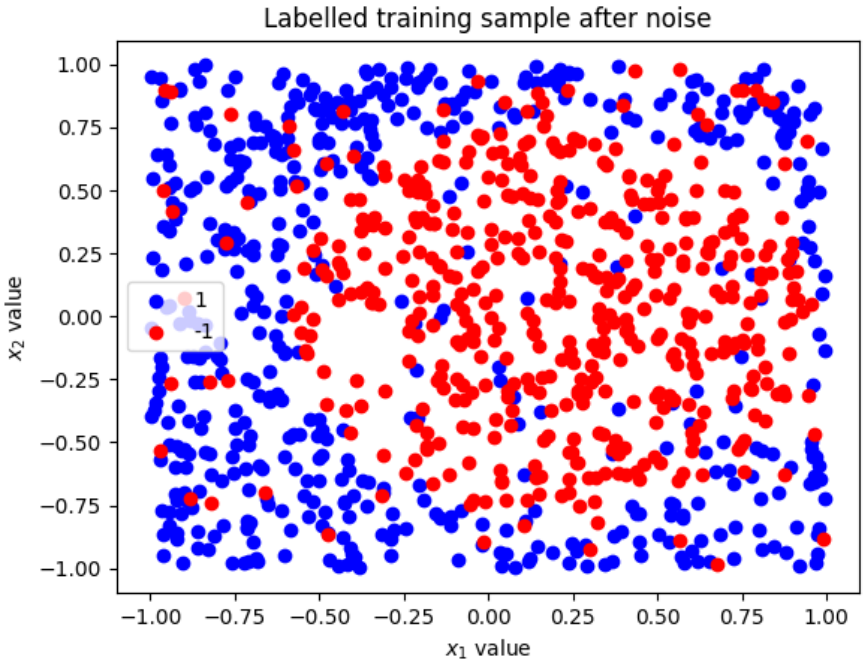


In order to introduce noise on the label we are going to change randomly the sign of the 10% of the labels obtained by b.

```
#labels
y = np.array( [f(x[0],x[1]) for x in training_sample ])

index = list(range(size_training_example))
np.random.shuffle(index)

percent_noisy_data = 10.0
size_noisy_data = int((size_training_example *percent_noisy_data)/ 100 )


noisy_y = np.copy(y)
for i in index[:size_noisy_data]:
    noisy_y[i] *= -1
```

As we can see the idea behind the snippet is simple: The noised labels would be a copy of the original one and 10% of the data would change their sign.

The final map is :



2.2.3 Estimate the fitting error of E_{in} using SGD

c

Using $(1, x_1, x_2)$ as feature vector, fit a linear regression model to the generated datasets and estimate the weights w. Estimate the fitting error of Ein using Stochastic Gradient Descent (SGD).

Having in mind the observation in the last subsection that the labels follows a circumference equation with a bit of noise, a linear regression model it is not going to be the best approach.

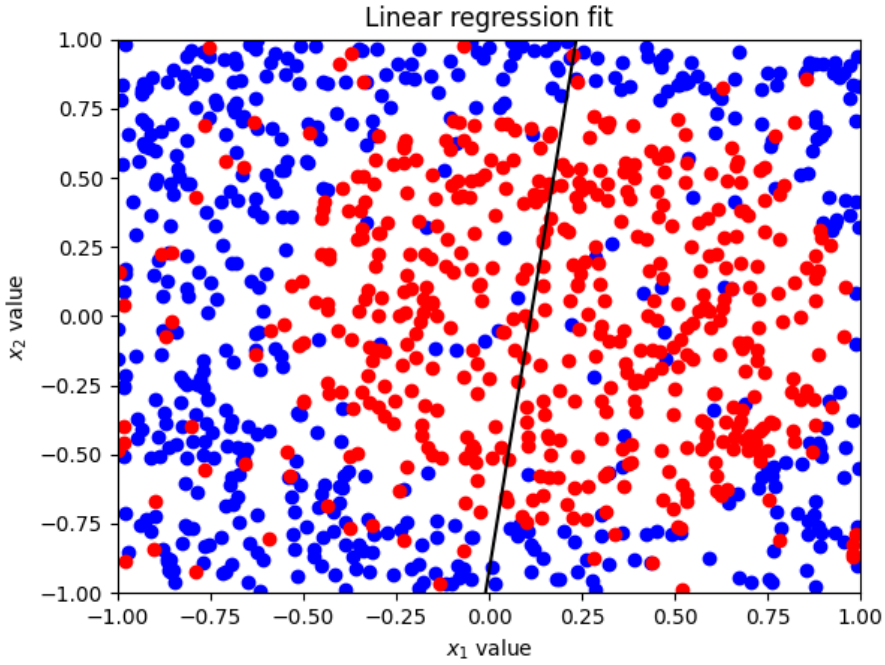
The experiment result are:

```
EXPERIMENT (c)

SGD, batch size 5
Ein:  0.9038395322567018

Evaluating output training data set
For w^T = [[ 0.05824863 -0.51637342  0.06313758]]
Input size:  1000
Bad negatives : 163
Bad positives : 212
Accuracy rate : 62.5 %
```

