

Personalized cancer diagnosis

1. Business Problem

1.1. Description

Source: <https://www.kaggle.com/c/msk-redefining-cancer-treatment/>

Data: Memorial Sloan Kettering Cancer Center (MSKCC)

Download training_variants.zip and training_text.zip from Kaggle.

Context:

Source: <https://www.kaggle.com/c/msk-redefining-cancer-treatment/discussion/35336#198462>

Problem statement :

Classify the given genetic variations/mutations based on evidence from text-based clinical literature.

1.2. Source/Useful Links

Some articles and reference blogs about the problem statement

1. <https://www.forbes.com/sites/matthewherper/2017/06/03/a-new-cancer-drug-helped-almost-everyone-who-took-it-almost-heres-what-it-teaches-us/#2a44ee2f6b25>
(<https://www.forbes.com/sites/matthewherper/2017/06/03/a-new-cancer-drug-helped-almost-everyone-who-took-it-almost-heres-what-it-teaches-us/#2a44ee2f6b25>)
2. <https://www.youtube.com/watch?v=UwbuW7oK8rk> (<https://www.youtube.com/watch?v=UwbuW7oK8rk>)
3. <https://www.youtube.com/watch?v=qxXRKVompl8> (<https://www.youtube.com/watch?v=qxXRKVompl8>)

1.3. Real-world/Business objectives and constraints.

- No low-latency requirement.
- Interpretability is important.
- Errors can be very costly.
- Probability of a data-point belonging to each class is needed.

2. Machine Learning Problem Formulation

2.1. Data

2.1.1. Data Overview

- Source: <https://www.kaggle.com/c/msk-redefining-cancer-treatment/data> (<https://www.kaggle.com/c/msk-redefining-cancer-treatment/data>)
- We have two data files: one contains the information about the genetic mutations and the other contains the clinical evidence (text) that human experts/pathologists use to classify the genetic mutations.
- Both these data files have a common column called ID
- Data file's information:
 - training_variants (ID , Gene, Variations, Class)
 - training_text (ID, Text)

2.1.2. Example Data Point

training_variants

ID, Gene, Variation, Class

0, FAM58A, Truncating Mutations, 1

1, CBL, W802*, 2

2, CBL, Q249E, 2

...

training_text

ID, Text

0||Cyclin-dependent kinases (CDKs) regulate a variety of fundamental cellular processes. CDK10 stands out as one of the last orphan CDKs for which no activating cyclin has been identified and no kinase activity revealed. Previous work has shown that CDK10 silencing increases ETS2 (v-ets erythroblastosis virus E26 oncogene homolog 2)-driven activation of the MAPK pathway, which confers tamoxifen resistance to breast cancer cells. The precise mechanisms by which CDK10 modulates ETS2 activity, and more generally the functions of CDK10, remain elusive. Here we demonstrate that CDK10 is a cyclin-dependent kinase by identifying cyclin M as an activating cyclin. Cyclin M, an orphan cyclin, is the product of FAM58A, whose mutations cause STAR syndrome, a human developmental anomaly whose features include toe syndactyly, telecanthus, and anogenital and renal malformations. We show that STAR syndrome-associated cyclin M mutants are unable to interact with CDK10. Cyclin M silencing phenocopies CDK10 silencing in increasing c-Raf and in conferring tamoxifen resistance to breast cancer cells. CDK10/cyclin M phosphorylates ETS2 in vitro, and in cells it positively controls ETS2 degradation by the proteasome. ETS2 protein levels are increased in cells derived from a STAR patient, and this increase is attributable to decreased cyclin M levels. Altogether, our results reveal an additional regulatory mechanism for ETS2, which plays key roles in cancer and development. They also shed light on the molecular mechanisms underlying STAR syndrome. Cyclin-dependent kinases (CDKs) play a pivotal role in the control of a number of fundamental cellular processes (1). The human genome contains 21 genes encoding proteins that can be considered as members of the CDK family owing to their sequence similarity with bona fide CDKs, those known to be activated by cyclins (2). Although discovered almost 20 y ago (3, 4), CDK10 remains one of the two CDKs without an identified cyclin partner. This knowledge gap has largely impeded the exploration of its biological functions. CDK10 can act as a positive cell cycle regulator in some cells (5, 6) or as a tumor suppressor in others (7, 8). CDK10 interacts with the ETS2 (v-ets erythroblastosis virus E26 oncogene homolog 2) transcription factor and inhibits its transcriptional activity through an unknown mechanism (9). CDK10 knockdown derepresses ETS2, which increases the expression of the c-Raf protein kinase, activates the MAPK pathway, and induces resistance of MCF7 cells to tamoxifen (6). ...

2.2. Mapping the real-world problem to an ML problem**2.2.1. Type of Machine Learning Problem**

There are nine different classes a genetic mutation can be classified into => Multi class classification problem

2.2.2. Performance Metric

Source: <https://www.kaggle.com/c/msk-redefining-cancer-treatment#evaluation> (<https://www.kaggle.com/c/msk-redefining-cancer-treatment#evaluation>)

Metric(s):

- Multi class log-loss
- Confusion matrix

2.2.3. Machine Learning Objectives and Constraints

Objective: Predict the probability of each data-point belonging to each of the nine classes.

Constraints:

- Interpretability
- Class probabilities are needed.
- Penalize the errors in class probabilities => Metric is Log-loss.
- No Latency constraints.

2.3. Train, CV and Test Datasets

Split the dataset randomly into three parts train, cross validation and test with 64%, 16%, 20% of data respectively

3. Exploratory Data Analysis

```
In [1]: import pandas as pd
import matplotlib.pyplot as plt
import re
import time
import warnings
import numpy as np
from nltk.corpus import stopwords
from sklearn.decomposition import TruncatedSVD
from sklearn.preprocessing import normalize
from sklearn.feature_extraction.text import CountVectorizer
from sklearn.manifold import TSNE
import seaborn as sns
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import confusion_matrix
from sklearn.metrics.classification import accuracy_score, log_loss
from sklearn.feature_extraction.text import TfidfVectorizer
from sklearn.linear_model import SGDClassifier
from imblearn.over_sampling import SMOTE
from collections import Counter
from scipy.sparse import hstack
from sklearn.multiclass import OneVsRestClassifier
from sklearn.svm import SVC
from sklearn.model_selection import StratifiedKFold
from collections import Counter, defaultdict
from sklearn.calibration import CalibratedClassifierCV
from sklearn.naive_bayes import MultinomialNB
from sklearn.naive_bayes import GaussianNB
from sklearn.model_selection import train_test_split
from sklearn.model_selection import GridSearchCV
import math
from sklearn.metrics import normalized_mutual_info_score
from sklearn.ensemble import RandomForestClassifier
warnings.filterwarnings("ignore")

from mlxtend.classifier import StackingClassifier

from sklearn import model_selection
from sklearn.linear_model import LogisticRegression
```

```

Using TensorFlow backend.
/usr/local/lib/python3.5/dist-packages/tensorflow/python/framework/dtypes.py:
516: FutureWarning: Passing (type, 1) or '1type' as a synonym of type is depr
ecated; in a future version of numpy, it will be understood as (type, (1,)) /
'(1,)type'.
    _np_qint8 = np.dtype [("qint8", np.int8, 1)]
/usr/local/lib/python3.5/dist-packages/tensorflow/python/framework/dtypes.py:
517: FutureWarning: Passing (type, 1) or '1type' as a synonym of type is depr
ecated; in a future version of numpy, it will be understood as (type, (1,)) /
'(1,)type'.
    _np_quint8 = np.dtype [("quint8", np.uint8, 1)]
/usr/local/lib/python3.5/dist-packages/tensorflow/python/framework/dtypes.py:
518: FutureWarning: Passing (type, 1) or '1type' as a synonym of type is depr
ecated; in a future version of numpy, it will be understood as (type, (1,)) /
'(1,)type'.
    _np_qint16 = np.dtype [("qint16", np.int16, 1)]
/usr/local/lib/python3.5/dist-packages/tensorflow/python/framework/dtypes.py:
519: FutureWarning: Passing (type, 1) or '1type' as a synonym of type is depr
ecated; in a future version of numpy, it will be understood as (type, (1,)) /
'(1,)type'.
    _np_quint16 = np.dtype [("quint16", np.uint16, 1)]
/usr/local/lib/python3.5/dist-packages/tensorflow/python/framework/dtypes.py:
520: FutureWarning: Passing (type, 1) or '1type' as a synonym of type is depr
ecated; in a future version of numpy, it will be understood as (type, (1,)) /
'(1,)type'.
    _np_qint32 = np.dtype [("qint32", np.int32, 1)]
/usr/local/lib/python3.5/dist-packages/tensorflow/python/framework/dtypes.py:
525: FutureWarning: Passing (type, 1) or '1type' as a synonym of type is depr
ecated; in a future version of numpy, it will be understood as (type, (1,)) /
'(1,)type'.
    np_resource = np.dtype [("resource", np.ubyte, 1)]
/usr/local/lib/python3.5/dist-packages/tensorboard/compat/tensorflow_stub/dty
pes.py:541: FutureWarning: Passing (type, 1) or '1type' as a synonym of type
is deprecated; in a future version of numpy, it will be understood as (type,
(1,)) / '(1,)type'.
    _np_qint8 = np.dtype [("qint8", np.int8, 1)]
/usr/local/lib/python3.5/dist-packages/tensorboard/compat/tensorflow_stub/dty
pes.py:542: FutureWarning: Passing (type, 1) or '1type' as a synonym of type
is deprecated; in a future version of numpy, it will be understood as (type,
(1,)) / '(1,)type'.
    _np_quint8 = np.dtype [("quint8", np.uint8, 1)]
/usr/local/lib/python3.5/dist-packages/tensorboard/compat/tensorflow_stub/dty
pes.py:543: FutureWarning: Passing (type, 1) or '1type' as a synonym of type
is deprecated; in a future version of numpy, it will be understood as (type,
(1,)) / '(1,)type'.
    _np_qint16 = np.dtype [("qint16", np.int16, 1)]
/usr/local/lib/python3.5/dist-packages/tensorboard/compat/tensorflow_stub/dty
pes.py:544: FutureWarning: Passing (type, 1) or '1type' as a synonym of type
is deprecated; in a future version of numpy, it will be understood as (type,
(1,)) / '(1,)type'.
    _np_quint16 = np.dtype [("quint16", np.uint16, 1)]
/usr/local/lib/python3.5/dist-packages/tensorboard/compat/tensorflow_stub/dty
pes.py:545: FutureWarning: Passing (type, 1) or '1type' as a synonym of type
is deprecated; in a future version of numpy, it will be understood as (type,
(1,)) / '(1,)type'.
    _np_qint32 = np.dtype [("qint32", np.int32, 1)]
/usr/local/lib/python3.5/dist-packages/tensorboard/compat/tensorflow_stub/dty

```

```

pes.py:550: FutureWarning: Passing (type, 1) or '1type' as a synonym of type
is deprecated; in a future version of numpy, it will be understood as (type,
(1,)) / '(1,)type'.
  np_resource = np.dtype([("resource", np.ubyte, 1)])

```

3.1. Reading Data

3.1.1. Reading Gene and Variation Data

```

In [2]: data = pd.read_csv('training_variants')
print('Number of data points : ', data.shape[0])
print('Number of features : ', data.shape[1])
print('Features : ', data.columns.values)
data.head()

```

```

Number of data points : 3321
Number of features : 4
Features : ['ID' 'Gene' 'Variation' 'Class']

```

Out[2]:

	ID	Gene	Variation	Class
0	0	FAM58A	Truncating Mutations	1
1	1	CBL	W802*	2
2	2	CBL	Q249E	2
3	3	CBL	N454D	3
4	4	CBL	L399V	4

training/training_variants is a comma separated file containing the description of the genetic mutations used for training.

Fields are

- **ID** : the id of the row used to link the mutation to the clinical evidence
- **Gene** : the gene where this genetic mutation is located
- **Variation** : the aminoacid change for this mutations
- **Class** : 1-9 the class this genetic mutation has been classified on

3.1.2. Reading Text Data

```
In [3]: # note the separator in this file
data_text = pd.read_csv("training_text", sep="\\|\\|", engine="python", names=["ID",
"TEXT"], skiprows=1)
print('Number of data points : ', data_text.shape[0])
print('Number of features : ', data_text.shape[1])
print('Features : ', data_text.columns.values)
data_text.head()
```

Number of data points : 3321

Number of features : 2

Features : ['ID' 'TEXT']

Out[3]:

	ID	TEXT
0	0	Cyclin-dependent kinases (CDKs) regulate a var...
1	1	Abstract Background Non-small cell lung canc...
2	2	Abstract Background Non-small cell lung canc...
3	3	Recent evidence has demonstrated that acquired...
4	4	Oncogenic mutations in the monomeric Casitas B...

3.1.3. Preprocessing of text

```
In [4]: # Loading stop words from nltk library
stop_words = set(stopwords.words('english'))

def nlp_preprocessing(total_text, index, column):
    if type(total_text) is not int:
        string = ""
        # replace every special char with space
        total_text = re.sub('[^a-zA-Z0-9\n]', ' ', total_text)
        # replace multiple spaces with single space
        total_text = re.sub('\s+', ' ', total_text)
        # converting all the chars into lower-case.
        total_text = total_text.lower()

        for word in total_text.split():
            # if the word is a not a stop word then retain that word from the data
            if not word in stop_words:
                string += word + " "

        data_text[column][index] = string
```



```
In [5]: #text processing stage.
start_time = time.clock()
for index, row in data_text.iterrows():
    if type(row['TEXT']) is str:
        nlp_preprocessing(row['TEXT'], index, 'TEXT')
    else:
        print("there is no text description for id:",index)
print('Time took for preprocessing the text :',time.clock() - start_time, "seconds")
```

```
there is no text description for id: 1109
there is no text description for id: 1277
there is no text description for id: 1407
there is no text description for id: 1639
there is no text description for id: 2755
Time took for preprocessing the text : 35.505905999999996 seconds
```

```
In [6]: #merging both gene_variations and text data based on ID
result = pd.merge(data, data_text,on='ID', how='left')
result.head()
```

Out[6]:

	ID	Gene	Variation	Class	TEXT
0	0	FAM58A	Truncating Mutations	1	cyclin dependent kinases cdks regulate variety...
1	1	CBL	W802*	2	abstract background non small cell lung cancer...
2	2	CBL	Q249E	2	abstract background non small cell lung cancer...
3	3	CBL	N454D	3	recent evidence demonstrated acquired uniparen...
4	4	CBL	L399V	4	oncogenic mutations monomeric casitas b lineag...

```
In [7]: result[result.isnull().any(axis=1)]
```

Out[7]:

	ID	Gene	Variation	Class	TEXT
1109	1109	FANCA	S1088F	1	NaN
1277	1277	ARID5B	Truncating Mutations	1	NaN
1407	1407	FGFR3	K508M	6	NaN
1639	1639	FLT1	Amplification	6	NaN
2755	2755	BRAF	G596C	7	NaN

```
In [8]: result.loc[result['TEXT'].isnull(), 'TEXT'] = result['Gene'] + ' '+result['Variation']
```

```
In [9]: result[result['ID']==1109]
```

Out[9]:

	ID	Gene	Variation	Class	TEXT
1109	1109	FANCA	S1088F	1	FANCA S1088F

3.1.4. Test, Train and Cross Validation Split

3.1.4.1. Splitting data into train, test and cross validation (64:20:16)

```
In [10]: y_true = result['Class'].values
result.Gene      = result.Gene.str.replace('\s+', '_')
result.Variation = result.Variation.str.replace('\s+', '_')

# split the data into test and train by maintaining same distribution of output variable 'y_true' [stratify=y_true]
X_train, test_df, y_train, y_test = train_test_split(result, y_true, stratify=y_true, test_size=0.2)
# split the train data into train and cross validation by maintaining same distribution of output variable 'y_train' [stratify=y_train]
train_df, cv_df, y_train, y_cv = train_test_split(X_train, y_train, stratify=y_train, test_size=0.2)
```

We split the data into train, test and cross validation data sets, preserving the ratio of class distribution in the original data set

```
In [11]: print('Number of data points in train data:', train_df.shape[0])
print('Number of data points in test data:', test_df.shape[0])
print('Number of data points in cross validation data:', cv_df.shape[0])

Number of data points in train data: 2124
Number of data points in test data: 665
Number of data points in cross validation data: 532
```

3.1.4.2. Distribution of y_i's in Train, Test and Cross Validation datasets

```

In [12]: # it returns a dict, keys as class labels and values as the number of data points in that class
train_class_distribution = train_df['Class'].value_counts().sort_index()
test_class_distribution = test_df['Class'].value_counts().sort_index()
cv_class_distribution = cv_df['Class'].value_counts().sort_index()

my_colors = 'rgbkymc'
train_class_distribution.plot(kind='bar')
plt.xlabel('Class')
plt.ylabel('Data points per Class')
plt.title('Distribution of yi in train data')
plt.grid()
plt.show()

# ref: argsort https://docs.scipy.org/doc/numpy/reference/generated/numpy.argsort.html
# -(train_class_distribution.values): the minus sign will give us in decreasing order
sorted_yi = np.argsort(-train_class_distribution.values)
for i in sorted_yi:
    print('Number of data points in class', i+1, ':', train_class_distribution.values[i], '(', np.round((train_class_distribution.values[i]/train_df.shape[0]*100), 3), '%)')

print('-'*80)
my_colors = 'rgbkymc'
test_class_distribution.plot(kind='bar')
plt.xlabel('Class')
plt.ylabel('Data points per Class')
plt.title('Distribution of yi in test data')
plt.grid()
plt.show()

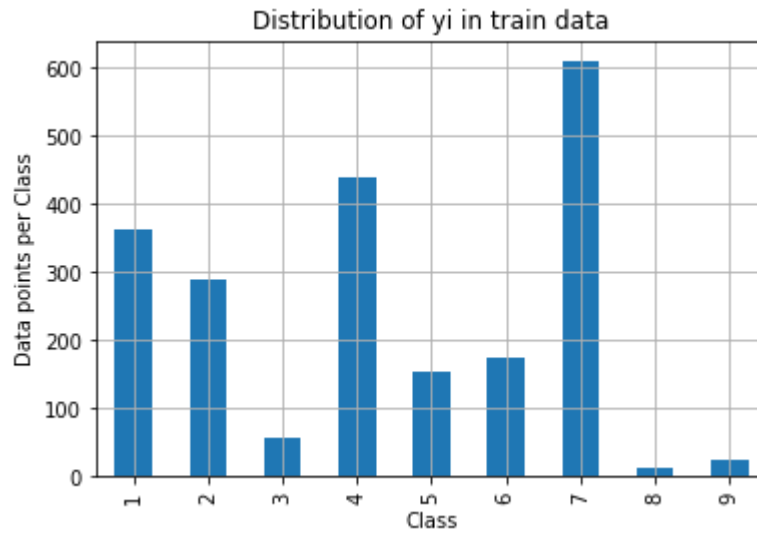
# ref: argsort https://docs.scipy.org/doc/numpy/reference/generated/numpy.argsort.html
# -(train_class_distribution.values): the minus sign will give us in decreasing order
sorted_yi = np.argsort(-test_class_distribution.values)
for i in sorted_yi:
    print('Number of data points in class', i+1, ':', test_class_distribution.values[i], '(', np.round((test_class_distribution.values[i]/test_df.shape[0]*100), 3), '%)')

print('-'*80)
my_colors = 'rgbkymc'
cv_class_distribution.plot(kind='bar')
plt.xlabel('Class')
plt.ylabel('Data points per Class')
plt.title('Distribution of yi in cross validation data')
plt.grid()
plt.show()

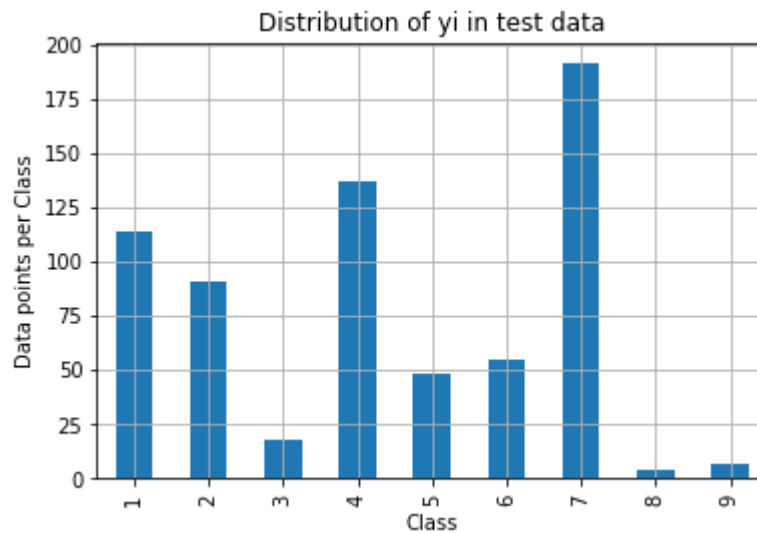
# ref: argsort https://docs.scipy.org/doc/numpy/reference/generated/numpy.argsort.html
# -(train_class_distribution.values): the minus sign will give us in decreasing order

```

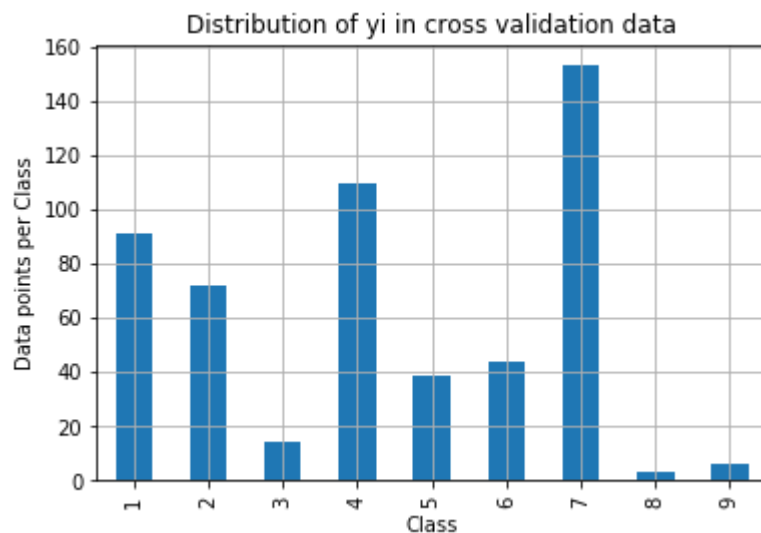
```
g order
sorted_yi = np.argsort(-train_class_distribution.values)
for i in sorted_yi:
    print('Number of data points in class', i+1, ':', cv_class_distribution.values[i], '(', np.round((cv_class_distribution.values[i]/cv_df.shape[0]*100), 3), '%)')
```



Number of data points in class 7 : 609 (28.672 %)
 Number of data points in class 4 : 439 (20.669 %)
 Number of data points in class 1 : 363 (17.09 %)
 Number of data points in class 2 : 289 (13.606 %)
 Number of data points in class 6 : 176 (8.286 %)
 Number of data points in class 5 : 155 (7.298 %)
 Number of data points in class 3 : 57 (2.684 %)
 Number of data points in class 9 : 24 (1.13 %)
 Number of data points in class 8 : 12 (0.565 %)



Number of data points in class 7 : 191 (28.722 %)
 Number of data points in class 4 : 137 (20.602 %)
 Number of data points in class 1 : 114 (17.143 %)
 Number of data points in class 2 : 91 (13.684 %)
 Number of data points in class 6 : 55 (8.271 %)
 Number of data points in class 5 : 48 (7.218 %)
 Number of data points in class 3 : 18 (2.707 %)
 Number of data points in class 9 : 7 (1.053 %)
 Number of data points in class 8 : 4 (0.602 %)



Number of data points in class 7 : 153 (28.759 %)
Number of data points in class 4 : 110 (20.677 %)
Number of data points in class 1 : 91 (17.105 %)
Number of data points in class 2 : 72 (13.534 %)
Number of data points in class 6 : 44 (8.271 %)
Number of data points in class 5 : 39 (7.331 %)
Number of data points in class 3 : 14 (2.632 %)
Number of data points in class 9 : 6 (1.128 %)
Number of data points in class 8 : 3 (0.564 %)

