9-1. Logistic Regression Scratch

September 17, 2020

0.0.1 Algorithm 1: Logistic Regression

Logistic regression is a binary classification algorithm by simply finding a best fitted line that separates two dataset. In order to squash the output to a value between 0 and 1, logistic regression used a function called logit function (or sigmoid function)

Steps are the followings:

1. Prepare your data
    - add intercept
    - X and y and w in the right shape
        - X (m, n)
        - y (m,)
        - w (n,)
    - train-test split
    - feature scale
    - clean out any missing data
    - (optional) feature engineering
2. Predict and calculate the loss
    - The loss function is the cross entropy defined as

    $$J = -\Sigma_{i=1}^{m} y^{(i)} log(h) + (1 - y^{(i)}) log(1 - h)$$

    where h is defined as the sigmoid function as

    $$h = \frac{1}{1 + e^{-\theta^T x}}$$

3. Calculate the gradient based on the loss
    - The gradient of θ_j is defined as

    $$\frac{\partial J}{\partial \theta_j} = \Sigma_{i=1}^{m} (h^{(i)} - y^{(i)}) x_j$$

    - This can be derived by knowing that

    $$J = y_1 logh + (1 - y_1) lg(1 - h)$$

    $$h = \frac{1}{1 + e^{-g}}$$

    $$g = \theta^T x$$

- Thus, gradient of J in respect to some θ_j is

$$\frac{\partial J}{\partial \theta_j} = \frac{\partial J}{\partial h}\frac{\partial h}{\partial g}\frac{\partial g}{\partial \theta_j}$$

  where

$$\frac{\partial J}{\partial h} = \frac{y_1 - h}{h(1-h)}$$

$$\frac{\partial h}{\partial g} = h(1-h)$$

$$\frac{\partial g}{\partial \theta_j} = x_j$$

- Thus,

$$\frac{\partial J}{\partial \theta_j} = \frac{\partial J}{\partial h}\frac{\partial h}{\partial g}\frac{\partial g}{\partial \theta_j}$$

$$= \frac{y_1 - h}{h(1-h)} * h(1-h) * x_j$$

$$= (y_1 - h)x_j$$

- We can then put negative sign in front to make it negative loglikelihood, thus

$$(h - y_i)x_j$$

4. Update the theta with this update rule

$$\theta_j := \theta_j - \alpha * \frac{\partial J}{\partial \theta_j}$$

   where α is a typical learning rate range between 0 and 1
5. Loop 2-4 until max_iter is reached, or the difference between old loss and new loss are smaller than some predefined threshold tol

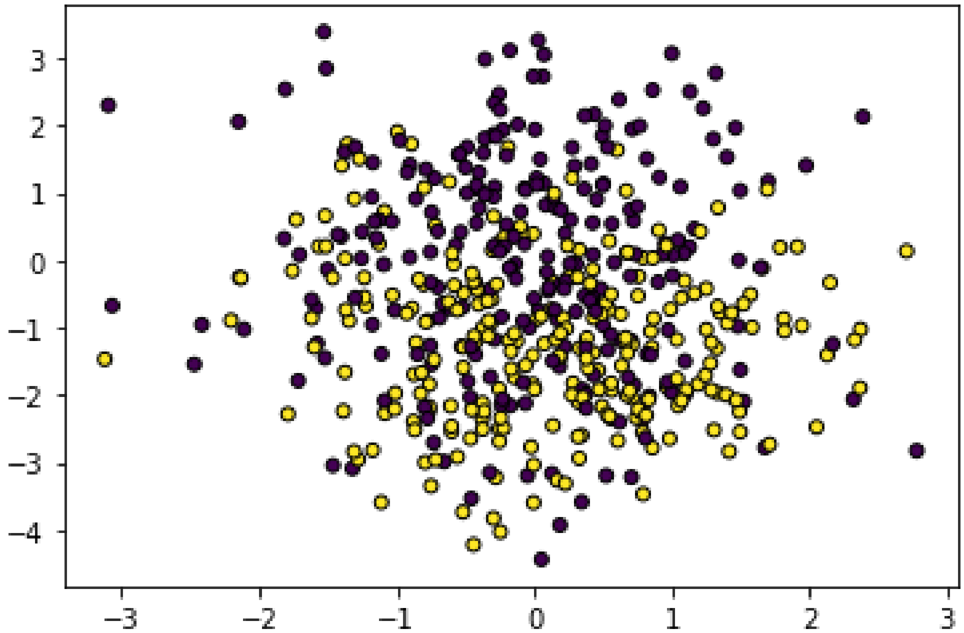
0.0.2 Step 1: Prepare your data

1.1 Get your X and y in the right shape

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn import linear_model

from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split

from sklearn.preprocessing import StandardScaler

#generate quite a lot of noise
#with only 4 informative features out of 10
#with 2 redundant features, overlapping with that 4 informative features
#and 4 noisy features
```