Remember that the bad negatives are the points that the regression classify in negative but they are positives and the bad positives are the negatives one that are classify as a positives.

Finally the accuracy rate was the corrected classify data divided by the input size, so it is not a good model due to the fact that the accuracy rate is so close to a random one, that it would theoretically have a 50% of accuracy rate.

A visual representation of the projection is



d) Repetition of the experiment

In order to see the last result was not hazaour we are going to repeat the experiment 1000 times, the result is:

```
EXPERIMENT (d), lineal regression

The mean value of E_in in all 1000 experiments is: 0.9270571984798377
The mean value of E_out in all 1000 experiments is: 0.9330084274789892
```

So as we can se the mean error is even worse hence, our linear regression is not a good one.

e) Quadratic adjustment

e) Assess how good you consider the fit with this linear model is according to the mean values obtained for Ein and Eout. Repeat the same previous experiment but using non-linear characteristics. Now, we will use the following feature vector: $\phi_2(x) = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$. Fit the new linear regression model and calculate the new vector of weights w. Calculate the average errors of Ein and Eout. Which model do you consider the most appropriate according to the average errors for Ein and Eout?

Now, instead of using a linear features vector, we are going to use a quadratic one

```
def quadraticFeatureVector(x_n):
      '''
      INPUT
       xn = (x1,x2) vector of coordinates

      '''
      return np.array([ 1,
                  x_n[0],
                  x_n[1],
                  x_n[0]*x_n[1],
                  x_n[0]* x_n[0],
                  x_n[1]* x_n[1]  ])
```

We know that the function is a circumference with a 10% of noise, so apriori we now that our target function is going to be

$$h(x,y) = (x-0.2)^2+y^2-0.6 = x^2-0.4x+0.04+y^2-0.6 = x^2+y^2-0.4x-0.56$$

What means that our target weight vector is goint to be

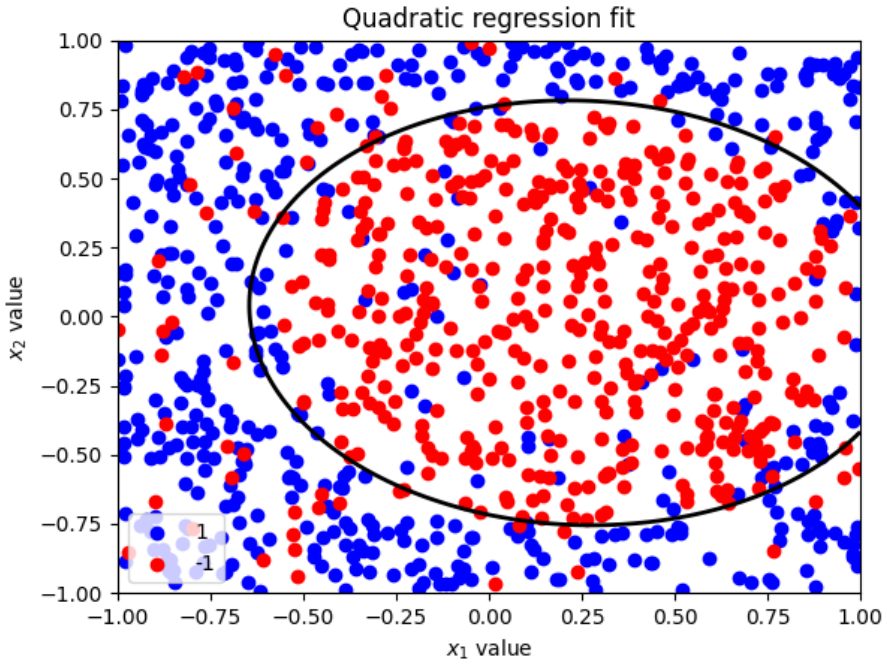
$$w_t = (-0.56, -0.4, 0, 0, 1, 1)$$

Moreover due to the fact that we are introducing 10% of noisy our accuracy level must be around 90%

