# Machine Learning: Assignment 3

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## 1 任务描述

- 实现逻辑回归算法
- 通过逻辑回归分类算法对 breast\_cancer 数据集进行预测

## 2 数据描述

- breast\_cancer 数据集一共包含 569 组数据,按照恶性 malignant 和良性 benign 分为两类,分别被标注为 0 和 1,每组数据包含 30 个特征
- 将特征数据和标签数据分别从 sklearn.datasets 中导出到变量 X,y 中
- breast\_cancer 数据集的一些信息如下

```
[1]: from sklearn import datasets
  import numpy as np
  cancer = datasets.load_breast_cancer()
  X = cancer.data
  y = cancer.target
  print('data_size:', len(X))
  print('feature_numbers:', len(X[0]))
  print('target_names:',cancer.target_names)
  print(cancer.DESCR)
```

```
data_size: 569
feature_numbers: 30
target_names: ['malignant' 'benign']
.. _breast_cancer_dataset:
Breast cancer wisconsin (diagnostic) dataset
```

#### \*\*Data Set Characteristics:\*\*

:Number of Instances: 569

:Number of Attributes: 30 numeric, predictive attributes and the class

#### :Attribute Information:

- radius (mean of distances from center to points on the perimeter)
- texture (standard deviation of gray-scale values)
- perimeter
- area
- smoothness (local variation in radius lengths)
- compactness (perimeter^2 / area 1.0)
- concavity (severity of concave portions of the contour)
- concave points (number of concave portions of the contour)
- symmetry
- fractal dimension ("coastline approximation" 1)

The mean, standard error, and "worst" or largest (mean of the three worst/largest values) of these features were computed for each image, resulting in 30 features. For instance, field 0 is Mean Radius, field 10 is Radius SE, field 20 is Worst Radius.

#### - class:

- WDBC-Malignant
- WDBC-Benign

### :Summary Statistics:

	=====	=====
	Min	Max
	=====	=====
radius (mean):	6.981	28.11
texture (mean):	9.71	39.28
perimeter (mean):	43.79	188.5
area (mean):	143.5	2501.0

```
smoothness (mean):
                                     0.053 0.163
compactness (mean):
                                     0.019 0.345
concavity (mean):
                                      0.0
                                            0.427
                                            0.201
concave points (mean):
                                     0.0
symmetry (mean):
                                     0.106 0.304
fractal dimension (mean):
                                     0.05
                                            0.097
radius (standard error):
                                     0.112 2.873
texture (standard error):
                                     0.36
                                            4.885
                                     0.757 21.98
perimeter (standard error):
area (standard error):
                                     6.802 542.2
smoothness (standard error):
                                     0.002 0.031
compactness (standard error):
                                     0.002 0.135
concavity (standard error):
                                      0.0
                                             0.396
concave points (standard error):
                                     0.0
                                             0.053
symmetry (standard error):
                                      0.008 0.079
fractal dimension (standard error):
                                     0.001 0.03
radius (worst):
                                     7.93
                                            36.04
texture (worst):
                                      12.02 49.54
perimeter (worst):
                                      50.41 251.2
area (worst):
                                      185.2 4254.0
                                     0.071 0.223
smoothness (worst):
compactness (worst):
                                     0.027 1.058
concavity (worst):
                                            1.252
                                     0.0
concave points (worst):
                                     0.0
                                            0.291
symmetry (worst):
                                     0.156 0.664
fractal dimension (worst):
                                     0.055 0.208
```

:Missing Attribute Values: None

:Class Distribution: 212 - Malignant, 357 - Benign

:Creator: Dr. William H. Wolberg, W. Nick Street, Olvi L. Mangasarian

:Donor: Nick Street

:Date: November, 1995

This is a copy of UCI ML Breast Cancer Wisconsin (Diagnostic) datasets. https://goo.gl/U2Uwz2

Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image.