```
#Also, make std wider using n_clusters=2
X, y = make_classification(n_samples=500, n_features=10, n_redundant=2,␣
↪n_informative=4,
                           n_clusters_per_class=2, random_state=14)
plt.scatter(X[:, 0], X[:, 1], marker='o', c=y,
            s=25, edgecolor='k')
```

[1]: <matplotlib.collections.PathCollection at 0x12c71d610>



1.2 Feature scale your data to reach faster convergence

[2]:
```
#feature scaling helps improve reach convergence faster
scaler = StandardScaler()
X = scaler.fit_transform(X)
```

1.3 Train test split your data

[3]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3)
```

1.4 Add intercepts

[4]:
```
intercept = np.ones((X_train.shape[0], 1))
X_train = np.concatenate((intercept, X_train), axis=1)  #add intercept
intercept = np.ones((X_test.shape[0], 1))
X_test = np.concatenate((intercept, X_test), axis=1)  #add intercept
```

0.0.3 Step 2: Fit your algorithm

1. Define your algorithm

[5]:
```
# Your code here

import numpy as np
from sklearn.metrics import average_precision_score, classification_report

#here I use mini-batch as a demonstration
#you are free to use any variants of gradient descent
def mini_batch_GD(X, y, max_iter=1000):
    w = np.zeros(X.shape[1])
    l_rate = 0.01
    #10% of data
    batch_size = int(0.1 * X.shape[0])
    for i in range(max_iter):
        ix = np.random.randint(0, X.shape[0])
        batch_X = X[ix:ix+batch_size]
        batch_y = y[ix:ix+batch_size]
        w = w - l_rate * grad(batch_X, batch_y, w)
    return w, i

def grad(X, y, w):
    m = X.shape[0]
    h = h_theta(X, w)
    error = h - y
    return (1/m) * np.dot(X.T, error)

def sigmoid(x):
    return 1 / (1 + np.exp(-x))

def h_theta(X, w):
    return sigmoid(X @ w)

def output(pred):
    return np.round(pred)

w, i = mini_batch_GD(X_train, y_train, max_iter=5000)
```

2. Compute accuracy

[6]:
```
yhat = output(h_theta(X_test, w))

print("APS: ", average_precision_score(y_test, yhat))
print("Report: ", classification_report(y_test, yhat))
```

```
APS:  0.7927592805204745
Report:                 precision    recall  f1-score   support
```

```
              0       0.77      0.89      0.83        72
              1       0.88      0.76      0.81        78

       accuracy                           0.82       150
      macro avg       0.83      0.82      0.82       150
   weighted avg       0.83      0.82      0.82       150
```

0.0.4 Algorithm 2: Multinomial Logistic Regression

This is logistic regression when number of classes are more than 2.

Steps are the followings:

The gradient descent has the following steps:

1. Prepare your data
   - add intercept
   - X and y in the right shape
     - X (m, n)
     - y (m, k)
     - w (n, k)
   - train-test split
   - feature scale
   - clean out any missing data
   - (optional) feature engineering
2. Predict and calculate the loss
   - The loss function is the cross entropy defined as

     $$-\Sigma_{i=1}^{m} y^{(i)} log(h)$$

     where h is defined as the softmax function as

     $$p(y = j \mid \theta^{(i)}) = \frac{e^{\theta^{(i)}}}{\Sigma_{j=1}^{k} e^{\theta_k^{(i)}}}$$

3. Calculate the gradient based on the loss
   - The gradient is defined as

     $$\frac{\partial J}{\partial \theta_j} = \Sigma_{i=1}^{m} (h^{(i)} - y^{(i)}) x_j$$

   - This gradient can be derived from the following simple examples:
     - Suppose given 2 classes (k = 2) and 3 features (n = 3), we have the loss function as

       $$J = -y_1 log h_1 - y_2 log h_2$$

       where h_1 and h_2 are

       $$h_1 = \frac{\exp(g_1)}{\exp(g_1) + \exp(g_2)}$$

       $$h_2 = \frac{\exp(g_2)}{\exp(g_1) + \exp(g_2)}$$

where g_1 and g_2 are

$$g_1 = w_{11}x_1 + w_{21}x_2 + w_{31}x_3$$

$$g_2 = w_{12}x_1 + w_{22}x_2 + w_{32}x_3$$

- For example, to find the gradient of J in respect to w_{21}, we simply can use the chain rule (or backpropagation) to calculate like this:

$$\frac{\partial J}{\partial w_{21}} = \frac{\partial J}{\partial h_1}\frac{\partial h_1}{\partial g_1}\frac{\partial g_1}{\partial w_{21}} + \frac{\partial J}{\partial h_2}\frac{\partial h_2}{\partial g_1}\frac{\partial g_1}{\partial w_{21}}$$

