Machine_learning_classification

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1 Machine Learning

Author: Jessica Cervi Expected time = 2.5 hours Total points = 80 points

1.1 Assignment Overview

In this assignment, we will begin considering the second category of supervised learning problems from our machine learning lectures -- classification problems. Specifically, we will use Scikit-Learn to implement and evaluate classification models on the MNIST handwritten digit dataset. This is to serve as a reminder and expansion of some earlier work. Later, you will explore how to apply these machine learning ideas to graphs.

This assignment is designed to build your familiarity and comfort coding in Python while also helping you review key topics from each module. As you progress through the assignment, answers will get increasingly complex. It is important that you adopt a data scientist's mindset when completing this assignment. Remember to run your code from each cell before submitting your assignment. Running your code beforehand will notify you of errors and give you a chance to fix your errors before submitting. You should view your Vocareum submission as if you are delivering a final project to your manager or client.

Vocareum Tips - Do not add arguments or options to functions unless you are specifically asked to. This will cause an error in Vocareum. - Do not use a library unless you are expicitly asked to in the question. - You can download the Grading Report after submitting the assignment. This will include feedback and hints on incorrect questions.

1.1.1 Learning Objectives

- Understand the main concepts behind classification problems
- Understand the difference between training and testing sets
- Understand dummy variables and dummy classifiers
- Measure the perormance of a classifier using the accuracy score or the confusion matrix
- Use the implementation of Logistic Regression in sklearn
- Use the decision tree classifier in sklearn

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1.3 Machine Learning

In this assignment, we will work with different dataset to understand and consolidate some of main concept behind an important class of machine learning algorithms: classification problems.

We will begin by splitting our data into a **training** and into a **testing** sets: the testing subset is for building your model. The testing subset is for using the model on unknown data to evaluate the performance of the model. Next, we learn how to use a dummy classifier. A **dummy classifier** is a type of classifier which does not generate any insight about the data and classifies the given data using only simple rules. The classifier's behavior is completely independent of the training data as the trends in the training data are completely ignored and instead uses one of the strategies to predict the class label. It is used only as a simple baseline for the other classifiers i.e. any other classifier is expected to perform better on the given dataset. Next, we will learn how to measure the accuracy of a classifier using two different metrics: the **accuracy score** and the **confusion matrix**. Finally, we will guide you through the usage of an important classifier implemented in the sk-learn library: Logistic Regression.

As usual, we will begin by importing the librarries that we will be needing for this module

```
In [90]: %matplotlib inline
    # Our standard data imports
    import pandas as pd
    import numpy as np
    import networkx as nx
    import matplotlib.pyplot as plt
    import seaborn as sns
    from sklearn.model_selection import train_test_split
    #this is used to grade the assignment
    import numpy.testing as npt
    import pandas.testing as pdt

#hide warnings
    import warnings
    warnings.filterwarnings('ignore')
```

In this assignment, we will work with a dataset from the library sklearn. The digit dataset dataset is made up of 1,797 8x8 images. Each image is an hand-written digit. In order to utilize an 8x8 figure like this, we'd have to first transform it into a feature vector with length 64.

You can find more information about the dataset here or by running the code cell below.

This is a copy of the test set of the UCI ML hand-written digits datasets https://archive.ics.uci.edu/ml/datasets/Optical+Recognition+of+Handwritten+Digits

The data set contains images of hand-written digits: 10 classes where each class refers to a digit.

Preprocessing programs made available by NIST were used to extract normalized bitmaps of handwritten digits from a preprinted form. From a total of 43 people, 30 contributed to the training set and different 13 to the test set. 32x32 bitmaps are divided into nonoverlapping blocks of 4x4 and the number of on pixels are counted in each block. This generates an input matrix of 8x8 where each element is an integer in the range 0..16. This reduces dimensionality and gives invariance to small distortions.

For info on NIST preprocessing routines, see M. D. Garris, J. L. Blue, G. T. Candela, D. L. Dimmick, J. Geist, P. J. Grother, S. A. Janet, and C. L. Wilson, NIST Form-Based Handprint Recognition System, NISTIR 5469, 1994.

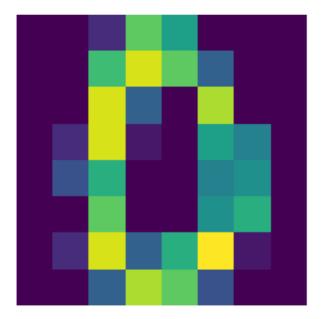
```
.. topic:: References
```

- C. Kaynak (1995) Methods of Combining Multiple Classifiers and Their Applications to Handwritten Digit Recognition, MSc Thesis, Institute of Graduate Studies in Science and Engineering, Bogazici University.
- E. Alpaydin, C. Kaynak (1998) Cascading Classifiers, Kybernetika.
- Ken Tang and Ponnuthurai N. Suganthan and Xi Yao and A. Kai Qin.
 Linear dimensionalityreduction using relevance weighted LDA. School of
 Electrical and Electronic Engineering Nanyang Technological University.
 2005
- Claudio Gentile. A New Approximate Maximal Margin Classification Algorithm. NIPS. 2000.

```
Input data shape: (1797, 64) Target data shape: (1797,)
```

To get a better feel of what the input data is, let's extract a row of 64 numbers, reshape it into an 8×8 array, and examine the resulting matrix by printing the numeric values & by plotting it as an image.

```
In [4]: k = 130
       im = X[k].reshape(8, 8)
       print(im)
       plt.imshow(im)
       plt.axis('off')
       print('y_{{}} = {}'.format(k, y[k]))
[[ 0. 0. 2. 12. 9. 0.
                             0.]
                         0.
ΓΟ.
      0. 11. 15. 12. 5.
                         0.
                             0.1
[ 0. 0. 15. 5. 0. 14.
                             0.1
[ 0. 2. 15.
                 0.
              1.
                     9.
[ 0. 4. 10. 0.
                 0. 7. 8. 0.]
[ 0. 0. 12. 0. 0. 8. 10.
                            0.1
[ 0. 2. 15. 5. 10. 16.
                         1. 0.]
[ 0. 0. 5. 14. 12. 4.
                        0. 0.]]
y_130 = 0
```



Apparently, row 130 of the matrix X (remember, indexed from zero, this is the 131st row from the top), when reshaped, yields the image above. The corresponding entry of the target vector y is 0 which means that this image is intended to represent the numeral 0. Whether this is obvious depends on the handwriting of the original author.