Separating plane described above was obtained using Multisurface Method-Tree (MSM-T) [K. P. Bennett, "Decision Tree Construction Via Linear Programming." Proceedings of the 4th Midwest Artificial Intelligence and Cognitive Science Society, pp. 97-101, 1992], a classification method which uses linear programming to construct a decision tree. Relevant features were selected using an exhaustive search in the space of 1-4 features and 1-3 separating planes.

The actual linear program used to obtain the separating plane in the 3-dimensional space is that described in:
[K. P. Bennett and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets", Optimization Methods and Software 1, 1992, 23-34].

This database is also available through the UW CS ftp server:

ftp ftp.cs.wisc.edu
cd math-prog/cpo-dataset/machine-learn/WDBC/

#### .. topic:: References

- W.N. Street, W.H. Wolberg and O.L. Mangasarian. Nuclear feature extraction for breast tumor diagnosis. IS&T/SPIE 1993 International Symposium on Electronic Imaging: Science and Technology, volume 1905, pages 861-870, San Jose, CA, 1993.
- O.L. Mangasarian, W.N. Street and W.H. Wolberg. Breast cancer diagnosis and prognosis via linear programming. Operations Research, 43(4), pages 570-577,

July-August 1995.

- W.H. Wolberg, W.N. Street, and O.L. Mangasarian. Machine learning techniques

to diagnose breast cancer from fine-needle aspirates. Cancer Letters 77 (1994)

163-171.

## 3 数据描述

• 通过观察各个特征的数值大小,可以发现各个特征之间数量级差距较大,故而需要进行归一 化处理

```
[2]: print(X[0])
from sklearn.preprocessing import MinMaxScaler
X = MinMaxScaler().fit_transform(X=X)
X = np.pad(X, ((0,0),(1,0)), 'constant', constant_values=(1)) # 为 X 填充
x_0=1
print(X[0])
```

- - 为对回归结果进行有效评估,将数据分割成训练集和测试集两部分,其中 70% 为训练集,30% 为测试集。

```
[3]: from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, □

→random_state=2021, shuffle=True)
```

print('数据集 size:\n', '训练集', X\_train.shape, y\_train.shape, '\n 测试集', □ →X\_test.shape, y\_test.shape)

数据集 size:

训练集 (398, 31) (398,) 测试集 (171, 31) (171,)

## 4 逻辑回归模型

## 4.1 模型回归概述

LogisticRegression 逻辑回归是一种分类模型,常用于二分类,它假设数据服从伯努利分布。相比于 LinearRegression 引入了 Sigmoid function 以加入非线性因素,从而解决二分类问题 ###模型推导 #### 符号规定  $x_j^{(i)}$  表示数据集第 i 个数据的第 j 个属性取值, $y^{(i)}$  表示数据集第 i 个数据的标签值, $\hat{y}^{(i)}$  表示第 i 组数据的计算预测值。数据集一共有 m 个数据,n 种属性。

矩阵形式表示, 
$$x_i = \begin{bmatrix} 1 & x_1^{(i)} & \cdots & x_n^{(i)} \end{bmatrix}$$
,  $X = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_n^{(1)} \\ 1 & x_1^{(2)} & \cdots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & x_1^{(m)} & \cdots & x_n^{(m)} \end{bmatrix}$ , 参数  $W = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{bmatrix}$ , 数据

集标签为 
$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

#### 4.1.1 模型目标

在二分类问题中,我们只需要一个线性判别函数  $f(x;w)=w^Tx$ ,其中 x,w 分别为增广特征向量和增广权重向量,特征空间  $\mathbb{R}^D$  中所有满足 f(x;w)=0 的点组成一个分割超平面(Hyperplane),称为决策边界(Decision Boundary)或决策平面(Decision Surface)。决策边界将特征空间一分为二,划分成两个区域,每个区域对应一个类别。

