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 differentiable 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 $w(t) \in \mathbb{R}^d$ $t \in \mathbb{N}$ 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 implements 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 based on purely practical observation [1].

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

```
def gradient_descent(initial_point, loss_function,
              gradient_function, eta, max_iter, target_error):
  111
  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
  111
  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)

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

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:

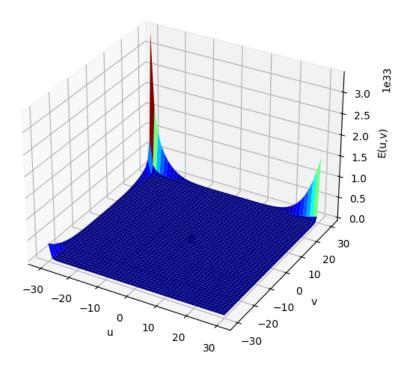
```
def dEu(u,v):
    111
    Partial derivate of E with respect to the variable u
    return np.float64(
        *( 3* u**2 * np.e**(v-2) + 2*v**2 * np.e**(-u) )
        *(u**3 * np.e**(v-2) - 2*v**2 * np.e**(-u))
    )
def dEv(u,v):
    Partial derivate of E with respect to the variable v
    return np.float64(
        (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:

The results are:

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

A 3d graph with the result is



1.1.5 Problem 2

Let's define the 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.

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

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

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.

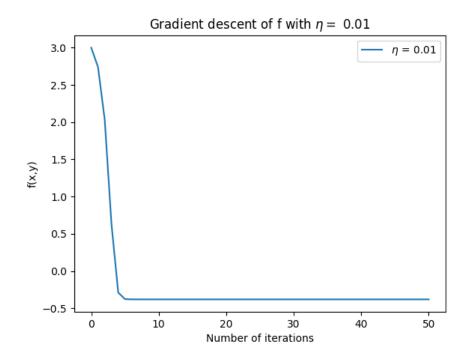
Now the new algorithm is

```
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:</pre>
      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

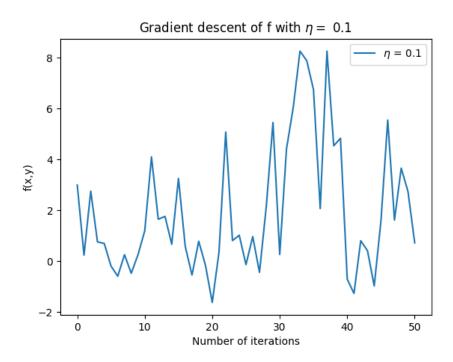
After 50 iterations for $\eta = 0.01$, the final coordinates are (-1.269, 1.287) and their value is -0.381. The graph which shows the relation between iterations and the function minimization is



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

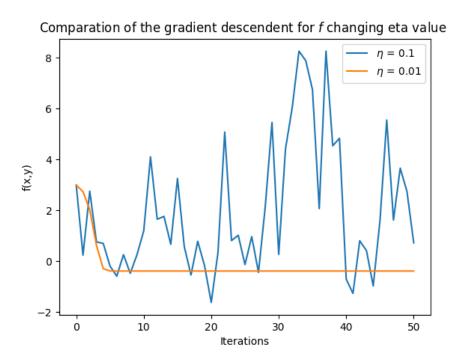
On the other hand, after 50 iterations for $\eta = 0.1$ the final coordinate is (-2.939, 1.608) and its value is f(-2.939, 1.608) = 0.724, so as we can see, this result is worse than the last one.

In the following graph we can see how the images' value fluctuates iteration by iteration.



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

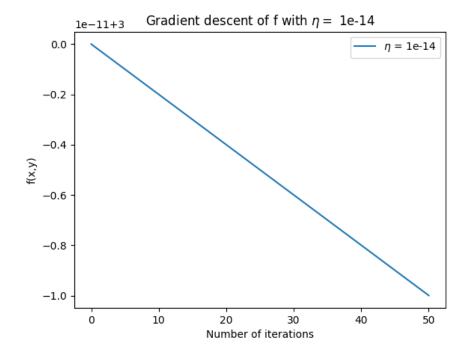
We can also compare the two experiment in the following graph.

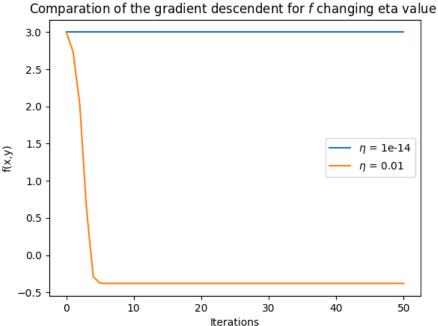


.

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's see a new example: now $\eta = 10^{-14}$, after 50 iterations 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's size, although it goes without oscillating.





As a conclusion, a priory, it is difficult to select a step's 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.

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.

Under a mathematical point of view, to study a function's monotony we need some more complex tools and conditions, such as solve equations; something that the majority of times is impossible. Fortunately, for the error functions such a the mean quadratic error, this is totally possible.

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

To sum up this first chapter, gradient descent's algorithm is a technique to minimize differentiable functions. It dramatically depends on the initial point and the learning rate. Moreover, it does not give global minimums 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 that can be successfully mimimized with used this algorithm are the mean quadratic's error or the logistic's function.

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.

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

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:

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

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

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

If X^TX is invertible, $w = X^{\dagger}y$ where $X^{\dagger} = (X^TX)^{-1}$ is the pseudo-inverse of X. The resulted 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^TX is invertible in most of the cases since N is often much more 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 ${\tt np.linalg.norm}$ [3] numpy function.

The gradient computation is direct too:

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

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

The mean squared error function $E: \mathbb{R}^d \longrightarrow \mathbb{R}_0^+$ measures the average of the squared difference between the estimated values and 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 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 computing the algorithm we obtain:

```
Ein: 0.07918658628900395
Eout: 0.1309538372005258

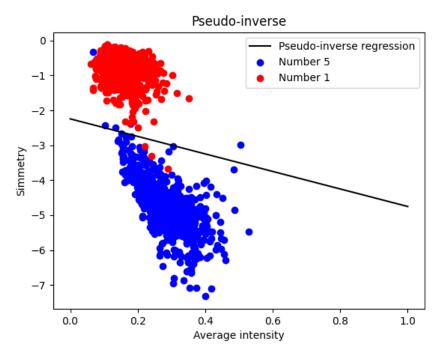
Evaluating output training data set
Input size: 1561
Bad negatives: 7
Bad positives: 3
Accuracy rate: 99.35938500960923 %

