Personalized cancer diagnosis

Problem statement :

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

Data

- Source: https://www.kaggle.com/c/msk-redefining-cancer-treatment/data
- We have two data files: one conatins 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 are have a common column called ID
- Data file's information:
  - training_variants (ID , Gene, Variations, Class)
  - training_text (ID, Text)

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). ...

Type of Machine Learning Problem

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

Performance Metric

Metric(s):

- Multi class log-loss
- Confusion matrix

Machine Learing 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 probabilites => Metric is Log-loss.
- No Latency constraints.

Exploratory Data Analysis

In [24]:

```python
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.cross_validation 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
```

Reading Data

Reading Gene and Variation Data

```
data = pd.read_csv('training/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

Reading Text Data

In [3]:

```
data_text =pd.read_csv("training/training_text",sep="\|\|",engine="python",names=["ID","TEXT"],skip
rows=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...

Preprocessing of text

In [4]:

```
stop words = set(stopwords.words('english'))
```

```python
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]:

```python
#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 : 211.52816454299833 seconds
```

In [13]:

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

Out[13]:

	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 [14]:

```python
result[result.isnull().any(axis=1)]
```

Out[14]:

	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

	ID	Gene	Variation	Class	TEXT
2755	2755	BRAF	G596C	7	NaN

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

In [16]:

```
result[result['ID']==1109]
```

Out[16]:

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

Test, Train and Cross Validation Split

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

In [17]:

```
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 varaible '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
varaible '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 [18]:

```
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
```

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

In [21]:

```
# 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().sortlevel()
test_class_distribution = test_df['Class'].value_counts().sortlevel()
cv_class_distribution = cv_df['Class'].value_counts().sortlevel()

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()

# -(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.ro
und((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()

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.rou
nd((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()

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), '%)')
```
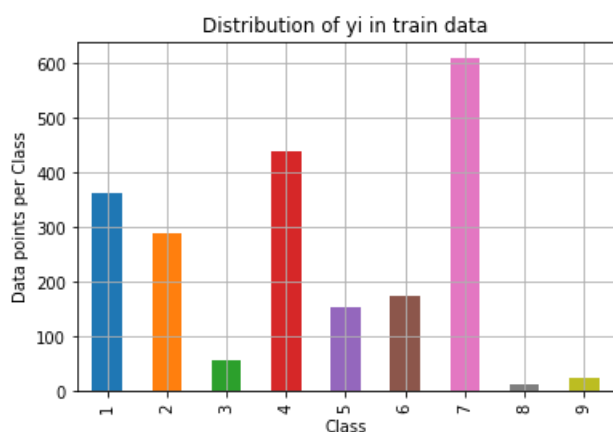

Distribution of yi in train data

```
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 %)
--------------------------------------------------------------------------------
```


Distribution of yi in test data
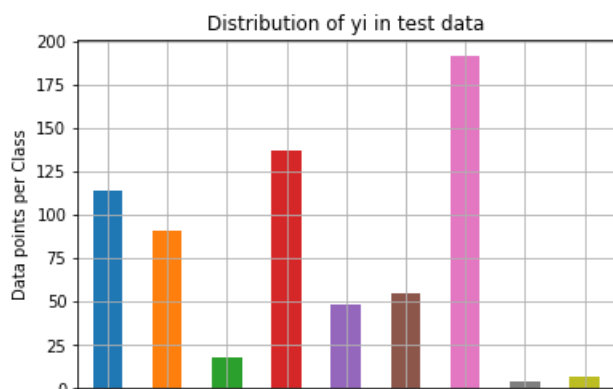
```
Number of data points in class 7 : 191 ( 28.722 %)
Number of data points in class 4 : 137 ( 20.602 %)
Number of data points in class 1 : 114 ( 17.143 %)
Number of data points in class 2 : 91 ( 13.684 %)
Number of data points in class 6 : 55 ( 8.271 %)
Number of data points in class 5 : 48 ( 7.218 %)
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 %)
--------------------------------------------------------------------------------
```
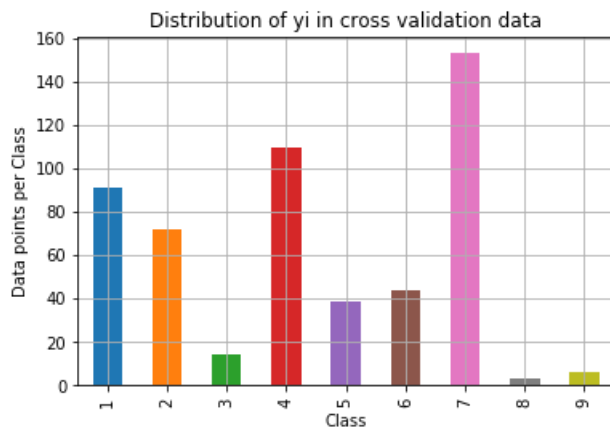


```
Number of data points in class 7 : 153 ( 28.759 %)
Number of data points in class 4 : 110 ( 20.677 %)
Number of data points in class 1 : 91 ( 17.105 %)
Number of data points in class 2 : 72 ( 13.534 %)
Number of data points in class 6 : 44 ( 8.271 %)
Number of data points in class 5 : 39 ( 7.331 %)
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 %)
```

Univariate Analysis

Univariate Analysis on Gene Feature

Gene is a categorical variable

In [28]:

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

```
Number of Unique Genes : 229
BRCA1     164
TP53       90
EGFR       88
PTEN       82
BRCA2      78
KIT        67
BRAF       51
ALK        48
ERBB2      46
PIK3CA     37
Name: Gene, dtype: int64
```

In [29]:

```
print("Ans: There are", unique_genes.shape[0] ,"different categories of genes in the train data, an
d they are distibuted as follows",)
```

Ans: There are 229 different categories of genes in the train data, and they are distibuted as fol
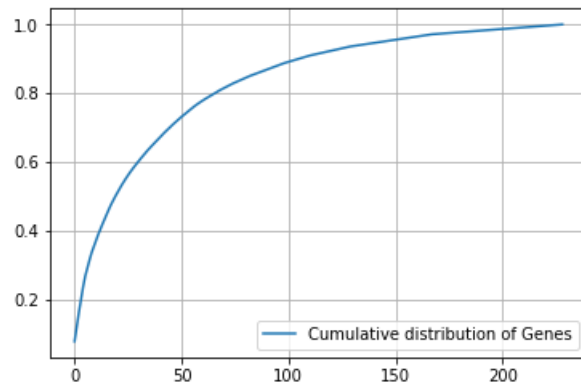lows

In [30]:

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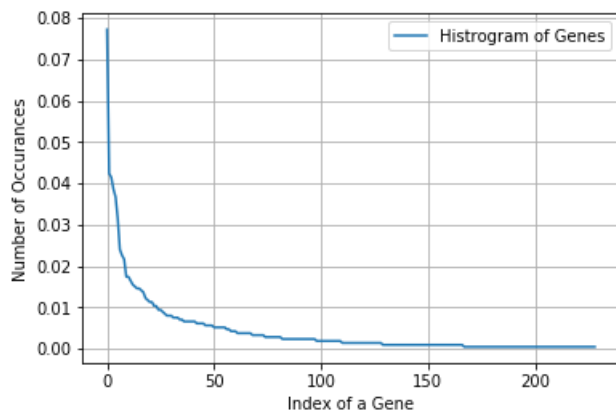

In [31]:

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


there are two ways we can featurize this variable

1. One hot Encoding

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 [33]:

```
print("train_gene_feature_responseCoding is converted feature using respone coding method. The sha
pe of gene feature:", train_gene_feature_responseCoding.shape)
```

train_gene_feature_responseCoding is converted feature using respone coding method. The shape of g
ene feature: (2124, 9)