也即,对于给定 N 个样本的训练集  $\mathcal{D}=\{(x^{(n)},y^{(n)})\}_{n=1}^N$ ,其中  $y^{(n)}\in\{0,1\}$ ,线性模型试图学习 到参数  $w^*$ ,使得对于每个样本  $(x^{(n)},y^{(n)})$  尽量满足

$$f(x^{(n)}; w^*) > \frac{1}{2}$$
 if  $y^{(n)} = 1 f(x^{(n)}; w^*) < \frac{1}{2}$  if  $y^{(n)} = 0$ 

#### 4.1.2 理论描述

而我们的线性模型是连续的,并不适合这种分类,所以我们需要引入非线性函数  $g:\mathbb{R}^D \to (0,1)$  来 预测类别标签的后验概率 p(y=1|x)

$$p(y = 1|x) = g(f(x; w))$$

其中  $g(\cdot)$  被称为激活函数,其作用是把线性函数的值域从实数区间挤压到了 (0,1) 之间,可以用来表示概率。在 LogisticRegression 中我们使用标准 Logistic 函数作为激活函数,因而标签 y=1 的后验概率为

$$p(y = 1|x) = \sigma(w^T x)$$

$$\triangleq \frac{1}{1 + exp(-w^T x)}$$

变换得到

$$w^{T}x = \ln \frac{p(y=1|x)}{1 - p(y=1|x)}$$
$$= \ln \frac{p(y=1|x)}{p(y=0|x)}$$

### 4.1.3 参数学习

在 LogisticRegression 中我们采用交叉熵作为损失函数,并使用梯度下降法对参数进行优化 > 信息量的大小与信息发生的概率成反比,因而用来表示所有信息量的期望的信息熵在分类问题中十分有效,交叉熵可以衡量同一个随机变量中两个不同概率分布的差异程度,在机器学习中就表示为概率分布与预测概率分布之间的差异。

#### @ref 交叉熵损失函数原理详解

给定 N 个训练样本  $\{(x^{(n)},y^{(n)})\}_{n=1}^N$ ,用 LogisticRegression 模型对每个样本  $x^{(n)}$  进行预测,输出其标签为 1 的后验概率,记为  $\hat{y}^{(n)}$ 

$$\hat{y}^{(n)} = \sigma(w^T x^{(n)}), \qquad 1 \le n \le N$$

由于  $y^{(n)} \in \{0,1\}$ , 样本  $(x^{(n)},y^{(n)})$  的真实条件概率可以表示为

$$p_r(y^{(n)} = 1|x^{(n)}) = y^{(n)}p_r(y^{(n)} = 0|x^{(n)}) = 1 - y^{(n)}$$

使用交叉熵损失函数, 其风险函数为

$$\mathcal{R}(w) = -\frac{1}{N} \sum_{n=1}^{N} \left( p_r(y^{(n)} = 1 | x^{(n)}) \log \hat{y}^{(n)} + p_r(y^{(n)} = 0 | x^{(n)}) \log(1 - \hat{y}^{(n)}) \right)$$
$$= -\frac{1}{N} \sum_{n=1}^{N} \left( y^{(n)} \log \hat{y}^{(n)} + (1 - y^{(n)}) \log(1 - \hat{y}^{(n)}) \right)$$

其关于参数 w 的偏导数为

$$\begin{split} \frac{\partial \mathcal{R}(w)}{\partial w} &= -\frac{1}{N} \sum_{n=1}^{N} \left( y^{(n)} \frac{\hat{y}^{(n)} (1 - \hat{y}^{(n)})}{\hat{y}^{(n)}} x^{(n)} - (1 - y^{(n)}) \frac{\hat{y}^{(n)} (1 - \hat{y}^{(n)})}{1 - \hat{y}^{(n)}} x^{(n)} \right) \\ &= -\frac{1}{N} \sum_{n=1}^{N} \left( y^{(n)} (1 - \hat{y}^{(n)}) x^{(n)} - (1 - y^{(n)}) \hat{y}^{(n)} x^{(n)} \right) \\ &= -\frac{1}{N} \sum_{n=1}^{N} x^{(n)} (y^{(n)} - \hat{y}^{(n)}) \end{split}$$