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 by the training data set has a $E_{in}(w)=0.079$ and by the test data $E_{out}(w)=0.131$, for our experiment it is a good fit, because it is closed enough to zero. In addition, if we evaluate the data classification, from 1561 training data it only misclassify 10 points, whereof 7 was truly positives. The accuracy rate $(\frac{\text{good classified data}}{\text{data cat size}})$ 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 is equal or better than the gradient descent, therefore in the next experiments 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 $w^T = (w_1, w_2, w_3)$, 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 equalize h(x, y) = 0 and from the infinity solutions we would compute two:

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
```

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

$$\max_{\text{iter}} \times \left[\frac{(\text{len(y)})}{\text{batch size}} \right]$$

```
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
        111
        #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 we are going to use this function:

```
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
111
#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)
```

return w

Due to the fact that this is a stochastic method and the gradient's descent does 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
```

return best_w

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

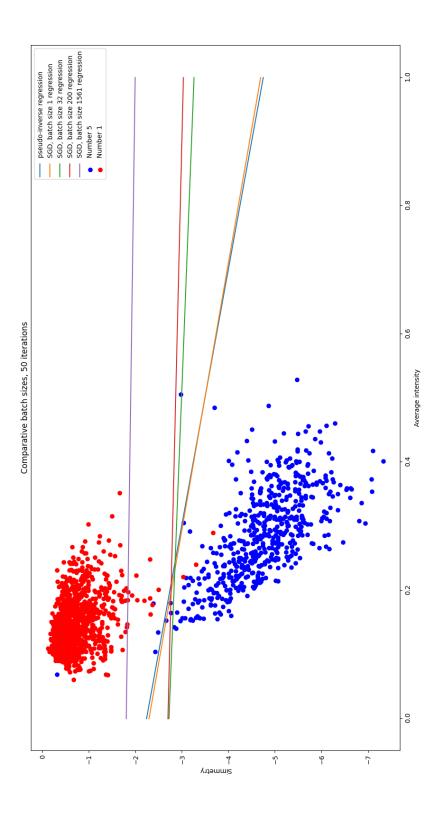
Initial point Another consideration is that as we know, it is really important the chosen of the initial point in gradient descendent. However, due to the fact that we are working with the mean quadratic error, we know that only exists one global minimum, so here the relevance of the initial point is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

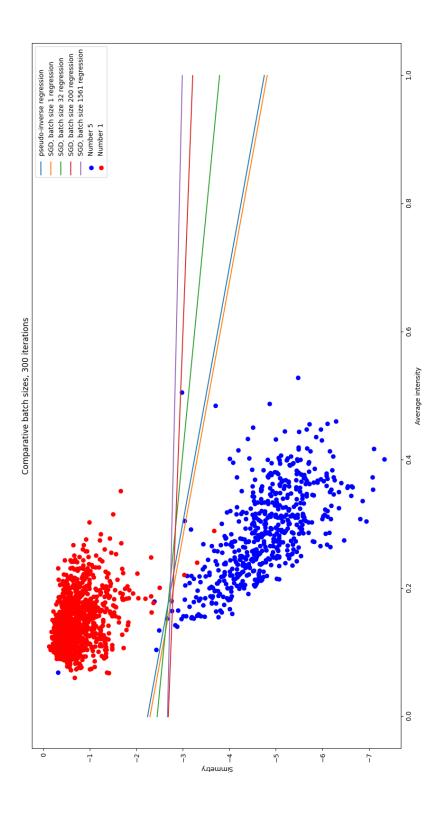
The experiment result We are going to execute the sgd algorithm (our version) with $\eta = 0.01$ batch sizes 1,32,200 and len(y) and the numbers of steps 50 and 300.

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's size 200 with bath's size 32. As we increase the numbers of iterations the general error decrease (see 300 steps).

Another interesting observation is that for batch's size one, 200 iterations is worse than 50, this is because we are oscillating over the solution. The algorithm we have described which saves the best w, sgd_save_w would solve this problem.





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 %

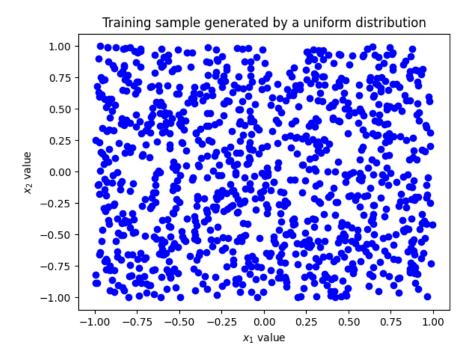
--- End of a section, press any enter to continue ---

2.2 Experiment

2.2.1 a) Generate a training sample

We are going to use a uniform generation:

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



2.2.2 b) Labels, noise and map

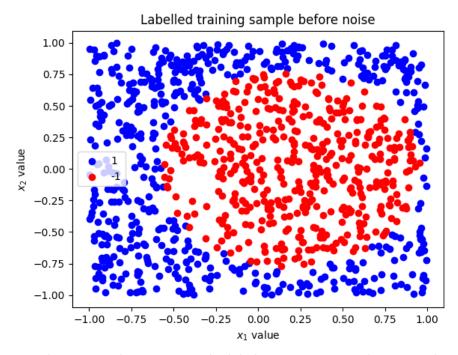
b) Let's consider the function $f(x_1, x_2) = sign((x_1 - 0.2)^2 + x_2^2 - 0.6)$ that we will use to assign a label to each point of the previous sample. We introduce noise on the labels, randomly changing the sign of 10 % of them. Draw the obtained labels map.

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.

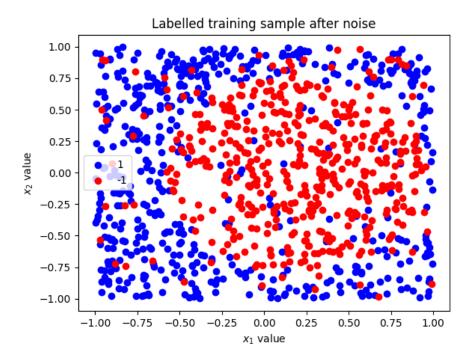
```
#labels
y = np.array( [f(x[0],x[1]) for x in training_sample ])
index = list(range(size_training_example))
np.random.shuffle(index)

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 ones 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

Experiment 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 follow a circumference's equation with a bit of noise, a linear regression model it is not going to be the best approach.