- If we know each of them, it is easy, where

$$\frac{\partial J}{\partial h_1} = -\frac{y_1}{h_1}$$

$$\frac{\partial J}{\partial h_2} = -\frac{y_2}{h_2}$$

$$\frac{\partial h_1}{\partial g_1} = \frac{\exp(g_1)}{\exp(g_1)+\exp(g_2)} - (\frac{\exp(g_1)}{\exp(g_1)+\exp(g_2)})^2 = h_1(1-h_1)$$

$$\frac{\partial h_2}{\partial g_1} = \frac{-exp(g_2)exp(g_1)}{(\exp(g_1)+\exp(g_2))^2} = -h_2h_1$$

$$\frac{\partial g_1}{\partial w_{21}} = x_2$$

- For those who forgets how to do third and fourth, recall that the quotient rule

$$(\frac{f}{g})' = \frac{f'g - fg'}{g^2}$$

- Putting everything together, we got

$$\frac{\partial J}{\partial w_{21}} = \frac{\partial J}{\partial h_1}\frac{\partial h_1}{\partial g_1}\frac{\partial g_1}{\partial w_{21}} + \frac{\partial J}{\partial h_2}\frac{\partial h_2}{\partial g_1}\frac{\partial g_1}{\partial w_{21}}$$

$$= -\frac{y_1}{h_1} * h_1(1-h_1) * x_2 + -\frac{y_2}{h_2} * -h_2h_1 * x_2$$

$$= x_2(-y_1 + y_1h_1 + y_2h_1)$$

$$= x_2(-y_1 + h_1(y_1+y_2))$$

$$= x_2(h_1 - y_1)$$

4. Update the theta with this update rule

$$\theta_j := \theta_j - \alpha * \frac{\partial J}{\partial \theta_j}$$

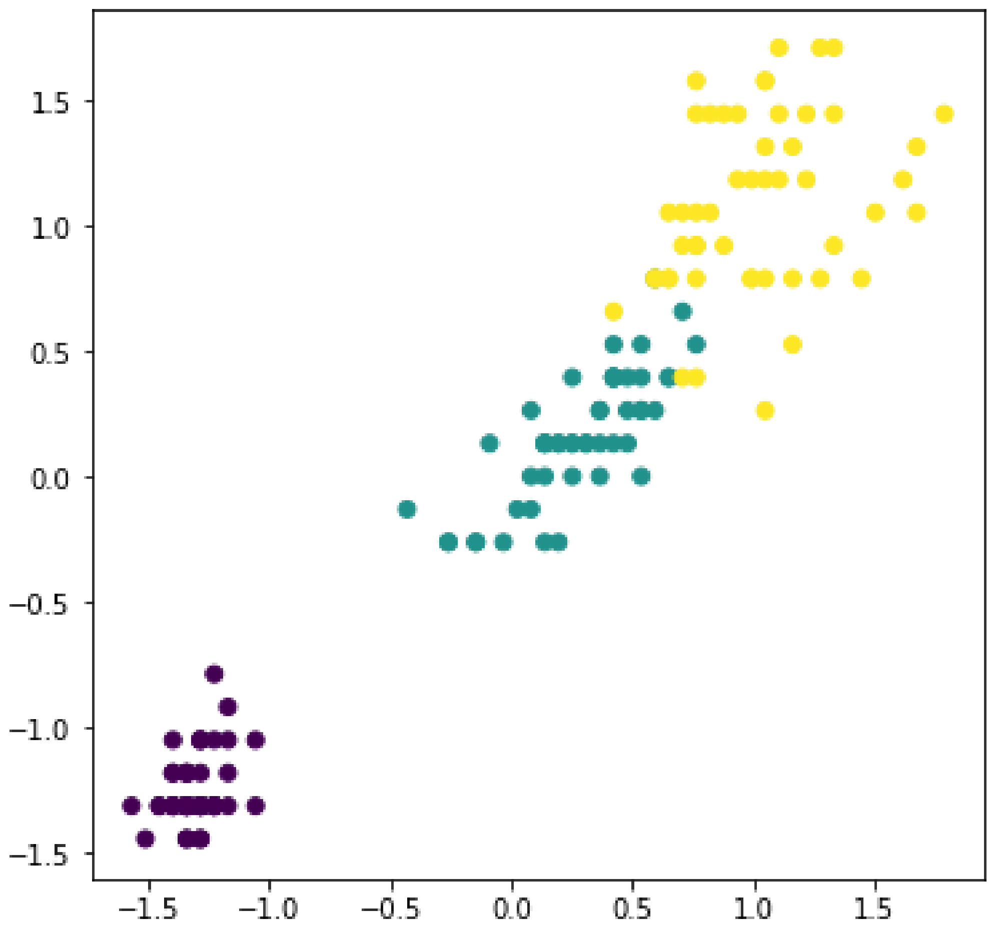
   where α is a typical learning rate range between 0 and 1
5. Loop 2-4 until max_iter is reached, or the difference between old loss and new loss are smaller than some predefined threshold tol