3.2 Prediction using a 'Random' Model

In a 'Random' Model, we generate the NINE class probabilities randomly such that they sum to 1.

```

In [13]: # This function plots the confusion matrices given y_i, y_i_hat.
def plot_confusion_matrix(test_y, predict_y):
    C = confusion_matrix(test_y, predict_y)
    # C = 9,9 matrix, each cell (i,j) represents number of points of class i a
    re predicted class j

    A = (((C.T)/(C.sum(axis=1))).T)
    #divid each element of the confusion matrix with the sum of elements in th
    at column

    # C = [[1, 2],
    #      [3, 4]]
    # C.T = [[1, 3],
    #        [2, 4]]
    # C.sum(axis = 1)  axis=0 corresponsds to columns and axis=1 corresponds to
    rows in two dimensional array
    # C.sum(axix =1) = [[3, 7]]
    # ((C.T)/(C.sum(axis=1))) = [[1/3, 3/7]
    #                             [2/3, 4/7]]

    # ((C.T)/(C.sum(axis=1))).T = [[1/3, 2/3]
    #                               [3/7, 4/7]]
    # sum of row elements = 1

    B = (C/C.sum(axis=0))
    #divid each element of the confusion matrix with the sum of elements in th
    at row

    # C = [[1, 2],
    #      [3, 4]]
    # C.sum(axis = 0)  axis=0 corresponsds to columns and axis=1 corresponds to
    rows in two dimensional array
    # C.sum(axix =0) = [[4, 6]]
    # (C/C.sum(axis=0)) = [[1/4, 2/6],
    #                       [3/4, 4/6]]

    labels = [1,2,3,4,5,6,7,8,9]
    # representing A in heatmap format
    print("-"*20, "Confusion matrix", "-"*20)
    plt.figure(figsize=(20,7))
    sns.heatmap(C, annot=True, cmap="YlGnBu", fmt=".3f", xticklabels=labels, y
    ticklabels=labels)
    plt.xlabel('Predicted Class')
    plt.ylabel('Original Class')
    plt.show()

    print("-"*20, "Precision matrix (Columm Sum=1)", "-"*20)
    plt.figure(figsize=(20,7))
    sns.heatmap(B, annot=True, cmap="YlGnBu", fmt=".3f", xticklabels=labels, y
    ticklabels=labels)
    plt.xlabel('Predicted Class')
    plt.ylabel('Original Class')
    plt.show()

    # representing B in heatmap format
    print("-"*20, "Recall matrix (Row sum=1)", "-"*20)
    plt.figure(figsize=(20,7))

```

```
sns.heatmap(A, annot=True, cmap="YlGnBu", fmt=".3f", xticklabels=labels, y  
ticklabels=labels)  
plt.xlabel('Predicted Class')  
plt.ylabel('Original Class')  
plt.show()
```



```
In [14]: # we need to generate 9 numbers and the sum of numbers should be 1
# one solution is to generate 9 numbers and divide each of the numbers by their sum
# ref: https://stackoverflow.com/a/18662466/4084039
test_data_len = test_df.shape[0]
cv_data_len = cv_df.shape[0]

# we create a output array that has exactly same size as the CV data
cv_predicted_y = np.zeros((cv_data_len,9))
for i in range(cv_data_len):
    rand_probs = np.random.rand(1,9)
    cv_predicted_y[i] = ((rand_probs/sum(sum(rand_probs))))[0])
print("Log loss on Cross Validation Data using Random Model",log_loss(y_cv,cv_predicted_y, eps=1e-15))

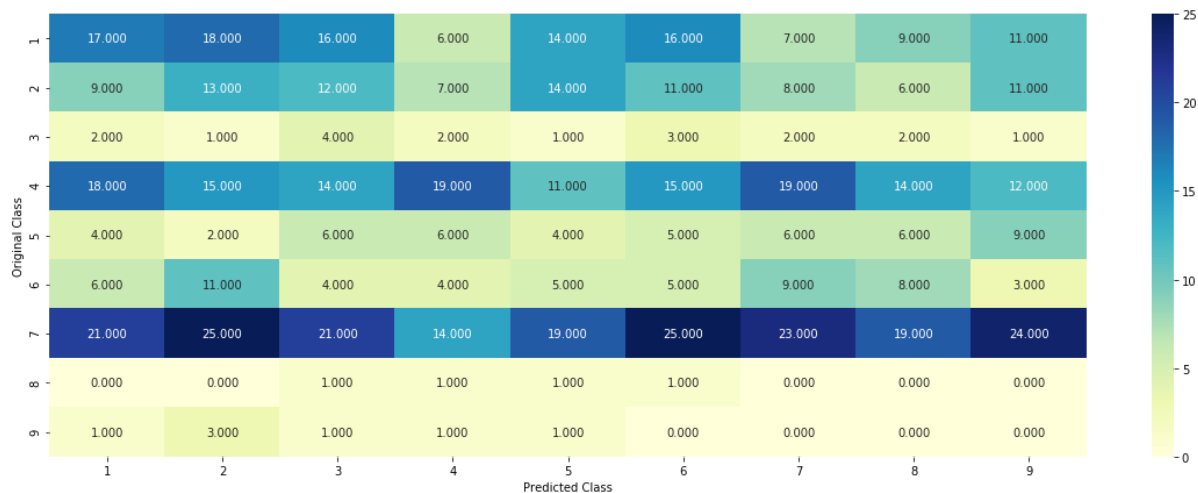
# Test-Set error.
#we create a output array that has exactly same as the test data
test_predicted_y = np.zeros((test_data_len,9))
for i in range(test_data_len):
    rand_probs = np.random.rand(1,9)
    test_predicted_y[i] = ((rand_probs/sum(sum(rand_probs))))[0])
print("Log loss on Test Data using Random Model",log_loss(y_test,test_predicted_y, eps=1e-15))

predicted_y =np.argmax(test_predicted_y, axis=1)
plot_confusion_matrix(y_test, predicted_y+1)
```

Log loss on Cross Validation Data using Random Model 2.496007849418387

Log loss on Test Data using Random Model 2.438241757580394

----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



3.3 Univariate Analysis


```

In [15]: # code for response coding with Laplace smoothing.
# alpha : used for Laplace smoothing
# feature: ['gene', 'variation']
# df: ['train_df', 'test_df', 'cv_df']
# algorithm
# -----
# Consider all unique values and the number of occurrences of given feature in
# train data dataframe
# build a vector (1*9) , the first element = (number of times it occurred in cl
# ass1 + 10*alpha / number of time it occurred in total data+90*alpha)
# gv_dict is like a look up table, for every gene it store a (1*9) representat
# ion of it
# for a value of feature in df:
# if it is in train data:
# we add the vector that was stored in 'gv_dict' Look up table to 'gv_fea'
# if it is not there is train:
# we add [1/9, 1/9, 1/9, 1/9,1/9, 1/9, 1/9, 1/9, 1/9] to 'gv_fea'
# return 'gv_fea'
# -----

# get_gv_fea_dict: Get Gene variation Feature Dict
def get_gv_fea_dict(alpha, feature, df):
    # value_count: it contains a dict like
    # print(train_df['Gene'].value_counts())
    # output:
    #          {BRCA1      174
    #           TP53      106
    #           EGFR       86
    #           BRCA2      75
    #           PTEN       69
    #           KIT        61
    #           BRAF        60
    #           ERBB2       47
    #           PDGFRA      46
    #           ...}
    # print(train_df['Variation'].value_counts())
    # output:
    # {
    # Truncating_Mutations      63
    # Deletion                   43
    # Amplification              43
    # Fusions                    22
    # Overexpression             3
    # E17K                       3
    # Q61L                       3
    # S222D                      2
    # P130S                      2
    # ...
    # }
    value_count = train_df[feature].value_counts()

    # gv_dict : Gene Variation Dict, which contains the probability array for
    # each gene/variation
    gv_dict = dict()

    # denominator will contain the number of time that particular feature occu

```

```

red in whole data
    for i, denominator in value_count.items():
        # vec will contain (p(yi=1/Gi) probability of gene/variation belongs
        to particular class
        # vec is 9 dimensional vector
        vec = []
        for k in range(1,10):
            # print(train_df.loc[(train_df['Class']==1) & (train_df['Gene']=
            = 'BRCA1')])
            #
            ID      Gene      Variation      Class
            # 2470  2470  BRCA1      S1715C      1
            # 2486  2486  BRCA1      S1841R      1
            # 2614  2614  BRCA1      M1R      1
            # 2432  2432  BRCA1      L1657P      1
            # 2567  2567  BRCA1      T1685A      1
            # 2583  2583  BRCA1      E1660G      1
            # 2634  2634  BRCA1      W1718L      1
            # cls_cnt.shape[0] will return the number of rows

            cls_cnt = train_df.loc[(train_df['Class']==k) & (train_df[feature]
            ==i)]

            # cls_cnt.shape[0](numerator) will contain the number of time that
            particular feature occurred in whole data
            vec.append((cls_cnt.shape[0] + alpha*10)/ (denominator + 90*alpha
            ))

            # we are adding the gene/variation to the dict as key and vec as value
            gv_dict[i]=vec
        return gv_dict

# Get Gene variation feature
def get_gv_feature(alpha, feature, df):
    # print(gv_dict)
    #
    # {'BRCA1': [0.20075757575757575, 0.03787878787878788, 0.06818181818181818, 0.13636363636363635, 0.25, 0.19318181818181818, 0.03787878787878788, 0.03787878787878788, 0.03787878787878788],
    #
    # 'TP53': [0.32142857142857145, 0.061224489795918366, 0.061224489795918366, 0.27040816326530615, 0.061224489795918366, 0.066326530612244902, 0.051020408163265307, 0.051020408163265307, 0.056122448979591837],
    #
    # 'EGFR': [0.056818181818181816, 0.21590909090909091, 0.0625, 0.068181818181818177, 0.068181818181818177, 0.0625, 0.34659090909090912, 0.0625, 0.056818181818181816],
    #
    # 'BRCA2': [0.13333333333333333, 0.060606060606060608, 0.060606060606060608, 0.078787878787878782, 0.13939393939393939, 0.34545454545454546, 0.060606060606060608, 0.060606060606060608, 0.060606060606060608],
    #
    # 'PTEN': [0.069182389937106917, 0.062893081761006289, 0.069182389937106917, 0.46540880503144655, 0.075471698113207544, 0.062893081761006289, 0.069182389937106917, 0.062893081761006289, 0.062893081761006289],
    #
    # 'KIT': [0.066225165562913912, 0.25165562913907286, 0.072847682119205295, 0.072847682119205295, 0.066225165562913912, 0.066225165562913912, 0.27152317880794702, 0.066225165562913912, 0.066225165562913912],
    #
    # 'BRAF': [0.066666666666666666, 0.17999999999999999, 0.07333333333333333, 0.07333333333333333, 0.09333333333333333, 0.080000000000000002, 0.29999999999999999, 0.066666666666666666, 0.066666666666666666],
    #
    # ...
    #
    }

```

```

gv_dict = get_gv_fea_dict(alpha, feature, df)
# value_count is similar in get_gv_fea_dict
value_count = train_df[feature].value_counts()

# gv_fea: Gene_variation feature, it will contain the feature for each fea
ture value in the data
gv_fea = []
# for every feature values in the given data frame we will check if it is
there in the train data then we will add the feature to gv_fea
# if not we will add [1/9,1/9,1/9,1/9,1/9,1/9,1/9,1/9,1/9] to gv_fea
for index, row in df.iterrows():
    if row[feature] in dict(value_count).keys():
        gv_fea.append(gv_dict[row[feature]])
    else:
        gv_fea.append([1/9,1/9,1/9,1/9,1/9,1/9,1/9,1/9,1/9])
#
return gv_fea

```

when we calculate the probability of a feature belongs to any particular class, we apply laplace smoothing

- $(\text{numerator} + 10 \cdot \alpha) / (\text{denominator} + 90 \cdot \alpha)$

3.2.1 Univariate Analysis on Gene Feature

Q1. Gene, What type of feature it is ?

Ans. Gene is a categorical variable

Q2. How many categories are there and How they are distributed?

```

In [16]: unique_genes = train_df['Gene'].value_counts()
print('Number of Unique Genes :', unique_genes.shape[0])
# the top 10 genes that occurred most
print(unique_genes.head(10))

```

```

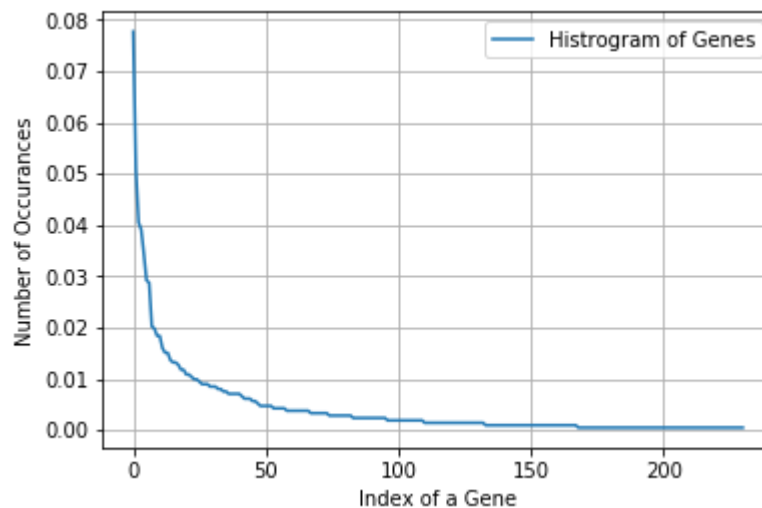
Number of Unique Genes : 231
BRCA1      165
TP53       108
PTEN        86
EGFR        83
BRCA2       73
BRAF        62
KIT         61
ALK         43
ERBB2       42
PIK3CA      39
Name: Gene, dtype: int64

```

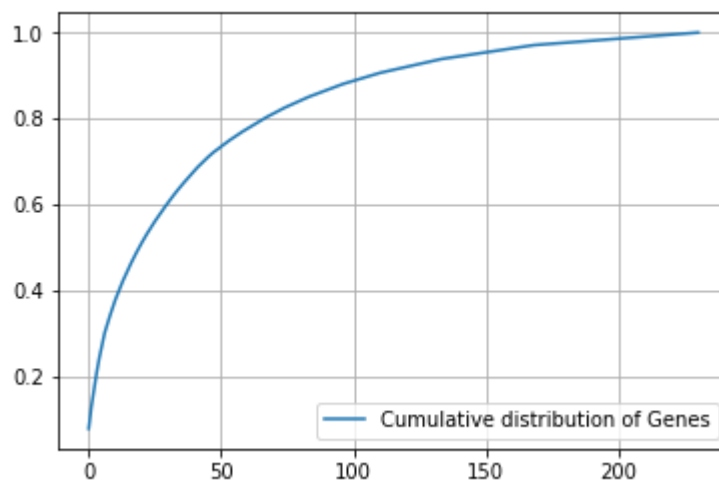
```
In [17]: print("Ans: There are", unique_genes.shape[0] , "different categories of genes  
in the train data, and they are distributed as follows",)
```

Ans: There are 231 different categories of genes in the train data, and they are distributed as follows

```
In [18]: s = sum(unique_genes.values);  
h = unique_genes.values/s;  
plt.plot(h, label="Histogram of Genes")  
plt.xlabel('Index of a Gene')  
plt.ylabel('Number of Occurances')  
plt.legend()  
plt.grid()  
plt.show()
```



```
In [19]: c = np.cumsum(h)  
plt.plot(c, label='Cumulative distribution of Genes')  
plt.grid()  
plt.legend()  
plt.show()
```



Q3. How to featurize this Gene feature ?

Ans.there are two ways we can featurize this variable check out this video:

<https://www.appliedaicourse.com/course/applied-ai-course-online/lessons/handling-categorical-and-numerical-features/>

1. One hot Encoding
2. Response coding

We will choose the appropriate featurization based on the ML model we use. For this problem of multi-class classification with categorical features, one-hot encoding is better for Logistic regression while response coding is better for Random Forests.

```
In [20]: #response-coding of the Gene feature
# alpha is used for Laplace smoothing
alpha = 1
# train gene feature
train_gene_feature_responseCoding = np.array(get_gv_feature(alpha, "Gene", train_df))
# test gene feature
test_gene_feature_responseCoding = np.array(get_gv_feature(alpha, "Gene", test_df))
# cross validation gene feature
cv_gene_feature_responseCoding = np.array(get_gv_feature(alpha, "Gene", cv_df))
```

```
In [21]: print("train_gene_feature_responseCoding is converted feature using response coding method. The shape of gene feature:", train_gene_feature_responseCoding.shape)
```

```
train_gene_feature_responseCoding is converted feature using response coding method. The shape of gene feature: (2124, 9)
```

```
In [22]: # one-hot encoding of Gene feature.
gene_vectorizer = CountVectorizer()
train_gene_feature_onehotCoding = gene_vectorizer.fit_transform(train_df['Gene'])
test_gene_feature_onehotCoding = gene_vectorizer.transform(test_df['Gene'])
cv_gene_feature_onehotCoding = gene_vectorizer.transform(cv_df['Gene'])
```

```
In [23]: train_df['Gene'].head()
```

```
Out[23]: 2780    BRCA2
1410    FGFR3
2165    PTEN
1973    CTNNB1
2944    KDR
Name: Gene, dtype: object
```



```
In [24]: gene_vectorizer.get_feature_names()
```

```
Out[24]: ['abl1',  
          'acvr1',  
          'ago2',  
          'akt1',  
          'akt2',  
          'akt3',  
          'alk',  
          'apc',  
          'ar',  
          'araf',  
          'arid1b',  
          'arid2',  
          'arid5b',  
          'asxl2',  
          'atm',  
          'atrx',  
          'aurka',  
          'aurkb',  
          'axl',  
          'b2m',  
          'bap1',  
          'bcl10',  
          'bcl2l11',  
          'bcor',  
          'braf',  
          'brca1',  
          'brca2',  
          'brd4',  
          'brip1',  
          'card11',  
          'carm1',  
          'casp8',  
          'cbl',  
          'ccnd1',  
          'ccnd2',  
          'ccnd3',  
          'cdh1',  
          'cdk12',  
          'cdk4',  
          'cdk6',  
          'cdkn1a',  
          'cdkn1b',  
          'cdkn2a',  
          'cdkn2b',  
          'cdkn2c',  
          'cebpa',  
          'chek2',  
          'cic',  
          'crebbp',  
          'ctcf',  
          'ctnnb1',  
          'ddr2',  
          'dicer1',  
          'dnmt3a',  
          'dnmt3b',  
          'egfr',  
          'eif1ax',
```

'elf3',
'ep300',
'epas1',
'epcam',
'erbb2',
'erbb3',
'erbb4',
'ercc2',
'ercc3',
'ercc4',
'erg',
'errfi1',
'esr1',
'etv1',
'etv6',
'ewsr1',
'ezh2',
'fanca',
'fancc',
'fat1',
'fbxw7',
'fgf19',
'fgf4',
'fgfr1',
'fgfr2',
'fgfr3',
'fgfr4',
'flt3',
'foxa1',
'foxl2',
'foxp1',
'fubp1',
'gata3',
'gli1',
'gnaq',
'gnas',
'h3f3a',
'hla',
'hnf1a',
'hras',
'idh1',
'idh2',
'igf1r',
'ikbke',
'il7r',
'jak1',
'jak2',
'kdm5c',
'kdm6a',
'kdr',
'keap1',
'kit',
'klf4',
'kmt2a',
'kmt2b',
'kmt2c',
'kmt2d',

'knstrn',
'kras',
'lats1',
'lats2',
'map2k1',
'map2k2',
'map2k4',
'map3k1',
'mapk1',
'mdm2',
'mdm4',
'med12',
'mef2b',
'met',
'mga',
'mlh1',
'mpl',
'msh2',
'msh6',
'mtor',
'myc',
'mycn',
'myd88',
'myod1',
'nf1',
'nf2',
'nfe2l2',
'nfkb1a',
'nkx2',
'notch1',
'notch2',
'npm1',
'nras',
'nsd1',
'ntrk1',
'ntrk2',
'ntrk3',
'nup93',
'pak1',
'pax8',
'pbrm1',
'pdgfra',
'pdgfrb',
'pik3ca',
'pik3cb',
'pik3cd',
'pik3r1',
'pik3r2',
'pik3r3',
'pim1',
'pms1',
'pms2',
'pole',
'ppp2r1a',
'ppp6c',
'prdm1',
'ptch1',

'pten',
'ptpn11',
'ptprd',
'ptprt',
'rac1',
'rad21',
'rad50',
'rad51c',
'rad54l',
'raf1',
'rara',
'rasa1',
'rb1',
'rbm10',
'ret',
'rheb',
'rhoa',
'rictor',
'rit1',
'rnf43',
'ros1',
'rras2',
'runx1',
'rxra',
'rybp',
'sdhc',
'setd2',
'sf3b1',
'shoc2',
'smad2',
'smad3',
'smad4',
'smarca4',
'smarcb1',
'smo',
'sos1',
'sox9',
'spop',
'src',
'stat3',
'stk11',
'tcf3',
'tert',
'tet1',
'tet2',
'tgfbr1',
'tgfbr2',
'tmprss2',
'tp53',
'tp53bp1',
'tsc1',
'tsc2',
'u2af1',
'vh1',
'whsc1',
'whsc1l1',
'xpo1',

```
'xrcc2',  
'yap1']
```

```
In [25]: print("train_gene_feature_onehotCoding is converted feature using one-hot encoding method. The shape of gene feature:", train_gene_feature_onehotCoding.shape)
```

```
train_gene_feature_onehotCoding is converted feature using one-hot encoding method. The shape of gene feature: (2124, 230)
```

Q4. How good is this gene feature in predicting y_i ?

There are many ways to estimate how good a feature is, in predicting y_i . One of the good methods is to build a proper ML model using just this feature. In this case, we will build a logistic regression model using only Gene feature (one hot encoded) to predict y_i .

```

In [26]: alpha = [10 ** x for x in range(-5, 1)] # hyperparam for SGD classifier.

# read more about SGDClassifier() at http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.SGDClassifier.html
# -----
# default parameters
# SGDClassifier(loss='hinge', penalty='l2', alpha=0.0001, l1_ratio=0.15, fit_intercept=True, max_iter=None, tol=None,
# shuffle=True, verbose=0, epsilon=0.1, n_jobs=1, random_state=None, learning_rate='optimal', eta0=0.0, power_t=0.5,
# class_weight=None, warm_start=False, average=False, n_iter=None)

# some of methods
# fit(X, y[, coef_init, intercept_init, ...])      Fit linear model with Stochastic Gradient Descent.
# predict(X)      Predict class labels for samples in X.

#-----
# video link:
#-----

cv_log_error_array=[]
for i in alpha:
    clf = SGDClassifier(alpha=i, penalty='l2', loss='log', random_state=42)
    clf.fit(train_gene_feature_onehotCoding, y_train)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_gene_feature_onehotCoding, y_train)
    predict_y = sig_clf.predict_proba(cv_gene_feature_onehotCoding)
    cv_log_error_array.append(log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
    print('For values of alpha = ', i, "The log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))

fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], np.round(txt, 3)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

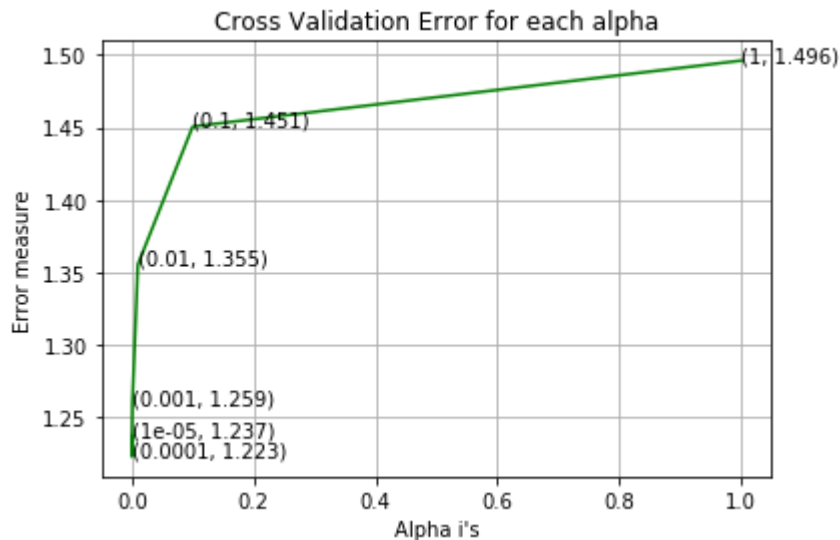
best_alpha = np.argmin(cv_log_error_array)
clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_state=42)
clf.fit(train_gene_feature_onehotCoding, y_train)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_gene_feature_onehotCoding, y_train)

predict_y = sig_clf.predict_proba(train_gene_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss is:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_gene_feature_onehotCoding)

```

```
print('For values of best alpha = ', alpha[best_alpha], "The cross validation
log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_gene_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss i
s:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))
```

For values of alpha = 1e-05 The log loss is: 1.2368745507768673
 For values of alpha = 0.0001 The log loss is: 1.2227028150130115
 For values of alpha = 0.001 The log loss is: 1.258731994752348
 For values of alpha = 0.01 The log loss is: 1.3552632355688468
 For values of alpha = 0.1 The log loss is: 1.4505687516968373
 For values of alpha = 1 The log loss is: 1.4960803362116422



For values of best alpha = 0.0001 The train log loss is: 0.9944723276058333
 For values of best alpha = 0.0001 The cross validation log loss is: 1.2227028150130115
 For values of best alpha = 0.0001 The test log loss is: 1.146286856683591

Q5. Is the Gene feature stable across all the data sets (Test, Train, Cross validation)?