The experiment results are:

EXPERIMENT (c)

SGD, batch size 5

Ein: 0.9038395322567018

Evaluating output training data set

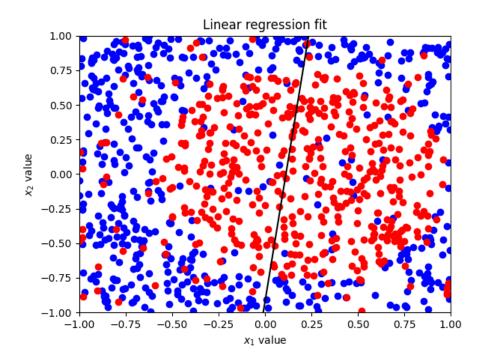
For $w^T = [[0.05824863 -0.51637342 0.06313758]]$

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 negative ones 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 that 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_{in} 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

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

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

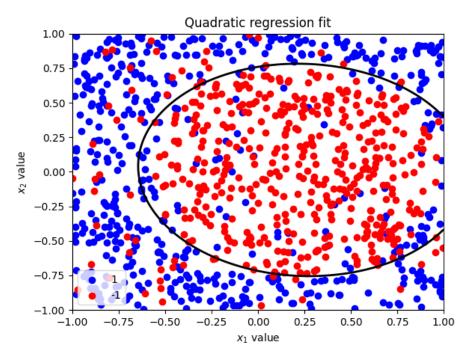
Moreover due to the fact that we are introducing 10% of noisy our accuracy level must be around 90%

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 than 1000, this is for the same reason we explained at exercise 1; we are minimazing the error, not the accuracy rate.

For one experiment:

SGD, batch size 5, number iterations 10

Ein: 0.96683465968506

Evaluating output training data set

For $w^T =$

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 $\sqrt{x} = [[-0.04576936 - 0.244725 - 0.00396614 0.015827 0.19350407 0.24068118]]$

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 $\sqrt{T} = [-0.16858105 - 0.3725849 - 0.01499836 0.02664101 0.30993404 0.4367047]]$

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 $w^T =$

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_{in} 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 does not happen).

Chapter 3

Newton's Method

3.1 Newton's method

3.1.1 Implementation

We are going to use the class algorithm:

Newton's Method: a cure for oscillation

• A new update rule for w based on the second order derivatives (Hessian)

$$f(x+\Delta x,y+\Delta y\,)\approx f(x,y)+\frac{\partial f}{\partial x}\Delta x+\frac{\partial f}{\partial y}\Delta y+\frac{1}{2}\bigg(\frac{\partial^2 f}{\partial x^2}\Delta x^2+\frac{\partial^2 f}{\partial y^2}\Delta y^2+\frac{\partial^2 f}{\partial y\partial x}\Delta x\Delta y+\frac{\partial^2 f}{\partial x\partial y}\Delta x\Delta y\bigg)$$

• Let's approach $E_{in}(\mathbf{w})$ up to second order.

$$g(\Delta \mathbf{w}) = E_{\rm in}(\mathbf{w}_0 + \Delta \mathbf{w}) \approx E_{\rm in}(\mathbf{w}_0) + \Delta \mathbf{w}^T \nabla E_{\rm in}(\mathbf{w}_0) + \frac{1}{2} \Delta \mathbf{w}^T \nabla^2 E_{\rm in}(\mathbf{w}_0) \Delta \mathbf{w}$$
$$\frac{\partial g(\Delta \mathbf{w})}{\partial \Delta \mathbf{w}} = \mathbf{0} \quad \rightarrow \quad \nabla E_{\rm in}(\mathbf{w}_0) + \underbrace{\nabla^2 E_{\rm in}(\mathbf{w}_0)}_{\mathbf{H}} \Delta \mathbf{w} = \mathbf{0}$$
$$\Delta \mathbf{w} = -\mathbf{H}^{-1} \nabla E_{\rm in}(\mathbf{w}_0)$$

Now the matrix **H** defines the advance on the gradient direction

The major complexity is to invert **H**

Hessian matrix

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

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

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

$$\frac{\partial^2}{\partial y \partial x}f = \frac{\partial^2}{\partial x \partial y}f = 8\pi^2 \cos(2\pi x)\cos(2\pi y)$$

$$\frac{\partial^2}{\partial y^2}f = 4 - 8\pi^2 \sin(2\pi x)\sin(2\pi y)$$

$$\frac{\partial^2}{\partial x^2}f = 2 - 8\pi^2 \sin(2\pi x)\sin(2\pi y)$$

Implementation

With eta = 0.01,

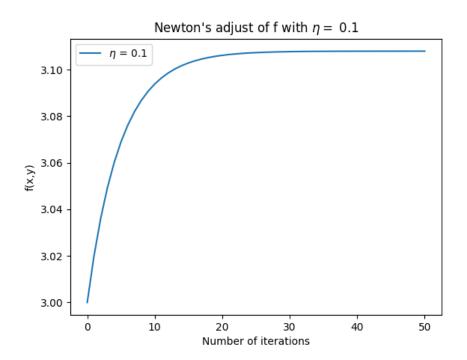
One implementation (really similar to the gradient_descent_trace

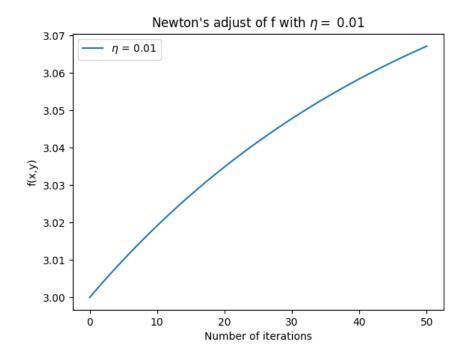
coordenates (x,y)=(-0.9793498427941949, 0.9893767407575305),

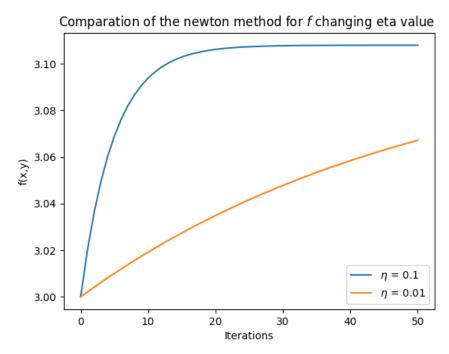
```
def newton_trace(initial_point, fun, grad_fun, hessian, eta, max_iter):
    """ Newton method
    INPUT
    - initial_point:
    - f: differential function
    - grad_fun: Gradient
    - hessian: hessian
    - eta: learning rate
    - max_iter: number of iterations
    OUTPUT
    w trace
    w = initial_point
    w_list = [initial_point]
    iterations = 0
    while iterations < max_iter:
        w = w - \text{eta } *\text{np.linalg.inv(hessian(w[0],w[1])).dot(grad_fun(w[0], w[1]))}
        w_list.append(w)
        iterations += 1
    return np.array(w_list)
   The results after run are
```

the number of iterations: 50 and the image is f(x,y) = 3.0671859515488302

With eta = 0.1, coordenates (x,y)=(-0.9463274028190676, 0.9717082373563009), the number of iterations: 50 and the image is f(x,y)=3.1079767229661335







As we see this method does not minimize the function independently of the learning rate and even worse than the initial point. This is because this algorithm is sensible about where the gradient is zero.