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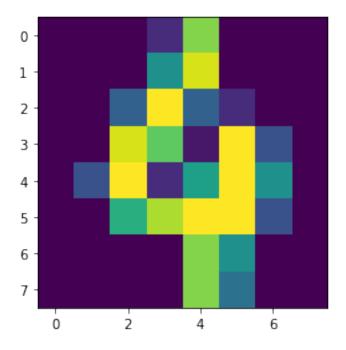
1.3.1 **Question 1**:

5 points

Plot the image from row 100 of the matrix X. What numeral does this image represent? Assign your response as an integer to the identifier ans_1.

In [5]: ### GRADED

```
k = 100
y = digits.target
### YOUR SOLUTION HERE
ans_1 = 4
#print(y[100])
###
### YOUR CODE HERE
###
image_digit = X[k].reshape(8, 8)
plt.imshow(image_digit)
plt.show()
print('This is an image of the digit {}.'.format(ans_1))
```



This is an image of the digit 4.

```
In [6]: ###
     ### AUTOGRADER TEST - DO NOT REMOVE
     ###
```

1.4 Target Variables

In classification problems, the labels (or targets) are *discrete* or *categorical* values (by contrast with regression problems). That being the case, we generally prefer the labeled data to be *balanced*; that is, we prefer having a uniform distribution of labels from which to build our models. For a binary classification problem (i.e., one with two classes), that would mean 50% of the data is from one class and 50% of the data from the other class. For a classification problem with k classes, that would mean each class is represented in $(100 \div k)\%$ of the data.

Examining the target vector y for the MNIST digits data, it appears that each numeral from the sequence 0 through 9 occurs in a random sequence:

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1.4.1 Question 2:

5 points

Your task here is to summarize how often each digit from 0 through 9 occurs in the vector y. The result be a Pandas Series with the integers 0 though 9 as the index (sorted in increasing order) and the corresponding counts as the data. Assign the result to the identifier digit_counts.

(Hint: the Pandas Series method value_counts can do this easily, as can the Numpy function unique).

```
In [8]: ### GRADED
        ### YOUR SOLUTION HERE
        digit_counts = pd.value_counts(y, sort=False)
        ### YOUR CODE HERE
        ###
        print(digit_counts)
0
     178
     182
1
2
     177
3
     183
4
     181
5
     182
6
     181
7
     179
8
     174
9
     180
dtype: int64
In [9]: ###
        ### AUTOGRADER TEST - DO NOT REMOVE
        ###
```

1.5 Train/Test Split

From question 2, it seems the MNIST digits data set is fairly balanced. Each of the 10 possible digits occurs roughly 180 times. As with regression problems, we want to divide the data into training and testing sets. The easiest way to do so is using the function train_test_split from the Scikit-Learn submodule sklearn.model_selection (you can consult the documentation to learn how to customize the behavior of this function).

```
In [10]: X_train, X_test, y_train, y_test = train_test_split(X, y, random_state = 42)
Section 1.2
```

1.5.1 **Question 3:**

5 points

Your task here is to create a Pandas DataFrame with the digits from 0 through 9 in ascending order as the index and with two columns: train_counts and test_counts. The entries of each row, then, are the number of occurrences of that digit in the training target y_train and the testing target y_test respectively. Bind the DataFrame to the identifier split_digit_counts.

```
In [11]: ### GRADED
         ### YOUR SOLUTION HERE
         bro = {'train_counts': pd.value_counts(y_train, sort=False),
                  'test_counts': pd.value_counts(y_test, sort=False)
         split_digit_counts = pd.DataFrame(bro)
         ###
         ### YOUR CODE HERE
         ###
         split_digit_counts
Out[11]:
            train_counts
                           test_counts
                      135
                                     43
         1
                      145
                                     37
         2
                      139
                                     38
         3
                      137
                                     46
                                     55
         4
                      126
         5
                      123
                                     59
         6
                      136
                                     45
         7
                                     41
                      138
         8
                      136
                                     38
         9
                      132
                                     48
In [12]: ###
         ### AUTOGRADER TEST - DO NOT REMOVE
         ###
```

1.6 Binary classification

To begin, we will turn this into a binary classification problem. We'll focus specifically on identifying all the occurrences of the digit 9. For this simpler binary classification problem, we need to change every value in the vector y to 1 or 0 according to whether it is 9 or not. That is, replace every occurrence of 9 in the vector y with the value 1 and replace all the other values with 0. This process is called *binarization*.

Section 1.2

1.6.1 Question 4:

5 points

Your task here is to create three new arrays: y_bin, y_bin_train, and y_bin_test. These will be binary vectors with 1s replacing 9s in y, y_train, and y_test respectively. All other entries will be replaced by 0s.