采用梯度下降法,LogisticRegression 的训练过程为: 初始化  $w \leftarrow 0$ ,然后通过下式来迭代更新参数:

$$w_{t+1} \leftarrow w_t + \alpha \frac{1}{N} \sum_{n=1}^{N} x^{(n)} (y^{(n)} - \hat{y}_{w_t}^{(n)})$$

其中  $\alpha$  为学习率, $\hat{y}_{w_t}^{(n)}$  为当参数为  $w_t$  时,LogisticRegression 模型的输出

## 4.2 模型实现

### 4.2.1 超参类

```
[4]:

class Hyperameters():

def __init__(self, feature_dimension, data_size, alpha=0.99,

max_epoch=1000, eps=0.0001):

self.feature_dimension = feature_dimension

self.data_size = data_size

self.alpha = alpha

self.max_epoch = max_epoch

self.eps = eps

def toString(self):

return str.format("feature_dimension:{0}, data_size:{1}\nalpha:{3},

→max_epoch:{4}", self.feature_dimension, self.data_size, self.alpha, self.

→max_epoch)
```

#### 4.2.2 逻辑回归类

```
[5]: class LogisticRegression():
    def __init__(self, hp):
        """Initialize variable matrix W
Args:
```

```
hp (Hyperameter)
       11 11 11
       self.hp = hp
       self.W = np.zeros((self.hp.feature_dimension, ))
       return
   def cal_loss(self, X, y):
       """calculate the loss function using input matrix X and vector y
       Args:
           X (numpy.array((sample_number, feature_dimension))): matrix X
           y (numpy.array((feature_dimension, ))): vector y
       Returns:
           [float]: the loss of the training data
           [numpy.array]: delta W
       .....
       m = X.shape[0]
       y_hat = self.predict(X)
       loss = np.sum((y*np.log(y_hat)+(1-y)*np.log(1-y_hat)))
       loss = - loss / m
       dw = - np.dot(X.T, (y - y_hat)) / m
       return loss, dw
   def train(self, X, y, loss_print=False, early_termination=True):
       """Use input matrix X and vector y to train the model.
       Args:
           X (numpy.array((sample_number, feature_dimension))): matrix X
           y (numpy.array((feature_dimension, ))): vector y
           learning_rate (float, optional): learning rate(may also called ⊔
\hookrightarrow alpha). Defaults to 0.99.
           iteration (int, optional): Number of iterations. Defaults to 1000.
           loss_print (bool, optional): True if want to print the loss.
\hookrightarrow Defaults to False.
```

```
11 11 11
       loss, dw = 0, 0
       history = []
       epoch_count = 0
       pre_loss = 0
       for _ in range(self.hp.max_epoch):
           epoch_count += 1
           pre_loss = loss
           loss, dw = self.cal_loss(X, y)
           self.W = self.W - self.hp.alpha * dw
           history.append(loss)
           if early_termination and np.abs(pre_loss - loss) < self.hp.eps:</pre>
               break
       if loss_print:
           import matplotlib.pyplot as plt
           plt.plot(range(epoch_count+1)[1:], history)
           plt.xlabel('iteration')
           plt.ylabel('loss')
           plt.show()
       return history, epoch_count
   def predict(self, X):
       """Use variable matrix W to predict the label result
       Args:
           X (numpy.array((test_sample, feature_dimension))): the input matrix\Box
\hookrightarrow X
       Returns:
            [float]: the prediction of the label result.
       return 1/(1 + np.exp(-X.dot(self.W)))
```