Ans. Yes, it is. Otherwise, the CV and Test errors would be significantly more than train error.


```
In [27]: print("Q6. How many data points in Test and CV datasets are covered by the ",
            unique_genes.shape[0], " genes in train dataset?")

test_coverage=test_df[test_df['Gene'].isin(list(set(train_df['Gene'])))].shape[0]
cv_coverage=cv_df[cv_df['Gene'].isin(list(set(train_df['Gene'])))].shape[0]

print('Ans\n1. In test data',test_coverage, 'out of',test_df.shape[0], ":",(test_coverage/test_df.shape[0])*100)
print('2. In cross validation data',cv_coverage, 'out of ',cv_df.shape[0],":",
      ,(cv_coverage/cv_df.shape[0])*100)
```

Q6. How many data points in Test and CV datasets are covered by the 231 genes in train dataset?

Ans

1. In test data 649 out of 665 : 97.59398496240601

2. In cross validation data 511 out of 532 : 96.05263157894737

3.2.2 Univariate Analysis on Variation Feature

Q7. Variation, What type of feature is it ?

Ans. Variation is a categorical variable

Q8. How many categories are there?

```
In [28]: unique_variations = train_df['Variation'].value_counts()
print('Number of Unique Variations :', unique_variations.shape[0])
# the top 10 variations that occurred most
print(unique_variations.head(10))
```

Number of Unique Variations : 1945

Truncating_Mutations 59

Amplification 47

Deletion 38

Fusions 22

G12V 4

G12S 2

Q61R 2

M1R 2

A146T 2

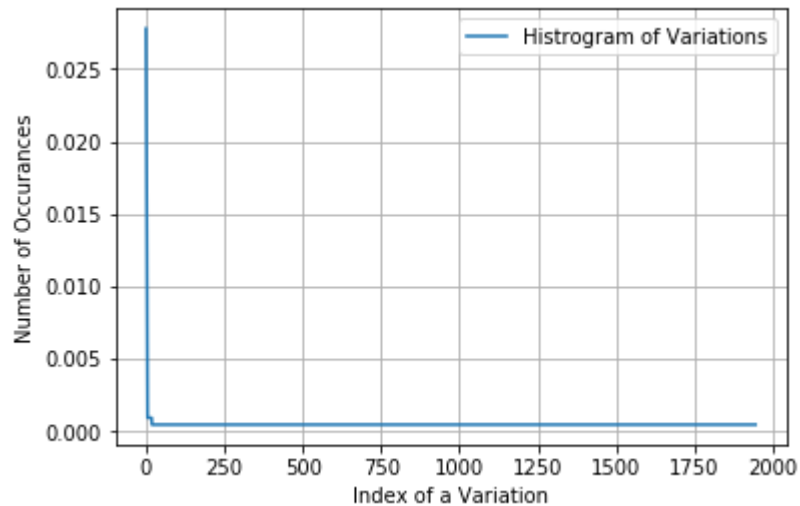
Q61L 2

Name: Variation, dtype: int64

```
In [29]: print("Ans: There are", unique_variations.shape[0] , "different categories of variations in the train data, and they are distributed as follows",)
```

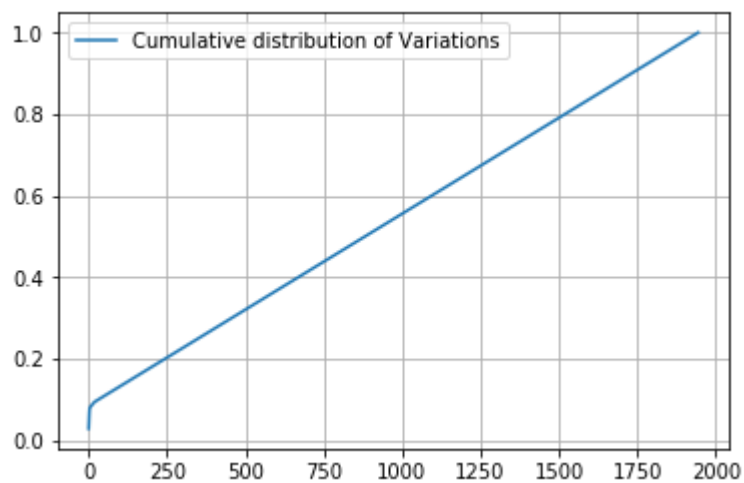
Ans: There are 1945 different categories of variations in the train data, and they are distributed as follows

```
In [30]: s = sum(unique_variations.values);
h = unique_variations.values/s;
plt.plot(h, label="Histogram of Variations")
plt.xlabel('Index of a Variation')
plt.ylabel('Number of Occurances')
plt.legend()
plt.grid()
plt.show()
```



```
In [31]: c = np.cumsum(h)
print(c)
plt.plot(c, label='Cumulative distribution of Variations')
plt.grid()
plt.legend()
plt.show()
```

```
[0.02777778 0.04990584 0.06779661 ... 0.99905838 0.99952919 1.          ]
```



Q9. How to featurize this Variation feature ?

Ans. There are two ways we can featurize this variable check out this video:

<https://www.appliedaicourse.com/course/applied-ai-course-online/lessons/handling-categorical-and-numerical-features/>

1. One hot Encoding
2. Response coding

We will be using both these methods to featurize the Variation Feature

```
In [32]: # alpha is used for Laplace smoothing
alpha = 1
# train gene feature
train_variation_feature_responseCoding = np.array(get_gv_feature(alpha, "Variation", train_df))
# test gene feature
test_variation_feature_responseCoding = np.array(get_gv_feature(alpha, "Variation", test_df))
# cross validation gene feature
cv_variation_feature_responseCoding = np.array(get_gv_feature(alpha, "Variation", cv_df))
```

```
In [33]: print("train_variation_feature_responseCoding is a converted feature using the response coding method. The shape of Variation feature:", train_variation_feature_responseCoding.shape)
```

train_variation_feature_responseCoding is a converted feature using the response coding method. The shape of Variation feature: (2124, 9)

```
In [34]: # one-hot encoding of variation feature.
variation_vectorizer = CountVectorizer()
train_variation_feature_onehotCoding = variation_vectorizer.fit_transform(train_df['Variation'])
test_variation_feature_onehotCoding = variation_vectorizer.transform(test_df['Variation'])
cv_variation_feature_onehotCoding = variation_vectorizer.transform(cv_df['Variation'])
```

```
In [35]: print("train_variation_feature_onehotEncoded is converted feature using the one-hot encoding method. The shape of Variation feature:", train_variation_feature_onehotCoding.shape)
```

train_variation_feature_onehotEncoded is converted feature using the one-hot encoding method. The shape of Variation feature: (2124, 1975)

Q10. How good is this Variation feature in predicting y_i?

Let's build a model just like the earlier!

```

In [36]: alpha = [10 ** x for x in range(-5, 1)]

cv_log_error_array=[]
for i in alpha:
    clf = SGDClassifier(alpha=i, penalty='l2', loss='log', random_state=42)
    clf.fit(train_variation_feature_onehotCoding, y_train)

    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_variation_feature_onehotCoding, y_train)
    predict_y = sig_clf.predict_proba(cv_variation_feature_onehotCoding)

    cv_log_error_array.append(log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
    print('For values of alpha = ', i, "The log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))

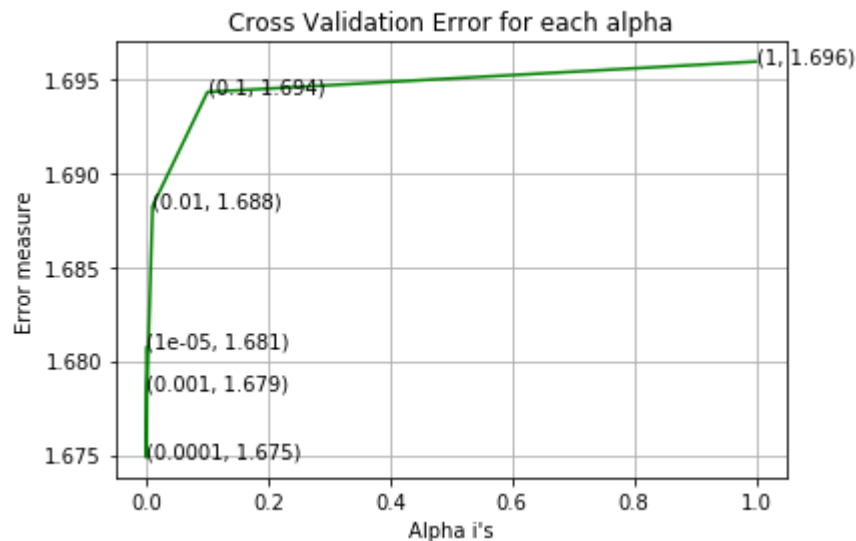
fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], np.round(txt, 3)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

best_alpha = np.argmin(cv_log_error_array)
clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_state=42)
clf.fit(train_variation_feature_onehotCoding, y_train)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_variation_feature_onehotCoding, y_train)

predict_y = sig_clf.predict_proba(train_variation_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss is:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_variation_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_variation_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss is:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

For values of alpha = 1e-05 The log loss is: 1.68070138569254
 For values of alpha = 0.0001 The log loss is: 1.6748495691271983
 For values of alpha = 0.001 The log loss is: 1.6785183675026936
 For values of alpha = 0.01 The log loss is: 1.68823786018618
 For values of alpha = 0.1 The log loss is: 1.6943130405613573
 For values of alpha = 1 The log loss is: 1.6959299685638511



For values of best alpha = 0.0001 The train log loss is: 0.7118918480630402
 For values of best alpha = 0.0001 The cross validation log loss is: 1.6748495691271983
 For values of best alpha = 0.0001 The test log loss is: 1.7125260608661488

Q11. Is the Variation feature stable across all the data sets (Test, Train, Cross validation)?

Ans. Not sure! But lets be very sure using the below analysis.

```
In [37]: print("Q12. How many data points are covered by total ", unique_variations.shape[0], " genes in test and cross validation data sets?")
test_coverage=test_df[test_df['Variation'].isin(list(set(train_df['Variation'])))].shape[0]
cv_coverage=cv_df[cv_df['Variation'].isin(list(set(train_df['Variation'])))].shape[0]
print('Ans\n1. In test data',test_coverage, 'out of',test_df.shape[0], ":",(test_coverage/test_df.shape[0])*100)
print('2. In cross validation data',cv_coverage, 'out of ',cv_df.shape[0],":", (cv_coverage/cv_df.shape[0])*100)
```

Q12. How many data points are covered by total 1945 genes in test and cross validation data sets?

Ans

1. In test data 74 out of 665 : 11.12781954887218
2. In cross validation data 67 out of 532 : 12.593984962406015

3.2.3 Univariate Analysis on Text Feature

1. How many unique words are present in train data?
2. How are word frequencies distributed?
3. How to featurize text field?
4. Is the text feature useful in predicting y_i ?
5. Is the text feature stable across train, test and CV datasets?

```
In [38]: # cls_text is a data frame
# for every row in data frame consider the 'TEXT'
# split the words by space
# make a dict with those words
# increment its count whenever we see that word

def extract_dictionary_paddle(cls_text):
    dictionary = defaultdict(int)
    for index, row in cls_text.iterrows():
        for word in row['TEXT'].split():
            dictionary[word] += 1
    return dictionary
```

```
In [39]: import math
#https://stackoverflow.com/a/1602964
def get_text_responsecoding(df):
    text_feature_responseCoding = np.zeros((df.shape[0],9))
    for i in range(0,9):
        row_index = 0
        for index, row in df.iterrows():
            sum_prob = 0
            for word in row['TEXT'].split():
                sum_prob += math.log(((dict_list[i].get(word,0)+10 )/(total_dictionary.get(word,0)+90)))
            text_feature_responseCoding[row_index][i] = math.exp(sum_prob/len(row['TEXT'].split()))
            row_index += 1
    return text_feature_responseCoding
```

```
In [40]: # building a CountVectorizer with all the words that occurred minimum 3 times in train data
text_vectorizer = TfidfVectorizer(ngram_range = (1,4), min_df=10, max_features=5000)
train_text_feature_onehotCoding = text_vectorizer.fit_transform(train_df['TEXT'])
# getting all the feature names (words)
train_text_features= text_vectorizer.get_feature_names()

# train_text_feature_onehotCoding.sum(axis=0).A1 will sum every row and returns (1*number of features) vector
train_text_fea_counts = train_text_feature_onehotCoding.sum(axis=0).A1

# zip(list(text_features),text_fea_counts) will zip a word with its number of times it occurred
text_fea_dict = dict(zip(list(train_text_features),train_text_fea_counts))

print("Total number of unique words in train data :", len(train_text_features))
```

Total number of unique words in train data : 5000

```
In [41]: dict_list = []
# dict_list =[] contains 9 dictionaries each corresponds to a class
for i in range(1,10):
    cls_text = train_df[train_df['Class']==i]
    # build a word dict based on the words in that class
    dict_list.append(extract_dictionary_paddle(cls_text))
    # append it to dict_list

# dict_list[i] is build on i'th class text data
# total_dict is build on whole training text data
total_dict = extract_dictionary_paddle(train_df)

confuse_array = []
for i in train_text_features:
    ratios = []
    max_val = -1
    for j in range(0,9):
        ratios.append((dict_list[j][i]+10)/(total_dict[i]+90))
    confuse_array.append(ratios)
confuse_array = np.array(confuse_array)
```

```
In [42]: #response coding of text features
train_text_feature_responseCoding = get_text_responsecoding(train_df)
test_text_feature_responseCoding = get_text_responsecoding(test_df)
cv_text_feature_responseCoding = get_text_responsecoding(cv_df)
```



```
In [43]: # https://stackoverflow.com/a/16202486
# we convert each row values such that they sum to 1
train_text_feature_responseCoding = (train_text_feature_responseCoding.T/train
_text_feature_responseCoding.sum(axis=1)).T
test_text_feature_responseCoding = (test_text_feature_responseCoding.T/test_t
xt_feature_responseCoding.sum(axis=1)).T
cv_text_feature_responseCoding = (cv_text_feature_responseCoding.T/cv_text_fea
ture_responseCoding.sum(axis=1)).T
```

```
In [44]: # don't forget to normalize every feature
train_text_feature_onehotCoding = normalize(train_text_feature_onehotCoding, a
xis=0)

# we use the same vectorizer that was trained on train data
test_text_feature_onehotCoding = text_vectorizer.transform(test_df['TEXT'])
# don't forget to normalize every feature
test_text_feature_onehotCoding = normalize(test_text_feature_onehotCoding, axi
s=0)

# we use the same vectorizer that was trained on train data
cv_text_feature_onehotCoding = text_vectorizer.transform(cv_df['TEXT'])
# don't forget to normalize every feature
cv_text_feature_onehotCoding = normalize(cv_text_feature_onehotCoding, axis=0)
```

```
In [45]: #https://stackoverflow.com/a/2258273/4084039
sorted_text_fea_dict = dict(sorted(text_fea_dict.items(), key=lambda x: x[1] ,
reverse=True))
sorted_text_occur = np.array(list(sorted_text_fea_dict.values()))
```

```
In [46]: # Number of words for a given frequency.  
print(Counter(sorted_text_occur))
```

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```

In [47]: # Train a Logistic regression+Calibration model using text features which are
on-hot encoded
alpha = [10 ** x for x in range(-5, 1)]

cv_log_error_array=[]
for i in alpha:
    clf = SGDClassifier(alpha=i, penalty='l2', loss='log', random_state=42)
    clf.fit(train_text_feature_onehotCoding, y_train)

    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_text_feature_onehotCoding, y_train)
    predict_y = sig_clf.predict_proba(cv_text_feature_onehotCoding)
    cv_log_error_array.append(log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
    print('For values of alpha = ', i, "The log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))

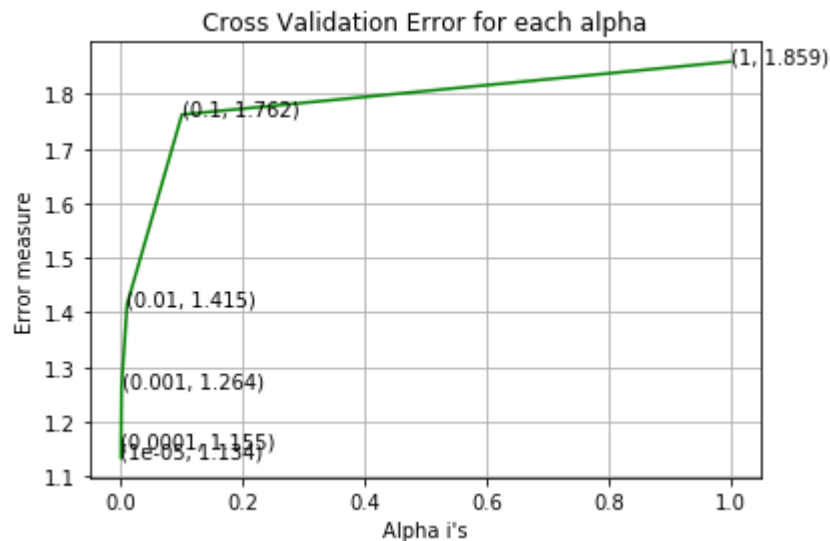
fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], np.round(txt, 3)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

best_alpha = np.argmin(cv_log_error_array)
clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_state=42)
clf.fit(train_text_feature_onehotCoding, y_train)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_text_feature_onehotCoding, y_train)

predict_y = sig_clf.predict_proba(train_text_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss is:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_text_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_text_feature_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss is:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

For values of alpha = 1e-05 The log loss is: 1.1339680227335633
 For values of alpha = 0.0001 The log loss is: 1.1548972359842409
 For values of alpha = 0.001 The log loss is: 1.2642637719707213
 For values of alpha = 0.01 The log loss is: 1.41484086363408
 For values of alpha = 0.1 The log loss is: 1.762350379931959
 For values of alpha = 1 The log loss is: 1.859327529546437



For values of best alpha = 1e-05 The train log loss is: 0.65114917839196
 For values of best alpha = 1e-05 The cross validation log loss is: 1.1339680227335633
 For values of best alpha = 1e-05 The test log loss is: 1.1786260735640253

Q. Is the Text feature stable across all the data sets (Test, Train, Cross validation)?

Ans. Yes, it seems like!

```
In [48]: def get_intersec_text(df):
df_text_vec = TfidfVectorizer(ngram_range = (1,4), min_df=10, max_features
=5000)
df_text_fea = df_text_vec.fit_transform(df['TEXT'])
df_text_features = df_text_vec.get_feature_names()

df_text_fea_counts = df_text_fea.sum(axis=0).A1
df_text_fea_dict = dict(zip(list(df_text_features),df_text_fea_counts))
len1 = len(set(df_text_features))
len2 = len(set(train_text_features) & set(df_text_features))
return len1,len2
```

```
In [49]: len1,len2 = get_intersec_text(test_df)
print(np.round((len2/len1)*100, 3), "% of word of test data appeared in train
data")
len1,len2 = get_intersec_text(cv_df)
print(np.round((len2/len1)*100, 3), "% of word of Cross Validation appeared in
train data")
```

91.08 % of word of test data appeared in train data
 90.84 % of word of Cross Validation appeared in train data

4. Machine Learning Models

```
In [50]: #Data preparation for ML models.

#Misc. functionns for ML models

def predict_and_plot_confusion_matrix(train_x, train_y, test_x, test_y, clf):
    clf.fit(train_x, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x, train_y)
    pred_y = sig_clf.predict(test_x)

    # for calculating log_loss we willl provide the array of probabilities bel
ongs to each class
    print("Log loss :", log_loss(test_y, sig_clf.predict_proba(test_x)))
    # calculating the number of data points that are misclassified
    print("Number of mis-classified points :", np.count_nonzero((pred_y- test_
y))/test_y.shape[0])
    plot_confusion_matrix(test_y, pred_y)
```

```
In [51]: def report_log_loss(train_x, train_y, test_x, test_y, clf):
    clf.fit(train_x, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x, train_y)
    sig_clf_probs = sig_clf.predict_proba(test_x)
    return log_loss(test_y, sig_clf_probs, eps=1e-15)
```

```

In [52]: # this function will be used just for naive bayes
# for the given indices, we will print the name of the features
# and we will check whether the feature present in the test point text or not
def get_impfeature_names(indices, text, gene, var, no_features):
    gene_count_vec = CountVectorizer()
    var_count_vec = CountVectorizer()
    text_count_vec = TfidfVectorizer(ngram_range = (1,4), min_df=10, max_features=5000)

    gene_vec = gene_count_vec.fit(train_df['Gene'])
    var_vec = var_count_vec.fit(train_df['Variation'])
    text_vec = text_count_vec.fit(train_df['TEXT'])

    fea1_len = len(gene_vec.get_feature_names())
    fea2_len = len(var_count_vec.get_feature_names())

    word_present = 0
    for i,v in enumerate(indices):
        if (v < fea1_len):
            word = gene_vec.get_feature_names()[v]
            yes_no = True if word == gene else False
            if yes_no:
                word_present += 1
                print(i, "Gene feature [{}] present in test data point [{}].format(word,yes_no))
            elif (v < fea1_len+fea2_len):
                word = var_vec.get_feature_names()[v-(fea1_len)]
                yes_no = True if word == var else False
                if yes_no:
                    word_present += 1
                    print(i, "variation feature [{}] present in test data point [{}].format(word,yes_no))
            else:
                word = text_vec.get_feature_names()[v-(fea1_len+fea2_len)]
                yes_no = True if word in text.split() else False
                if yes_no:
                    word_present += 1
                    print(i, "Text feature [{}] present in test data point [{}].format(word,yes_no))

    print("Out of the top ",no_features," features ", word_present, "are present in query point")

```

Stacking the three types of features

```
In [53]: # merging gene, variance and text features

# building train, test and cross validation data sets
# a = [[1, 2],
#       [3, 4]]
# b = [[4, 5],
#       [6, 7]]
# hstack(a, b) = [[1, 2, 4, 5],
#                 [ 3, 4, 6, 7]]

train_gene_var_onehotCoding = hstack((train_gene_feature_onehotCoding, train_variation_feature_onehotCoding))
test_gene_var_onehotCoding = hstack((test_gene_feature_onehotCoding, test_variation_feature_onehotCoding))
cv_gene_var_onehotCoding = hstack((cv_gene_feature_onehotCoding, cv_variation_feature_onehotCoding))

train_x_onehotCoding = hstack((train_gene_var_onehotCoding, train_text_feature_onehotCoding)).tocsr()
train_y = np.array(list(train_df['Class']))

test_x_onehotCoding = hstack((test_gene_var_onehotCoding, test_text_feature_onehotCoding)).tocsr()
test_y = np.array(list(test_df['Class']))

cv_x_onehotCoding = hstack((cv_gene_var_onehotCoding, cv_text_feature_onehotCoding)).tocsr()
cv_y = np.array(list(cv_df['Class']))

train_gene_var_responseCoding = np.hstack((train_gene_feature_responseCoding, train_variation_feature_responseCoding))
test_gene_var_responseCoding = np.hstack((test_gene_feature_responseCoding, test_variation_feature_responseCoding))
cv_gene_var_responseCoding = np.hstack((cv_gene_feature_responseCoding, cv_variation_feature_responseCoding))

train_x_responseCoding = np.hstack((train_gene_var_responseCoding, train_text_feature_responseCoding))
test_x_responseCoding = np.hstack((test_gene_var_responseCoding, test_text_feature_responseCoding))
cv_x_responseCoding = np.hstack((cv_gene_var_responseCoding, cv_text_feature_responseCoding))
```



```
In [54]: print("One hot encoding features :")
print("(number of data points * number of features) in train data = ", train_x_
_onehotCoding.shape)
print("(number of data points * number of features) in test data = ", test_x_o
nehotCoding.shape)
print("(number of data points * number of features) in cross validation data
=", cv_x_onehotCoding.shape)
```

```
One hot encoding features :
(number of data points * number of features) in train data = (2124, 7205)
(number of data points * number of features) in test data = (665, 7205)
(number of data points * number of features) in cross validation data = (532,
7205)
```

```
In [55]: print(" Response encoding features :")
print("(number of data points * number of features) in train data = ", train_x
_responseCoding.shape)
print("(number of data points * number of features) in test data = ", test_x_r
esponseCoding.shape)
print("(number of data points * number of features) in cross validation data
=", cv_x_responseCoding.shape)
```

```
Response encoding features :
(number of data points * number of features) in train data = (2124, 27)
(number of data points * number of features) in test data = (665, 27)
(number of data points * number of features) in cross validation data = (532,
27)
```

4.1. Base Line Model

4.1.1. Naive Bayes

4.1.1.1. Hyper parameter tuning

```

In [98]: alpha = [0.00001, 0.0001, 0.001, 0.1, 1, 10, 100,1000]
cv_log_error_array = []
for i in alpha:
    print("for alpha =", i)
    clf = MultinomialNB(alpha=i)
    clf.fit(train_x_onehotCoding, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x_onehotCoding, train_y)
    sig_clf_probs = sig_clf.predict_proba(cv_x_onehotCoding)
    cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes_
_, eps=1e-15))
    # to avoid rounding error while multiplying probabilities we use log-probability estimates
    print("Log Loss :",log_loss(cv_y, sig_clf_probs))

fig, ax = plt.subplots()
ax.plot(np.log10(alpha), cv_log_error_array,c='g')
for i, txt in enumerate(np.round(cv_log_error_array,3)):
    ax.annotate((alpha[i],str(txt)), (np.log10(alpha[i]),cv_log_error_array[i
]))
plt.grid()
plt.xticks(np.log10(alpha))
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

best_alpha = np.argmin(cv_log_error_array)
clf = MultinomialNB(alpha=alpha[best_alpha])
clf.fit(train_x_onehotCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_onehotCoding, train_y)