So in this case the algorithm get trapped in a saddle point.

However if the function is convex it would be more precise even though the selection of the learning rating was bigger.

Different initial points

Initial point	Final coordinates	Final value
(-0.5 - 0.5)	(-0.9463274, 0.97170824)	3.10798
(1, 1)	[1.067, 0.911]	11.345
(2.1, -2.1)	(3.261, -3.118)	78.711
(-3, 3)	(-3.0536726, 3.02829176)	3.108
(-2, 2)	(-2, 2)	0

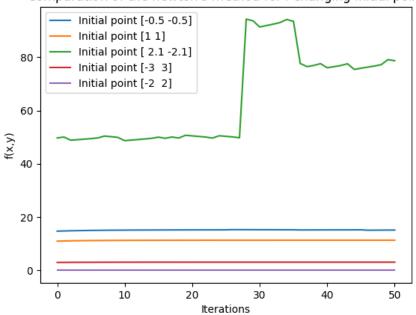
If we compare with the gradient descendant's algorithm

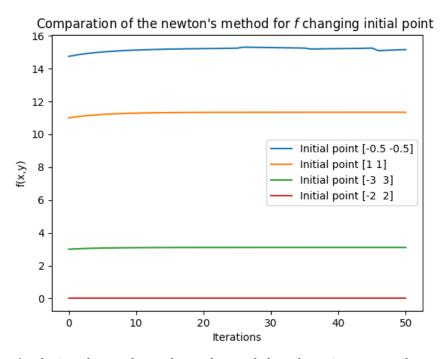
Initial point	Final coordinates	Final value
(-0.5 - 0.5)	(-0.793 -0.126)	9.125
(1 1)	$(0.677 \ 1.29)$	6.437
(2.1 - 2.1)	(0.149 - 0.096)	12.491
$(-3\ 3)$	$(-2.7315\ 2.713)$	-0.381
(-2 2)	(-2. 2.)	0

So apart form the first one and the last point (which is a solution) the Newton's method is worse.

Let's see what is happening by plotting their traces.

Comparation of the newton's method for f changing initial point





Analysing the results we have observed that the points get easily trapped in a point, this may be because this algorithm is sensitive to the hessian. If we compute these points' gradients and hessian we see that:

```
For (-0.38067878, -0.52778221)
The gradient value is [ 1.64133153 -1.67813744]
The inverse hessian is [[-0.00432244 0.01843361]
 [ 0.01843361 -0.00367461]]
For (1.06677195, 0.91078249)
The gradient value is [ 0.03180694 -0.02149455]
The inverse hessian is [[-0.00634209 0.01835718]
 [ 0.01835718 -0.00574093]]
For (3.26077803, -3.11750721)
The gradient value is [ 11.09387996 -11.19723696]
The inverse hessian is [[0.0182662 0.00126589]
 [0.00126589 0.0176255 ]]
For (-2.0, 2.0)
The gradient value is [-6.15574622e-15 6.15574622e-15]
The inverse hessian is [[-0.00064245 0.01268142]
 [ 0.01268142 -0.00032122]]
```

As we thought the hessians of all these points are *close* the null matrix.

Conclusions

This algorithm minimizes correctly the gradient but not the function. Therefore, if a function have saddle points this algorithm would not be as useful as the gradient descendent. Moreover, other problem is that the function should be twice differentiable.

Bibliography

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- [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.

Chapter 4

Appendix

4.1 Code

```
# -*- coding: utf-8 -*-
HHH
TRABAJO 1.
Autor Blanca Cano Camarero
Grupo 2
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D # to display 3d function
np.random.seed(1)
def STOP_EXECUTION_TO_SEE_RESULT():
        input('\n--- End of a section, press any enter to continue ---\n')
print('GRADIENT DESCENDENT\n')
print('Exercise 1\n')
## 1
def gradient_descent(initial_point, loss_function, gradient_function, eta, max_iter, tar
    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
    111
   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
def E(u,v):
   Function to minimize
   return np.float64(
       (u**3 * np.e**(v-2) - 2*v**2 * np.e**(-u))**2
   )
def dEu(u,v):
   111
   Partial derivate of E with respect to the variable u
   return np.float64(
       *(u**3 * np.e**(v-2) - 2*v**2 * np.e**(-u))
       *( 3* u**2 * np.e**(v-2) + 2*v**2 * np.e**(-u))
```

```
)
def dEv(u,v):
    111
    Partial derivate of E with respect to the variable v
   return np.float64(
        *( 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)])
###### conditions
eta = 0.1
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 )
# DISPLAY FIGURE
x = np.linspace(-30, 30, 50)
y = np.linspace(-30, 30, 50)
X, Y = np.meshgrid(x, y)
Z = E(X, Y) \#E_w([X, Y])
fig = plt.figure()
ax = Axes3D(fig)
surf = ax.plot_surface(X, Y, Z, edgecolor='none', rstride=1,
                        cstride=1, cmap='jet')
min_point = np.array([w[0],w[1]])
min_point_ = min_point[:, np.newaxis]
ax.plot(min_point_[0], min_point_[1], E(min_point_[0], min_point_[1]), 'r*', markersize=1
ax.set(title='Ejercicio 1.2. Función sobre la que se calcula el descenso de gradiente')
ax.set_xlabel('u')
```

```
ax.set_ylabel('v')
ax.set_zlabel('E(u,v)')
plt.show()
####### Exercise 1, part 2 answers #####
print('2 a) Function: E(u,v) = (u^3 e^{(v-s)} - 2* v^2 e^{-u})^2'
print('dE_u = 2(u^3 e^{(v-s)} - 2* v^2 e^{-u})(3u^2e^{(v-2)} + 2 v^2 e^{-u}), '
print( 'dE_v = 2(u^3 e^{(v-s)}) - 2* v^2 e^{-u}(u^3 e^{(v-2)}) - 4 v e^{-u}')
print ('So de gradient is: \n nabla E(u,v) = (2(u^3 e^{(v-s)} - 2* v^2 e^{-u}))(3u^2 + u^2)
print ('2b) Numbers of iterations : ', it)
print ('2c) Final coodinates: (', w[0], ', ', w[1],')')
def f(x,y):
   111
   Function to minimize
   return np.float64(
       (x+2)**2 + 2*(y-2)**2 + 2* np.sin( 2* np.pi * x)* np.sin( 2* np.pi * y)
   )
def dfx(x,y):
   Partial derivate of f with respect to the variable x
   return np.float64(
       2*( x+2 ) + 4* np.pi* np.cos( 2* np.pi * x )* np.sin(2* np.pi * y)
   )
def dfy(x,y):
   Partial derivate of f with respect to the variable y
   return np.float64(
       4*(y-2) + 4* np.pi* np.cos(2* np.pi * y)* np.sin(2* np.pi * x)
```

```
4.1. CODE
                                                         55
   )
def gradF(x,y):
      gradient of E
   return np.array([dfx(x,y), dfy(x,y)])
def gradient_descent_trace(initial_point, loss_function, gradient_function, eta, max_ite
   111
   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
    111
   iterations = 0
   error = loss_function( initial_point[0], initial_point[1])
   w = [initial_point]
   while iterations < max_iter:</pre>
       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