In [34]:

```
# 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 [35]:

```
train_df['Gene'].head()
```

Out[35]:

```
2988        KIT
1718     KNSTRN
2076       TET2
751       ERBB2
462        TP53
Name: Gene, dtype: object
```

In [36]:

```
gene_vectorizer.get_feature_names()
```

Out[36]:

```
['abl1',
 'acvr1',
 'ago2',
 'akt1',
 'akt2',
 'akt3',
 'alk',
 'apc',
 'ar',
 'araf',
 'arid1a',
 'arid2',
 'arid5b',
 'asxl1',
 'atm',
 'atr',
 'atrx',
 'aurka',
 'axl',
 'b2m',
 'bap1',
 'bcl10',
 'bcl2l11',
 'bcor',
 'braf',
 'brca1',
 'brca2',
 'brd4',
 'brip1',
 'btk',
 'card11',
 'carm1',
 'casp8',
 'cbl',
 'ccnd1',
 'ccnd2',
 'ccnd3',
 'ccne1',
 'cdh1',
 'cdk12',
 'cdk4',
 'cdk6',
 'cdk8',
 'cdkn1a',
 'cdkn1b',
 'cdkn2a',
 'cdkn2b',
 'cdkn2c',
 'cebpa',
```

```
'chek2',
'cic',
'crebbp',
'ctcf',
'ctnnb1',
'ddr2',
'dicer1',
'dnmt3a',
'dnmt3b',
'dusp4',
'egfr',
'elf3',
'ep300',
'epas1',
'epcam',
'erbb2',
'erbb3',
'erbb4',
'ercc2',
'ercc3',
'ercc4',
'erg',
'esr1',
'etv1',
'etv6',
'ewsr1',
'ezh2',
'fanca',
'fancc',
'fat1',
'fbxw7',
'fgf19',
'fgf3',
'fgfr1',
'fgfr2',
'fgfr3',
'fgfr4',
'flt3',
'foxa1',
'foxl2',
'foxo1',
'foxp1',
'gata3',
'gna11',
'gnaq',
'gnas',
'h3f3a',
'hist1h1c',
'hla',
'hnf1a',
'hras',
'idh1',
'idh2',
'igf1r',
'ikzf1',
'jak1',
'jak2',
'jun',
'kdm5a',
'kdm5c',
'kdm6a',
'kdr',
'keap1',
'kit',
'kmt2a',
'kmt2b',
'kmt2c',
'kmt2d',
'knstrn',
'kras',
'lats1',
'map2k1',
'map2k2',
'map2k4',
'map3k1',
'mapk1',
'mdm4',
```

```
'med12',
'mef2b',
'met',
'mga',
'mlh1',
'mpl',
'msh2',
'msh6',
'mtor',
'myc',
'mycn',
'myd88',
'myod1',
'ncor1',
'nf1',
'nf2',
'nfe2l2',
'nfkbia',
'nkx2',
'notch1',
'npm1',
'nras',
'nsd1',
'ntrk1',
'ntrk3',
'nup93',
'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',
'rad51b',
'rad51c',
'rad54l',
'raf1',
'rasa1',
'rb1',
'rbm10',
'ret',
'rheb',
'rhoa',
'rit1',
'rnf43',
'ros1',
'rras2',
'runx1',
'rxra',
'rybp',
'sdhb',
'sdhc',
'setd2',
'sf3b1',
'shq1',
'smad2',
'smad3',
'smad4',
'smarca4',
```

```
 'smarcb1',
 'smo',
 'sos1',
 'sox9',
 'spop',
 'src',
 'stag2',
 'stat3',
 'stk11',
 'tcf7l2',
 'tert',
 'tet1',
 'tet2',
 'tgfbr1',
 'tgfbr2',
 'tmprss2',
 'tp53',
 'tp53bp1',
 'tsc1',
 'tsc2',
 'u2af1',
 'vhl',
 'whsc1',
 'xpo1',
 'xrcc2',
 'yap1']
```

In [37]:

```python
print("train_gene_feature_onehotCoding is converted feature using one-hot encoding method. The sha
pe of gene feature:", train_gene_feature_onehotCoding.shape)
```

```
train_gene_feature_onehotCoding is converted feature using one-hot encoding method. The shape of g
ene feature: (2124, 229)
```

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 [38]:

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


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.clas
ses_, 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
```

```
print( for Variation 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_lo
ss(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 is:",log_loss(y_test, p
redict_y, labels=clf.classes_, eps=1e-15))
```

```
For values of alpha =  1e-05 The log loss is: 1.418841767162939
For values of alpha =  0.0001 The log loss is: 1.2325868001617826
For values of alpha =  0.001 The log loss is: 1.2503129272158073
For values of alpha =  0.01 The log loss is: 1.360379976757511
For values of alpha =  0.1 The log loss is: 1.4314392521126913
For values of alpha =  1 The log loss is: 1.4659143358159061
```
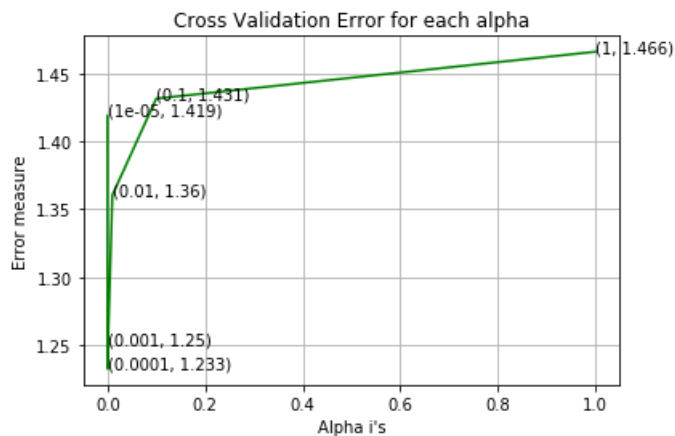


```
For values of best alpha =  0.0001 The train log loss is: 1.0425604300119806
For values of best alpha =  0.0001 The cross validation log loss is: 1.2325868001617826
For values of best alpha =  0.0001 The test log loss is: 1.200905436534172
```

Univariate Analysis on Variation Feature

Variation is a categorical variable

In [40]:

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

```
Number of Unique Variations : 1924
Truncating_Mutations         59
Deletion                     49
Amplification                47
Fusions                      23
E17K                          3
Overexpression                3
Q22K                          2
Promoter_Hypermethylation     2
G13D                          2
T73I                          2
Name: Variation, dtype: int64
```

In [41]:

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

```
Ans: There are 1924 different categories of variations in the train data, and they are distibuted
as follows
```

In [42]:

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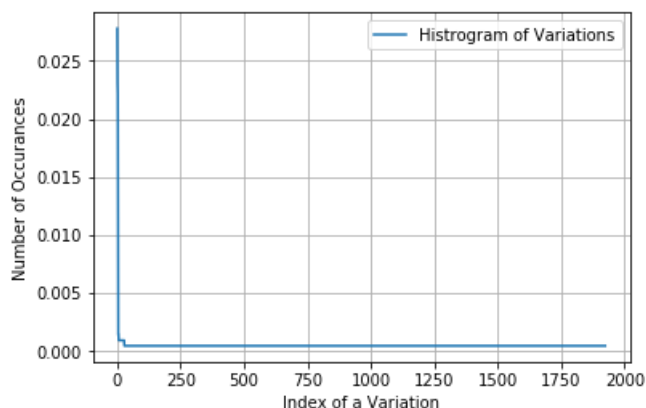

In [43]:

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

```
[0.02777778 0.05084746 0.07297552 ... 0.99905838 0.99952919 1.        ]
```
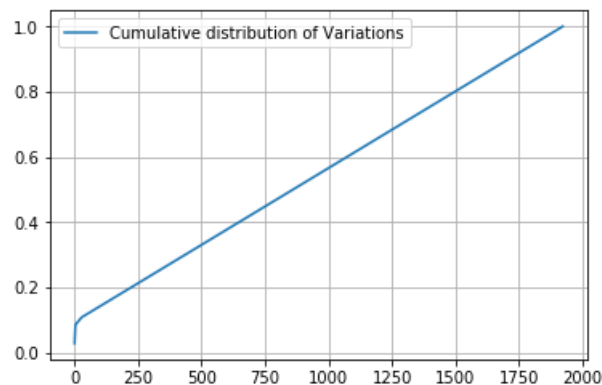

In [46]:

```
# 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 [47]:

```
print("train_variation_feature_onehotEncoded is converted feature using the onne-hot encoding meth
od. The shape of Variation feature:", train_variation_feature_onehotCoding.shape)
```

```
train_variation_feature_onehotEncoded is converted feature using the onne-hot encoding method. The
shape of Variation feature: (2124, 1960)
```

Let's build a model just like the earlier!

In [48]:

```
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.clas
ses_, 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_lo
ss(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, p
redict_y, labels=clf.classes_, eps=1e-15))
```
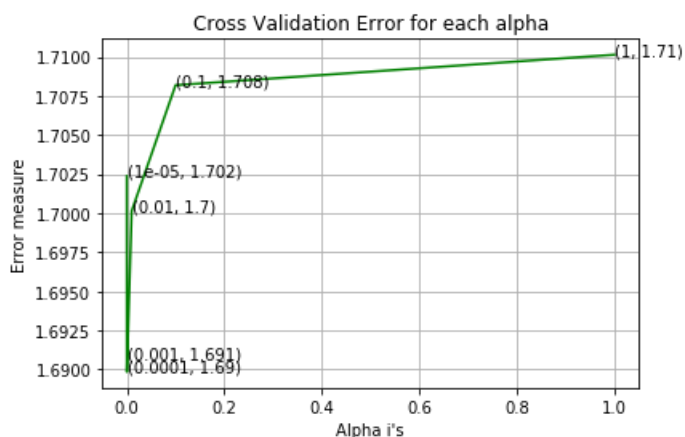
```
For values of alpha =  1e-05 The log loss is: 1.7023621747765858
For values of alpha =  0.0001 The log loss is: 1.689842322110077
For values of alpha =  0.001 The log loss is: 1.6907130717518253
For values of alpha =  0.01 The log loss is: 1.7001345396142153
For values of alpha =  0.1 The log loss is: 1.7081826775989355
For values of alpha =  1 The log loss is: 1.710131025593559
```



```
For values of best alpha =  0.0001 The train log loss is: 0.8255455900343496
For values of best alpha =  0.0001 The cross validation log loss is: 1.689842322110077
For values of best alpha =  0.0001 The test log loss is: 1.7362385768757977
```

Univariate Analysis on Text Feature

In [50]:

```python
# cls_text is a data frame
# for every row in data fram 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 [51]:

```python
import math

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_dict.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 [52]:

```python
# building a CountVectorizer with all the words that occured minimum 3 times in train data
text_vectorizer = CountVectorizer(min_df=3)
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 featu
res) 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 occured
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 : 54850

In [56]:

```python
train_text_feature_onehotCoding = normalize(train_text_feature_onehotCoding, axis=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, axis=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 [59]:

```python
# Train a Logistic regression+Calibration model using text features whicha re on-hot encoded
alpha = [10 ** x for x in range(-5, 1)]
```

```python
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.clas
ses_, 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_lo
ss(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, p
redict_y, labels=clf.classes_, eps=1e-15))
```
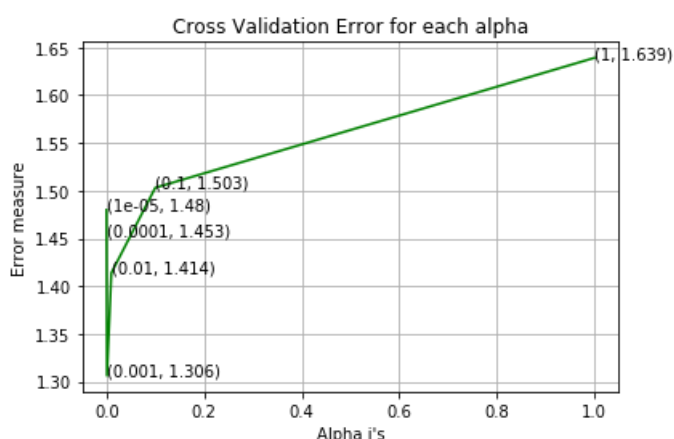
```
For values of alpha =  1e-05 The log loss is: 1.4798785760828574
For values of alpha =  0.0001 The log loss is: 1.4534937808292785
For values of alpha =  0.001 The log loss is: 1.3062465612808916
For values of alpha =  0.01 The log loss is: 1.4138930975129917
For values of alpha =  0.1 The log loss is: 1.5031084843525189
For values of alpha =  1 The log loss is: 1.6391636597237738
```



```
For values of best alpha =  0.001 The train log loss is: 0.7614133457365512
For values of best alpha =  0.001 The cross validation log loss is: 1.3062465612808916
For values of best alpha =  0.001 The test log loss is: 1.1902669954542044
```

Machine Learning Models

In [62]:

```
#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 belongs 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 [63]:

```
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 [64]:

```
# 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 = CountVectorizer(min_df=3)

    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_n
o))
        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 [65]:

```
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)).tocs
r()
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 [66]:

```
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_onehotCoding.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, 57039)
(number of data points * number of features) in test data =  (665, 57039)
(number of data points * number of features) in cross validation data = (532, 57039)
```

In [67]:

```
print(" Response encoding features :")
print("(number of data points * number of features) in train data = ", train_x_responseCoding.shap
e)
print("(number of data points * number of features) in test data = ", test_x_responseCoding.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)
```

Base Line Model

Naive Bayes

Hyper parameter tuning

In [68]:

```
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 probabilites 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 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 alpha = ', alpha[best_alpha], "The cross validation log loss is:",log_lo
ss(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 is:",log_loss(y_test, p
redict_y, labels=clf.classes_, eps=1e-15))
```

```
for alpha = 1e-05
Log Loss : 1.3655537837941127
for alpha = 0.0001
Log Loss : 1.3711793514758466
for alpha = 0.001
Log Loss : 1.3696542195047903
for alpha = 0.1
Log Loss : 1.3509235125982695
for alpha = 1
Log Loss : 1.3591155403248767
for alpha = 10
Log Loss : 1.4299766791532638
for alpha = 100
Log Loss : 1.451360452876549
for alpha = 1000
Log Loss : 1.4099515277732073
```
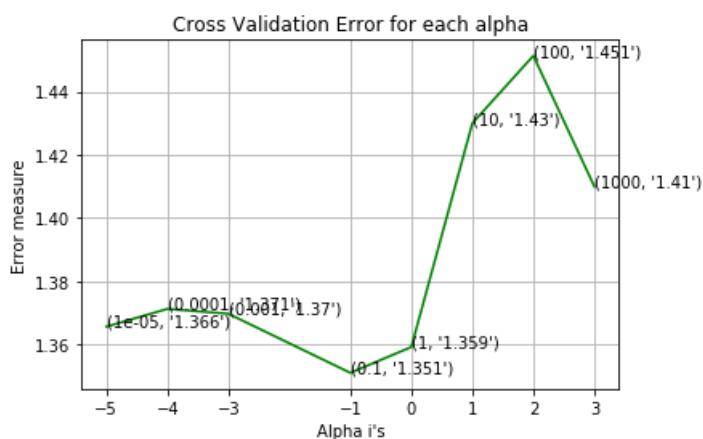