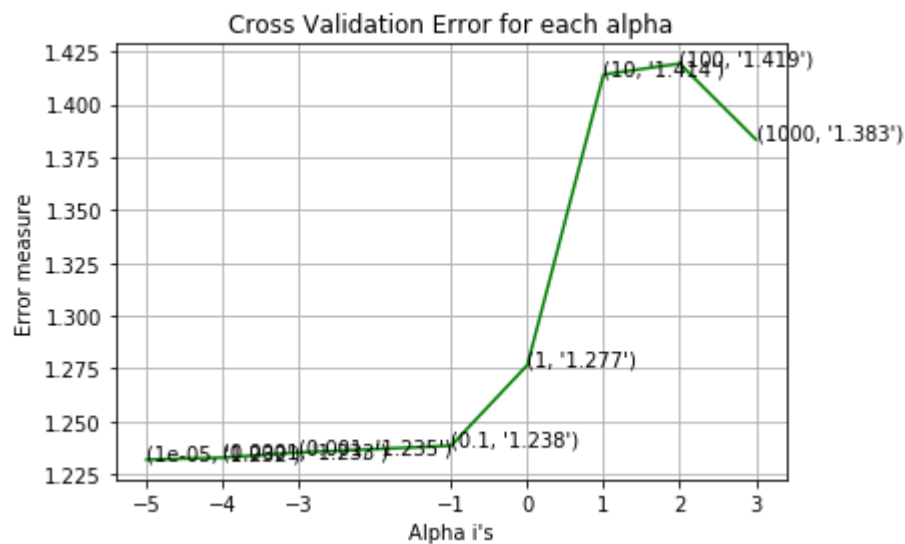
predict_y = sig_clf.predict_proba(train_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss i
s:",log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation
log loss is:",log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss i
s:",log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

```

for alpha = 1e-05
Log Loss : 1.2318129246635912
for alpha = 0.0001
Log Loss : 1.232785201993066
for alpha = 0.001
Log Loss : 1.235205053367683
for alpha = 0.1
Log Loss : 1.2384152725001947
for alpha = 1
Log Loss : 1.2765966711360812
for alpha = 10
Log Loss : 1.4141490525487528
for alpha = 100
Log Loss : 1.4193139479314296
for alpha = 1000
Log Loss : 1.3833884669045606

```



For values of best alpha = 1e-05 The train log loss is: 0.6749756701031507
 For values of best alpha = 1e-05 The cross validation log loss is: 1.2318129246635912
 For values of best alpha = 1e-05 The test log loss is: 1.1754148928058274

4.1.1.2. Testing the model with best hyper paramters

```
In [101]: clf = MultinomialNB(alpha=alpha[best_alpha])
clf.fit(train_x_onehotCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_onehotCoding, train_y)
sig_clf_probs = sig_clf.predict_proba(test_x_onehotCoding)
# to avoid rounding error while multiplying probabilities we use log-probability estimates
print("Log Loss :", log_loss(test_y, sig_clf_probs))
print("Number of misclassified point :", np.count_nonzero((sig_clf.predict(test_x_onehotCoding) - test_y))/test_y.shape[0])
plot_confusion_matrix(test_y, sig_clf.predict(test_x_onehotCoding.toarray()))
```

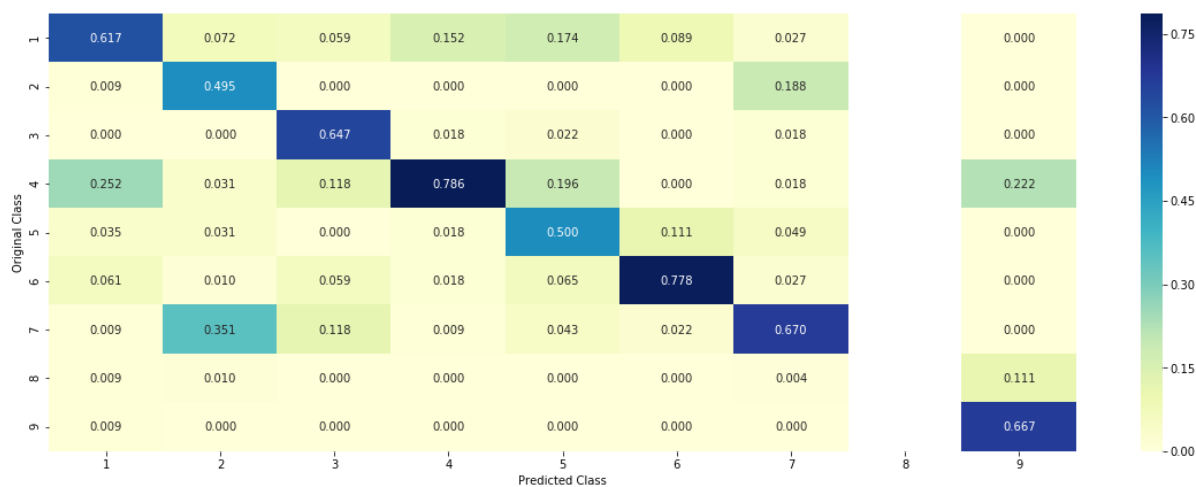
Log Loss : 1.1754148928058274

Number of missclassified point : 0.35037593984962406

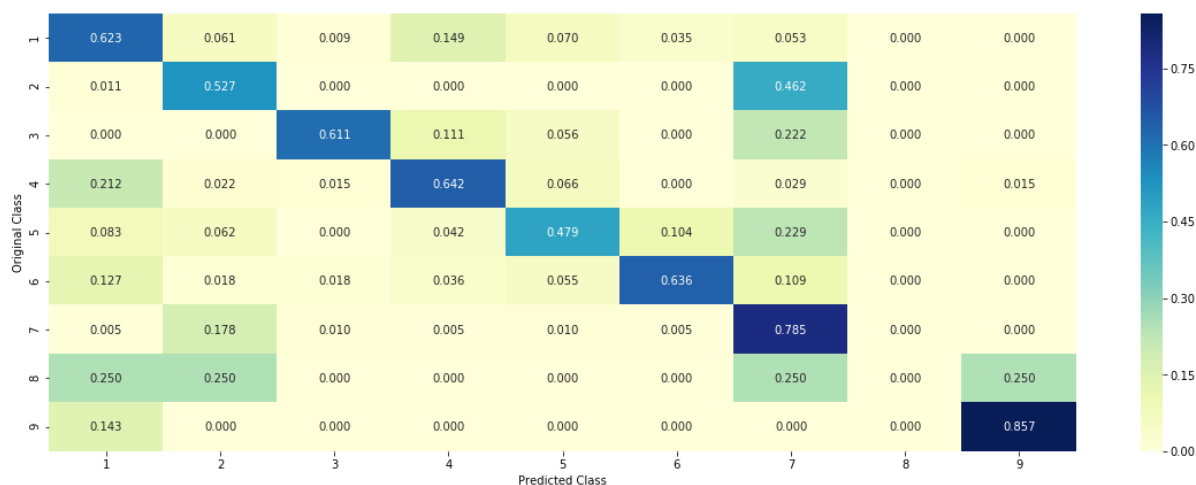
----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.1.1.3. Feature Importance, Correctly classified point

```
In [58]: test_point_index = 11
no_feature = 100
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:,no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_d
f['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_point_index],
no_feature)
```

Predicted Class : 4

Predicted Class Probabilities: [[0.0695 0.0559 0.0164 0.6976 0.037 0.036 0.0809 0.0042 0.0023]]

Actual Class : 4

11 Text feature [activity] present in test data point [True]
12 Text feature [protein] present in test data point [True]
13 Text feature [proteins] present in test data point [True]
18 Text feature [experiments] present in test data point [True]
19 Text feature [function] present in test data point [True]
20 Text feature [ability] present in test data point [True]
24 Text feature [results] present in test data point [True]
27 Text feature [acid] present in test data point [True]
28 Text feature [loss] present in test data point [True]
29 Text feature [functions] present in test data point [True]
31 Text feature [determined] present in test data point [True]
32 Text feature [shown] present in test data point [True]
34 Text feature [whether] present in test data point [True]
35 Text feature [suppressor] present in test data point [True]
36 Text feature [important] present in test data point [True]
37 Text feature [missense] present in test data point [True]
38 Text feature [described] present in test data point [True]
40 Text feature [bind] present in test data point [True]
41 Text feature [amino] present in test data point [True]
43 Text feature [also] present in test data point [True]
44 Text feature [type] present in test data point [True]
45 Text feature [mutations] present in test data point [True]
46 Text feature [two] present in test data point [True]
47 Text feature [indicate] present in test data point [True]
50 Text feature [functional] present in test data point [True]
51 Text feature [partially] present in test data point [True]
52 Text feature [retained] present in test data point [True]
53 Text feature [indicated] present in test data point [True]
56 Text feature [although] present in test data point [True]
57 Text feature [may] present in test data point [True]
59 Text feature [wild] present in test data point [True]
60 Text feature [levels] present in test data point [True]
62 Text feature [either] present in test data point [True]
67 Text feature [containing] present in test data point [True]
68 Text feature [purified] present in test data point [True]
69 Text feature [expressed] present in test data point [True]
70 Text feature [incubated] present in test data point [True]
72 Text feature [determine] present in test data point [True]
73 Text feature [analyzed] present in test data point [True]
75 Text feature [30] present in test data point [True]
77 Text feature [thus] present in test data point [True]
80 Text feature [vitro] present in test data point [True]
81 Text feature [buffer] present in test data point [True]
85 Text feature [tris] present in test data point [True]
86 Text feature [general] present in test data point [True]
88 Text feature [sds] present in test data point [True]
89 Text feature [terminal] present in test data point [True]
90 Text feature [previously] present in test data point [True]
91 Text feature [reduced] present in test data point [True]
92 Text feature [hcl] present in test data point [True]
93 Text feature [show] present in test data point [True]
96 Text feature [lack] present in test data point [True]

97 Text feature [lower] present in test data point [True]
98 Text feature [three] present in test data point [True]
99 Text feature [possible] present in test data point [True]
Out of the top 100 features 55 are present in query point

4.1.1.4. Feature Importance, Incorrectly classified point


```
In [60]: test_point_index = 5
no_feature = 100
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:,no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_d
f['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_point_index],
no_feature)
```

Predicted Class : 2

Predicted Class Probabilities: [[0.094 0.4288 0.0222 0.0968 0.0499 0.0488 0.2508 0.0057 0.0031]]

Actual Class : 6

13 Text feature [patients] present in test data point [True]
14 Text feature [treatment] present in test data point [True]
15 Text feature [clinical] present in test data point [True]
16 Text feature [time] present in test data point [True]
17 Text feature [response] present in test data point [True]
18 Text feature [first] present in test data point [True]
19 Text feature [molecular] present in test data point [True]
21 Text feature [study] present in test data point [True]
22 Text feature [therapy] present in test data point [True]
23 Text feature [recently] present in test data point [True]
24 Text feature [including] present in test data point [True]
25 Text feature [15] present in test data point [True]
26 Text feature [also] present in test data point [True]
27 Text feature [using] present in test data point [True]
28 Text feature [achieved] present in test data point [True]
29 Text feature [13] present in test data point [True]
30 Text feature [identified] present in test data point [True]
31 Text feature [10] present in test data point [True]
32 Text feature [common] present in test data point [True]
33 Text feature [therapeutic] present in test data point [True]
34 Text feature [initial] present in test data point [True]
35 Text feature [analysis] present in test data point [True]
36 Text feature [11] present in test data point [True]
37 Text feature [kinase] present in test data point [True]
38 Text feature [observed] present in test data point [True]
39 Text feature [may] present in test data point [True]
40 Text feature [harbor] present in test data point [True]
41 Text feature [18] present in test data point [True]
42 Text feature [12] present in test data point [True]
43 Text feature [reported] present in test data point [True]
44 Text feature [however] present in test data point [True]
45 Text feature [mutation] present in test data point [True]
46 Text feature [one] present in test data point [True]
47 Text feature [months] present in test data point [True]
48 Text feature [different] present in test data point [True]
49 Text feature [mutations] present in test data point [True]
50 Text feature [respectively] present in test data point [True]
51 Text feature [confirmed] present in test data point [True]
52 Text feature [gene] present in test data point [True]
53 Text feature [performed] present in test data point [True]
54 Text feature [identification] present in test data point [True]
55 Text feature [described] present in test data point [True]
56 Text feature [harboring] present in test data point [True]
57 Text feature [small] present in test data point [True]
58 Text feature [table] present in test data point [True]
59 Text feature [16] present in test data point [True]
60 Text feature [another] present in test data point [True]
61 Text feature [detection] present in test data point [True]
62 Text feature [previously] present in test data point [True]
63 Text feature [found] present in test data point [True]
64 Text feature [19] present in test data point [True]
65 Text feature [median] present in test data point [True]

```
66 Text feature [demonstrated] present in test data point [True]
67 Text feature [17] present in test data point [True]
68 Text feature [pcr] present in test data point [True]
69 Text feature [20] present in test data point [True]
70 Text feature [treated] present in test data point [True]
71 Text feature [although] present in test data point [True]
72 Text feature [present] present in test data point [True]
73 Text feature [novel] present in test data point [True]
74 Text feature [similar] present in test data point [True]
75 Text feature [well] present in test data point [True]
76 Text feature [higher] present in test data point [True]
77 Text feature [two] present in test data point [True]
78 Text feature [single] present in test data point [True]
79 Text feature [tissue] present in test data point [True]
80 Text feature [discussion] present in test data point [True]
81 Text feature [case] present in test data point [True]
82 Text feature [advanced] present in test data point [True]
83 Text feature [chronic] present in test data point [True]
84 Text feature [number] present in test data point [True]
85 Text feature [positive] present in test data point [True]
86 Text feature [complete] present in test data point [True]
87 Text feature [approved] present in test data point [True]
88 Text feature [studies] present in test data point [True]
89 Text feature [samples] present in test data point [True]
90 Text feature [62] present in test data point [True]
91 Text feature [due] present in test data point [True]
93 Text feature [overall] present in test data point [True]
94 Text feature [three] present in test data point [True]
95 Text feature [clinically] present in test data point [True]
96 Text feature [cases] present in test data point [True]
97 Text feature [total] present in test data point [True]
98 Text feature [sequencing] present in test data point [True]
Out of the top 100 features 84 are present in query point
```

4.2. K Nearest Neighbour Classification

4.2.1. Hyper parameter tuning

```

In [102]: # find more about KNeighborsClassifier() here http://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html
# -----
# default parameter
# KNeighborsClassifier(n_neighbors=5, weights='uniform', algorithm='auto', leaf_size=30, p=2,
# metric='minkowski', metric_params=None, n_jobs=1, **kwargs)

# methods of
# fit(X, y) : Fit the model using X as training data and y as target values
# predict(X):Predict the class labels for the provided data
# predict_proba(X):Return probability estimates for the test data X.
#-----

# video link: https://www.appliedaicourse.com/course/applied-ai-course-online/Lessons/k-nearest-neighbors-geometric-intuition-with-a-toy-example-1/
#-----

# find more about CalibratedClassifierCV here at http://scikit-learn.org/stable/modules/generated/sklearn.calibration.CalibratedClassifierCV.html
# -----
# default paramters
# sklearn.calibration.CalibratedClassifierCV(base_estimator=None, method='sigmoid', cv=3)
#
# some of the methods of CalibratedClassifierCV()
# fit(X, y[, sample_weight]) Fit the calibrated model
# get_params([deep]) Get parameters for this estimator.
# predict(X) Predict the target of new samples.
# predict_proba(X) Posterior probabilities of classification
#-----
# video link:
#-----

alpha = [5, 11, 15, 21, 31, 41, 51, 99]
cv_log_error_array = []
for i in alpha:
    print("for alpha =", i)
    clf = KNeighborsClassifier(n_neighbors=i)
    clf.fit(train_x_responseCoding, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x_responseCoding, train_y)
    sig_clf_probs = sig_clf.predict_proba(cv_x_responseCoding)
    cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes_, eps=1e-15))
    # to avoid rounding error while multiplying probabilities we use log-probability estimates
    print("Log Loss :", log_loss(cv_y, sig_clf_probs))

fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], str(txt)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")

```

```
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

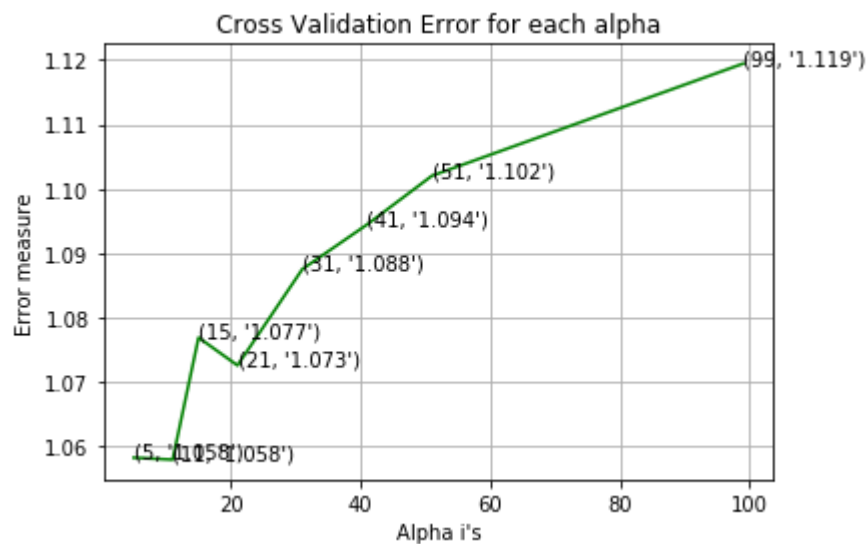
best_alpha = np.argmin(cv_log_error_array)
clf = KNeighborsClassifier(n_neighbors=alpha[best_alpha])
clf.fit(train_x_responseCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_responseCoding, train_y)

predict_y = sig_clf.predict_proba(train_x_responseCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss is:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_responseCoding)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_responseCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss is:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))
```

```

for alpha = 5
Log Loss : 1.0582459242255784
for alpha = 11
Log Loss : 1.0579427663391208
for alpha = 15
Log Loss : 1.076898953532393
for alpha = 21
Log Loss : 1.0725700152579816
for alpha = 31
Log Loss : 1.0875091676128672
for alpha = 41
Log Loss : 1.09444953427156
for alpha = 51
Log Loss : 1.102014333634802
for alpha = 99
Log Loss : 1.1194267408852046

```



For values of best alpha = 11 The train log loss is: 0.6492554707867186
 For values of best alpha = 11 The cross validation log loss is: 1.0579427663391208
 For values of best alpha = 11 The test log loss is: 0.9886585809459049

4.2.2. Testing the model with best hyper paramters

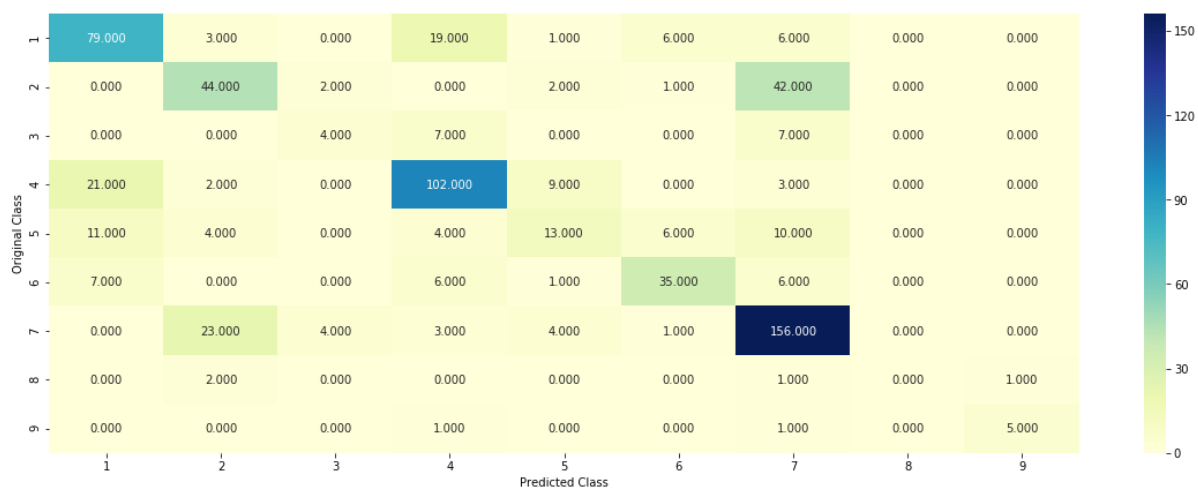
```
In [103]: # find more about KNeighborsClassifier() here http://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html
# -----
# default parameter
# KNeighborsClassifier(n_neighbors=5, weights='uniform', algorithm='auto', leaf_size=30, p=2,
# metric='minkowski', metric_params=None, n_jobs=1, **kwargs)

# methods of
# fit(X, y) : Fit the model using X as training data and y as target values
# predict(X):Predict the class labels for the provided data
# predict_proba(X):Return probability estimates for the test data X.
#-----
# video link: https://www.appliedaicourse.com/course/applied-ai-course-online/lessons/k-nearest-neighbors-geometric-intuition-with-a-toy-example-1/
#-----
clf = KNeighborsClassifier(n_neighbors=alpha[best_alpha])
predict_and_plot_confusion_matrix(train_x_responseCoding, train_y, test_x_responseCoding, test_y, clf)
```

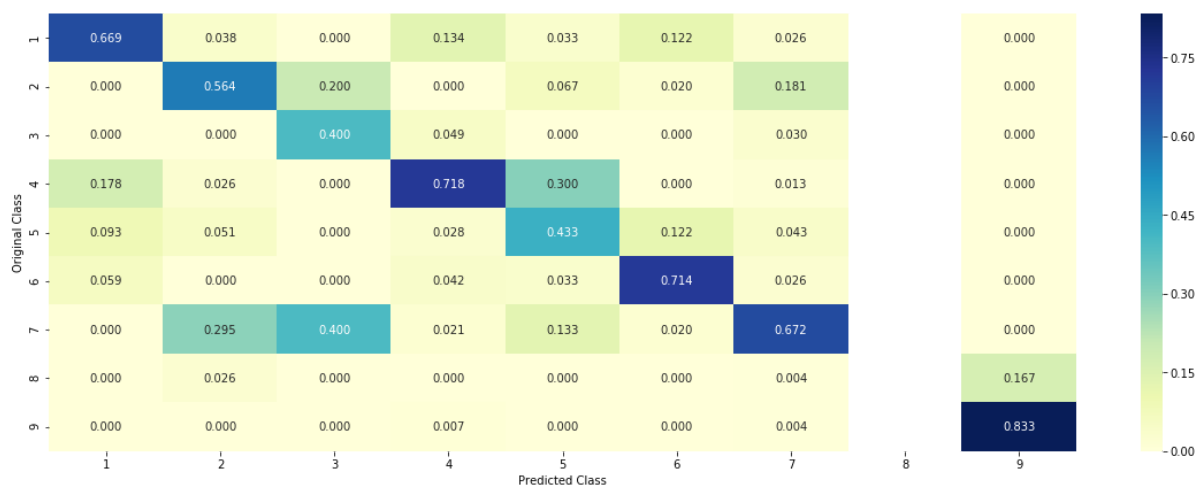
Log loss : 0.9886585809459049

Number of mis-classified points : 0.34135338345864663

----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.2.3.Sample Query point -1


```
In [63]: clf = KNeighborsClassifier(n_neighbors=alpha[best_alpha])
clf.fit(train_x_responseCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_responseCoding, train_y)

test_point_index = 1
predicted_cls = sig_clf.predict(test_x_responseCoding[0].reshape(1,-1))
print("Predicted Class :", predicted_cls[0])
print("Actual Class :", test_y[test_point_index])
neighbors = clf.kneighbors(test_x_responseCoding[test_point_index].reshape(1,
-1), alpha[best_alpha])
print("The ",alpha[best_alpha]," nearest neighbours of the test points belongs
to classes",train_y[neighbors[1][0]])
print("Fequency of nearest points :",Counter(train_y[neighbors[1][0]]))

Predicted Class : 7
Actual Class : 7
The 11 nearest neighbours of the test points belongs to classes [7 7 7 7 7
7 7 7 7 2 2]
Fequency of nearest points : Counter({7: 9, 2: 2})
```