(Hint: The Numpy function where is very useful in this context).

```
In [13]: ### GRADED

### YOUR SOLUTION HERE

y_bin = np.where(y < 9, 0,(np.where(y == 9, 1,y)))
y_bin_train = np.where(y_train < 9, 0,(np.where(y_train == 9, 1,y_train)))
y_bin_test = np.where(y_test < 9, 0,(np.where(y_test == 9, 1,y_test)))

###

### YOUR CODE HERE
###

In [14]: ###

### AUTOGRADER TEST - DO NOT REMOVE
###</pre>
```

1.6.2 DummyClassifier

To begin, we'll apply the built-in <code>DummyClassifier</code> class from <code>sklearn.dummy</code> to set a baseline for performance of our future models. This classifier does not actually use the feature matrix <code>X</code>. Classification decisions are made using the target vector <code>y</code> only. There are a few permissible strategies, but we'll start with the <code>'most_frequent'</code> strategy. That is, the <code>predict</code> method always returns the majority class. For our binary digit classification problem, this would be <code>0</code> (because the <code>1</code> classification is reserved for <code>9s</code> and most of the digits are not <code>9s</code>).

Having applied the fit method to the training data, we can use the predict method to see how this estimator classifies the data. Unsurprisingly, it returns a vector of all 0s (because that is the majority class for this data).

We can compute the fraction of correct classifications using the method score with the test data:

The fraction of correct classifications is: 0.89333333333333333

Using dummy.score is equivalent to explicitly comparing the entries of y_bin_pred to y_bin_test, counting the number of correct classifications, and dividing by the number of classifications in total.

For classification problems, a *confusion matrix* is a more detailed description of the accuracy of a classifier. It contains entries for the actual values as rows and predicted values as columns. This means we have:

	predicted 0	predicted 1	
	predicted 0	predicted 1	
actual 0	true negative	false positive	
actual 1	false negative	true positive	

In *Scikit-Learn*, the confusion_matrix function takes as arguments the actual labels followed by the predicted labels (labeled in ascending order according to the class labels). From the documentation:

```
sklearn.metrics.confusion_matrix(y_true, y_pred, labels=None,
sample_weight=None)
```

Compute a confusion matrix to evaluate the accuracy of a classification

By definition a confusion matrix C is such that $C_{i,j}$ is equal to the number of observations known to be in group i but predicted to be in group j.

Thus in a binary classification, the count of true negatives is $C_{0,0}$, false negatives is $C_{1,0}$, true positives is $C_{1,1}$, and false positives is $C_{0,1}$.

Section 1.2

1.6.3 **Question 5**:

10 points

Generate the confusion matrix associated with the test data for this digits binary classification problem (i.e., computing which images correspond to the digit 9 and which do not).

Use the training data (X_train, y_bin_train) to fit a DummyClassifier class instance to the training data as we did above. Then, construct a prediction from the test input features X_test and, by comparing to the test labels y_bin_test, build the corresponding confusion matrix. Assign the resulting 2D Numpy array to the identifier bin_confusion_mat.

You can do so explicitly or you can use the function confusion_matrix from sklearn.metrics according to your preference.

```
In [36]: ### GRADED

from sklearn.metrics import confusion_matrix

    ## YOUR SOLUTION HERE
    dummy.fit(X_train, y_bin_train)
    pred = dummy.predict(X_test)
    bin_confusion_mat = confusion_matrix(y_bin_test,pred, labels=None, sample_weight=None
    ###
    ### YOUR CODE HERE
    ###
    #bin_confusion_mat
In [37]: ###
### AUTOGRADER TEST - DO NOT REMOVE
###
```

1.7 Accuracy

The most basic way to assess our performance is to compare how many predictions we were right on out of the total number of observations. We refer to this as **accuracy**. Using the diagram of our confusion matrix above, we have the formula

$$accuracy = \frac{tp + tn}{tn + tp + fn + fp}$$

where tp is the number of true positives, tn is the number of true negatives, fp is the number of false positives, and fn is the number of false negatives.

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1.7.1 **Question 6:**

5 points

Your task here is to compose a function accuracy_score that implements the preceding formula. The input to the function is a (previously computed) confusion matrix and the output is an accuracy score.

1.8 Logistic Regression

We move on now to estimators for classification problems that actually use the input data (unlike the DummyClassifier). To begin, let's examine the LogisticRegression estimator. In order to determine a logistic regression model, a nonlinear system of equations needs to be solved iteratively. Thus, when we instantiate the estimator, we can specify the solver and the maximum number of iterations. For instance:

```
>>> from sklearn.linear_model import LogisticRegression
>>> clf = LogisticRegression(solver='newton-cg', max_iter=1000)
```

Don't worry about what these particular optional parameters mean. Although other choices exist, we'll use these for now.

As with other *Scikit-Learn*'s estimator classes, the .fit and .predict methods are used to construct the model and make predictions.

For classifications, we can also access the *probabilities* of correctness. That is, for a given observation (i.e., row of X), there is not only the class prediction (i.e., corresponding row of y), but there are associated *probabilities* of that observation belonging to each class. These probabilities are accessible by the method predict_proba. For each observation, this returns a row vector of nonnegative values that sum to 1 where the entry in column k is the probability of belonging to class k. Thus, for this binary classification problem, after fitting a classifier (e.g., LogisticRegression) to the training data, the method predict_proba returns an $n_{\text{test}} \times 2$ matrix of probabilities (where n_{test} is the number of observations in the testing set) whose rows all sum to one.

```
In [40]: # Column O: probability of class O
         # Column 1: probability of class 1
         clf.predict_proba(X_test)[335:350]
Out[40]: array([[9.99999959e-01, 4.11013670e-08],
                [9.99999993e-01, 7.12261056e-09],
                [2.96714441e-05, 9.99970329e-01],
                [9.99360921e-01, 6.39079380e-04],
                [1.00000000e+00, 2.37463349e-13],
                [9.9999999e-01, 8.59748534e-10],
                [1.00000000e+00, 8.11193166e-20],
                [1.00000000e+00, 1.32088362e-18],
                [1.00000000e+00, 1.04422574e-13],
                [9.99833323e-01, 1.66676925e-04],
                [6.20574701e-06, 9.99993794e-01],
                [9.99999998e-01, 1.90976911e-09],
                [8.90567392e-06, 9.99991094e-01],
                [9.99999910e-01, 9.00940355e-08],
                [1.00000000e+00, 7.59870641e-11]])
```