```
###### conditions
smaller_eta = 0.01
bigger_eta = 0.1
max_iter = 50
initial_point = np.array([-1.0,1.0])
#### run
smaller_w, smaller_it = gradient_descent_trace( initial_point,f, gradF, smaller_e
bigger_w, bigger_it = gradient_descent_trace(initial_point,f, gradF, bigger_eta_
images_smaller_eta = [f(x[0],x[1]) \text{ for } x \text{ in smaller_w}]
images\_bigger\_eta = [ f(x[0],x[1]) for x in bigger\_w]
print(f'With eta = {smaller_eta}, coordenates (x,y)= {(smaller_w[-1][0],smaller_w
print(f'With eta = {bigger_eta}, coordenates (x,y)={(bigger_w[-1][0],bigger_w[-1]
######## PLOTTING
x_label = 'Number of iterations'
y_{abel} = 'f(x,y)'
bigger_eta_label = '$\eta$ = '+str(bigger_eta)
smaller_eta_label = '$\eta$ = '+str(smaller_eta)
## bigger eta ####
plt.clf()
plt.plot(images_bigger_eta, label=bigger_eta_label)
plt.xlabel(x_label)
plt.ylabel(y_label)
plt.title(f'Gradient descent of f with $\eta =$ {bigger_eta}')
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
## smaller eta ###
plt.plot(images_smaller_eta, label=smaller_eta_label)
plt.xlabel(x_label)
plt.ylabel(y_label)
plt.title(f'Gradient descent of f with $\eta =$ {smaller_eta}')
```

```
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
## comparation ###
plt.clf()
plt.plot(images_bigger_eta, label=r"$\eta$ = 0.1")
plt.plot( images_smaller_eta, label=r"$\eta$ = 0.01")
plt.xlabel('Iterations')
plt.ylabel('f(x,y)')
plt.title("Comparation of the gradient descendent for $f$ changing eta value ")
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
### exta experimental ####
epsilon_eta = 1e-14
max_iter = 50
initial_point = np.array([-1.0,1.0])
epsilon_eta_label = '$\eta$ = '+str(epsilon_eta)
#### run
epsilon_w, epsilon_it = gradient_descent_trace( initial_point,f, gradF, epsilon_eta, max_
images_epsilon_eta = [f(x[0],x[1]) for x in epsilon_w]
print(f'With eta = {epsilon_eta}, coordenates (x,y)={(epsilon_w[-1][0],epsilon_w[-1][1])}
STOP_EXECUTION_TO_SEE_RESULT()
plt.plot(images_epsilon_eta, label=epsilon_eta_label)
plt.xlabel(x_label)
plt.ylabel(y_label)
plt.title(f'Gradient descent of f with $\eta =$ {epsilon_eta}')
```

```
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
## smaller eta and tiny one ###
plt.clf()
plt.plot(images_epsilon_eta, label=epsilon_eta_label)
plt.plot( images_smaller_eta, label=r"$\eta$ = 0.01")
plt.xlabel('Iterations')
plt.ylabel('f(x,y)')
plt.title("Comparation of the gradient descendent for $f$ changing eta value ")
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
#### exercise 3.b
initial_points = map(np.array, [[-.5, -.5],[1, 1], [2.1, -2.1], [-3,3], [-2, 2]]
minimum_value = np.Infinity
print('{:^17} {:^17} {:^9}'.format('Initial', 'Final', 'Value'))
for initial in initial_points:
  w, _ = gradient_descent_trace(initial, f, gradF, 0.01, 50)
  local_minimum = w[-1]
  local_value = f(local_minimum[0], local_minimum[1])
 print('{} {} {: 1.5f}'.format(initial, local_minimum, local_value))
STOP_EXECUTION_TO_SEE_RESULT()
11 11 11
Exercise 2
```

```
Author: Blanca Cano Camarero
def STOP_EXECUTION_TO_SEE_RESULT():
        input('\n--- End of a section, press any enter to continue ---\n')
print('____LINEAR REGRESSION EXERCISE _____\n')
print('Exercise 1')
input('\n Enter to start\n')
label5 = 1
label1 = -1
def readData(file_x, file_y):
        function for read data
        # reads files
        datax = np.load(file_x)
        datay = np.load(file_y)
        y = []
        x = []
        # Solo guardamos los datos cuya clase sea la 1 o la 5
        for i in range(0,datay.size):
                if datay[i] == 5 or datay[i] == 1:
                        if datay[i] == 5:
                                y.append(label5)
                        else:
                                y.append(label1)
                        x.append(np.array([1, datax[i][0], datax[i][1]]))
        x = np.array(x, np.float64)
        y = np.array(y, np.float64)
       return x, y
def Error(x,y,w):
    '''quadratic error
    INPUT
    x: input data matrix
    y: target vector
```

```
w: vector to
    OUTPUT
    quadratic error >= 0
    111
    error_times_n = np.float64(np.linalg.norm(x.dot(w) - y.reshape(-1,1))**2)
    return np.float64(error_times_n/len(x))
def dError(x,y,w):
    ''' gradient
    OUTPUT
    column vector
    111
    return 2/len(x)*(x.T.dot(x.dot(w) - y.reshape(-1,1)))
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
        111
        #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
def sgd_exact_number_iter(x,y, eta = 0.01, max_iter = 1000, batch_size = 32, error = 10**
        Stochastic gradient descent
        INPUT
        x: data set
        y: target vector
        eta: learning rate
        max_iter
        OUTPUT
        w: weight vector
        111
        #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
def pseudoInverseMatrix ( X ):
    INPUT
    X: is a matrix (must be a np.array) to use transpose and dot method
    hat matrix
    111
    \#S = (X \cap TX) \cap \{-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)
# Pseudoinverse
def pseudoInverse(X, Y):
    111
    INPUT
    X is the feature matrix
    Y is the target vector (y_1, \ldots, y_m)
    OUTPUT:
    w: weight vector
    111
    X_pseudo_inverse = pseudoInverseMatrix ( X )
    Y_transposed = Y.reshape(-1, 1)
    w = X_pseudo_inverse.dot( Y_transposed)
    return w
```