4.2.4. Sample Query Point-2

```
In [65]: clf = KNeighborsClassifier(n_neighbors=alpha[best_alpha])
clf.fit(train_x_responseCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_responseCoding, train_y)

test_point_index = 5

predicted_cls = sig_clf.predict(test_x_responseCoding[test_point_index].reshap
e(1,-1))
print("Predicted Class :", predicted_cls[0])
print("Actual Class :", test_y[test_point_index])
neighbors = clf.kneighbors(test_x_responseCoding[test_point_index].reshape(1,
-1), alpha[best_alpha])
print("the k value for knn is",alpha[best_alpha],"and the nearest neighbours o
f the test points belongs to classes",train_y[neighbors[1][0]])
print("Fequency of nearest points :",Counter(train_y[neighbors[1][0]]))

Predicted Class : 7
Actual Class : 6
the k value for knn is 11 and the nearest neighbours of the test points belon
gs to classes [6 7 7 7 2 7 7 6 2 7 7]
Fequency of nearest points : Counter({7: 7, 2: 2, 6: 2})
```

4.3. Logistic Regression

4.3.1. With Class balancing

4.3.1.1. Hyper paramter tuning

```

In [104]: # read more about SGDClassifier() at http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.SGDClassifier.html
# -----
# default parameters
# SGDClassifier(loss='hinge', penalty='l2', alpha=0.0001, l1_ratio=0.15, fit_intercept=True, max_iter=None, tol=None,
# shuffle=True, verbose=0, epsilon=0.1, n_jobs=1, random_state=None, learning_rate='optimal', eta0=0.0, power_t=0.5,
# class_weight=None, warm_start=False, average=False, n_iter=None)

# some of methods
# fit(X, y[, coef_init, intercept_init, ...])      Fit linear model with Stochastic Gradient Descent.
# predict(X)      Predict class labels for samples in X.

#-----
# video link: https://www.appliedaicourse.com/course/applied-ai-course-online/lessons/geometric-intuition-1/
#-----

# find more about CalibratedClassifierCV here at http://scikit-learn.org/stable/modules/generated/sklearn.calibration.CalibratedClassifierCV.html
# -----
# default paramters
# sklearn.calibration.CalibratedClassifierCV(base_estimator=None, method='sigmoid', cv=3)
#
# some of the methods of CalibratedClassifierCV()
# fit(X, y[, sample_weight])      Fit the calibrated model
# get_params([deep])      Get parameters for this estimator.
# predict(X)      Predict the target of new samples.
# predict_proba(X)      Posterior probabilities of classification
#-----
# video link:
#-----

alpha = [10 ** x for x in range(-6, 3)]
cv_log_error_array = []
for i in alpha:
    print("for alpha =", i)
    clf = SGDClassifier(class_weight='balanced', alpha=i, penalty='l2', loss='log', random_state=42)
    clf.fit(train_x_onehotCoding, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x_onehotCoding, train_y)
    sig_clf_probs = sig_clf.predict_proba(cv_x_onehotCoding)
    cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes_, eps=1e-15))
    # to avoid rounding error while multiplying probabilities we use log-probability estimates
    print("Log Loss :", log_loss(cv_y, sig_clf_probs))

fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):

```

```
ax.annotate((alpha[i],str(txt)), (alpha[i],cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

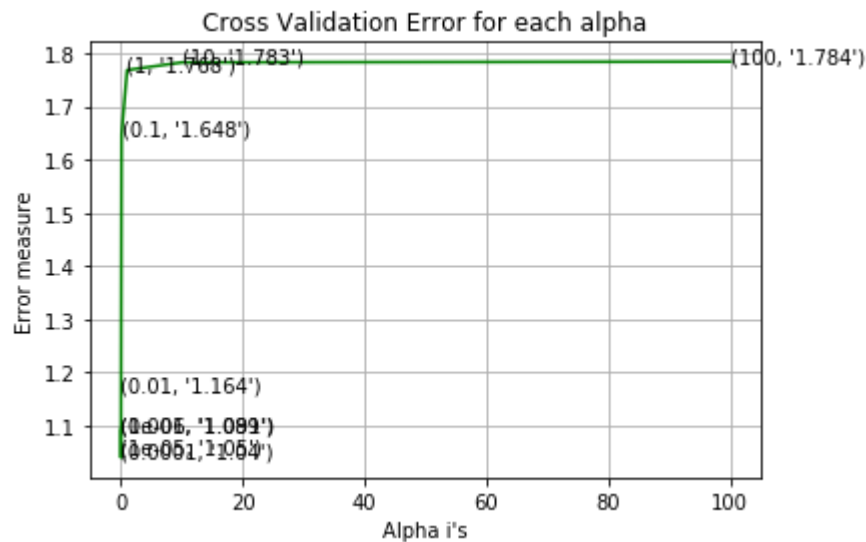
best_alpha = np.argmin(cv_log_error_array)
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty=
'12', loss='log', random_state=42)
clf.fit(train_x_onehotCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_onehotCoding, train_y)

predict_y = sig_clf.predict_proba(train_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss i
s:",log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation
log loss is:",log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss i
s:",log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))
```

```

for alpha = 1e-06
Log Loss : 1.0914491187749007
for alpha = 1e-05
Log Loss : 1.049706811580974
for alpha = 0.0001
Log Loss : 1.0396964861215026
for alpha = 0.001
Log Loss : 1.0893686813836045
for alpha = 0.01
Log Loss : 1.1637505157598274
for alpha = 0.1
Log Loss : 1.6476310666813305
for alpha = 1
Log Loss : 1.7681793697081507
for alpha = 10
Log Loss : 1.782553230134367
for alpha = 100
Log Loss : 1.7840827605565979

```



For values of best alpha = 0.0001 The train log loss is: 0.414428606953632
 For values of best alpha = 0.0001 The cross validation log loss is: 1.0396964861215026
 For values of best alpha = 0.0001 The test log loss is: 0.9860566892998761

4.3.1.2. Testing the model with best hyper paramters

```
In [105]: # read more about SGDClassifier() at http://scikit-learn.org/stable/modules/generated/sklearn.linear\_model.SGDClassifier.html
# -----
# default parameters
# SGDClassifier(loss='hinge', penalty='l2', alpha=0.0001, l1_ratio=0.15, fit_intercept=True, max_iter=None, tol=None,
# shuffle=True, verbose=0, epsilon=0.1, n_jobs=1, random_state=None, learning_rate='optimal', eta0=0.0, power_t=0.5,
# class_weight=None, warm_start=False, average=False, n_iter=None)

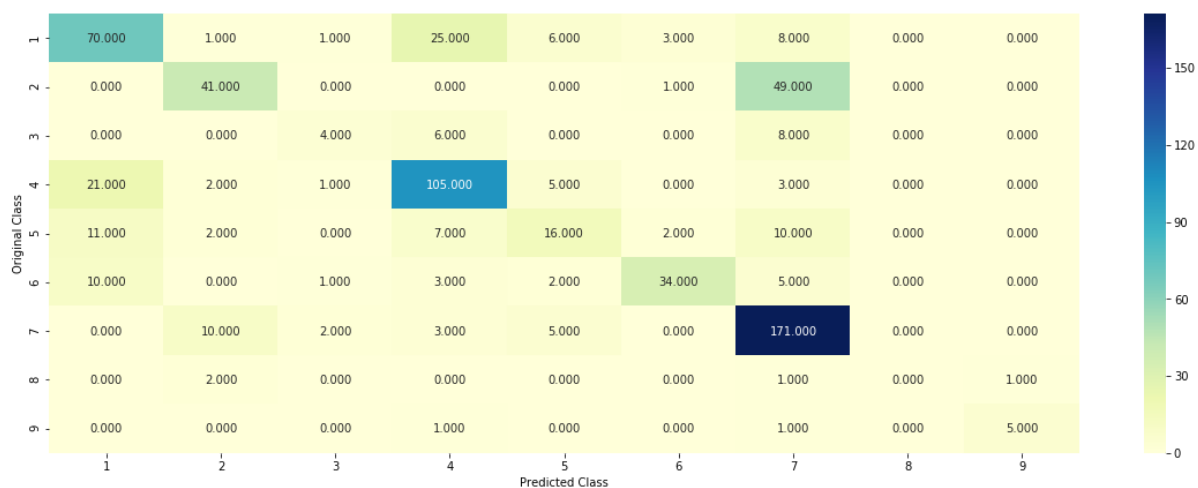
# some of methods
# fit(X, y[, coef_init, intercept_init, ...])    Fit linear model with Stochastic Gradient Descent.
# predict(X)    Predict class labels for samples in X.

#-----
# video link: https://www.appliedaicourse.com/course/applied-ai-course-online/lessons/geometric-intuition-1/
#-----
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty='l2', loss='log', random_state=42)
predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y, test_x_onehotCoding, test_y, clf)
```

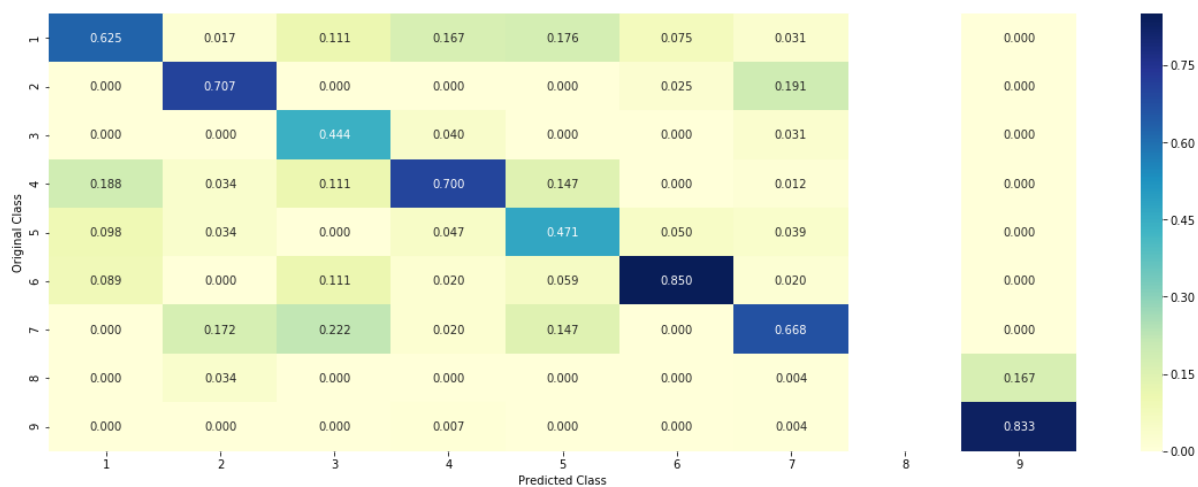
Log loss : 0.9860566892998761

Number of mis-classified points : 0.3293233082706767

----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.3.1.3. Feature Importance

```

In [68]: def get_imp_feature_names(text, indices, removed_ind = []):
    word_present = 0
    tabulte_list = []
    incresingorder_ind = 0
    for i in indices:
        if i < train_gene_feature_onehotCoding.shape[1]:
            tabulte_list.append([incresingorder_ind, "Gene", "Yes"])
        elif i < 18:
            tabulte_list.append([incresingorder_ind, "Variation", "Yes"])
        if ((i > 17) & (i not in removed_ind)) :
            word = train_text_features[i]
            yes_no = True if word in text.split() else False
            if yes_no:
                word_present += 1
            tabulte_list.append([incresingorder_ind, train_text_features[i], yes_no])
        incresingorder_ind += 1
    print(word_present, "most important features are present in our query point")
    print("-"*50)
    print("The features that are most important of the ", predicted_cls[0], " class:")
    print(tabulate(tabulte_list, headers=["Index", 'Feature name', 'Present or Not']))

```

4.3.1.3.1. Correctly Classified point


```
In [70]: # from tabulate import tabulate
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty=
'12', loss='log', random_state=42)
clf.fit(train_x_onehotCoding,train_y)
test_point_index = 11
no_feature = 300
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:,:no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_d
f['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_point_index],
no_feature)
```

Predicted Class : 4

Predicted Class Probabilities: [[1.54e-01 1.23e-02 6.60e-03 8.06e-01 9.50e-03
6.10e-03 3.90e-03 9.00e-04
8.00e-04]]

Actual Class : 4

```
-----
142 Text feature [inactivating] present in test data point [True]
147 Text feature [suppressor] present in test data point [True]
191 Text feature [inactivation] present in test data point [True]
218 Text feature [stabilization] present in test data point [True]
229 Text feature [bind] present in test data point [True]
237 Text feature [subcellular] present in test data point [True]
240 Text feature [spectra] present in test data point [True]
263 Text feature [consequence] present in test data point [True]
270 Text feature [asp] present in test data point [True]
295 Text feature [nonsense] present in test data point [True]
Out of the top 300 features 10 are present in query point
```

4.3.1.3.2. Incorrectly Classified point

```
In [71]: test_point_index = 5
no_feature = 300
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:,no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_d
f['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_point_index],
no_feature)
```

Predicted Class : 7

Predicted Class Probabilities: [[1.000e-03 4.321e-01 1.200e-03 4.000e-04 3.50
0e-03 1.920e-02 5.419e-01
4.000e-04 2.000e-04]]

Actual Class : 6

```
-----
53 Text feature [cross] present in test data point [True]
56 Text feature [nude] present in test data point [True]
62 Text feature [downstream] present in test data point [True]
65 Text feature [adenocarcinomas] present in test data point [True]
88 Text feature [activated] present in test data point [True]
98 Text feature [doses] present in test data point [True]
112 Text feature [overexpression] present in test data point [True]
129 Text feature [enhance] present in test data point [True]
130 Text feature [constitutive] present in test data point [True]
131 Text feature [nf] present in test data point [True]
132 Text feature [virus] present in test data point [True]
138 Text feature [untreated] present in test data point [True]
139 Text feature [rarely] present in test data point [True]
148 Text feature [activation] present in test data point [True]
156 Text feature [receptors] present in test data point [True]
161 Text feature [transformed] present in test data point [True]
162 Text feature [remain] present in test data point [True]
167 Text feature [ligand] present in test data point [True]
185 Text feature [lipid] present in test data point [True]
196 Text feature [enhanced] present in test data point [True]
201 Text feature [intrinsic] present in test data point [True]
202 Text feature [3t3] present in test data point [True]
216 Text feature [independently] present in test data point [True]
244 Text feature [pediatric] present in test data point [True]
247 Text feature [overcome] present in test data point [True]
254 Text feature [term] present in test data point [True]
259 Text feature [lymphomas] present in test data point [True]
279 Text feature [91] present in test data point [True]
280 Text feature [month] present in test data point [True]
288 Text feature [heterogeneous] present in test data point [True]
295 Text feature [inhibitor] present in test data point [True]
297 Text feature [extent] present in test data point [True]
Out of the top 300 features 32 are present in query point
```

4.3.2. Without Class balancing

4.3.2.1. Hyper paramter tuning

```

In [106]: alpha = [10 ** x for x in range(-6, 1)]
cv_log_error_array = []
for i in alpha:
    print("for alpha =", i)
    clf = SGDClassifier(alpha=i, penalty='l2', loss='log', random_state=42)
    clf.fit(train_x_onehotCoding, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x_onehotCoding, train_y)
    sig_clf_probs = sig_clf.predict_proba(cv_x_onehotCoding)
    cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes_,
    _, eps=1e-15))
    print("Log Loss :", log_loss(cv_y, sig_clf_probs))

fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], str(txt)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

best_alpha = np.argmin(cv_log_error_array)
clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_
state=42)
clf.fit(train_x_onehotCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_onehotCoding, train_y)

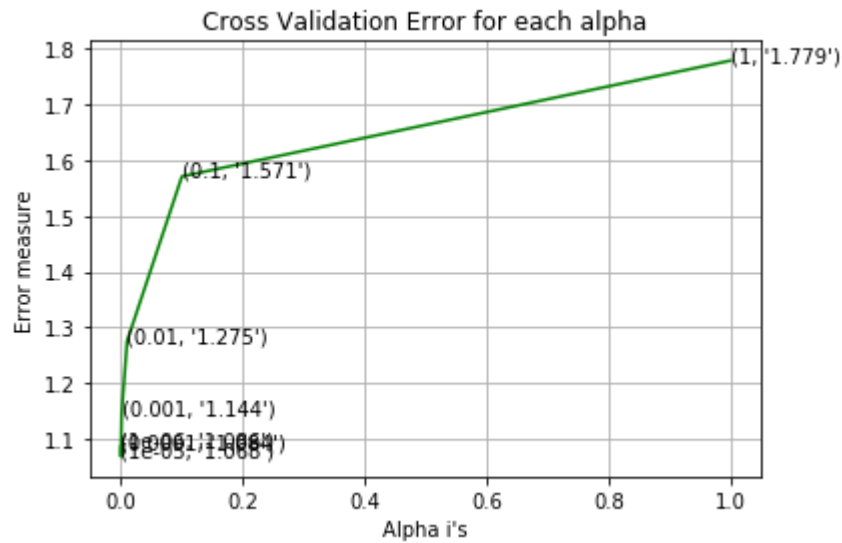
predict_y = sig_clf.predict_proba(train_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss i
s:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation
log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss i
s:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

```

for alpha = 1e-06
Log Loss : 1.0857713172441734
for alpha = 1e-05
Log Loss : 1.0681720993905723
for alpha = 0.0001
Log Loss : 1.084079097351972
for alpha = 0.001
Log Loss : 1.143514987529129
for alpha = 0.01
Log Loss : 1.2754641684278205
for alpha = 0.1
Log Loss : 1.5711867818815803
for alpha = 1
Log Loss : 1.7790023232702894

```



For values of best alpha = 1e-05 The train log loss is: 0.46574530399776204
 For values of best alpha = 1e-05 The cross validation log loss is: 1.0681720993905723
 For values of best alpha = 1e-05 The test log loss is: 1.0843585331668242

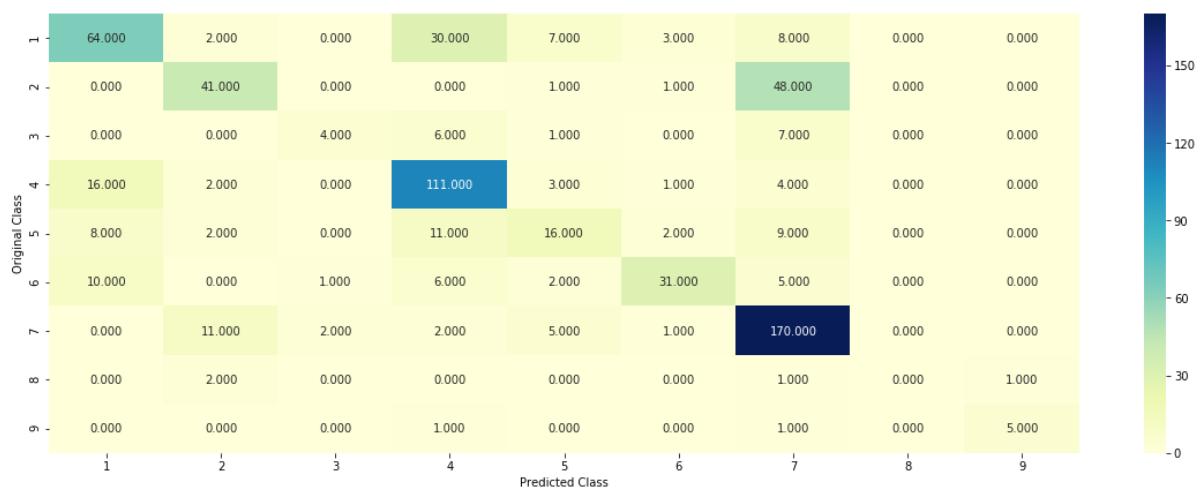
4.3.2.2. Testing model with best hyper parameters

```
In [107]: clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_
state=42)
predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y, test_x_onehot
Coding, test_y, clf)
```

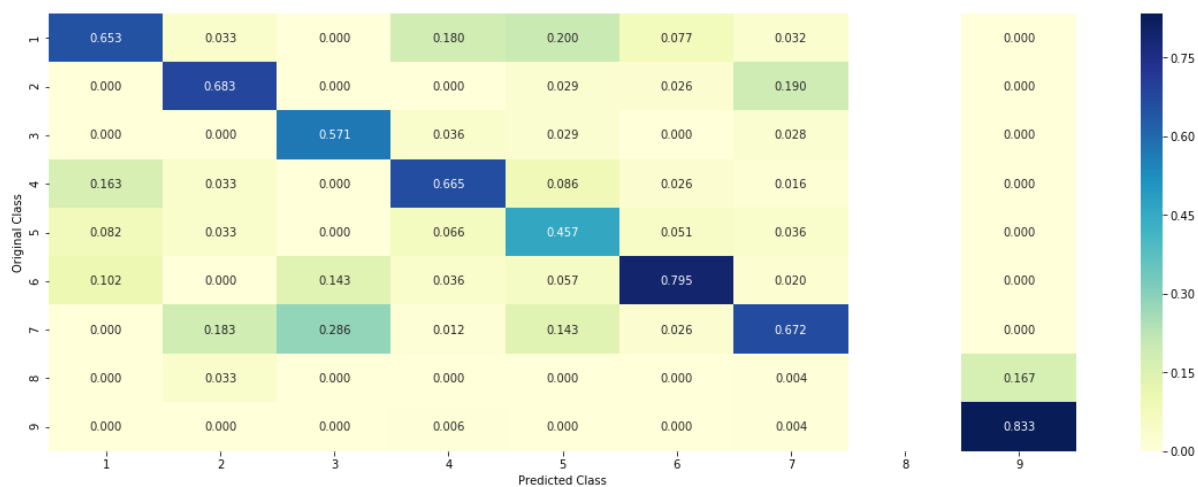
Log loss : 1.0843585331668242

Number of mis-classified points : 0.33533834586466166

----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.3.2.3. Feature Importance, Correctly Classified point

```
In [74]: clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_
state=42)
clf.fit(train_x_onehotCoding,train_y)
test_point_index = 11
no_feature = 300
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:,no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_d
f['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_point_index],
no_feature)
```

Predicted Class : 4

Predicted Class Probabilities: [[1.241e-01 2.390e-02 1.120e-02 7.668e-01 3.64
0e-02 2.450e-02 1.080e-02
1.700e-03 6.000e-04]]

Actual Class : 4

80 Text feature [asp] present in test data point [True]
275 Text feature [iii] present in test data point [True]
283 Text feature [spectra] present in test data point [True]
Out of the top 300 features 3 are present in query point

4.3.2.4. Feature Importance, Inorrectly Classified point


```
In [75]: test_point_index = 5
no_feature = 300
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:,no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_d
f['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_point_index],
no_feature)
```

Predicted Class : 7

Predicted Class Probabilities: [[2.800e-03 3.743e-01 3.800e-03 1.100e-03 1.12
0e-02 1.940e-02 5.861e-01
1.300e-03 1.000e-04]]

Actual Class : 6

```
-----
54 Text feature [adenocarcinomas] present in test data point [True]
56 Text feature [cross] present in test data point [True]
81 Text feature [remain] present in test data point [True]
84 Text feature [nude] present in test data point [True]
87 Text feature [term] present in test data point [True]
101 Text feature [downstream] present in test data point [True]
112 Text feature [untreated] present in test data point [True]
114 Text feature [overexpression] present in test data point [True]
118 Text feature [independently] present in test data point [True]
144 Text feature [advanced] present in test data point [True]
162 Text feature [rarely] present in test data point [True]
167 Text feature [91] present in test data point [True]
174 Text feature [us] present in test data point [True]
179 Text feature [lipid] present in test data point [True]
183 Text feature [lesions] present in test data point [True]
184 Text feature [metastases] present in test data point [True]
216 Text feature [inhibitor] present in test data point [True]
224 Text feature [heterogeneous] present in test data point [True]
227 Text feature [86] present in test data point [True]
241 Text feature [intrinsic] present in test data point [True]
Out of the top 300 features 20 are present in query point
```

4.4. Linear Support Vector Machines

4.4.1. Hyper paramter tuning

```

In [108]: alpha = [10 ** x for x in range(-5, 3)]
cv_log_error_array = []
for i in alpha:
    print("for C =", i)
    # clf = SVC(C=i, kernel='linear', probability=True, class_weight='balanced')
    clf = SGDClassifier(class_weight='balanced', alpha=i, penalty='l2', loss=
'hinge', random_state=42)
    clf.fit(train_x_onehotCoding, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x_onehotCoding, train_y)
    sig_clf_probs = sig_clf.predict_proba(cv_x_onehotCoding)
    cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes
_, eps=1e-15))
    print("Log Loss :", log_loss(cv_y, sig_clf_probs))

fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], str(txt)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

best_alpha = np.argmin(cv_log_error_array)
# clf = SVC(C=i, kernel='linear', probability=True, class_weight='balanced')
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty=
'l2', loss='hinge', random_state=42)
clf.fit(train_x_onehotCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_onehotCoding, train_y)