Here we have constructed a function prob_table encapsulating the previous computations. This function accepts the test data X_test, and y_test, followed by a classifier (e.g., DummyClassifier, LogisticRegression, etc.) as arguments. The classifier should already have been fit to data (e.g., classifier.fit(X_train, y_train) should already have been invoked). The result returned should be a DataFrame:

	prob_0	prob_1	predicted_value	actual_value
0	p_0	$(1 - p_0)$ $(1 - p_1)$	$y_0^{ m pred}$	$y_0^{ m test}$
1	p_1	$(1 - p_1)$	$y_1^{ m pred}$	$y_1^{ m test}$
:	:	:	· 13	:

1.9 Standardizing the data

Prior to fitting a given estimator to data, we usually want to *standardize* the data. This is usually done by replacing features with their respective *z-scores*. That is, we translate and rescale the data so that the *k*th feature x_k is replaced according to the substitution $x_k \leftarrow (x_k - \mu_k)/\sigma_k$ where μ_k is the (empirical) mean of the *k*th feature and σ_k is the (empirical) standard deviation of the *k*th feature. When working with testing and training data sets, the values of μ_k and σ_k are determined using the training data and those same values are used to standardize the test data when validating the resulting estimator.

All of the above can be achieved using the StandardScaler class from sklearn.preprocessing. Instances of this class can accept a matrix of observations and return the corresponding z-scores down each column (remember, the rows are observations and the columns are the features). The resulting StandardScalar object, once fit to the training data, can be used to transform the testing data as well.

Here's an example of how to use the StandardScaler class to transform data:

```
>>> from sklearn.preprocessing import StandardScaler
>>> data = np.array([[0, 0], [0, 1], [1, 1], [1, 1]]) # Create 4x2 array of data
>>> scaler = StandardScaler() # Instantiate StandardScaler object
>>> scaler.fit(data)
                             # Use columns from data to define transformation
>>> print(scaler.mean_) # means of 2 columns from data
[0.5 \quad 0.75]
>>> print(scaler.var_)
                            # variances of 2 columns from data
>>> print(scaler.transform(data)) # Applying transformation to data
\Gamma\Gamma-1.
            -1.73205081
 Γ-1.
              0.57735027]
 Γ1.
              0.57735027]
              0.57735027]]
>>> print(scaler.transform([[2, 2]])) # Applying transformation to new observation
[[3.
            2.88675135]]
```

As an alternative to applying the methods fit and then transform, there is a fit_transform method that combines the two into a single step.

Section 1.2

1.9.1 **Question 7**:

10 points

Your task here is to standardize the data using the StandardScalar class as above. You'll define the transformation to the training feature matrix X_train with the fit method. You'll apply the resulting transformation to X_train and X_test to yield standardized data for both the training and testing sets. From there, you'll define a LogisticRegression classifier and fit that to the standardized training feature matrix and the binary labels y_bin_train. Set the arguments max_iter equal to 1000 and solver equal to newton-cg inside the LogisticRegression classifier.

Finally, you'll use the function prob_table from above to create a DataFrame prob_table_standardized that shows the classifications using the standardized test data as compared to the actual classifications with their corresponding probabilities.

```
In [42]: ### GRADED
         from sklearn.preprocessing import StandardScaler
         ### YOUR SOLUTION HERE
         scaler = StandardScaler() # Instantiate StandardScaler object
         scaler.fit(X_train)
         scaler.mean_
         scaler.var_
                                   # Use columns from data to define transformation
         scaler.transform(X_train)
         scaler.transform(X_test)
         classifier = LogisticRegression(solver = 'newton-cg', max_iter=1000)
         classifier.fit(X_train, y_bin_train)
         prob_table_standardized = prob_table(X_test, y_test, classifier)
         ###
         ### YOUR CODE HERE
         ###
         # prob_table_standardized
Out [42]:
              probab_0
                            probab_1 predicted_value actual_value
             1.000000 3.245542e-09
         0
                                                    0
                                                                   6
         1
             0.000027 9.999734e-01
                                                    1
                                                                  9
         2
             0.999997 2.593555e-06
                                                    0
                                                                   3
             0.989060 1.094016e-02
         3
                                                    0
                                                                  7
         4
              1.000000 5.865655e-13
                                                    0
                                                                   2
         445 1.000000 3.273137e-09
                                                    0
                                                                   3
         446 1.000000 1.641273e-21
                                                    0
                                                                   6
                                                                   2
         447 1.000000 4.354151e-16
                                                    0
         448
             1.000000 2.015757e-17
                                                    0
                                                                  6
```

0

449 1.000000 2.370787e-19

```
[450 rows x 4 columns]
In [27]: ###
### AUTOGRADER TEST - DO NOT REMOVE
###
```

1.9.2 Using Pipelines

Many modeling tasks involve the combination of preprocessing steps that are fed into an estimator. As such, *Scikit-Learn* comes with a handy Pipeline module that allows us to combine *transformers* (e.g., StandardScaler) and *estimators* (e.g., LinearRegression, LogisticRegression, etc.) in a single object. The Pipeline expects a sequence of transformers -- objects that have methods fit, transform, & fit_transform -- and ends with an estimator -- objects that have methods fit, predict, & fit_predict. For example, we could have a Pipeline that scales our data and subsequently fits a LogisticRegression model as follows:

```
pipe = Pipeline([('scaler', StandardScaler()), ('clf', LogisticRegression(max_iter=1000, solve.
```

Notice that the Pipeline object is instantiated using a list of tuples. All the tuples consist of a string identifier followed by an instance of one of Scikit-Learn's transformer classes except the last tuple (which has an estimator class instance instead). The resulting Pipeline object behaves like an estimator (i.e., it has methods fit, predict, and fit_predict).