```
# Evaluating the autput
def performanceMeasurement(x,y,w):
    '''Evaluating the output binary case
    TNPUT
    X is the feature matrix
    Y is the target vector (y_1, \ldots, y_m)
    OUTPUT:
    w: weight vector
    OUTPUT:
    bad_negative, bad_positives, input_size
    111
    # defference between the sign of the regression and the target vector
    sign_column = np.sign(x.dot(w)) - y.reshape(-1,1)
    bad_positives = 0
   bad_negatives = 0
    for sign in sign_column[:,0]:
        if sign > 0:
                bad_positives += 1
        elif sign < 0 :</pre>
                bad_negatives += 1
    input_size = len(y)
    return bad_negatives, bad_positives, input_size
def evaluationMetrics (x,y,w, label = None):
    '''PRINT THE PERFORMANCE MEASUREMENT
   bad_negatives, bad_positives, input_size = performanceMeasurement(x,y,w)
    accuracy = ( input_size-(bad_negatives +bad_positives))*100 / input_size
    if label :
        print(label)
   print (f'For w^T = \{w.reshape(1,-1)\}')
   print ( 'Input size: ', input_size )
```

```
print( 'Bad negatives :', bad_negatives)
   print( 'Bad positives :', bad_positives)
   print( 'Accuracy rate :', accuracy, '%')
## Draw de result
### scatter plot
def plotResults (x,y,w, title = None):
        label_5 = 1
        label_1 = -1
        labels = (label_5, label_1)
        colors = {label_5: 'b', label_1: 'r'}
        values = {label_5: 'Number 5', label_1: 'Number 1'}
        plt.clf()
        # data set plot
        for number_label in labels:
                index = np.where(y == number_label)
                plt.scatter(x[index, 1], x[index, 2], c=colors[number_label], lab
        # 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
        if title :
                plt.title(title)
        plt.xlabel('Average intensity')
        plt.ylabel('Simmetry')
```

```
plt.legend()
        plt.show()
def plotResultMultiplesLines(x,y,multiple_w, main_title = None, multiples_title = None):
        INPUT
        x featue matrx
        y labels vector
        multiple_w vector of different weight vector
        multiple_titles
        label_5 = 1
        label_1 = -1
        labels = (label_5, label_1)
        colors = {label_5: 'b', label_1: 'r'}
        values = {label_5: 'Number 5', label_1: 'Number 1'}
       plt.clf()
        # data set plot
        for number_label in labels:
                index = np.where(y == number_label)
                plt.scatter(x[index, 1], x[index, 2], c=colors[number_label], label=value
        for i in range(len(multiple_w)):
                w = multiple_w[i]
                title = multiple_title[i]
                # 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'))
```

```
if main_title :
                                         plt.title(main_title)
                    plt.xlabel('Average intensity')
                    plt.ylabel('Simmetry')
                    plt.legend()
                    plt.show()
### _____ DATA _____
# Reading training data set
x, y = readData('datos/X_train.npy', 'datos/y_train.npy')
# Reading test data set
x_test, y_test = readData('datos/X_test.npy', 'datos/y_test.npy')
w_pseudoinverse = pseudoInverse(x, y)
print("\n___ Goodness of the Pseudo-inverse fit ___\n")
print(" Ein: ", Error(x, y, w_pseudoinverse))
print(" Eout: ", Error(x_test, y_test, w_pseudoinverse))
evaluationMetrics (x,y,w_pseudoinverse, '\nEvaluating output training data set')
evaluationMetrics (x_test, y_test, w_pseudoinverse, '\nEvaluating output test data
plotResults(x,y,w_pseudoinverse, title = 'Pseudo-inverse')
print(f'\nThe weight vector is {w_pseudoinverse}')
STOP_EXECUTION_TO_SEE_RESULT()
print("\n__ Goodness of the Stochastic Gradient Descendt (SGD) fit ___\n")
batch_sizes =[1,32,200,len(y)] #batch sizes compared in the experiment
n_{iterations} = [50,300]
for iteration in n_iterations:
                    multiple_w = [w_pseudoinverse]
                    multiple_title = ['pseudo-inverse']
                    for _batch_size in batch_sizes:
                                         w = sgd(x,y, eta = 0.01, max_iter = iteration, batch_size = _batch_size 
                                         _title = f'SGD, batch size {_batch_size}'
                                         print( '\n\t'+_title)
```

```
print ("Ein: ", Error(x,y,w))
                print ("Eout: ", Error(x_test, y_test, w))
                evaluationMetrics (x,y,w, '\nEvaluating output training data set')
                evaluationMetrics (x_test, y_test, w, '\nEvaluating output test data set'
                \#plotResults(x,y,w, title = _title)
                multiple_w.append(w)
                multiple_title.append(_title)
                STOP_EXECUTION_TO_SEE_RESULT()
        plotResultMultiplesLines(x,y,multiple_w,f'Comparative batch sizes, {iteration} it
STOP_EXECUTION_TO_SEE_RESULT()
print ('Exercise 2\n')
#### EXPERIMIENTS #########
## a)
print('\nEXPERIMENT (a) \n')
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))
### data
size_training_example = 1000
dimension = 2
square_half_size = 1
training_sample = simula_unif( size_training_example,
                               dimension,
                               square_half_size)
```

```
STOP_EXECUTION_TO_SEE_RESULT()
plt.clf()
plt.scatter(training_sample[:, 0], training_sample[:, 1], c='b')
plt.title('Muestra de entrenamiento generada por una distribución uniforme')
plt.title('Training sample generated by a uniform distribution')
plt.xlabel('$x_1$ value')
plt.ylabel('$x_2$ value')
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
## b)
print('\nEXPERIMENT (b) \n')
def f(x1, x2):
        return np.sign(
            (x1 -0.2)**2
            x2**2 -0.6
        )
def noisyVector(y, percent_noisy_data):
        y target vector to introduce noise
        size_training_example: number of point generated in each experiment,
        percent\_noisy\_data
        len_y = len(y)
        index = list(range(len_y))
        np.random.shuffle(index)
        size_noisy_data = int((len_y*percent_noisy_data)/ 100 )
        noisy_y = np.copy(y)
        for i in index[:size_noisy_data]:
                noisy_y[i] *= -1
        return noisy_y
#labels
```