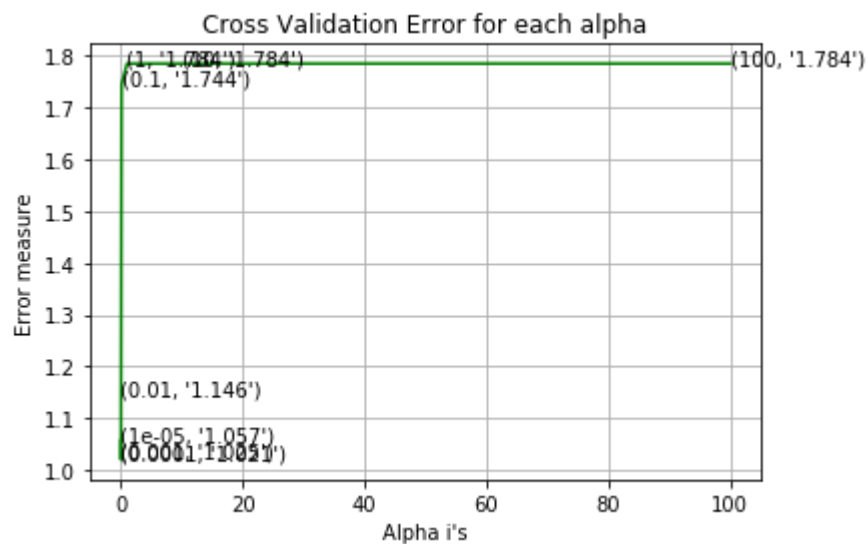
predict_y = sig_clf.predict_proba(train_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss i
s:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation
log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_onehotCoding)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss i
s:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

```

for C = 1e-05
Log Loss : 1.0570465653544852
for C = 0.0001
Log Loss : 1.0205552821213693
for C = 0.001
Log Loss : 1.024986214599474
for C = 0.01
Log Loss : 1.1457297182312518
for C = 0.1
Log Loss : 1.7443270987369555
for C = 1
Log Loss : 1.7844082347530408
for C = 10
Log Loss : 1.7844082284792935
for C = 100
Log Loss : 1.7844082176585756

```



For values of best alpha = 0.0001 The train log loss is: 0.4000688840166313
 For values of best alpha = 0.0001 The cross validation log loss is: 1.0205552821213693
 For values of best alpha = 0.0001 The test log loss is: 1.0451559188685706

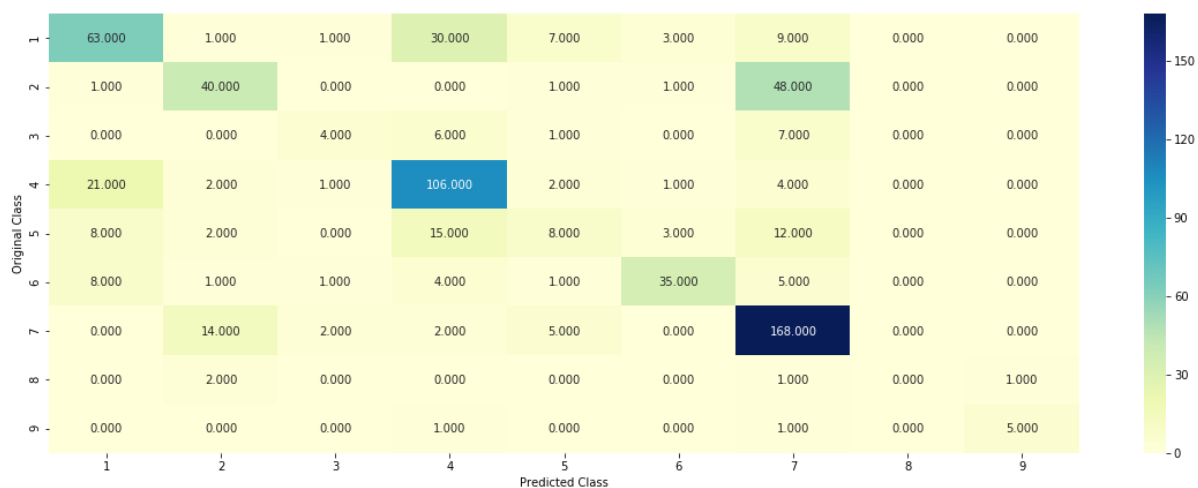
4.4.2. Testing model with best hyper parameters

```
In [109]: clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='hinge', random_state=42, class_weight='balanced')
          predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y, test_x_onehotCoding, test_y, clf)
```

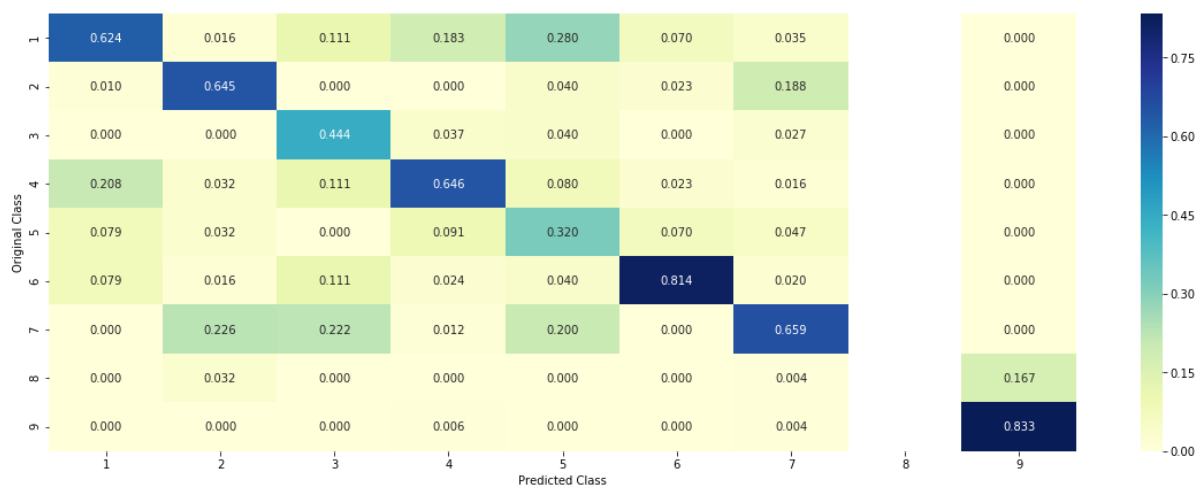
Log loss : 1.0451559188685706

Number of mis-classified points : 0.3548872180451128

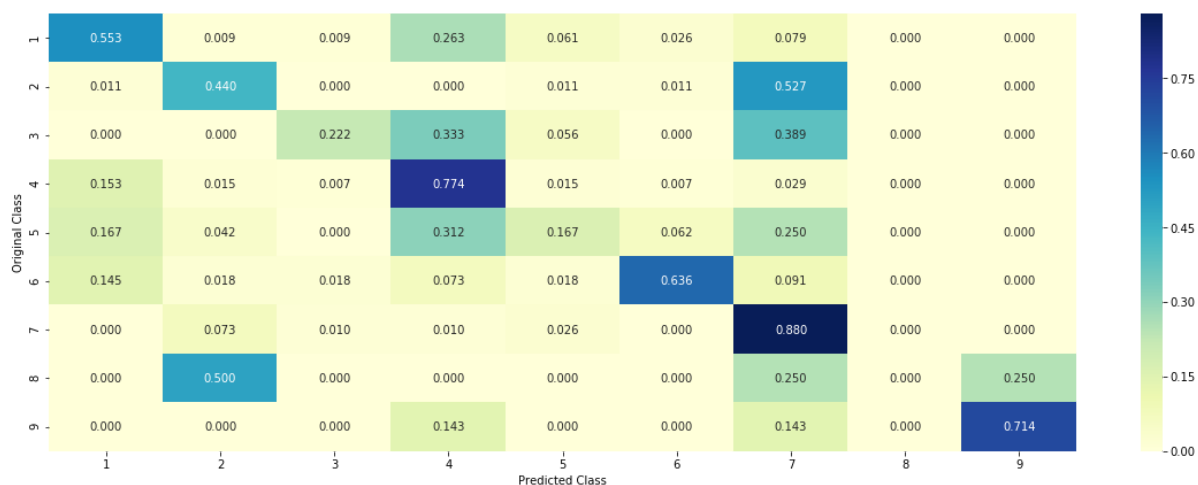
----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.3.3. Feature Importance

4.3.3.1. For Correctly classified point

```
In [78]: clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='hinge', random_state=42)
clf.fit(train_x_onehotCoding, train_y)
test_point_index = 11
# test_point_index = 100
no_feature = 300
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_onehotCoding[test_point_index]), 4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:, :no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index], test_df['Gene'].iloc[test_point_index], test_df['Variation'].iloc[test_point_index], no_feature)
```

Predicted Class : 4

Predicted Class Probabilities: [[0.1269 0.0377 0.0099 0.7484 0.0472 0.0163 0.0113 0.0011 0.0012]]

Actual Class : 4

```
-----
203 Text feature [stabilization] present in test data point [True]
208 Text feature [inactivating] present in test data point [True]
213 Text feature [bind] present in test data point [True]
215 Text feature [asp] present in test data point [True]
216 Text feature [glu] present in test data point [True]
220 Text feature [consequence] present in test data point [True]
Out of the top 300 features 6 are present in query point
```

4.3.3.2. For Incorrectly classified point

```
In [79]: test_point_index = 5
no_feature = 300
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.coef_)[predicted_cls-1][:,no_feature]
print("-"*50)
get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_d
f['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_point_index],
no_feature)
```

Predicted Class : 7

Predicted Class Probabilities: [[1.600e-03 4.272e-01 2.600e-03 1.900e-03 1.88
0e-02 2.730e-02 5.195e-01
6.000e-04 5.000e-04]]

Actual Class : 6

```
-----
120 Text feature [overexpression] present in test data point [True]
121 Text feature [nude] present in test data point [True]
126 Text feature [independently] present in test data point [True]
127 Text feature [heterogeneous] present in test data point [True]
128 Text feature [remain] present in test data point [True]
129 Text feature [downstream] present in test data point [True]
131 Text feature [cross] present in test data point [True]
219 Text feature [adenocarcinomas] present in test data point [True]
222 Text feature [untreated] present in test data point [True]
231 Text feature [treating] present in test data point [True]
233 Text feature [doses] present in test data point [True]
236 Text feature [3t3] present in test data point [True]
239 Text feature [virus] present in test data point [True]
242 Text feature [enhance] present in test data point [True]
253 Text feature [cancers] present in test data point [True]
255 Text feature [activated] present in test data point [True]
261 Text feature [protocol] present in test data point [True]
263 Text feature [overcome] present in test data point [True]
267 Text feature [ligands] present in test data point [True]
270 Text feature [enhanced] present in test data point [True]
272 Text feature [rarely] present in test data point [True]
274 Text feature [91] present in test data point [True]
279 Text feature [intrinsic] present in test data point [True]
282 Text feature [parameters] present in test data point [True]
Out of the top 300 features 24 are present in query point
```

4.5 Random Forest Classifier

4.5.1. Hyper paramter tuning (With One hot Encoding)

```

In [110]: alpha = [100,200,500,1000,2000]
max_depth = [5, 10]
cv_log_error_array = []
for i in alpha:
    for j in max_depth:
        print("for n_estimators =", i,"and max depth = ", j)
        clf = RandomForestClassifier(n_estimators=i, criterion='gini', max_depth=j, random_state=42, n_jobs=-1)
        clf.fit(train_x_onehotCoding, train_y)
        sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
        sig_clf.fit(train_x_onehotCoding, train_y)
        sig_clf_probs = sig_clf.predict_proba(cv_x_onehotCoding)
        cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes_, eps=1e-15))
        print("Log Loss :",log_loss(cv_y, sig_clf_probs))

'''fig, ax = plt.subplots()
features = np.dot(np.array(alpha)[: ,None],np.array(max_depth)[None]).ravel()
ax.plot(features, cv_log_error_array,c='g')
for i, txt in enumerate(np.round(cv_log_error_array,3)):
    ax.annotate((alpha[int(i/2)],max_depth[int(i%2)],str(txt)), (features[i],cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()
'''

best_alpha = np.argmin(cv_log_error_array)
clf = RandomForestClassifier(n_estimators=alpha[int(best_alpha/2)], criterion='gini', max_depth=max_depth[int(best_alpha%2)], random_state=42, n_jobs=-1)
clf.fit(train_x_onehotCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_onehotCoding, train_y)

predict_y = sig_clf.predict_proba(train_x_onehotCoding)
print('For values of best estimator = ', alpha[int(best_alpha/2)], "The train log loss is:",log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_onehotCoding)
print('For values of best estimator = ', alpha[int(best_alpha/2)], "The cross validation log loss is:",log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_onehotCoding)
print('For values of best estimator = ', alpha[int(best_alpha/2)], "The test log loss is:",log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```



```
for n_estimators = 100 and max depth = 5
Log Loss : 1.2150018049530225
for n_estimators = 100 and max depth = 10
Log Loss : 1.1760807589148536
for n_estimators = 200 and max depth = 5
Log Loss : 1.1963578774840096
for n_estimators = 200 and max depth = 10
Log Loss : 1.1595625527864588
for n_estimators = 500 and max depth = 5
Log Loss : 1.1890810814033
for n_estimators = 500 and max depth = 10
Log Loss : 1.161460992507832
for n_estimators = 1000 and max depth = 5
Log Loss : 1.1864263879386292
for n_estimators = 1000 and max depth = 10
Log Loss : 1.1629487705124686
for n_estimators = 2000 and max depth = 5
Log Loss : 1.184558232717106
for n_estimators = 2000 and max depth = 10
Log Loss : 1.1602360970350871
For values of best estimator = 200 The train log loss is: 0.5923182491087172
For values of best estimator = 200 The cross validation log loss is: 1.15956
25527864586
For values of best estimator = 200 The test log loss is: 1.1074529416264431
```

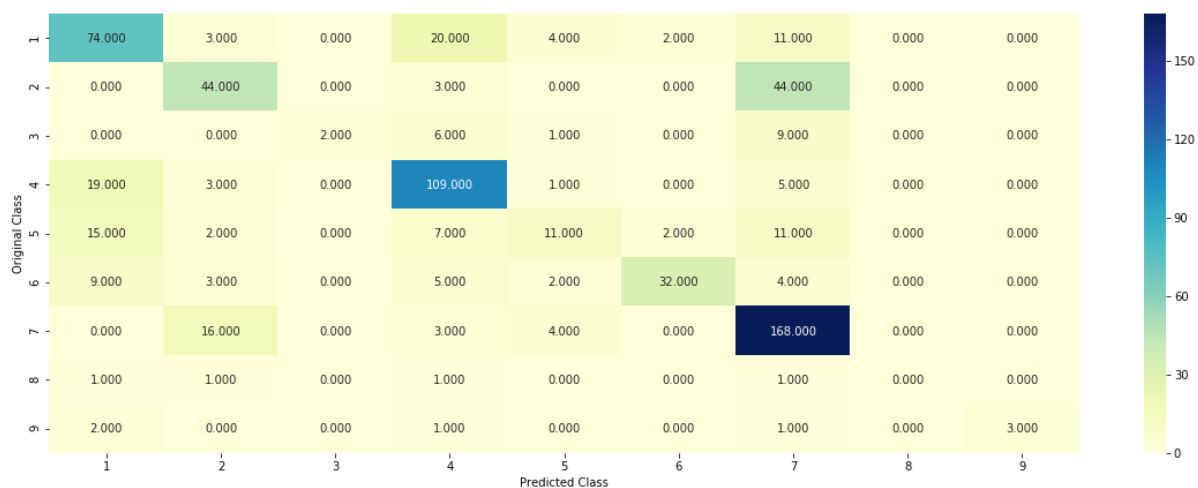
4.5.2. Testing model with best hyper parameters (One Hot Encoding)

```
In [111]: clf = RandomForestClassifier(n_estimators=alpha[int(best_alpha/2)], criterion=  
      'gini', max_depth=max_depth[int(best_alpha%2)], random_state=42, n_jobs=-1)  
      predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y, test_x_onehotC  
      oding, test_y, clf)
```

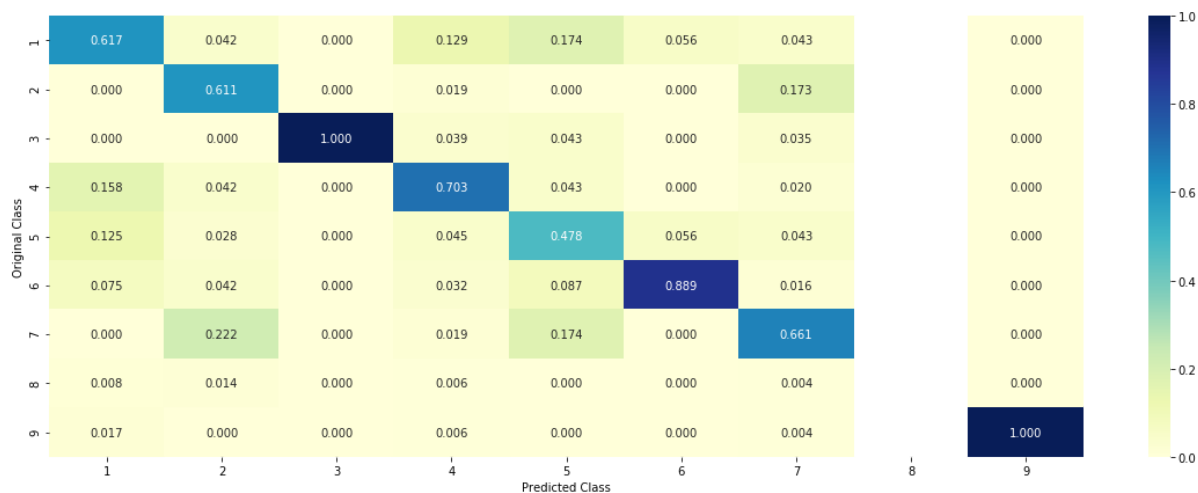
Log loss : 1.1074529416264431

Number of mis-classified points : 0.33383458646616543

----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.5.3. Feature Importance

4.5.3.1. Correctly Classified point

```
In [82]: # test_point_index = 10
clf = RandomForestClassifier(n_estimators=alpha[int(best_alpha/2)], criterion=
'gini', max_depth=max_depth[int(best_alpha%2)], random_state=42, n_jobs=-1)
clf.fit(train_x_onehotCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_onehotCoding, train_y)

test_point_index = 11
no_feature = 100
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.feature_importances_)
print("-"*50)
get_impfeature_names(indices[:no_feature], test_df['TEXT'].iloc[test_point_ind
ex],test_df['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_poin
t_index], no_feature)
```

Predicted Class : 4

Predicted Class Probabilities: [[0.1392 0.0461 0.0183 0.6725 0.0357 0.0303 0.0494 0.0036 0.0047]]

Actual Class : 4

```
-----
0 Text feature [kinase] present in test data point [True]
3 Text feature [activated] present in test data point [True]
8 Text feature [phosphorylation] present in test data point [True]
10 Text feature [inhibitors] present in test data point [True]
11 Text feature [suppressor] present in test data point [True]
13 Text feature [missense] present in test data point [True]
14 Text feature [activation] present in test data point [True]
17 Text feature [function] present in test data point [True]
26 Text feature [activating] present in test data point [True]
27 Text feature [protein] present in test data point [True]
28 Text feature [loss] present in test data point [True]
29 Text feature [growth] present in test data point [True]
31 Text feature [nonsense] present in test data point [True]
38 Text feature [cells] present in test data point [True]
40 Text feature [functional] present in test data point [True]
43 Text feature [inhibition] present in test data point [True]
54 Text feature [proteins] present in test data point [True]
61 Text feature [cell] present in test data point [True]
85 Text feature [functions] present in test data point [True]
87 Text feature [activity] present in test data point [True]
96 Text feature [11] present in test data point [True]
97 Text feature [inhibited] present in test data point [True]
98 Text feature [lines] present in test data point [True]
99 Text feature [defective] present in test data point [True]
Out of the top 100 features 24 are present in query point
```

4.5.3.2. Inorrectly Classified point

```
In [83]: test_point_index = 5
no_feature = 100
predicted_cls = sig_clf.predict(test_x_onehotCoding[test_point_index])
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
onehotCoding[test_point_index]),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.feature_importances_)
print("-"*50)
get_impfeature_names(indices[:no_feature], test_df['TEXT'].iloc[test_point_ind
ex],test_df['Gene'].iloc[test_point_index],test_df['Variation'].iloc[test_poin
t_index], no_feature)
```

Predicted Class : 7

Predicted Class Probabilities: [[0.0673 0.1727 0.0187 0.0361 0.0371 0.0421 0.6162 0.0041 0.0057]]

Actual Class : 6

0 Text feature [kinase] present in test data point [True]
3 Text feature [activated] present in test data point [True]
6 Text feature [tyrosine] present in test data point [True]
7 Text feature [constitutive] present in test data point [True]
8 Text feature [phosphorylation] present in test data point [True]
10 Text feature [inhibitors] present in test data point [True]
11 Text feature [suppressor] present in test data point [True]
12 Text feature [treatment] present in test data point [True]
13 Text feature [missense] present in test data point [True]
14 Text feature [activation] present in test data point [True]
15 Text feature [pten] present in test data point [True]
16 Text feature [inhibitor] present in test data point [True]
17 Text feature [function] present in test data point [True]
18 Text feature [erk] present in test data point [True]
21 Text feature [oncogenic] present in test data point [True]
22 Text feature [treated] present in test data point [True]
23 Text feature [activate] present in test data point [True]
24 Text feature [ic50] present in test data point [True]
26 Text feature [activating] present in test data point [True]
27 Text feature [protein] present in test data point [True]
28 Text feature [loss] present in test data point [True]
29 Text feature [growth] present in test data point [True]
32 Text feature [signaling] present in test data point [True]
34 Text feature [months] present in test data point [True]
36 Text feature [clinical] present in test data point [True]
38 Text feature [cells] present in test data point [True]
40 Text feature [functional] present in test data point [True]
43 Text feature [inhibition] present in test data point [True]
49 Text feature [response] present in test data point [True]
50 Text feature [receptor] present in test data point [True]
54 Text feature [proteins] present in test data point [True]
56 Text feature [therapeutic] present in test data point [True]
60 Text feature [akt] present in test data point [True]
61 Text feature [cell] present in test data point [True]
64 Text feature [serum] present in test data point [True]
66 Text feature [advanced] present in test data point [True]
69 Text feature [potential] present in test data point [True]
71 Text feature [mek] present in test data point [True]
75 Text feature [amplification] present in test data point [True]
77 Text feature [repair] present in test data point [True]
81 Text feature [downstream] present in test data point [True]
82 Text feature [drug] present in test data point [True]
85 Text feature [functions] present in test data point [True]
87 Text feature [activity] present in test data point [True]
90 Text feature [transforming] present in test data point [True]
95 Text feature [therapy] present in test data point [True]
96 Text feature [11] present in test data point [True]
97 Text feature [inhibited] present in test data point [True]
98 Text feature [lines] present in test data point [True]
Out of the top 100 features 49 are present in query point

4.5.3 Hyperparameter tuning (With Response Coding)


```

In [112]: alpha = [10,50,100,200,500,1000]
max_depth = [2,3,5,10]
cv_log_error_array = []
for i in alpha:
    for j in max_depth:
        print("for n_estimators =", i,"and max depth = ", j)
        clf = RandomForestClassifier(n_estimators=i, criterion='gini', max_depth=j, random_state=42, n_jobs=-1)
        clf.fit(train_x_responseCoding, train_y)
        sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
        sig_clf.fit(train_x_responseCoding, train_y)
        sig_clf_probs = sig_clf.predict_proba(cv_x_responseCoding)
        cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes_, eps=1e-15))
        print("Log Loss :",log_loss(cv_y, sig_clf_probs))
    ...

fig, ax = plt.subplots()
features = np.dot(np.array(alpha)[: ,None],np.array(max_depth)[None]).ravel()
ax.plot(features, cv_log_error_array,c='g')
for i, txt in enumerate(np.round(cv_log_error_array,3)):
    ax.annotate((alpha[int(i/4)],max_depth[int(i%4)],str(txt)), (features[i],cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()
...