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1.9.3 **Question 8:**

5 points

Your task here is to construct a Pipeline object as described above for a binary classification problem. We'll load and prepare the data X and y for you (y is a binary vector distinguishing the digit 3 from all other digits).

Construct a pipeline object called pipe combining a StandardScaler transformation with a LogisticRegression estimator. Fit the resulting pipelined estimator's to the training data X_train and y_train (provided) and construct a vector y_pred using the predict method of the Pipeline.

Be sure your solution binds a suitable Pipeline object to the identifier pipe and a Numpy array to the identifier y_pred.

```
In [43]: ### GRADED
```

```
from sklearn.pipeline import Pipeline
digits = load_digits()
X, y = digits.data, np.where(digits.target==3, 1, 0)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state = 42)
### YOUR SOLUTION HERE
pipe = Pipeline([('scaler', StandardScaler()), ('clf', LogisticRegression(max_iter=10)
pipe.fit(X_train, y_train)
y_pred = pipe.predict(X_test)
###
### YOUR CODE HERE
###
```

1.10 Regularization

As with linear regression, we can use *regularization* in conjunction with logistic regression. That is, we can modify the objective function being minimized to construct the estimator with a penalty term. From the Scikit-Learn User guide:

As an optimization problem, binary class *L*2 penalized logistic regression minimizes the following cost function:

$$\min_{w,c} \frac{1}{2} w^T w + C \sum_{i=1}^n \log \left(\exp \left(-y_i \left(X_i^T w + c \right) \right) + 1 \right).$$

Similarly, L1 regularized logistic regression solves the following optimization problem

$$\min_{w,c} \|w\|_1 + C \sum_{i=1}^n \log \left(\exp \left(-y_i \left(X_i^T w + c \right) \right) + 1 \right).$$

Note that, in this notation, it's assumed that the observation y_i takes values in the set $\{-1,1\}$ at trial.

Ignoring the mathematical details of all the terms in these objective functions, the regularization parameter in the Scikit-Learn LogisticRegression estimator is labeled C consistent with the parameter C in the equations above. Loosely speaking, C controls the relative importance of the penalty term (the terms w^Tw or $\|w\|_1$ in each of the objective functions) and the unpenalized objective (the expression preceded by C). So, when C is small, the coefficients in w that determine the logistic regressor are penalized more strongly forcing the penalty term to be smaller.

In practice with *Scikit-Learn*, we instantiate a LogisticRegression instance using the keyword option C. For our purposes, this means (when we use the max_iter and solver parameters as before) the following code for instantiation:

```
>>> clf = LogisticRegression(C=100, max_iter=1000, solver='newton-cg')
```

Below, we have defined a function , log_reg_gridsearch, that accepts as input arguments the input feature matrix X, the target vector y, and a list C_vals of positive scalar values (for the regularization parameter C in regularized logistic regression).

The input data is split into training & test sets with a fixed random parameter 42.

This function loops over the values c_val within the list C_vals. For each value, it: - instantiate a Pipeline object with a StandardScaler object followed by a LogisticRegression object

- instantiate the LogisticRegression estimator with keyword arguments solver='newton-cg', max_iter=1000, and C=c_val.
- fit the Pipeline to the training data X_train & y_train
- uses the Pipeline to predict target values from the test data X_test

The result returned by the function is a DataFrame with two columns: 'C' and 'accuracy'. The column 'C' contains the elements of the input list C_vals. The column 'accuracy' contains the corresponding accuracy score as computed in the loop just described.

1.11 Decision Trees

Now, we turn to a different classifier -- the DecisionTreeClassifier. The aim is to compare its performance to that of our LogisticRegression classifier. As with LogisticRegression and other estimators, the specific performance and behavior of the DecisionTreeClassifier can be tuned by specifying certain *hyperparameters* upon instantiation. Some useful hyperparameters for the DecisionTreeClassifier are:

- criterion: 'gini' (default) for the Gini impurity or 'entropy' for the information gain
- max_depth: depth of tree (default None; expands until all nodes are pure)
- min_samples_split: minimum number of samples required to split a node (default 2)

We also would like to search over different hyperparameters relevant to this classifier as well. In the problem below, you are asked to fit a DecisionTreeClassifier and search over the three hyperparameters listed above.

Here, we build a function decision_tree_gridsearch similar to log_reg_gridsearch. The function decision_tree_gridsearch accepts as input arguments the input feature matrix X, the target vector y, a list criteria of strings (either 'gini' or 'entropy' or both), a list depths of positive integers, and a list min_splits of positive integers.

The input data is split into training & test sets with a fixed random parameter 42.