```
y = np.array([f(x[0],x[1]) for x in training_sample])
percent_noisy_data = 10.0
y = noisyVector(y, percent_noisy_data)
## draw
labels = (1, -1)
colors = {1: 'blue', -1: 'red'}
plt.clf()
for l in labels:
        index = np.where(y == 1)
        plt.scatter(training_sample[index, 0],
                    training_sample[index,1],
                    c=colors[1],
                    label=str(1))
plt.title('Labelled training sample before noise')
plt.xlabel('$x_1$ value')
plt.ylabel('$x_2$ value')
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
plt.clf()
for l in labels:
        index = np.where(y == 1)
        plt.scatter(training_sample[index, 0],
                    training_sample[index,1],
                    c=colors[1],
                    label=str(1))
plt.title('Labelled training sample after noise')
plt.xlabel('$x_1$ value')
plt.ylabel('$x_2$ value')
plt.legend()
```

```
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
#### C
print('\nEXPERIMENT (c) \n')
eta = 0.01
batch_size = 5
maximum_number_iterations = 1000
x = np.array([
        np.array([ 1, x_n[0], x_n[1] ])
        for x_n in training_sample
])
y = np.array([f(x_n[0],x_n[1]) for x_n in training_sample])
y = noisyVector(y, percent_noisy_data)
w = sgd_exact_number_iter(x, y, eta, maximum_number_iterations, batch_size )
_title = f'SGD, batch size {batch_size}'
print( '\n\t'+_title)
print ("Ein: ", Error(x,y,w))
evaluationMetrics (x,y,w, '\nEvaluating output training data set')
STOP_EXECUTION_TO_SEE_RESULT()
plt.clf()
for l in labels:
        index = np.where(y == 1)
        plt.scatter(training_sample[index, 0],
                    training_sample[index,1],
                    c=colors[1],
                    label=str(1))
plt.title('Linear regression fit')
plt.xlabel('$x_1$ value')
plt.ylabel('$x_2$ value')
```

```
# regression line
\# x_0 = -1
y_0 = (w[1] - w[0]) / w[2]
\#x_1 = 1
y_1 = -(w[1]+w[0])/w[2]
plt.plot([-1, 1], [y_0, y_1], 'k-', label=('SGD regression'))
plt.xlim([-1,1])
plt.ylim([-1,1])
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
## d
print('\n EXPERIMENT (d), lineal regression\n')
def experiment(featureVector,
               number_of_repetitions = 1000,
               size_training_example = 1000,
               percent_noisy_data = 10.0
        111
        INPUT
        featureVector: function that return np.array
        number_of_repetitions: experiment repetitions ,
        size_training_example: number of point generated in each experiment,
        percent_noisy_data:
        OUTPUT
        (error_in, error_out)
        total_in_error = 0
        total_out_error = 0
        for _ in range( number_of_repetitions):
        ## data generation
                training_sample = simula_unif( size_training_example,
                                                dimension,
                                                square_half_size)
                test_sample = simula_unif( size_training_example,
                                            dimension,
                                            square_half_size)
```

 $test_y = np.array([f(x[0],x[1]) for x in test_sample])$

```
test_y = noisyVector(test_y, percent_noisy_data)
                y = np.array([f(x[0],x[1]) for x in training_sample])
                y = noisyVector(y, percent_noisy_data)
                # fit
                x = np.array([
                        featureVector(x_n)
                        for x_n in training_sample
                ])
                x_test = np.array( [
                        featureVector(x_n)
                        for x_n in test_sample
                ])
                w = sgd_exact_number_iter(x, y, eta, maximum_number_iterations, )
                total_in_error += Error(x,y,w)
                total_out_error += Error(x_test, test_y, w)
        error_in = float(total_in_error / number_of_repetitions)
        error_out = float(total_out_error / number_of_repetitions)
       return error_in, error_out
def linearFeatureVector(x_n):
        return np.array([
               1,
               x_n[0],
                x_n[1]
               ])
_number_of_repetitions = 1000
error_in, error_out = experiment( linearFeatureVector,
                                  number_of_repetitions = _number_of_repetitions
                                  size_training_example = 1000,
                                  percent_noisy_data = 10.0
               )
print(f'The mean value of E_in in all {_number_of_repetitions} experiments is: {e
```

```
print(f'The mean value of E_out in all {_number_of_repetitions} experiments is: {error_ou
STOP_EXECUTION_TO_SEE_RESULT()
# e)
print('\nEXPERIMENT (e)\n' )
eta = 0.01
batch\_size = 5
maximum_number_iterations = 1000
def quadraticFeatureVector(x_n):
        I \cdot I \cdot I
        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] )
x = np.array([
        quadraticFeatureVector(x_n)
        for x_n in training_sample
])
y = np.array([f(x[0],x[1]) for x in training_sample])
y = noisyVector(y, percent_noisy_data)
for i in [10, 50, 100, 200, 500, 700, 1000]:
        maximum_number_iterations = i
        w = sgd_exact_number_iter(x, y, eta, maximum_number_iterations , batch_size = 17)
        print('\nFor one experiment:')
        _title = f'SGD, batch size {batch_size}, number iterations {maximum_number_iterat
        print( '\n',_title)
        print ("Ein: ", Error(x,y,w))
        evaluationMetrics (x,y,w, '\nEvaluating output training data set')
print('')
STOP_EXECUTION_TO_SEE_RESULT()
```

```
## plotting
def equation (x,y,w):
        INPUT
        x coordinate
        y coodinate
        w weights vector
        OUTPUT
        Real number, the scalar product of features vector dot weights vector
        return ( w[0,0]
                 + w[1,0] * x
                 + w[2,0] * y
                 + w[3,0] * x * y
                 + w[4,0] * x**2
                + w[5,0] * y**2
PLOTING LINEAR REGRESSION
We are going to plot the (x,y) \in [-1,-1]^2 that their value after
the linear regression for classification is near to 0.
That means that they are in the limit area.
error = 10**(-2.1)
space = np.linspace(-1,1,100)
z = [[ equation(i,j,w) for i in space] for j in space ]
plt.contour(space, space, z, 0, colors=['black'],linewidths=2 )
for l in labels:
        index = np.where(y == 1)
        plt.scatter(training_sample[index, 0],
                    training_sample[index,1],
                    c=colors[1],
```

label=str(1))