best_alpha = np.argmin(cv_log_error_array)
clf = RandomForestClassifier(n_estimators=alpha[int(best_alpha/4)], criterion='gini', max_depth=max_depth[int(best_alpha%4)], random_state=42, n_jobs=-1)
clf.fit(train_x_responseCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_responseCoding, train_y)

predict_y = sig_clf.predict_proba(train_x_responseCoding)
print('For values of best alpha = ', alpha[int(best_alpha/4)], "The train log loss is:",log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_responseCoding)
print('For values of best alpha = ', alpha[int(best_alpha/4)], "The cross validation log loss is:",log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_responseCoding)
print('For values of best alpha = ', alpha[int(best_alpha/4)], "The test log loss is:",log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

```

for n_estimators = 10 and max depth = 2
Log Loss : 2.2225779734772373
for n_estimators = 10 and max depth = 3
Log Loss : 1.7205643127841401
for n_estimators = 10 and max depth = 5
Log Loss : 1.4313599952830258
for n_estimators = 10 and max depth = 10
Log Loss : 1.865315410801488
for n_estimators = 50 and max depth = 2
Log Loss : 1.7375381419207148
for n_estimators = 50 and max depth = 3
Log Loss : 1.516699182666602
for n_estimators = 50 and max depth = 5
Log Loss : 1.3321330206327053
for n_estimators = 50 and max depth = 10
Log Loss : 1.6803327946441324
for n_estimators = 100 and max depth = 2
Log Loss : 1.6406706721132633
for n_estimators = 100 and max depth = 3
Log Loss : 1.5708347788634307
for n_estimators = 100 and max depth = 5
Log Loss : 1.3422163832378395
for n_estimators = 100 and max depth = 10
Log Loss : 1.6488195514062143
for n_estimators = 200 and max depth = 2
Log Loss : 1.6307137336295923
for n_estimators = 200 and max depth = 3
Log Loss : 1.5231411902051564
for n_estimators = 200 and max depth = 5
Log Loss : 1.3780173129537336
for n_estimators = 200 and max depth = 10
Log Loss : 1.6362521928538065
for n_estimators = 500 and max depth = 2
Log Loss : 1.6896906921532182
for n_estimators = 500 and max depth = 3
Log Loss : 1.5740439497618555
for n_estimators = 500 and max depth = 5
Log Loss : 1.4000628388519205
for n_estimators = 500 and max depth = 10
Log Loss : 1.6472567423500535
for n_estimators = 1000 and max depth = 2
Log Loss : 1.6568070311872165
for n_estimators = 1000 and max depth = 3
Log Loss : 1.5869373610621338
for n_estimators = 1000 and max depth = 5
Log Loss : 1.3829784042888842
for n_estimators = 1000 and max depth = 10
Log Loss : 1.6206387569050444
For values of best alpha = 50 The train log loss is: 0.05489681179369581
For values of best alpha = 50 The cross validation log loss is: 1.3321330206
327051
For values of best alpha = 50 The test log loss is: 1.3411921240569868

```

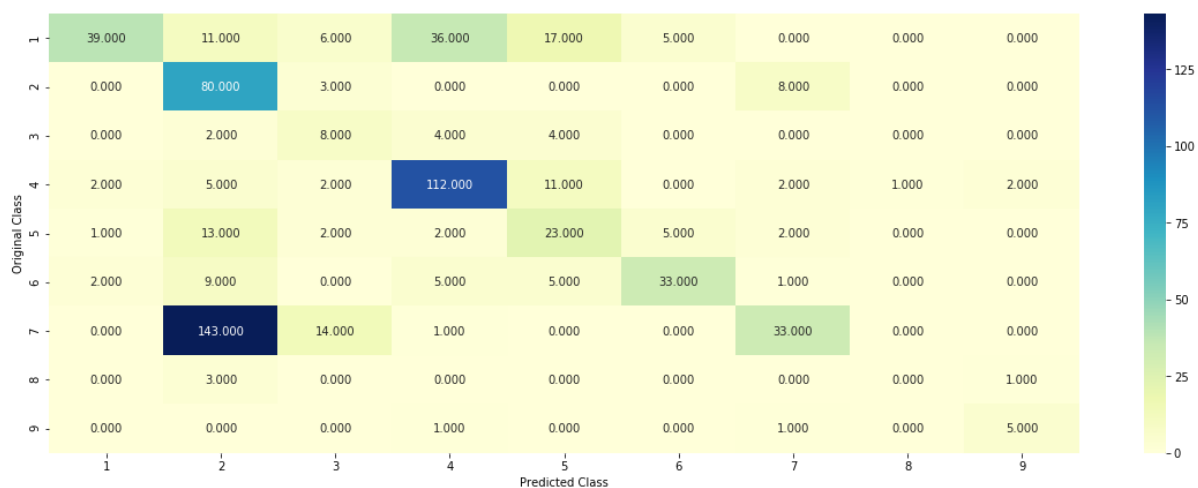
4.5.4. Testing model with best hyper parameters (Response Coding)

```
In [113]: clf = RandomForestClassifier(max_depth=max_depth[int(best_alpha%4)], n_estimators=alpha[int(best_alpha/4)], criterion='gini', max_features='auto', random_state=42)
predict_and_plot_confusion_matrix(train_x_responseCoding, train_y, test_x_responseCoding, test_y, clf)
```

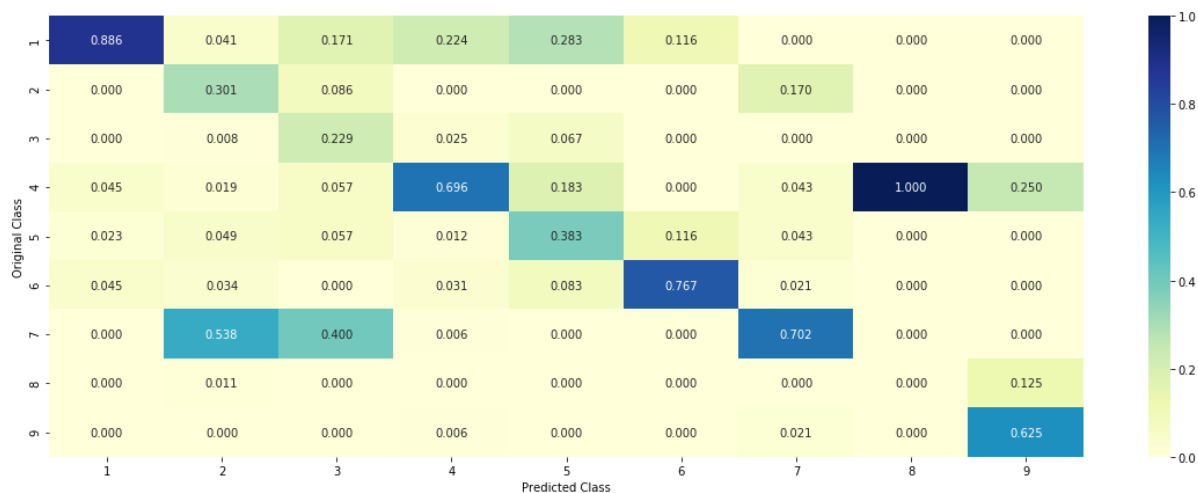
Log loss : 1.3411921240569866

Number of mis-classified points : 0.4992481203007519

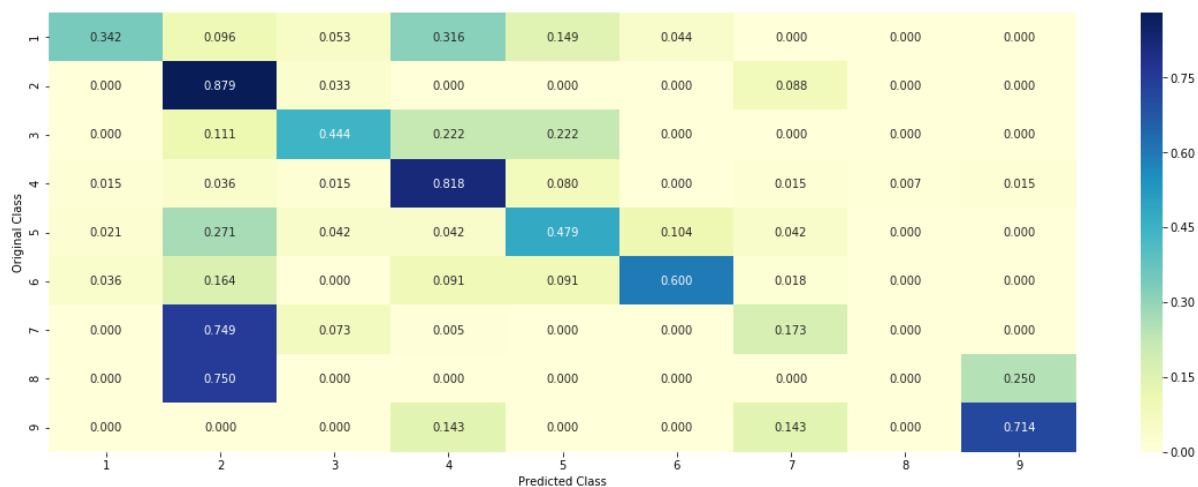
----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.5.5. Feature Importance

4.5.5.1. Correctly Classified point

```
In [86]: clf = RandomForestClassifier(n_estimators=alpha[int(best_alpha/4)], criterion=
'gini', max_depth=max_depth[int(best_alpha%4)], random_state=42, n_jobs=-1)
clf.fit(train_x_responseCoding, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_responseCoding, train_y)

test_point_index = 11
no_feature = 27
predicted_cls = sig_clf.predict(test_x_responseCoding[test_point_index].reshape(1,-1))
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_
responseCoding[test_point_index].reshape(1,-1)),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.feature_importances_)
print("-"*50)
for i in indices:
    if i<9:
        print("Gene is important feature")
    elif i<18:
        print("Variation is important feature")
    else:
        print("Text is important feature")
```

Predicted Class : 4

Predicted Class Probabilities: [[0.0235 0.0235 0.1762 0.698 0.0241 0.0223 0.0038 0.0127 0.0159]]

Actual Class : 4

Variation is important feature
Variation is important feature
Variation is important feature
Gene is important feature
Variation is important feature
Variation is important feature
Variation is important feature
Text is important feature
Text is important feature
Text is important feature
Text is important feature
Gene is important feature
Text is important feature
Variation is important feature
Gene is important feature
Gene is important feature
Text is important feature
Gene is important feature
Gene is important feature
Variation is important feature
Gene is important feature
Text is important feature
Text is important feature
Variation is important feature
Gene is important feature
Text is important feature
Gene is important feature

4.5.5.2. Incorrectly Classified point

```
In [87]: test_point_index = 5
predicted_cls = sig_clf.predict(test_x_responseCoding[test_point_index].reshape(1,-1))
print("Predicted Class :", predicted_cls[0])
print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_responseCoding[test_point_index].reshape(1,-1)),4))
print("Actual Class :", test_y[test_point_index])
indices = np.argsort(-clf.feature_importances_)
print("-"*50)
for i in indices:
    if i<9:
        print("Gene is important feature")
    elif i<18:
        print("Variation is important feature")
    else:
        print("Text is important feature")
```

Predicted Class : 2

Predicted Class Probabilities: [[0.0015 0.5003 0.0012 0.0025 0.0008 0.0093 0.4817 0.0016 0.0012]]

Actual Class : 6

```
-----
Variation is important feature
Variation is important feature
Variation is important feature
Gene is important feature
Variation is important feature
Variation is important feature
Variation is important feature
Text is important feature
Text is important feature
Text is important feature
Text is important feature
Text is important feature
Gene is important feature
Text is important feature
Variation is important feature
Gene is important feature
Gene is important feature
Text is important feature
Gene is important feature
Gene is important feature
Variation is important feature
Gene is important feature
Text is important feature
Text is important feature
Variation is important feature
Gene is important feature
Text is important feature
Gene is important feature
```

4.7 Stack the models

4.7.1 testing with hyper parameter tuning

```
In [88]: clf1 = SGDClassifier(alpha=0.001, penalty='l2', loss='log', class_weight='balanced', random_state=0)
clf1.fit(train_x_onehotCoding, train_y)
sig_clf1 = CalibratedClassifierCV(clf1, method="sigmoid")

clf2 = SGDClassifier(alpha=1, penalty='l2', loss='hinge', class_weight='balanced', random_state=0)
clf2.fit(train_x_onehotCoding, train_y)
sig_clf2 = CalibratedClassifierCV(clf2, method="sigmoid")

clf3 = MultinomialNB(alpha=0.001)
clf3.fit(train_x_onehotCoding, train_y)
sig_clf3 = CalibratedClassifierCV(clf3, method="sigmoid")

sig_clf1.fit(train_x_onehotCoding, train_y)
print("Logistic Regression : Log Loss: %0.2f" % (log_loss(cv_y, sig_clf1.predict_proba(cv_x_onehotCoding))))
sig_clf2.fit(train_x_onehotCoding, train_y)
print("Support vector machines : Log Loss: %0.2f" % (log_loss(cv_y, sig_clf2.predict_proba(cv_x_onehotCoding))))
sig_clf3.fit(train_x_onehotCoding, train_y)
print("Naïve Bayes : Log Loss: %0.2f" % (log_loss(cv_y, sig_clf3.predict_proba(cv_x_onehotCoding))))
print("-"*50)
alpha = [0.0001,0.001,0.01,0.1,1,10]
best_alpha = 999
for i in alpha:
    lr = LogisticRegression(C=i)
    scf = StackingClassifier(classifiers=[sig_clf1, sig_clf2, sig_clf3], meta_classifier=lr, use_probabilities=True)
    scf.fit(train_x_onehotCoding, train_y)
    print("Stacking Classifier : for the value of alpha: %f Log Loss: %0.3f" % (i, log_loss(cv_y, scf.predict_proba(cv_x_onehotCoding))))
    log_error = log_loss(cv_y, scf.predict_proba(cv_x_onehotCoding))
    if best_alpha > log_error:
        best_alpha = log_error
```

```
Logistic Regression : Log Loss: 1.09
Support vector machines : Log Loss: 1.78
Naïve Bayes : Log Loss: 1.24
```

```
-----
Stacking Classifier : for the value of alpha: 0.000100 Log Loss: 2.177
Stacking Classifier : for the value of alpha: 0.001000 Log Loss: 2.028
Stacking Classifier : for the value of alpha: 0.010000 Log Loss: 1.484
Stacking Classifier : for the value of alpha: 0.100000 Log Loss: 1.128
Stacking Classifier : for the value of alpha: 1.000000 Log Loss: 1.259
Stacking Classifier : for the value of alpha: 10.000000 Log Loss: 1.529
```

4.7.2 testing the model with the best hyper parameters

```
In [89]: lr = LogisticRegression(C=0.1)
sclf = StackingClassifier(classifiers=[sig_clf1, sig_clf2, sig_clf3], meta_classifier=lr, use_probabilities=True)
sclf.fit(train_x_onehotCoding, train_y)

log_error = log_loss(train_y, sclf.predict_proba(train_x_onehotCoding))
print("Log loss (train) on the stacking classifier :", log_error)

log_error = log_loss(cv_y, sclf.predict_proba(cv_x_onehotCoding))
print("Log loss (CV) on the stacking classifier :", log_error)

log_error = log_loss(test_y, sclf.predict_proba(test_x_onehotCoding))
print("Log loss (test) on the stacking classifier :", log_error)

print("Number of misclassified points :", np.count_nonzero((sclf.predict(test_x_onehotCoding) - test_y).sum(axis=1)))
plot_confusion_matrix(test_y=test_y, predict_y=sclf.predict(test_x_onehotCoding))
```

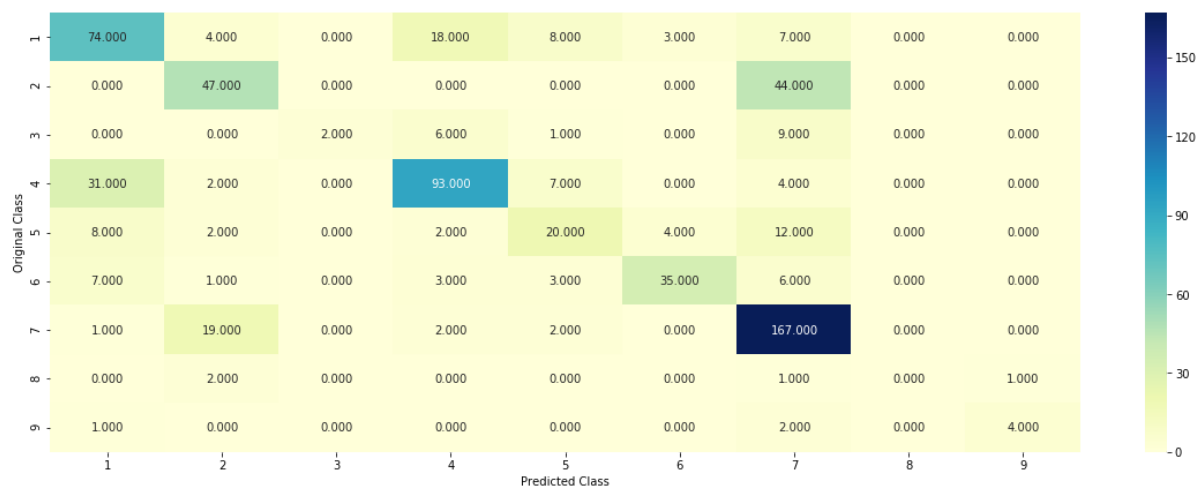
Log loss (train) on the stacking classifier : 0.6505369477610267

Log loss (CV) on the stacking classifier : 1.1281110077906034

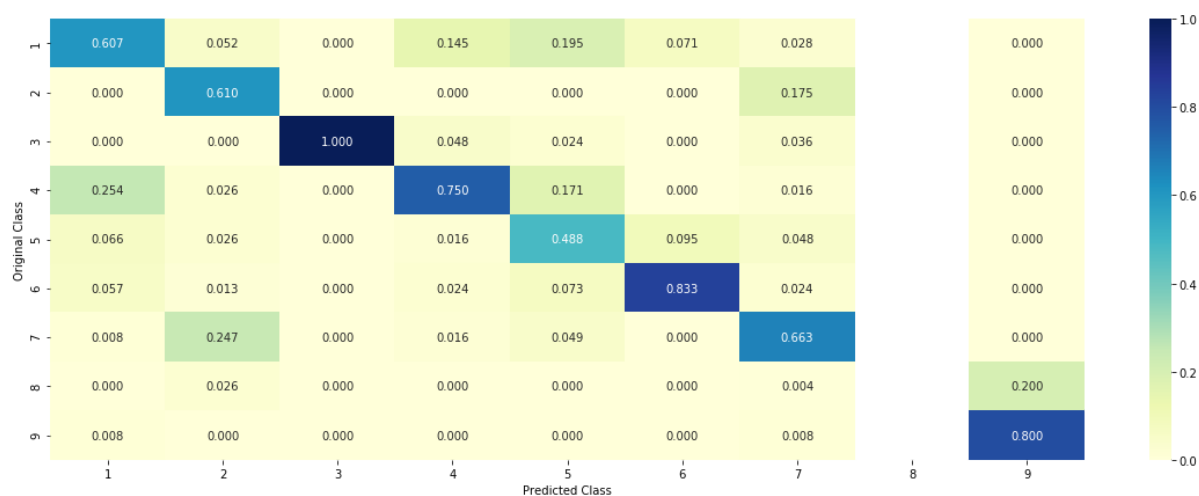
Log loss (test) on the stacking classifier : 1.0854815320633013

Number of missclassified point : 0.33533834586466166

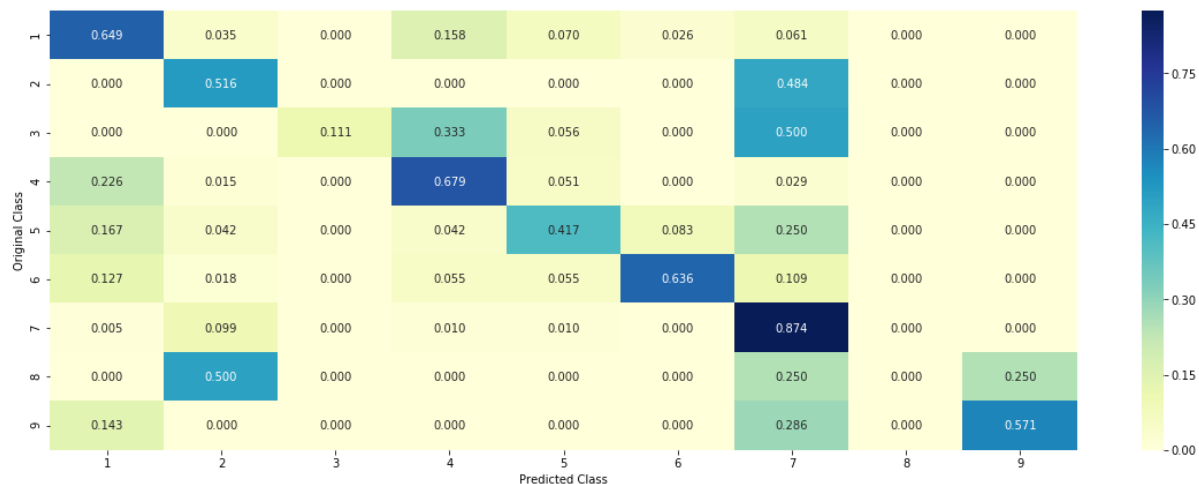
----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



4.7.3 Maximum Voting classifier

```
In [90]: #Refer:http://scikit-Learn.org/stable/modules/generated/sklearn.ensemble.VotingClassifier.html
from sklearn.ensemble import VotingClassifier
vclf = VotingClassifier(estimators=[('lr', sig_clf1), ('svc', sig_clf2), ('rf', sig_clf3)], voting='soft')
vclf.fit(train_x_onehotCoding, train_y)
print("Log loss (train) on the VotingClassifier :", log_loss(train_y, vclf.predict_proba(train_x_onehotCoding)))
print("Log loss (CV) on the VotingClassifier :", log_loss(cv_y, vclf.predict_proba(cv_x_onehotCoding)))
print("Log loss (test) on the VotingClassifier :", log_loss(test_y, vclf.predict_proba(test_x_onehotCoding)))
print("Number of missclassified point :", np.count_nonzero((vclf.predict(test_x_onehotCoding)- test_y))/test_y.shape[0])
plot_confusion_matrix(test_y=test_y, predict_y=vclf.predict(test_x_onehotCoding))
```

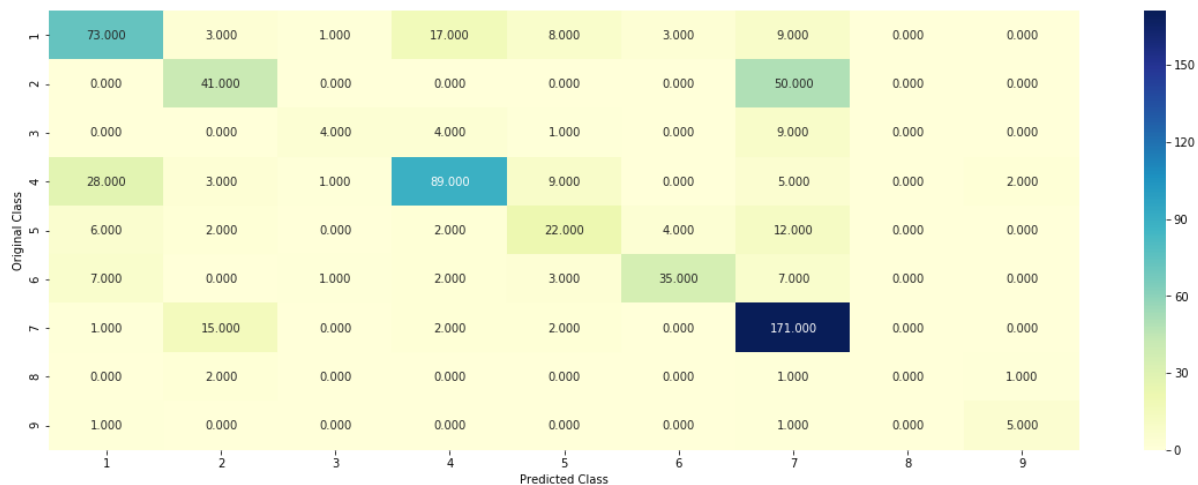
Log loss (train) on the VotingClassifier : 0.8707642892936034

Log loss (CV) on the VotingClassifier : 1.1697311290457197

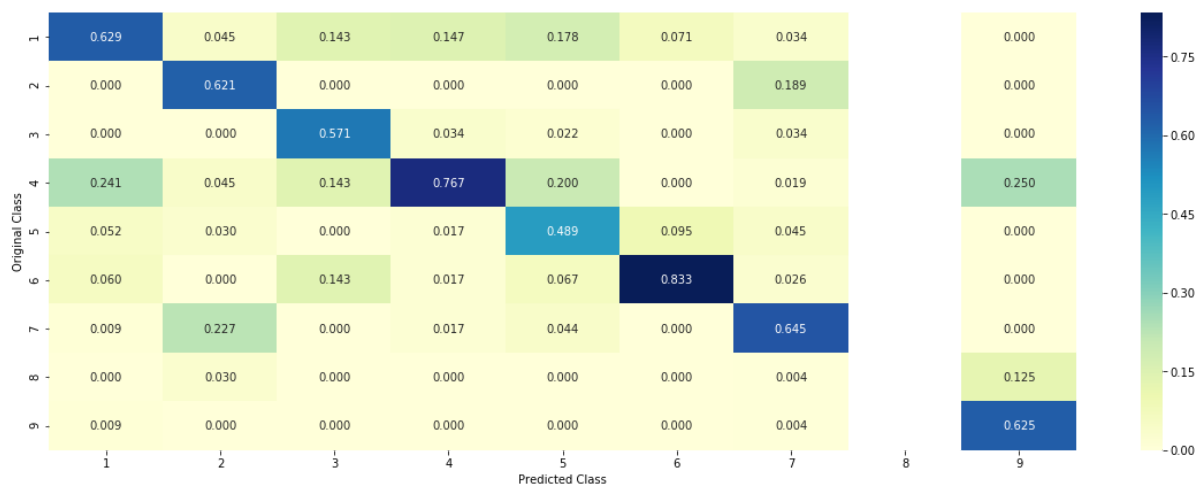
Log loss (test) on the VotingClassifier : 1.1224887055347923