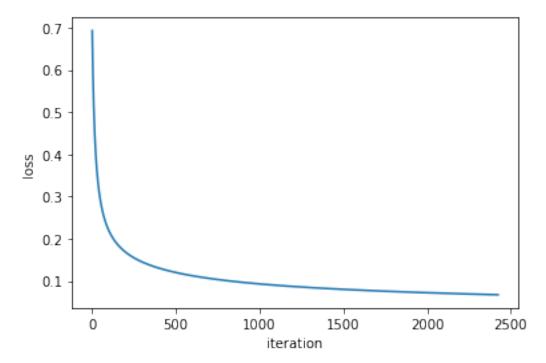
## 4.3 模型结果

利用训练出的模型对测试集中的数据进行预测,若预测值超过 0.5 则认为为标签 1,否则为标签 0,根据预测正确的数量比上总测试数据数量得到正确率。分别用分割训练集和 kFold 算法方式进行检验。

```
[6]: def score(test_result, y_test):
         counter = 0
         acc = 0
         for (pred_label, true_label) in zip(test_result, y_test):
             counter += 1
             if pred_label == true_label:
                 acc += 1
         return acc/counter
     from sklearn.model_selection import KFold
     def score_with_kfold(X, y, model):
         kf = KFold(n splits=10, shuffle=True, random state=2021)
         scores = []
         for train_index, test_index in kf.split(X):
             X_train = X[train_index]
            y_train = y[train_index]
             X_test = X[test_index]
             y_test = y[test_index]
             model.train(X_train, y_train)
             test_result = model.predict(X_test).round()
             scores.append(score(test_result, y_test))
         return np.mean(scores)
    hp = Hyperameters(X_train.shape[1], X_test.shape[0], alpha=0.9,__
     →max_epoch=10000, eps=0.00001)
     lr = LogisticRegression(hp)
     _, epoch_count = lr.train(X_train, y_train, loss_print=True)
     test_result = lr.predict(X_test).round()
     print('Logistic regression with %d iterations test score: %.4f' % (epoch_count,_
     ⇔score(test_result, y_test)))
    kfold_lr = LogisticRegression(hp)
```

```
print('Logistic regression with kFold algorithm get score: %.4f' %⊔

⇒score_with_kfold(X, y, kfold_lr))
```



Logistic regression with 2424 iterations test score: 0.9649 Logistic regression with kFold algorithm get score: 0.9842

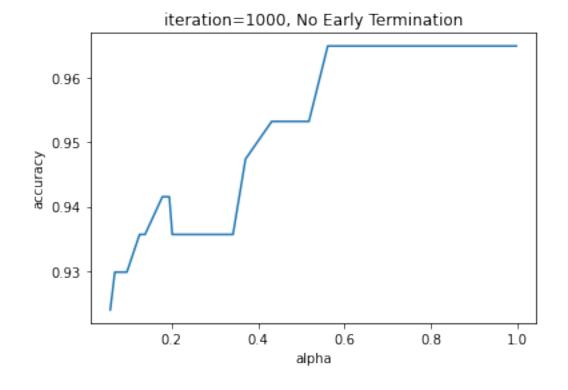
## 4.4 模型调参

接下来我们通过调参比较正确率的方式找到合适的超参

```
_, epoch_count = lr.train(X_train, y_train, loss_print=False,__
→early_termination=False)

test_result = lr.predict(X_test).round()
scores.append(score(test_result, y_test))

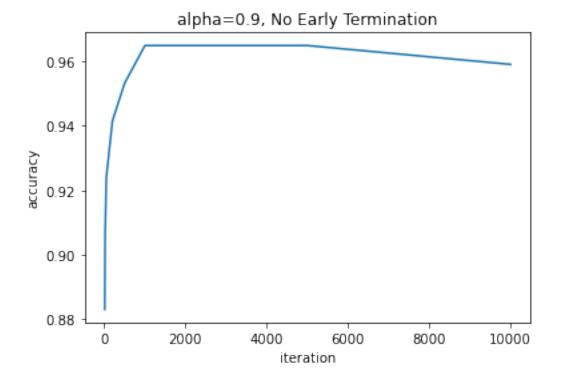
# print('Logistic regression with %d iterations using learning rate %.4fu
→gets test score: %.4f' % (epoch_count, alpha, score(test_result, y_test)))
```