```
plt.title('Quadratic regression fit')
plt.xlabel('$x_1$ value')
plt.ylabel('$x_2$ value')
plt.legend( loc = 'lower left')
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
## EXPERIMENT
error_in, error_out = experiment( quadraticFeatureVector,
                                 number_of_repetitions = _number_of_repetitions,
                                 size_training_example = 1000,
                                 percent_noisy_data = 10.0
print(f'The mean value of E_in in all {_number_of_repetitions} experiments is: {error_in}
print(f'The mean value of E_out in all {_number_of_repetitions} experiments is: {error_ou
print('======="')
STOP_EXECUTION_TO_SEE_RESULT()
HHHH
Exercise 3
Author: Blanca Cano Camarero
11 11 11
def f(x,y):
   Function to minimize
   return np.float64(
        (x+2)**2 + 2*(y-2)**2 + 2* np.sin( 2* np.pi * x)* np.sin( 2* np.pi * y)
    )
def dfx(x,y):
    111
   Partial derivate of f with respect to the variable x
   return np.float64(
       2*( x+2 ) + 4* np.pi* np.cos( 2* np.pi * x )* np.sin(2* np.pi * y)
   )
```

```
def dfy(x,y):
    Partial derivate of f with respect to the variable y
    return np.float64(
        4*(y-2) + 4* np.pi* np.cos(2* np.pi* y)* np.sin(2* np.pi* x)
    )
def gradf(x,y):
       gradient of E
    return np.array([dfx(x,y), dfy(x,y)])
def ddfxx(x,y):
    return 2 - 8*np.pi**2*np.sin(2*np.pi*x)*np.sin(2*np.pi*y)
def ddfyy(x,y):
    return 4 - 8*np.pi**2*np.sin(2*np.pi*x)*np.sin(2*np.pi*y)
def ddfxy(x,y):
    return 8*np.pi**2*np.cos(2*np.pi*x)*np.cos(2*np.pi*y)
def hessianf(x, y):
    return np.array([
        ddfxx(x,y),
        ddfxy(x,y),
        ddfxy(x,y),
        ddfyy(x,y),
    ]).reshape((2, 2))
def newton_trace(initial_point, fun, grad_fun, hessian, eta, max_iter):
   """ Newton method
    INPUT
    - initial_point:
    - f: differential function
    - grad_fun: Gradient
    - hessian: hessian
    - eta: learning rate
    - max_iter: number of iterations
```

```
OUTPUT
    w trace
    11 11 11
    w = initial_point
    w_list = [initial_point]
    iterations = 0
    while iterations < max_iter:</pre>
        w = w - \text{eta *np.linalg.inv(hessian(w[0],w[1])).dot(grad_fun(w[0], w[1]))}
        w_list.append(w)
        iterations += 1
    return np.array(w_list)
# Dicrease with the x-axis
## Exercise 1
###### conditions
smaller_eta = 0.01
bigger_eta = 0.1
max_iter = 50
initial_point = np.array([-1.0,1.0])
smaller_w = newton_trace( initial_point,f, gradf, hessianf, smaller_eta, max_iter)
bigger_w = newton_trace( initial_point,f, gradf, hessianf, bigger_eta, max_iter)
images\_smaller\_eta = [ f(x[0],x[1]) for x in smaller\_w ]
images_bigger_eta = [f(x[0],x[1]) \text{ for } x \text{ in bigger_w}]
print(f'With eta = {smaller_eta}, coordenates (x,y)= {(smaller_w[-1][0],smaller_w[-1][1])
print(f'With eta = {bigger_eta}, coordenates (x,y)={(bigger_w[-1][0],bigger_w[-1][1])}, t
######## PLOTTING
x_label = 'Number of iterations'
y_{abel} = 'f(x,y)'
```

```
bigger_eta_label = '$\eta$ = '+str(bigger_eta)
smaller_eta_label = '$\eta$ = '+str(smaller_eta)
## bigger eta ####
plt.clf()
plt.plot(images_bigger_eta, label=bigger_eta_label)
plt.xlabel(x_label)
plt.ylabel(y_label)
plt.title(f"Newton's adjust of f with $\eta =$ {bigger_eta}")
plt.legend()
plt.show()
## smaller eta ###
plt.clf()
plt.plot(images_smaller_eta, label=smaller_eta_label)
plt.xlabel(x_label)
plt.ylabel(y_label)
plt.title(f"Newton's adjust of f with $\eta =$ {smaller_eta}")
plt.legend()
plt.show()
## comparation ###
plt.clf()
plt.plot(images_bigger_eta, label=r"$\eta$ = 0.1")
plt.plot( images_smaller_eta, label=r"$\eta$ = 0.01")
plt.xlabel('Iterations')
plt.ylabel('f(x,y)')
plt.title("Comparation of the newton's method for $f$ changing eta value ")
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
```

```
#### exercise 3.b
eta = 0.1
max_iter = 50
initial_points = map(np.array, [[-.5, -.5],[1, 1], [2.1, -2.1], [-3,3], [-2, 2]])
minimum_value = np.Infinity
plt.clf()
print('{:^17} {:^17} {:^9}'.format('Initial', 'Final', 'Value'))
for initial in initial_points:
 w = newton_trace( initial,f, gradf, hessianf, eta, max_iter)
 local_minimum = w[-1]
  local_value = f(local_minimum[0], local_minimum[1])
  #plot
  images = [f(x[0],x[1]) \text{ for } x \text{ in } w]
 plt.plot(images, label=f'Initial point {initial}')
 print('{} {} {: 1.5f}'.format(initial, local_minimum, local_value))
plt.xlabel('Iterations')
plt.ylabel('f(x,y)')
plt.title("Comparation of the newton's method for $f$ changing initial point ")
plt.legend()
plt.show()
## without the biggest
initial_points = map(np.array, [[-.5, -.5],[1, 1], [-3,3], [-2, 2]])
minimum_value = np.Infinity
plt.clf()
print('{:^17} {:^17} {:^9}'.format('Initial', 'Final', 'Value'))
for initial in initial_points:
 w = newton_trace( initial,f, gradf, hessianf, eta, max_iter)
```

```
local_minimum = w[-1]
  local_value = f(local_minimum[0], local_minimum[1])
  #plot
  images = [f(x[0],x[1]) for x in w]
  plt.plot(images, label=f'Initial point {initial}')
  print('{} {} {: 1.5f}'.format(initial, local_minimum, local_value))
plt.xlabel('Iterations')
plt.ylabel('f(x,y)')
plt.title("Comparation of the newton's method for $f$ changing initial point ")
plt.legend()
plt.show()
STOP_EXECUTION_TO_SEE_RESULT()
# let see gradient values
points = [[-0.38067878, -0.52778221],
           [1.06677195, 0.91078249],
           [ 3.26077803, -3.11750721] ,
           [-2., 2.]]
for x,y in points :
    print(f'For {(x,y)}')
    print(f'\tThe gradient value is {gradf(x,y)}')
    print(f'\tThe inverse hessian is {np.linalg.inv(hessianf(x,y))}\n')
STOP_EXECUTION_TO_SEE_RESULT()
```