```
For values of best alpha =  0.1 The train log loss is: 0.9033118479519152
For values of best alpha =  0.1 The cross validation log loss is: 1.3509235125982695
For values of best alpha =  0.1 The test log loss is: 1.2784897724659714
```

Testing the model with best hyper paramters

In [69]:

```
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(cv_x_onehotCoding)
# to avoid rounding error while multiplying probabilites we use log-probability estimates
print("Log Loss :",log_loss(cv_y, sig_clf_probs))
print("Number of missclassified point :", np.count_nonzero((sig_clf.predict(cv_x_onehotCoding)- cv
_y))/cv_y.shape[0])
plot_confusion_matrix(cv_y, sig_clf.predict(cv_x_onehotCoding.toarray()))
```
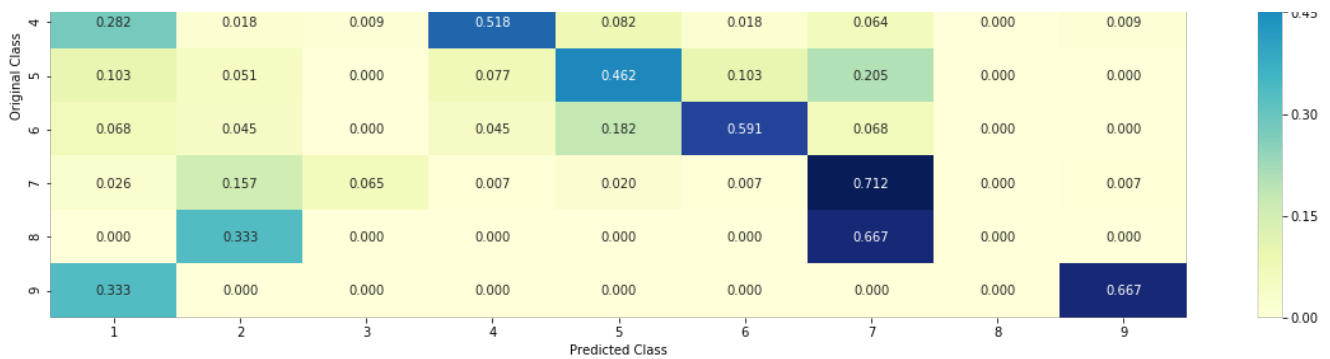
```
Log Loss : 1.3509235125982695
Number of missclassified point : 0.44360902255639095
-------------------- Confusion matrix --------------------
```



```
-------------------- Precision matrix (Columm Sum=1) --------------------
```



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

Feature Importance, Correctly classified point

In [70]:

```python
test_point_index = 1
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_df['Gene'].iloc[test_point_index],test_df['Variation']
.iloc[test_point_index], no_feature)
```

```
Predicted Class : 7
Predicted Class Probabilities: [[0.0911 0.1284 0.0141 0.1119 0.0334 0.0365 0.5764 0.0057 0.0025]]
Actual Class : 7
--------------------------------------------------
16 Text feature [presence] present in test data point [True]
17 Text feature [kinase] present in test data point [True]
18 Text feature [well] present in test data point [True]
19 Text feature [activating] present in test data point [True]
20 Text feature [downstream] present in test data point [True]
21 Text feature [cell] present in test data point [True]
22 Text feature [inhibitor] present in test data point [True]
23 Text feature [cells] present in test data point [True]
24 Text feature [independent] present in test data point [True]
25 Text feature [contrast] present in test data point [True]
26 Text feature [recently] present in test data point [True]
29 Text feature [shown] present in test data point [True]
30 Text feature [potential] present in test data point [True]
31 Text feature [also] present in test data point [True]
32 Text feature [obtained] present in test data point [True]
33 Text feature [growth] present in test data point [True]
34 Text feature [activation] present in test data point [True]
35 Text feature [suggest] present in test data point [True]
36 Text feature [showed] present in test data point [True]
37 Text feature [however] present in test data point [True]
38 Text feature [expressing] present in test data point [True]
39 Text feature [addition] present in test data point [True]
40 Text feature [found] present in test data point [True]
41 Text feature [10] present in test data point [True]
42 Text feature [previously] present in test data point [True]
43 Text feature [factor] present in test data point [True]
44 Text feature [compared] present in test data point [True]
45 Text feature [treated] present in test data point [True]
46 Text feature [inhibition] present in test data point [True]
47 Text feature [higher] present in test data point [True]
48 Text feature [observed] present in test data point [True]
49 Text feature [described] present in test data point [True]
50 Text feature [may] present in test data point [True]
51 Text feature [similar] present in test data point [True]
52 Text feature [total] present in test data point [True]
53 Text feature [furthermore] present in test data point [True]
54 Text feature [studies] present in test data point [True]
55 Text feature [using] present in test data point [True]
56 Text feature [without] present in test data point [True]
57 Text feature [concentrations] present in test data point [True]
```

```
58 Text feature [1a] present in test data point [True]
59 Text feature [various] present in test data point [True]
60 Text feature [including] present in test data point [True]
61 Text feature [mutations] present in test data point [True]
62 Text feature [respectively] present in test data point [True]
63 Text feature [12] present in test data point [True]
64 Text feature [followed] present in test data point [True]
65 Text feature [enhanced] present in test data point [True]
66 Text feature [although] present in test data point [True]
67 Text feature [interestingly] present in test data point [True]
68 Text feature [phosphorylation] present in test data point [True]
70 Text feature [new] present in test data point [True]
71 Text feature [inhibited] present in test data point [True]
72 Text feature [constitutively] present in test data point [True]
75 Text feature [1b] present in test data point [True]
76 Text feature [reported] present in test data point [True]
77 Text feature [confirmed] present in test data point [True]
78 Text feature [inhibitors] present in test data point [True]
79 Text feature [proliferation] present in test data point [True]
80 Text feature [report] present in test data point [True]
81 Text feature [either] present in test data point [True]
82 Text feature [molecular] present in test data point [True]
83 Text feature [15] present in test data point [True]
84 Text feature [thus] present in test data point [True]
85 Text feature [recent] present in test data point [True]
86 Text feature [3b] present in test data point [True]
87 Text feature [fig] present in test data point [True]
88 Text feature [results] present in test data point [True]
89 Text feature [occur] present in test data point [True]
90 Text feature [small] present in test data point [True]
91 Text feature [3a] present in test data point [True]
92 Text feature [approximately] present in test data point [True]
93 Text feature [hours] present in test data point [True]
94 Text feature [consistent] present in test data point [True]
95 Text feature [figure] present in test data point [True]
97 Text feature [suggests] present in test data point [True]
98 Text feature [absence] present in test data point [True]
99 Text feature [measured] present in test data point [True]
Out of the top  100   features  78 are present in query point
```

Feature Importance, Incorrectly classified point

In [71]:

```
test_point_index = 100
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_df['Gene'].iloc[test_point_index],test_df['Variation']
.iloc[test_point_index], no_feature)
```