由此可以看到应让学习率为接近1的值,在之后的讨论中会使用0.9的学习率。接下来再考察不同 迭代次数的影响,此处会禁用提前终止。

```
[9]: hp_list = []
scores = []
epoch_list = [10, 20, 50, 100, 200, 500, 1000, 2000, 5000, 10000]
for item in epoch_list:
    hp_list.append(Hyperameters(X_train.shape[1], X_test.shape[0], alpha=0.9, \( \)
    \times max_epoch=item))
for epoch, item in zip(epoch_list, hp_list):
    lr = LogisticRegression(item)
    _, epoch_count = lr.train(X_train, y_train, loss_print=False, \( \)
    \times early_termination=False)
    test_result = lr.predict(X_test).round()
    scores.append(score(test_result, y_test))
```

```
[10]: plt.xlabel('iteration')
   plt.ylabel('accuracy')
   plt.title('alpha=0.9, No Early Termination')
   plt.plot(epoch_list, scores)
   plt.show()
```



由此可以看出迭代次数在 2000-6000 时有较好的效果, 迭代次数太多也并不好, 可能会出现过拟合而导致准确率下降。

## 4.5 模型优化

与 LinearRegression 类似,LogisticRegression 也可以通过引入 L1,L2 正则化进行优化,从而降低过拟合的概率,使得结果更可信。#### L1 正则化实现

```
[11]: class LogisticRegressionL1(LogisticRegression):
    def __init__(self, hp, lambdaI):
        super().__init__(hp)
        self.lambdaI = lambdaI

    def cal_loss(self, X, y):
        loss, dw = super().cal_loss(X, y)
        l = self.lambdaI
        w = self.W
        loss += 1 * np.sum(np.power(w, 2))
        dw += 2 * 1 * w
        return loss, dw
```

### 4.5.1 L2 正则化实现

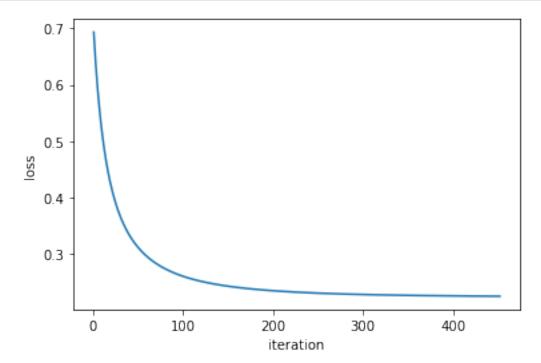
```
class LogisticRegressionL2(LogisticRegression):
    def __init__(self, hp, lambdaI):
        super().__init__(hp)
        self.lambdaI = lambdaI

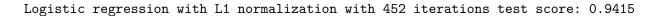
    def cal_loss(self, X, y):
        loss, dw = super().cal_loss(X, y)
        l = self.lambdaI
        w = self.W
        dw += l*(len(w)-len(w[w < 0]))
        return loss, dw</pre>
```