0.0.5 Step 2: Fit your algorithm

1. Define your algorithm

[7]:
```python
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LogisticRegression
from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler

#Step 1: Prepare data

# import some data to play with
iris = datasets.load_iris()
X = iris.data[:, 2:]  # we only take the first two features.
y = iris.target  #now our y is three classes thus require multinomial

#feature scaling helps improve reach convergence faster
scaler = StandardScaler()
X = scaler.fit_transform(X)

#data split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3)

#add intercept to our X
intercept = np.ones((X_train.shape[0], 1))
X_train = np.concatenate((intercept, X_train), axis=1)  #add intercept
intercept = np.ones((X_test.shape[0], 1))
X_test = np.concatenate((intercept, X_test), axis=1)  #add intercept

#make sure our y is in the shape of (n, k)
#we will convert our output vector in
#matrix where no of columns is equal to the no of classes.
#The values in the matrix will be 0 or 1. For instance the rows
#where we have output 2 the column 2 will contain 1 and rest all 0.
#in simple words, y will be of shape (m, k)
k = len(set(y))  #no. of class  (can also use np.unique)
m = X_train.shape[0]  #no.of samples
n = X_train.shape[1]  #no. of features
y_train_encoded = np.zeros((m, k))
for each_class in range(k):
    cond = y_train==each_class
    y_train_encoded[np.where(cond), each_class] = 1
```

[8]:
```python
#Step 1.1 (optional): Visualize our data

#your code here
plt.figure(figsize=(6,6))
plt.scatter(X[:, 0], X[:, 1], label='class 0', c=y)
plt.show()
```



[9]:
```
#Step 2: Fit your data

import numpy as np
from sklearn.metrics import average_precision_score, classification_report
from sklearn.preprocessing import StandardScaler

def logistic_regression_GD(X, y, k, n, max_iter=1000):
    '''
    Inputs:
        X shape: (m, n)
        w shape: (n, k)
    '''
    w = np.random.rand(n, k)
    l_rate = 0.01
    for i in range(max_iter):
        cost, grad =  gradient(X, y, w)
        w = w - l_rate * grad
    return w, i
```

```python
#for those who tend to feel overwhelmed with lots of code
#I recommend you to write each part of the code separately as function
#it helps!
def gradient(X, y, w):
    m = X.shape[0]
    h = h_theta(X, w)
    cost = np.sum(-y * np.log(h) - (1 - y) * np.log(1 - h)) / m
    error = h - y
    grad = softmax_grad(X, error)
    return cost, grad

def softmax(x):
    return np.exp(x) / np.sum(np.exp(x), axis=1, keepdims=True)

def softmax_grad(X, error):
    return  X.T @ error

def h_theta(X, w):
    '''
    Input:
        X shape: (m, n)
        w shape: (n, k)
    Returns:
        yhat shape: (m, k)
    '''
#     print("X@w: ", (X @ w)[:5])
#     print("Softmax: ", softmax(X @ w)[:5])
    return softmax(X @ w)

w, i = logistic_regression_GD(X_train, y_train_encoded, k, X_train.shape[1],␣
↪max_iter=5000)

pred = np.argmax(h_theta(X_test, w), axis=1)

print("Report: ", classification_report(y_test, pred))
```

```
Report:                precision    recall  f1-score   support

           0       1.00      1.00      1.00        16
           1       1.00      0.87      0.93        15
           2       0.88      1.00      0.93        14

    accuracy                           0.96        45
   macro avg       0.96      0.96      0.95        45
weighted avg       0.96      0.96      0.96        45
```

```
[ ]:
```