This function will loop over all the hyperparameter values within the three input lists. For each hyperparameter combination, it: - Instantiate a DecisionTreeClassifier object

• Instantiate the DecisionTreeClassifier estimator with hyperparameters criterion, max_depth, andmin_samples_split determined from the input

- Fit the DecisionTreeClassifier to the training data X_train & y_train
- Uses the DecisionTreeClassifier to predict target values from the test data X_test

The result returned by the function is a DataFrame with four columns: 'criterion', 'max_depth', 'min_samples_split', and 'accuracy'. The first three columns contain all combinations of the hyperparameter values from the input lists. The column 'accuracy' contains the corresponding accuracy score as computed in the loop just described.

```
In [45]: def decision_tree_gridsearch(X, y, criteria, max_depths, min_splits):
             Input: predictor X values, target y values, and lists criteria,
                    max_depths, & min_splits of hyperparameter values for
                    the DecisionTreeClassifier.
             Output: DataFrame with accuracy scores & hyperparameter values;
                     column headings as follows:
                     | 'criterion' | 'max_depth' | 'min_samples_split' | 'accuracy' |
             ,,,
             # DO NOT CHANGE NEXT LINE
             X_train_, X_test_, y_train_, y_test_ = train_test_split(X, y, random_state=42)
             results = []
             crit = []
             mdepth = []
             minspl = []
             for criterion in criteria:
                 for max_depth in max_depths:
                     for min_samples_split in min_splits:
                         kwargs = {'criterion':criterion,
                                    'max_depth':max_depth,
                                    'min_samples_split':min_samples_split}
                         clf_ = DecisionTreeClassifier(**kwargs)
                         clf_.fit(X_train_, y_train_)
                         results.append(clf_.score(X_test_, y_test_))
                         crit.append(criterion)
                         mdepth.append(max_depth)
                         minspl.append(min_samples_split)
             df = pd.DataFrame({'criterion':crit, 'max_depth':mdepth,
                                 'min_samples_split':minspl, 'accuracy': results})
             df = df.sort_values(by=['criterion', 'max_depth', 'min_samples_split']).reset_ind
             return df
```

1.12 Machine Learning on Graphs

In this part of the assignment, we investigate how to apply some basic machine learning concepts to graph structures. This involves structuring data from a graph in familiar tabular format. We will begin by looking at a classic graph from Zachary's Karate Club. This is built in to networkx and has an attribute called club associated with each node.

```
In [46]: #create the graph
         K = nx.karate_club_graph()
In [47]: #print info
         print(nx.info(K))
Name: Zachary's Karate Club
Type: Graph
Number of nodes: 34
Number of edges: 78
Average degree:
                 4.5882
In [48]: K.nodes
Out[48]: NodeView((0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 2
In [49]: # checking node structure
         K.nodes[5]
Out[49]: {'club': 'Mr. Hi'}
In [50]: # node attributes
         K.nodes[5]['club']
Out[50]: 'Mr. Hi'
In [51]: # extract the value
         K.nodes[0]['club']
Out[51]: 'Mr. Hi'
   From this graph, we can construct a DataFrame object using the nodes as indices. Then, we
will map the attributes of the nodes 'club' values to a new column.
In [52]: karate = pd.DataFrame(index=K.nodes)
In [53]: karate['club'] = [K.nodes[i]['club'] for i in karate.index]
In [54]: karate.head()
Out [54]:
              club
         0 Mr. Hi
         1 Mr. Hi
         2 Mr. Hi
         3 Mr. Hi
         4 Mr. Hi
In [55]: karate.club.value_counts()
Out[55]: Mr. Hi
                    17
         Officer
                    17
         Name: club, dtype: int64
   Section 1.2
```

1.12.1 Question 09:

5 points

After we have the club feature established, we aim to use features of the graph to translate into new features in our DataFrame. To start, we can determine the degree of each vertex and incorporate these as features in our data.

In the karate dataframe, create a new feature named degree and fill it with the degree of each vertex.

```
In [107]: K.degree()
Out[107]: DegreeView({0: 16, 1: 9, 2: 10, 3: 6, 4: 3, 5: 4, 6: 4, 7: 4, 8: 5, 9: 2, 10: 3, 11:
In [78]: ### GRADED
         ### YOUR SOLUTION HERE
         karate['degree'] = [K.degree[i] for i in karate.index]
         ###
         ### YOUR CODE HERE
         ###
         #type(K.degree())
         # karate.head()
Out[78]:
              club degree cluster_coef
         0 Mr. Hi
                        16
                                       0
         1 Mr. Hi
                        9
                                       1
                                       2
         2 Mr. Hi
                        10
         3 Mr. Hi
                                       3
                         6
         4 Mr. Hi
In [44]: ###
         ### AUTOGRADER TEST - DO NOT REMOVE
         ###
<img src = "https://upload.wikimedia.org/wikipedia/commons/thumb/5/5a/Complete_graph_K3.svg/32</pre>
```

From Wikipedia:

</center>

"In graph theory, a clustering coefficient is a measure of the degree to which nodes in a graph tend to cluster together. Evidence suggests that in most real-world networks, and in particular social networks, nodes tend to create tightly knit groups characterized by a relatively high density of ties. This likelihood tends to be greater than the average probability of a tie randomly established between two nodes"

$$C = \frac{3 \times \text{number of triangles}}{\text{number of all triplets}}$$

In networkx, we can execute this computation using the function nx.clustering:

Notice that the output of nx.clustering is a Python dict with the node labels as keys and the corresponding clustering coefficients as values. Observe also that this function iterates over the entire graph and computes all the clustering coefficients at once (this will be relevant later when you have to work with a relatively large graph).

Section 1.2

1.12.2 Question 10:

5 points

Add a feature 'cluster_coef' to the karate dataframe below using the nx.clustering() method.