Number of missclassified point : 0.3383458646616541

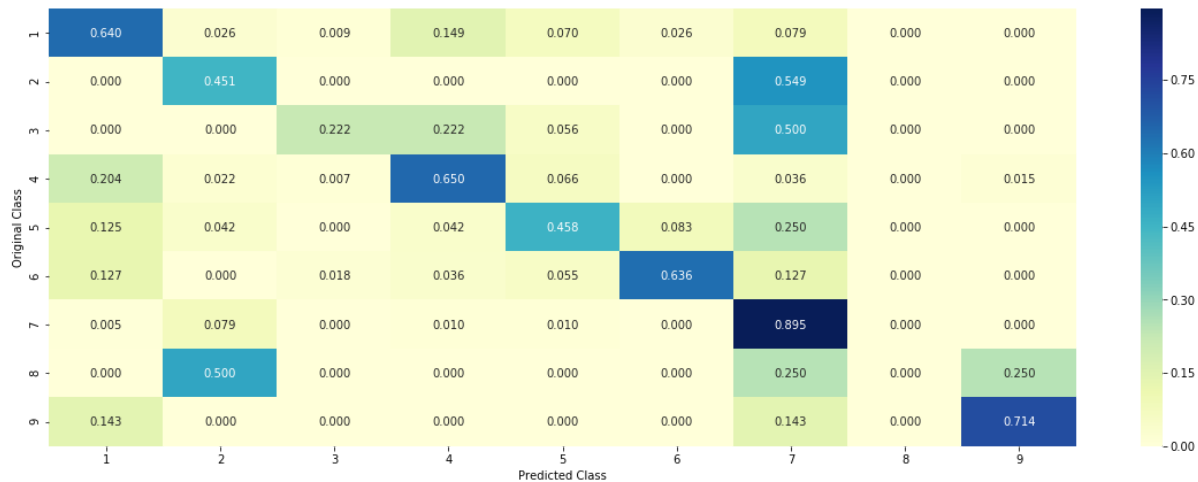
----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



Loaistic Rearession

```
In [114]: text_vectorizer = CountVectorizer(ngram_range=(1,1),min_df=5, max_features=10000)
train_text_feature_unigram = text_vectorizer.fit_transform(train_df['TEXT'])

train_text_feature_unigram = normalize(train_text_feature_unigram, axis=0)

# we use the same vectorizer that was trained on train data
test_text_feature_unigram = text_vectorizer.transform(test_df['TEXT'])
# don't forget to normalize every feature
test_text_feature_unigram = normalize(test_text_feature_unigram, axis=0)

# we use the same vectorizer that was trained on train data
cv_text_feature_unigram = text_vectorizer.transform(cv_df['TEXT'])
# don't forget to normalize every feature
cv_text_feature_unigram = normalize(cv_text_feature_unigram, axis=0)

train_gene_var_unigram = hstack((train_gene_feature_onehotCoding,train_variation_
on_feature_onehotCoding))
test_gene_var_unigram = hstack((test_gene_feature_onehotCoding,test_variation_
feature_onehotCoding))
cv_gene_var_unigram = hstack((cv_gene_feature_onehotCoding,cv_variation_featur
e_onehotCoding))

train_x_unigram = hstack((train_gene_var_unigram, train_text_feature_unigram))
.tocsr()
train_y = np.array(list(train_df['Class']))

test_x_unigram = hstack((test_gene_var_unigram, test_text_feature_unigram)).to
csr()
test_y = np.array(list(test_df['Class']))

cv_x_unigram = hstack((cv_gene_var_unigram, cv_text_feature_unigram)).tocsr()
cv_y = np.array(list(cv_df['Class']))
```



```
In [117]: text_vectorizer = CountVectorizer(ngram_range=(1,2),min_df=5, max_features=10000)
train_text_feature_bigram = text_vectorizer.fit_transform(train_df['TEXT'])

train_text_feature_bigram = normalize(train_text_feature_bigram, axis=0)

# we use the same vectorizer that was trained on train data
test_text_feature_bigram = text_vectorizer.transform(test_df['TEXT'])
# don't forget to normalize every feature
test_text_feature_bigram = normalize(test_text_feature_bigram, axis=0)

# we use the same vectorizer that was trained on train data
cv_text_feature_bigram = text_vectorizer.transform(cv_df['TEXT'])
# don't forget to normalize every feature
cv_text_feature_bigram = normalize(cv_text_feature_bigram, axis=0)

train_gene_var_bigram = hstack((train_gene_feature_onehotCoding,train_variation_feature_onehotCoding))
test_gene_var_bigram = hstack((test_gene_feature_onehotCoding,test_variation_feature_onehotCoding))
cv_gene_var_bigram = hstack((cv_gene_feature_onehotCoding,cv_variation_feature_onehotCoding))

train_x_bigram = hstack((train_gene_var_bigram, train_text_feature_bigram)).to_csr()
train_y = np.array(list(train_df['Class']))

test_x_bigram = hstack((test_gene_var_bigram, test_text_feature_bigram)).to_csr()
test_y = np.array(list(test_df['Class']))

cv_x_bigram = hstack((cv_gene_var_bigram, cv_text_feature_bigram)).to_csr()
cv_y = np.array(list(cv_df['Class']))
```

```

In [118]: alpha = [10 ** x for x in range(-6, 3)]
cv_log_error_array = []
for i in alpha:
    print("for alpha =", i)
    clf = SGDClassifier(class_weight='balanced', alpha=i, penalty='l2', loss=
'log', random_state=42)
    clf.fit(train_x_unigram, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x_unigram, train_y)
    sig_clf_probs = sig_clf.predict_proba(cv_x_unigram)
    cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes
_, eps=1e-15))
    # to avoid rounding error while multiplying probabilities we use log-probab
ility estimates
    print("Log Loss :", log_loss(cv_y, sig_clf_probs))

fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], str(txt)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

best_alpha = np.argmin(cv_log_error_array)
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty=
'l2', loss='log', random_state=42)
clf.fit(train_x_unigram, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_unigram, train_y)

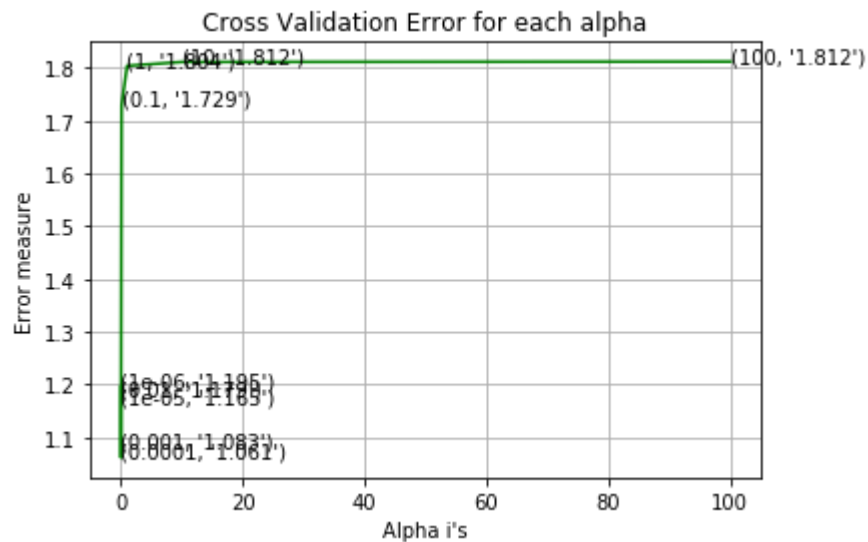
predict_y = sig_clf.predict_proba(train_x_unigram)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss i
s:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_unigram)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation
log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_unigram)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss i
s:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

```

for alpha = 1e-06
Log Loss : 1.1949383643558178
for alpha = 1e-05
Log Loss : 1.165489778569634
for alpha = 0.0001
Log Loss : 1.0610850670679761
for alpha = 0.001
Log Loss : 1.0828092303937074
for alpha = 0.01
Log Loss : 1.1786977642016547
for alpha = 0.1
Log Loss : 1.7293653389622106
for alpha = 1
Log Loss : 1.804358397090669
for alpha = 10
Log Loss : 1.8116113961676308
for alpha = 100
Log Loss : 1.8123467625178002

```



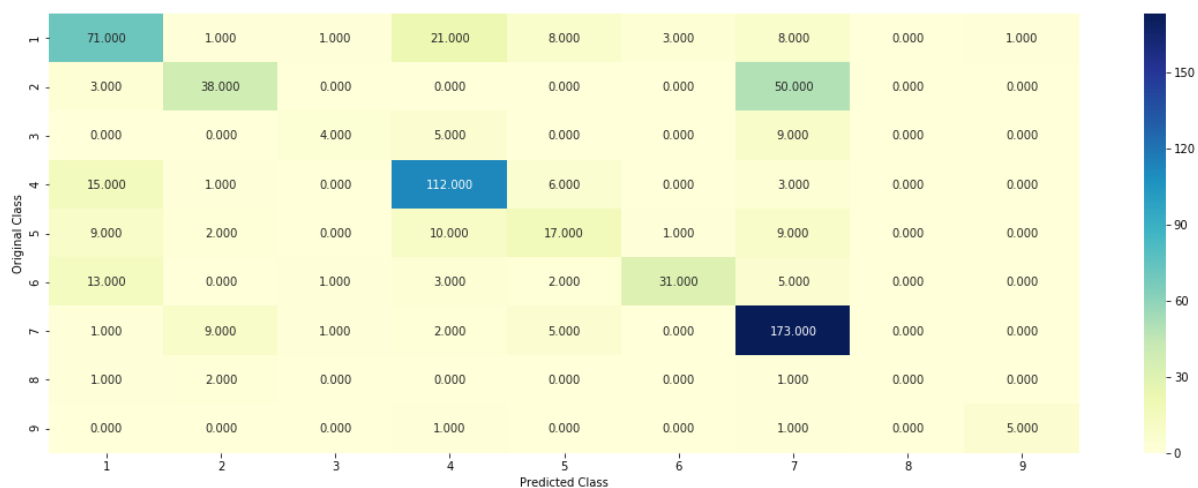
For values of best alpha = 0.0001 The train log loss is: 0.44632183198180686
 For values of best alpha = 0.0001 The cross validation log loss is: 1.0610850670679761
 For values of best alpha = 0.0001 The test log loss is: 0.9744348565967921

```
In [119]: clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty=  
          'l2', loss='log', random_state=42)  
          predict_and_plot_confusion_matrix(train_x_unigram, train_y, test_x_unigram, te  
          st_y, clf)
```

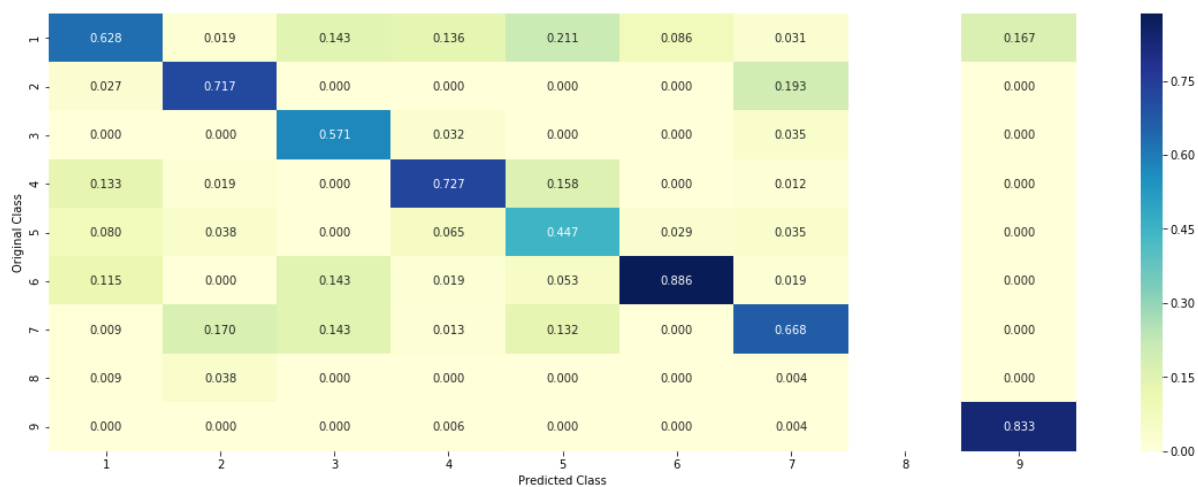
Log loss : 0.9744348565967921

Number of mis-classified points : 0.3218045112781955

----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



```

In [120]: alpha = [10 ** x for x in range(-6, 3)]
cv_log_error_array = []
for i in alpha:
    print("for alpha =", i)
    clf = SGDClassifier(class_weight='balanced', alpha=i, penalty='l2', loss=
'log', random_state=42)
    clf.fit(train_x_bigram, train_y)
    sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
    sig_clf.fit(train_x_bigram, train_y)
    sig_clf_probs = sig_clf.predict_proba(cv_x_bigram)
    cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes
_, eps=1e-15))
    # to avoid rounding error while multiplying probabilities we use log-probab
ility estimates
    print("Log Loss :", log_loss(cv_y, sig_clf_probs))

fig, ax = plt.subplots()
ax.plot(alpha, cv_log_error_array, c='g')
for i, txt in enumerate(np.round(cv_log_error_array, 3)):
    ax.annotate((alpha[i], str(txt)), (alpha[i], cv_log_error_array[i]))
plt.grid()
plt.title("Cross Validation Error for each alpha")
plt.xlabel("Alpha i's")
plt.ylabel("Error measure")
plt.show()

best_alpha = np.argmin(cv_log_error_array)
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty=
'l2', loss='log', random_state=42)
clf.fit(train_x_bigram, train_y)
sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
sig_clf.fit(train_x_bigram, train_y)

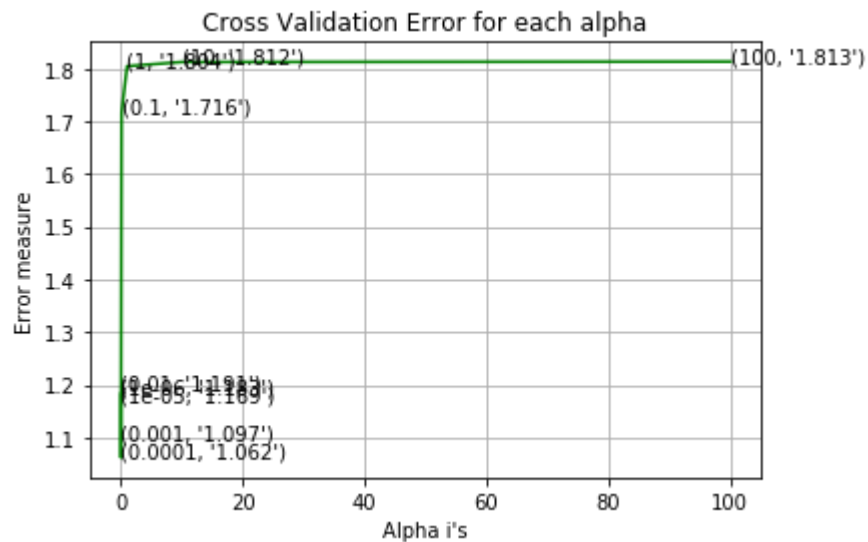
predict_y = sig_clf.predict_proba(train_x_bigram)
print('For values of best alpha = ', alpha[best_alpha], "The train log loss i
s:", log_loss(y_train, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(cv_x_bigram)
print('For values of best alpha = ', alpha[best_alpha], "The cross validation
log loss is:", log_loss(y_cv, predict_y, labels=clf.classes_, eps=1e-15))
predict_y = sig_clf.predict_proba(test_x_bigram)
print('For values of best alpha = ', alpha[best_alpha], "The test log loss i
s:", log_loss(y_test, predict_y, labels=clf.classes_, eps=1e-15))

```

```

for alpha = 1e-06
Log Loss : 1.182867276805894
for alpha = 1e-05
Log Loss : 1.1690440227982835
for alpha = 0.0001
Log Loss : 1.0619137518668915
for alpha = 0.001
Log Loss : 1.0966656377534192
for alpha = 0.01
Log Loss : 1.19131272270934
for alpha = 0.1
Log Loss : 1.716401732973238
for alpha = 1
Log Loss : 1.8043443836645345
for alpha = 10
Log Loss : 1.8121772333911041
for alpha = 100
Log Loss : 1.8129913612599509

```



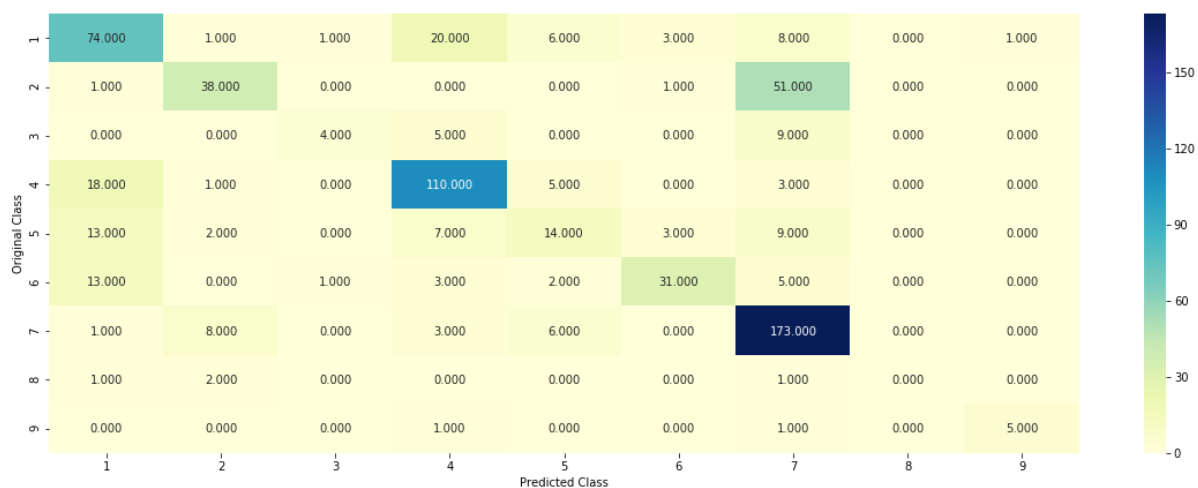
For values of best alpha = 0.0001 The train log loss is: 0.44273374532206616
 For values of best alpha = 0.0001 The cross validation log loss is: 1.0619137518668915
 For values of best alpha = 0.0001 The test log loss is: 0.9905961612433127

```
In [121]: clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty=  
        'l2', loss='log', random_state=42)  
        predict_and_plot_confusion_matrix(train_x_bigram, train_y, test_x_bigram, test  
        _y, clf)
```

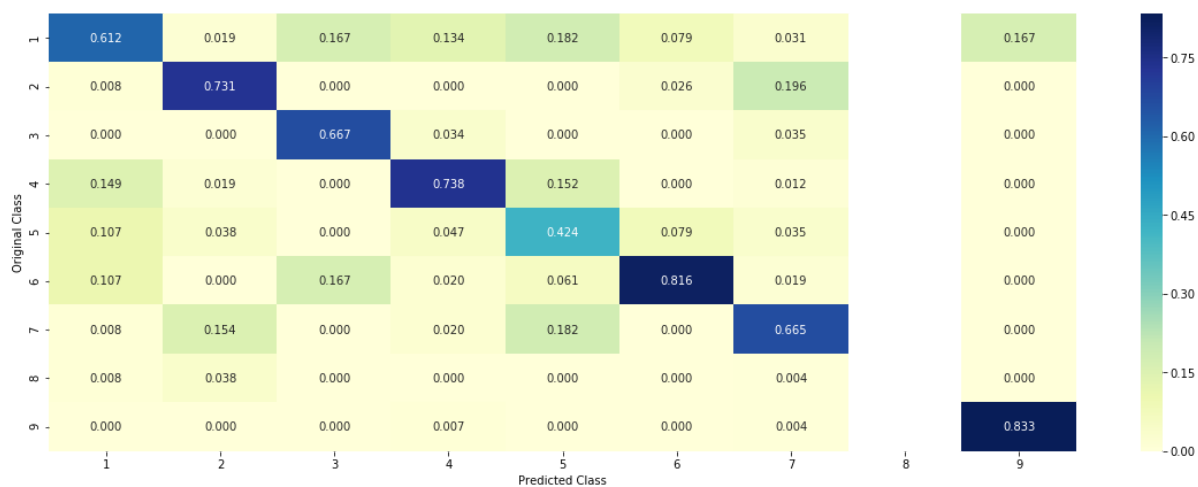

Log loss : 0.9905961612433127

Number of mis-classified points : 0.324812030075188

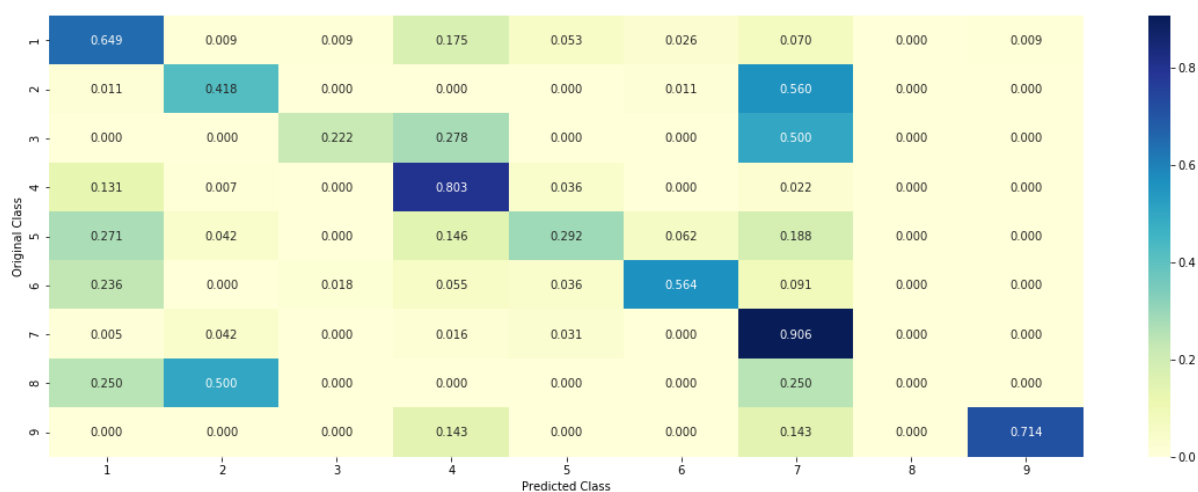
----- Confusion matrix -----



----- Precision matrix (Column Sum=1) -----



----- Recall matrix (Row sum=1) -----



```
In [3]: # Please compare all your models using Prettytable library
from prettytable import PrettyTable
x = PrettyTable()
columns = ["Model", "Train log-loss", "CV log-loss", "Test log-loss"]
x.add_column(columns[0], ["Naive Bayes", "KNN", "Logistic Regression(Class balancing)", "Logistic Regression(no Class balancing)", \
    "Linear SVM", "Random Forest(1-hot encoding)", "Random Forest(Response Coding)", "Maximum Voting", \
    "Logistic Regression(uni-gram)", "Logistic Regression (bi-gram)"])
x.add_column(columns[1], ["0.675", "0.649", "0.414", "0.465", "0.400", "0.592", "0.054", "0.870", "0.446", "0.442"])
x.add_column(columns[2], ["1.232", "1.058", "1.039", "1.068", "1.020", "1.159", "1.332", "1.169", "1.061", "1.061"])
x.add_column(columns[3], ["1.175", "0.988", "0.986", "1.084", "1.045", "1.107", "1.341", "1.122", "0.974", "0.990"])
print(x)
```

Model	Train log-loss	CV log-loss	Test log-loss
Naive Bayes	0.675	1.232	1.175
KNN	0.649	1.058	0.988
Logistic Regression(Class balancing)	0.414	1.039	0.986
Logistic Regression(no Class balancing)	0.465	1.068	1.084
Linear SVM	0.400	1.020	1.045
Random Forest(1-hot encoding)	0.592	1.159	1.107
Random Forest(Response Coding)	0.054	1.332	1.341
Maximum Voting	0.870	1.169	1.122
Logistic Regression(uni-gram)	0.446	1.061	0.974
Logistic Regression(bi-gram)	0.442	1.061	0.990

Conclusion:

1. After trying bi,3,4,5-grams TfidfVectorization for text feature, 4-grams model is concluded as the best due to its low log-loss.
2. Under 4-grams, KNN, LR, Linear SVM has low log-loss and these models doesn't seem to overfit either.
3. By using uni,bi-gram for Logistic Regression, we were able to get the lowest log-loss without the risk of overfitting.

5. Assignments

1. Apply All the models with tf-idf features (Replace CountVectorizer with tfidfVectorizer and run the same cells)
2. Instead of using all the words in the dataset, use only the top 1000 words based of tf-idf values
3. Apply Logistic regression with CountVectorizer Features, including both unigrams and bigrams
4. Try any of the feature engineering techniques discussed in the course to reduce the CV and test log-loss to a value less than 1.0