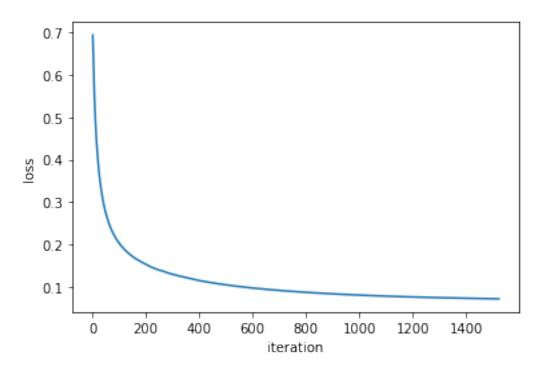
#### 4.5.2 优化结果

```
[13]: hp = Hyperameters(X_train.shape[1], X_test.shape[0], alpha=0.9,__
      →max_epoch=10000, eps=0.00001)
      lr 11 = LogisticRegressionL1(hp, lambdaI=0.001)
      lr_12 = LogisticRegressionL2(hp, lambdaI=0.001)
      _, epoch_count = lr_l1.train(X_train, y_train, loss_print=True)
      test_result = lr_l1.predict(X_test).round()
      print('Logistic regression with L1 normalization with %d iterations test score:
      →%.4f' % (epoch_count, score(test_result, y_test)))
      _, epoch_count = lr_l2.train(X_train, y_train, loss_print=True)
      test_result = lr_l2.predict(X_test).round()
      print('Logistic regression with L2 normalization with %d iterations test score:
      →%.4f' % (epoch_count, score(test_result, y_test)))
      kfold_lr_l1 = LogisticRegressionL1(hp, lambdaI=0.001)
      print('Logistic regression with L1 normalization with kFold algorithm get score:
      → %.4f' % score_with_kfold(X, y, kfold_lr_l1))
     kfold lr 12 = LogisticRegressionL2(hp, lambdaI=0.001)
      print('Logistic regression with L2 normalization with kFold algorithm get score:

→ %.4f' % score_with_kfold(X, y, kfold_lr_12))
```







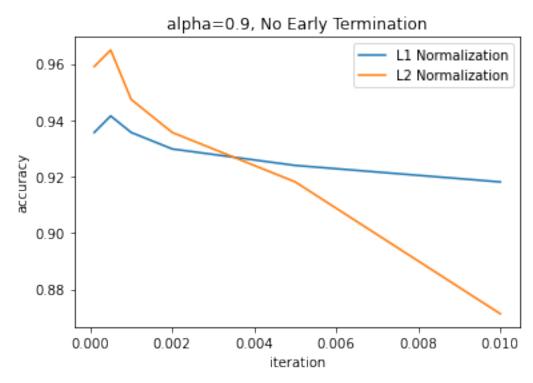
Logistic regression with L2 normalization with 1522 iterations test score: 0.9649

Logistic regression with L1 normalization with kFold algorithm get score: 0.9596 Logistic regression with L2 normalization with kFold algorithm get score: 0.9666

```
[14]: lambda_list = [0.01, 0.005, 0.002, 0.001, 0.0005, 0.0001]
scores_l1 = []
scores_l2 = []
hp = Hyperameters(X_train.shape[1], X_test.shape[0], alpha=0.9, max_epoch=10000)
for item in lambda_list:
    lr_l1 = LogisticRegressionL1(hp, item)
    lr_l2 = LogisticRegressionL2(hp, item)
    _, epoch_count_l1 = lr_l1.train(X_train, y_train, loss_print=False,u
early_termination=True)
    _, epoch_count_l2 = lr_l2.train(X_train, y_train, loss_print=False,u
early_termination=True)
```

```
test_result = lr_l1.predict(X_test).round()
scores_l1.append(score(test_result, y_test))
test_result = lr_l2.predict(X_test).round()
scores_l2.append(score(test_result, y_test))

plt.xlabel('iteration')
plt.ylabel('accuracy')
plt.title('alpha=0.9, No Early Termination')
plt.plot(lambda_list, scores_l1, label='L1 Normalization')
plt.plot(lambda_list, scores_l2, label='L2 Normalization')
plt.legend()
plt.show()
```



可以看出,在加入正则化后,模型经过更少的迭代次数即可达到较稳定的 1oss 值,这表明模型更加稳定了。并且加入两种正则化后仍保持了极高的准确率,在学习率很小时 L2 正则化的准确率略高于 L1 正则化。

## 5 总结

通过训练逻辑回归模型,对 breast\_cancer 数据集进行了性能优秀的二分类。通过为防止过拟合问题,采用了归一化的方式进行数据预处理,引入 L1,L2 正则化以使模型更稳定,通过提前终止的方式提前结束迭代防止过拟合。并通过控制变量考察了各个超参的最佳选取范围。最终分类的准确率达到 0.96 左右。