HINT: Use the method values to fill your dataframe

```
In [168]: ### GRADED
          ### YOUR SOLUTION HERE
          karate['cluster_coef'] = nx.clustering(K).values()
           ###
           ### YOUR CODE HERE
           ###
          karate['cluster_coef']
Out[168]: 0
                 0.150000
                 0.333333
          2
                 0.244444
          3
                 0.666667
          4
                 0.666667
          5
                 0.500000
          6
                 0.500000
          7
                 1.000000
          8
                 0.500000
          9
                 0.000000
          10
                 0.666667
          11
                 0.000000
          12
                 1.000000
          13
                 0.600000
          14
                 1.000000
          15
                 1.000000
          16
                 1.000000
          17
                 1.000000
          18
                 1.000000
          19
                 0.333333
          20
                 1.000000
```

```
21
                 1.000000
          22
                 1.000000
          23
                 0.400000
          24
                 0.333333
          25
                 0.333333
          26
                 1.000000
          27
                 0.166667
          28
                 0.333333
          29
                 0.666667
          30
                 0.500000
          31
                 0.200000
          32
                 0.196970
          33
                 0.110294
          Name: cluster_coef, dtype: float64
In [82]: ###
         ### AUTOGRADER TEST - DO NOT REMOVE
         ###
```

The scenario for our karate club involves a rift in the members, and subsequent splitting into two clubs. Here we want to predict who will join the club. Another feature that could be helpful involves the distance each node is from the two protagonists. These individuals correspond to the two nodes of the highest degree in the graph.

Below we identify the two nodes with the highest degree and save their indices in order to sensei_1 and sensei_2.

```
In [83]: sensei_1, sensei_2 = karate.degree.nlargest(2).index
In [143]: K.nodes[sensei_2]['club']
Out[143]: 'Mr. Hi'
    Section 1.2
```

1.12.3 Question 11:

5 points

We will identify the highest degree node (i.e., sensei_1) as Officer and the second highest (i.e., sensei_2) as Mr. Hi. Subsequently, we want to measure the distance from each as our final features. To do so, we can use **Djikstra's** shortest path algorithm with the .djikstra_path_length() method for each of the influencers.

Add a feature dist_officer that includes the length of the shortest path from each vertex to the highest degree vertex.

```
In [148]: ### GRADED

### YOUR SOLUTION HERE
karate['dist_officer'] = [nx.dijkstra_path_length(K, sensei_1, member) for member in
### YOUR CODE HERE
###
```

Let's have a look at our dataframe

4 Mr. Hi

```
In [150]: karate.head()
Out[150]:
               club
                    degree cluster_coef dist_officer
          0 Mr. Hi
                                                                  0
                         16
                                         0
                                                       2
          1 Mr. Hi
                          9
                                         1
                                                       2
                                                                  1
          2 Mr. Hi
                                                       2
                         10
                                         2
                                                                  1
          3 Mr. Hi
                          6
                                         3
                                                       2
                                                                  1
          4 Mr. Hi
                                                                  1
```

Here we repeat the computation from the preceding question by computing the shortest path distance (as measured by number of edges) from each member to Mr. Hi (i.e., sensei_2, the node of second highest degree).

Next, we add a feature dist_mrh to the datarame karate that is the length of the shortest path from each vertex to the second highest degree vertex.

```
In [151]: karate['dist_mrh'] = [nx.dijkstra_path_length(K, sensei_2, member) for member in K.n.dijkstra_path_length(K, sensei_
```

```
In [100]: karate.head()
Out[100]:
               club degree cluster_coef dist_officer dist_mrh
          0 Mr. Hi
                         16
                                        0
                                                      2
          1 Mr. Hi
                         9
                                                      2
                                                                1
                                        1
          2 Mr. Hi
                                        2
                                                      2
                         10
                                                                1
          3 Mr. Hi
                          6
                                        3
                                                      2
                                                                1
```

After building our features, we can see if we are in fact able to predict the club feature using a LogisticRegression classifier.

```
In [155]: clf.score(X_test, y_test)
Out[155]: 1.0
In [156]: from sklearn.model_selection import cross_val_score
In [157]: cross_val_score(clf, X_train, y_train, cv = 4)
Out[157]: array([0.85714286, 1. , 1. , 0.66666667])
Section 1.2
```

1.12.4 Question 12:

5 points

Use cross-validation as above but add arguments to group data based on y and to use 5 folds. Save your results to ans12 below.

```
In [110]: ### GRADED

### YOUR SOLUTION HERE
ans12= cross_val_score(clf, X_train, y_train, cv = 5)
###
### YOUR CODE HERE
###

In [111]: ###
### AUTOGRADER TEST - DO NOT REMOVE
###
```

Section ??

In our Karate Club example, we were dealing with a very small community sample. Now, we move to investigate an email network containing information about salary and department. Here, we have a larger dataset as well as one additional attribute for each node that we can incorporate into our model.

```
In [112]: G = nx.read_gpickle('data/email_prediction.gpickle')
In [113]: print(nx.info(G))
Name:
Type: Graph
Number of nodes: 1005
Number of edges: 16706
Average degree: 33.2458
In [114]: G.nodes[0]
Out[114]: {'Department': 1, 'ManagementSalary': 0.0}
Section 1.2
```

1.12.5 Question 13:

5 points

Your goal is to predict salaries for the nodes missing data. We proceed by splitting the data into two sets; labeled and not_labeled.