After 1000 iterations we obtain:

```
 SGD, batch size 5, number iterations 1000
Ein:  0.5724680127717665

Evaluating output training data set
For w^T =
[[-0.67345368 -0.45209455 -0.0521589   0.07569398  0.92011803  1.23673771]]
Input size:  1000
```

```
Bad negatives : 94
Bad positives : 55
Accuracy rate : 85.1 %
```



The results are close to our first approach,
but apriori, for 1000 iterations they seen a bit bad.

However if we analyse how the error, accuracy rate and w are evoluting over $10, 50, 100, 200, 500, 700, 1000$ we clearly see that the error is improving, so the iterations were not enought.

Something interesting is that the 700 iterations have better accuracy rate, this is for the same reason explained at exercise 1.

```
For one experiment:

 SGD, batch size 5, number iterations 10
Ein:  0.96683465968506

Evaluating output training data set
For w^T =
[[ 0.02353559 -0.04212481 -0.00067979  0.00785992  0.02654321  0.03756063]]
Input size:  1000
Bad negatives : 0
```

```
Bad positives : 474
Accuracy rate : 52.6 %

For one experiment:

 SGD, batch size 5, number iterations 50
Ein:  0.8964601273439083

Evaluating output training data set
For w^T =
 [[-0.00103819 -0.136871   -0.01033269  0.00363211  0.1056979   0.14178948]]
Input size:  1000
Bad negatives : 34
Bad positives : 266
Accuracy rate : 70.0 %

For one experiment:

 SGD, batch size 5, number iterations 100
Ein:  0.8337613668693657

Evaluating output training data set
For w^T = [[-0.04576936 -0.244725   -0.00396614  0.015827    0.19350407  0.24068118]]
Input size:  1000
Bad negatives : 64
Bad positives : 198
Accuracy rate : 73.8 %

For one experiment:

 SGD, batch size 5, number iterations 200
Ein:  0.751970586436338

Evaluating output training data set
For w^T = [[-0.16858105 -0.3725849  -0.01499836  0.02664101  0.30993404  0.4367047 ]]
Input size:  1000
Bad negatives : 93
Bad positives : 121
Accuracy rate : 78.6 %

For one experiment:

 SGD, batch size 5, number iterations 500
Ein:  0.6352766784644138
```

```
Evaluating output training data set
For w^T =
[[-0.41975341 -0.46092311 -0.02902233  0.06514428  0.6286317   0.84761192]]
Input size:  1000
Bad negatives : 80
Bad positives : 72
Accuracy rate : 84.8 %

For one experiment:

 SGD, batch size 5, number iterations 700
Ein:  0.5997408279310205

Evaluating output training data set
For w^T =
[[-0.53430804 -0.46110075 -0.0464511   0.06892706  0.76915291  1.04094009]]
Input size:  1000
Bad negatives : 78
Bad positives : 63
Accuracy rate : 85.9 %

For one experiment:

 SGD, batch size 5, number iterations 1000
Ein:  0.5724680127717665

Evaluating output training data set
For w^T =
[[-0.67345368 -0.45209455 -0.0521589   0.07569398  0.92011803  1.23673771]]
Input size:  1000
Bad negatives : 94
Bad positives : 55
Accuracy rate : 85.1 %
```

Mean error and conclusion

In order to see the last result was not hazaour we are going to repeat the experiment 1000 times, the result is:

```
The mean value of E_in in all 1000 experiments is: 0.600107053636983
The mean value of E_out in all 1000 experiments is: 0.6058641910896161
```

More or less the error is the same, so we can trust that a good adjustment is a quadratic one.

Something which we have known a priori, because we knew our target vector (something that in real life do not happen).

Bibliography

[1] Hsuan-Tien Lin Yaser S. Abu-Mostafa, Malik Magdon-Ismail. *Learing From Data. A Short Course*. AMLbook, 2012.

[2] Numpy documentation. Numpy basic data types documentation, 2021.

[3] Numpy documentation. norm, documentation, 2021.

[4] wikipedia. Mean squared error wikipedia, 2021.

[5] Numpy documentation. Numpy pseudo-inverse matrix, documentation, 2021.