Using the DataFrame loaded below, create two subsets of the frame determined by if the management_salary is NaN or not. Assign the new dataframes to labeled and not_labeled, respectively.

```
In [177]: ### GRADED

salaries = pd.read_csv('data/salary_clean.csv', index_col = 0)
    ### YOUR SOLUTION HERE
    labeled = salaries['management_salary'].dropna() # DataFrame of observations with m
    not_labeled = salaries['management_salary'].isna() # DataFrame of observations missi

###
    ### YOUR CODE HERE
    ###

In [178]: ###
    ### AUTOGRADER TEST - DO NOT REMOVE
    ###
```

Now, you can build a basic LogisticRegression model on our data. Note that you build a split on the labeled data only, and reserve the unlabeled data for later.

During handling of the above exception, another exception occurred:

KeyError: 1

```
Traceback (most recent call last)
```

```
<ipython-input-180-b6b14aebeed8> in <module>
----> 1 X_train, X_test, y_train, y_test = train_test_split(labeled.drop('management_salar
                                                             labeled['management_salary'], :
    /usr/lib/python3.7/site-packages/pandas/core/series.py in drop(self, labels, axis, independent)
   4502
                    level=level,
   4503
                    inplace=inplace,
-> 4504
                    errors=errors,
                )
   4505
   4506
    /usr/lib/python3.7/site-packages/pandas/core/generic.py in drop(self, labels, axis, in-
                    if index is not None or columns is not None:
   3869
   3870
                        raise ValueError("Cannot specify both 'labels' and 'index'/'column
-> 3871
                    axis_name = self._get_axis_name(axis)
                    axes = {axis name: labels}
   3872
   3873
                elif index is not None or columns is not None:
    /usr/lib/python3.7/site-packages/pandas/core/generic.py in _get_axis_name(cls, axis)
    372
            @classmethod
    373
            def _get_axis_name(cls, axis: Axis) -> str:
--> 374
                axis_number = cls._get_axis_number(axis)
                return cls._AXIS_ORDERS[axis_number]
    375
    376
    /usr/lib/python3.7/site-packages/pandas/core/generic.py in _get_axis_number(cls, axis)
    368
                    return cls._AXIS_TO_AXIS_NUMBER[axis]
                except KeyError:
    369
--> 370
                    raise ValueError(f"No axis named {axis} for object type {cls.__name__}
    371
    372
            @classmethod
```

ValueError: No axis named 1 for object type Series

Next, we create a basic LogisticRegression classifier on the X_train and y_train sets. After using the function predict() we compute the roc_auc score from this estimator and assign it to the variable score.

ValueError

```
preds = lgr.predict(X_test)
      score = roc_auc_score(y_test, preds)
     print("Your roc_auc_score is : {:8.6f}".format(score))
   ValueError
                                              Traceback (most recent call last)
    <ipython-input-174-66f9ba19a8ce> in <module>
     2 lgr.fit(X_train, y_train)
     3 preds = lgr.predict(X_test)
---> 4 score = roc_auc_score(y_test, preds)
     6 print("Your roc_auc_score is : {:8.6f}".format(score))
    /usr/lib/python3.7/site-packages/sklearn/metrics/_ranking.py in roc_auc_score(y_true, ;
   347
            y_type = type_of_target(y_true)
           y_true = check_array(y_true, ensure_2d=False, dtype=None)
   348
--> 349
           y_score = check_array(y_score, ensure_2d=False)
   350
   351
           if y_type == "multiclass" or (y_type == "binary" and
   /usr/lib/python3.7/site-packages/sklearn/utils/validation.py in check_array(array, acc
   513
                            array = array.astype(dtype, casting="unsafe", copy=False)
   514
                        else:
                            array = np.asarray(array, order=order, dtype=dtype)
--> 515
                    except ComplexWarning:
   516
   517
                        raise ValueError("Complex data not supported\n"
    /usr/lib/python3.7/site-packages/numpy/core/_asarray.py in asarray(a, dtype, order)
    81
    82
           return array(a, dtype, copy=False, order=order)
---> 83
    84
    85
   ValueError: could not convert string to float: 'Mr. Hi'
```

1.12.6 Bagging Classifiers

From the documentation:

A Bagging classifier is an ensemble meta-estimator that fits base classifiers each on random subsets of the original dataset and then aggregate their individual predictions (either by voting or by averaging) to form a final prediction. Such a meta-estimator can typically be used as a way to reduce the variance of a black-box estimator (e.g., a decision tree), by introducing randomization into its construction procedure and then making an ensemble out of it.

1.12.7 Question 14:

5 points

Fit the data with a bagged KNearestNeighbor estimator and save your cross-validated roc_auc score average to bag_knn. below.

```
In [173]: ### GRADED
          ### YOUR SOLUTION HERE
          # bagging classifier
          bag = BaggingClassifier(knn, random_state = 24)
          bag knn = cross_val_score(bag, X_train, y_train, scoring = 'roc_auc')
          print(bag_knn)
          ###
          ### YOUR CODE HERE
          # print('Your roc_auc_score is : {:8.6f}'.format(bag_knn))
[1.
            0.66666667 1.
                                             0.83333333]
                                  1.
In []: ###
        ### AUTOGRADER TEST - DO NOT REMOVE
        ###
In [ ]: from sklearn.tree import DecisionTreeClassifier
        from sklearn.ensemble import RandomForestClassifier
```

1.12.8 Boosting Classifiers

From the documentation:

An AdaBoost classifier is a meta-estimator that begins by fitting a classifier on the original dataset and then fits additional copies of the classifier on the same dataset but where the weights of incorrectly classified instances are adjusted such that subsequent classifiers focus more on difficult cases.

By default, the classifier is a DecisionTreeClassifier. Below is an example from the user guide. We will use the AdaBoostClassifier and the GradientBoostingClassifier here. These boostings adjust themselves in different manners. AdaBoost focuses on misclassified data on each iteration and the GradientBoost focuses on the gradient of a loss function.