```
Predicted Class : 7
Predicted Class Probabilities: [[0.0876 0.0895 0.0136 0.1069 0.0322 0.0356 0.6267 0.0055 0.0024]]
Actual Class : 7
--------------------------------------------------
17 Text feature [kinase] present in test data point [True]
18 Text feature [well] present in test data point [True]
19 Text feature [activating] present in test data point [True]
20 Text feature [downstream] present in test data point [True]
21 Text feature [cell] present in test data point [True]
23 Text feature [cells] present in test data point [True]
24 Text feature [independent] present in test data point [True]
25 Text feature [contrast] present in test data point [True]
26 Text feature [recently] present in test data point [True]
29 Text feature [shown] present in test data point [True]
30 Text feature [potential] present in test data point [True]
31 Text feature [also] present in test data point [True]
33 Text feature [growth] present in test data point [True]
34 Text feature [activation] present in test data point [True]
```

34 Text feature [activation] present in test data point [True]
35 Text feature [suggest] present in test data point [True]
36 Text feature [showed] present in test data point [True]
37 Text feature [however] present in test data point [True]
39 Text feature [addition] present in test data point [True]
40 Text feature [found] present in test data point [True]
41 Text feature [10] present in test data point [True]
42 Text feature [previously] present in test data point [True]
44 Text feature [compared] present in test data point [True]
46 Text feature [inhibition] present in test data point [True]
47 Text feature [higher] present in test data point [True]
48 Text feature [observed] present in test data point [True]
50 Text feature [may] present in test data point [True]
51 Text feature [similar] present in test data point [True]
54 Text feature [studies] present in test data point [True]
55 Text feature [using] present in test data point [True]
56 Text feature [without] present in test data point [True]
58 Text feature [1a] present in test data point [True]
60 Text feature [including] present in test data point [True]
61 Text feature [mutations] present in test data point [True]
62 Text feature [respectively] present in test data point [True]
63 Text feature [12] present in test data point [True]
64 Text feature [followed] present in test data point [True]
65 Text feature [enhanced] present in test data point [True]
66 Text feature [although] present in test data point [True]
68 Text feature [phosphorylation] present in test data point [True]
69 Text feature [activated] present in test data point [True]
70 Text feature [new] present in test data point [True]
71 Text feature [inhibited] present in test data point [True]
72 Text feature [constitutively] present in test data point [True]
75 Text feature [1b] present in test data point [True]
78 Text feature [inhibitors] present in test data point [True]
79 Text feature [proliferation] present in test data point [True]
81 Text feature [either] present in test data point [True]
82 Text feature [molecular] present in test data point [True]
83 Text feature [15] present in test data point [True]
85 Text feature [recent] present in test data point [True]
86 Text feature [3b] present in test data point [True]
87 Text feature [fig] present in test data point [True]
88 Text feature [results] present in test data point [True]
89 Text feature [occur] present in test data point [True]
90 Text feature [small] present in test data point [True]
91 Text feature [3a] present in test data point [True]
94 Text feature [consistent] present in test data point [True]
95 Text feature [figure] present in test data point [True]
97 Text feature [suggests] present in test data point [True]
98 Text feature [absence] present in test data point [True]
Out of the top 100 features 60 are present in query point

Logistic Regression

With Class balancing

Hyper paramter tuning

In [76]:

```python
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 probabilites 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='l2', loss='log', ran
dom_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 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 alpha = ', alpha[best_alpha], "The cross validation log loss is:",log_lo
ss(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 is:",log_loss(y_test, p
redict_y, labels=clf.classes_, eps=1e-15))
```

```
for alpha = 1e-06
Log Loss : 1.4554353198842396
for alpha = 1e-05
Log Loss : 1.4602144866667575
for alpha = 0.0001
Log Loss : 1.358469527280309
for alpha = 0.001
Log Loss : 1.217324457704446
for alpha = 0.01
Log Loss : 1.3437838209291793
for alpha = 0.1
Log Loss : 1.5457557924182381
for alpha = 1
Log Loss : 1.706360520395438
for alpha = 10
Log Loss : 1.7261917214695601
for alpha = 100
Log Loss : 1.7282505302427342
```
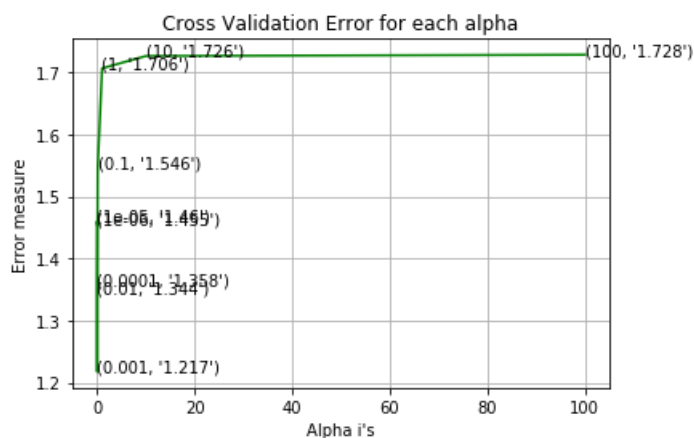


```
For values of best alpha =  0.001 The train log loss is: 0.6153177097029675
For values of best alpha =  0.001 The cross validation log loss is: 1.217324457704446
For values of best alpha =  0.001 The test log loss is: 1.1047257743181136
```
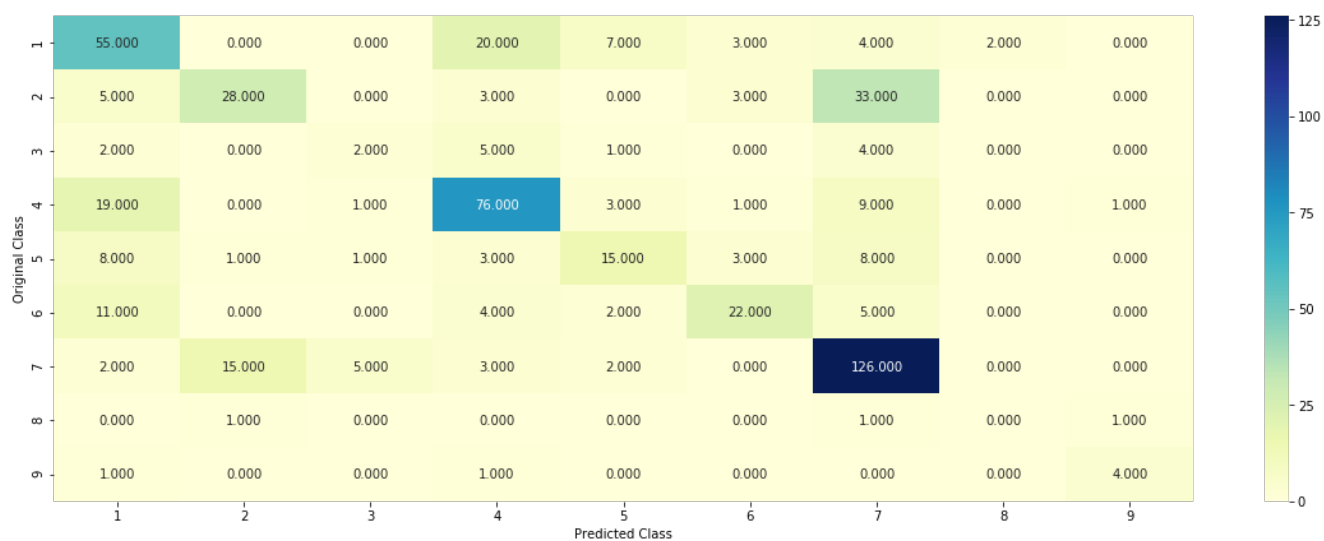
Testing the model with best hyper paramters
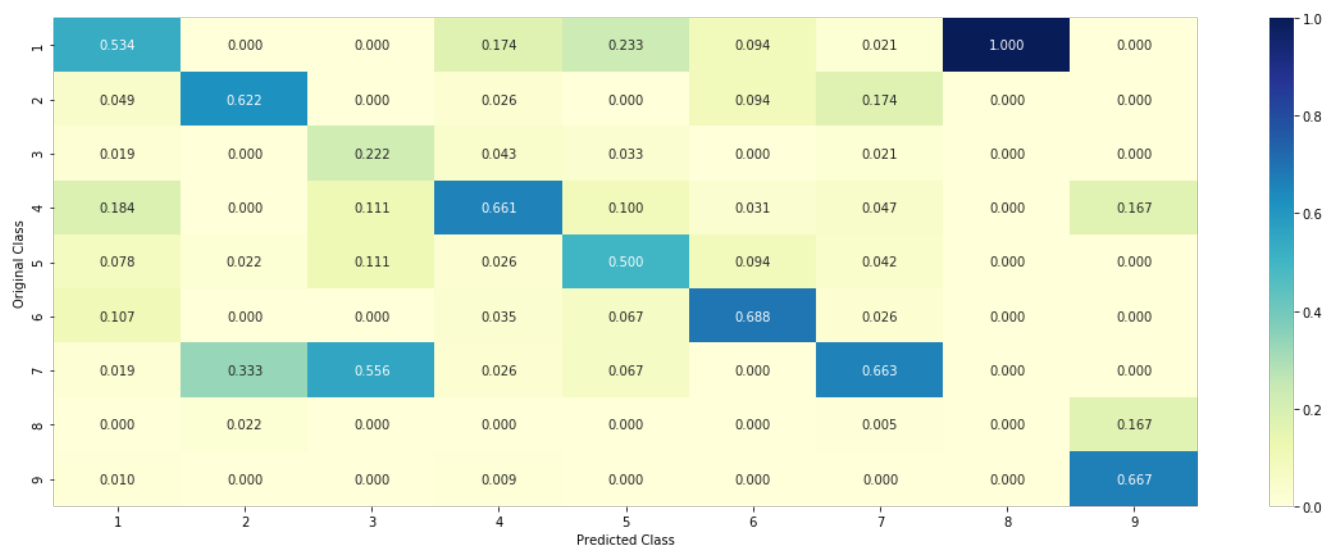
In [77]:

```
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty='l2', loss='log', ran
dom_state=42)
predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y, cv_x_onehotCoding, cv_y, clf)
```

```
Log loss : 1.217324457704446
Number of mis-classified points : 0.38345864661654133
-------------------- Confusion matrix --------------------
```



```
-------------------- Precision matrix (Columm Sum=1) --------------------
```



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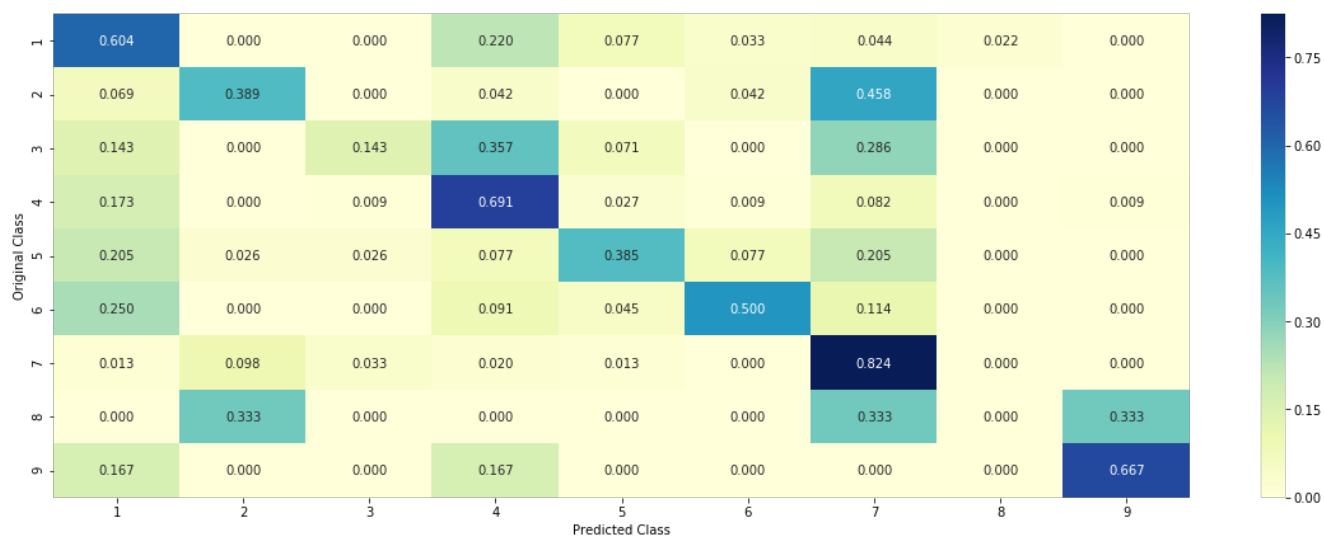

Feature Importance

In [78]:

```python
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 importent features are present in our query point")
    print("-"*50)
    print("The features that are most importent of the ",predicted_cls[0]," class:")
    print (tabulate(tabulte_list, headers=["Index",'Feature name', 'Present or Not']))
```

Correctly Classified point

In [79]:

```python
# from tabulate import tabulate
clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty='l2', loss='log', ran
dom_state=42)
clf.fit(train_x_onehotCoding,train_y)
test_point_index = 1
no_feature = 500
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 : 7
Predicted Class Probabilities: [[0.0045 0.1905 0.0012 0.0012 0.0047 0.0014 0.7872 0.0076 0.0017]]
Actual Class : 7
--------------------------------------------
23 Text feature [constitutively] present in test data point [True]
39 Text feature [flt1] present in test data point [True]
79 Text feature [oncogene] present in test data point [True]
80 Text feature [oncogenes] present in test data point [True]
84 Text feature [cysteine] present in test data point [True]
89 Text feature [inhibited] present in test data point [True]
137 Text feature [technology] present in test data point [True]
160 Text feature [dramatic] present in test data point [True]
162 Text feature [gaiix] present in test data point [True]
166 Text feature [ligand] present in test data point [True]
177 Text feature [downstream] present in test data point [True]
181 Text feature [concentrations] present in test data point [True]
182 Text feature [thyroid] present in test data point [True]
187 Text feature [expressing] present in test data point [True]
217 Text feature [activating] present in test data point [True]
241 Text feature [cdnas] present in test data point [True]
250 Text feature [manageable] present in test data point [True]
265 Text feature [axilla] present in test data point [True]
302 Text feature [inhibitor] present in test data point [True]
311 Text feature [cot] present in test data point [True]
313 Text feature [viability] present in test data point [True]
334 Text feature [activation] present in test data point [True]
352 Text feature [forced] present in test data point [True]
368 Text feature [subcutaneous] present in test data point [True]
371 Text feature [melanocyte] present in test data point [True]
376 Text feature [erk1] present in test data point [True]
388 Text feature [hours] present in test data point [True]
```

```
388 Text feature [hours] present in test data point [True]
446 Text feature [procure] present in test data point [True]
448 Text feature [doses] present in test data point [True]
480 Text feature [mapk] present in test data point [True]
Out of the top  500  features  30 are present in query point
```

Incorrectly Classified point

In [80]:

```
test_point_index = 100
no_feature = 500
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 : 7
Predicted Class Probabilities: [[0.0482 0.2032 0.0108 0.0446 0.071  0.0164 0.5932 0.0078 0.0046]]
Actual Class : 7
--------------------------------------------------
23 Text feature [constitutively] present in test data point [True]
29 Text feature [constitutive] present in test data point [True]
47 Text feature [activated] present in test data point [True]
79 Text feature [oncogene] present in test data point [True]
89 Text feature [inhibited] present in test data point [True]
93 Text feature [transforming] present in test data point [True]
108 Text feature [transform] present in test data point [True]
148 Text feature [receptors] present in test data point [True]
177 Text feature [downstream] present in test data point [True]
210 Text feature [isozyme] present in test data point [True]
217 Text feature [activating] present in test data point [True]
232 Text feature [exchange] present in test data point [True]
326 Text feature [murine] present in test data point [True]
333 Text feature [agar] present in test data point [True]
334 Text feature [activation] present in test data point [True]
Out of the top  500  features  15 are present in query point
```

Without Class balancing

Hyper paramter tuning

In [81]:

```
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()
```

```python
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 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 alpha = ', alpha[best_alpha], "The cross validation log loss is:",log_lo
ss(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 is:",log_loss(y_test, p
redict_y, labels=clf.classes_, eps=1e-15))
```
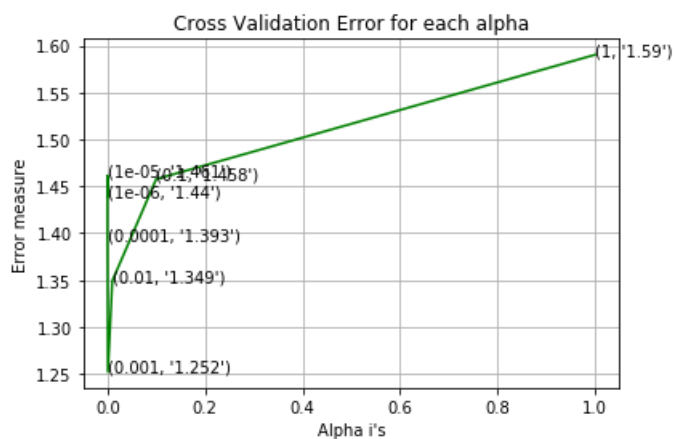
```
for alpha = 1e-06
Log Loss : 1.4395190222240433
for alpha = 1e-05
Log Loss : 1.4613951945118617
for alpha = 0.0001
Log Loss : 1.392640595913179
for alpha = 0.001
Log Loss : 1.2521811628755943
for alpha = 0.01
Log Loss : 1.349151219922669
for alpha = 0.1
Log Loss : 1.457591708320943
for alpha = 1
Log Loss : 1.5902258764770603
```



```
For values of best alpha =  0.001 The train log loss is: 0.6257422677412771
For values of best alpha =  0.001 The cross validation log loss is: 1.2521811628755943
For values of best alpha =  0.001 The test log loss is: 1.1306020069615057
```

Testing model with best hyper parameters
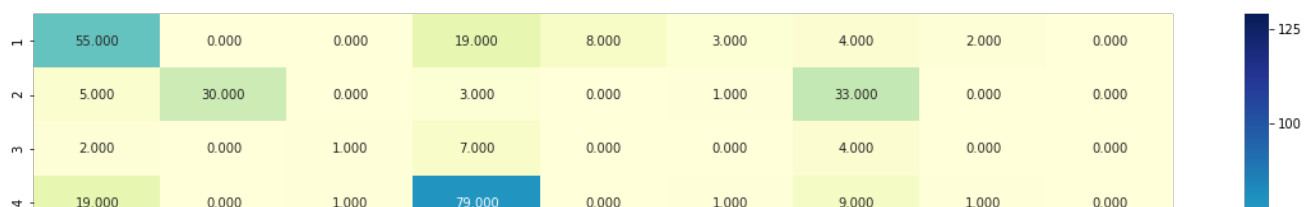
```python
clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_state=42)
predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y, cv_x_onehotCoding, cv_y, clf)
```
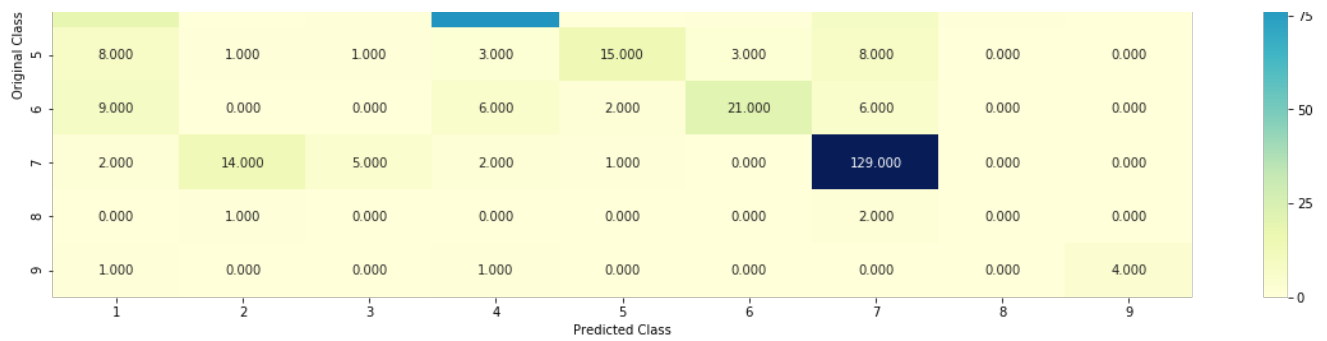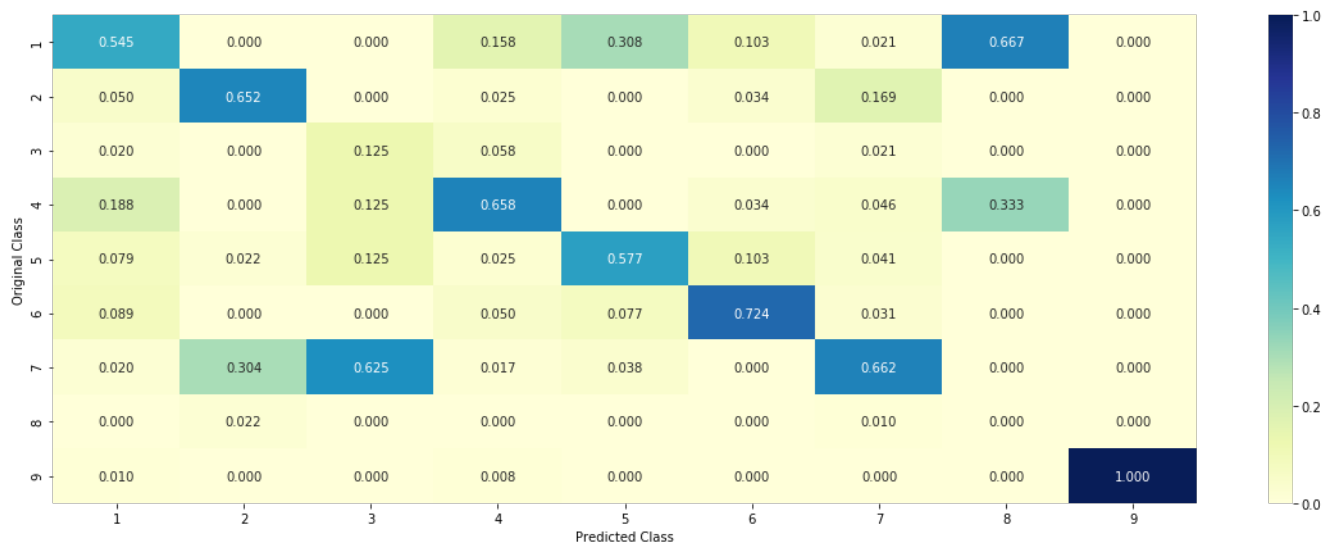
```
Log loss : 1.2521811628755943
Number of mis-classified points : 0.37218045112781956
------------------- Confusion matrix -------------------
```
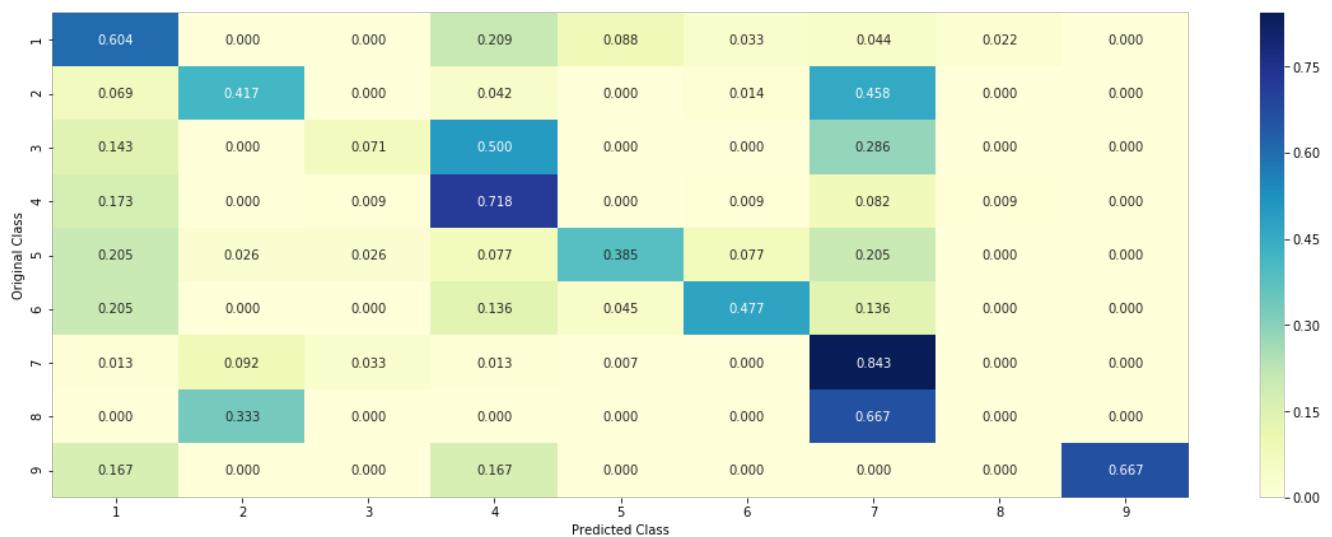
Original Class \ Predicted Class	1	2	3	4	5	6	7	8	9
5	8.000	1.000	1.000	3.000	15.000	3.000	8.000	0.000	0.000
6	9.000	0.000	0.000	6.000	2.000	21.000	6.000	0.000	0.000
7	2.000	14.000	5.000	2.000	1.000	0.000	129.000	0.000	0.000
8	0.000	1.000	0.000	0.000	0.000	0.000	2.000	0.000	0.000
9	1.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	4.000

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

Original Class \ Predicted Class	1	2	3	4	5	6	7	8	9
1	0.545	0.000	0.000	0.158	0.308	0.103	0.021	0.667	0.000
2	0.050	0.652	0.000	0.025	0.000	0.034	0.169	0.000	0.000
3	0.020	0.000	0.125	0.058	0.000	0.000	0.021	0.000	0.000
4	0.188	0.000	0.125	0.658	0.000	0.034	0.046	0.333	0.000
5	0.079	0.022	0.125	0.025	0.577	0.103	0.041	0.000	0.000
6	0.089	0.000	0.000	0.050	0.077	0.724	0.031	0.000	0.000
7	0.020	0.304	0.625	0.017	0.038	0.000	0.662	0.000	0.000
8	0.000	0.022	0.000	0.000	0.000	0.000	0.010	0.000	0.000
9	0.010	0.000	0.000	0.008	0.000	0.000	0.000	0.000	1.000

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

Original Class \ Predicted Class	1	2	3	4	5	6	7	8	9
1	0.604	0.000	0.000	0.209	0.088	0.033	0.044	0.022	0.000
2	0.069	0.417	0.000	0.042	0.000	0.014	0.458	0.000	0.000
3	0.143	0.000	0.071	0.500	0.000	0.000	0.286	0.000	0.000
4	0.173	0.000	0.009	0.718	0.000	0.009	0.082	0.009	0.000
5	0.205	0.026	0.026	0.077	0.385	0.077	0.205	0.000	0.000
6	0.205	0.000	0.000	0.136	0.045	0.477	0.136	0.000	0.000
7	0.013	0.092	0.033	0.013	0.007	0.000	0.843	0.000	0.000
8	0.000	0.333	0.000	0.000	0.000	0.000	0.667	0.000	0.000
9	0.167	0.000	0.000	0.167	0.000	0.000	0.000	0.000	0.667

Feature Importance, Correctly Classified point

In [83]:

```
clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='log', random_state=42)
clf.fit(train_x_onehotCoding,train_y)
test_point_index = 1
no_feature = 500
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 : 7
Predicted Class Probabilities: [[5.100e-03 1.255e-01 2.000e-04 1.300e-03 2.300e-03 1.400e-03 8.556
e-01
  8.500e-03 1.000e-04]]
Actual Class : 7
-------------------------------------------------
60 Text feature [constitutively] present in test data point [True]
107 Text feature [flt1] present in test data point [True]
124 Text feature [cysteine] present in test data point [True]
157 Text feature [oncogenes] present in test data point [True]
158 Text feature [inhibited] present in test data point [True]
195 Text feature [activating] present in test data point [True]
200 Text feature [ligand] present in test data point [True]
203 Text feature [oncogene] present in test data point [True]
204 Text feature [technology] present in test data point [True]
257 Text feature [gaiix] present in test data point [True]
260 Text feature [concentrations] present in test data point [True]
265 Text feature [downstream] present in test data point [True]
314 Text feature [hki] present in test data point [True]
316 Text feature [dramatic] present in test data point [True]
323 Text feature [expressing] present in test data point [True]
371 Text feature [cdnas] present in test data point [True]
380 Text feature [viability] present in test data point [True]
412 Text feature [thyroid] present in test data point [True]
459 Text feature [activation] present in test data point [True]
461 Text feature [manageable] present in test data point [True]
462 Text feature [ser473] present in test data point [True]
468 Text feature [axilla] present in test data point [True]
495 Text feature [extracellular] present in test data point [True]
Out of the top  500  features  23 are present in query point
```

Feature Importance, Inorrectly Classified point

In [84]:

```
test_point_index = 100
no_feature = 500
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 : 7
Predicted Class Probabilities: [[0.0485 0.1851 0.0052 0.0442 0.0617 0.0143 0.6317 0.0072 0.0022]]
Actual Class : 7
-------------------------------------------------
60 Text feature [constitutively] present in test data point [True]
89 Text feature [constitutive] present in test data point [True]
116 Text feature [activated] present in test data point [True]
158 Text feature [inhibited] present in test data point [True]
159 Text feature [transforming] present in test data point [True]
193 Text feature [receptors] present in test data point [True]
195 Text feature [activating] present in test data point [True]
203 Text feature [oncogene] present in test data point [True]
226 Text feature [transform] present in test data point [True]
241 Text feature [isozyme] present in test data point [True]
265 Text feature [downstream] present in test data point [True]
377 Text feature [agar] present in test data point [True]
442 Text feature [interatomic] present in test data point [True]
459 Text feature [activation] present in test data point [True]
Out of the top  500  features  14 are present in query point
```

Linear Support Vector Machines

Hyper paramter tuning

In [85]:

```python
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', r
andom_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 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 alpha = ', alpha[best_alpha], "The cross validation log loss is:",log_lo
ss(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 is:",log_loss(y_test, p
redict_y, labels=clf.classes_, eps=1e-15))
```
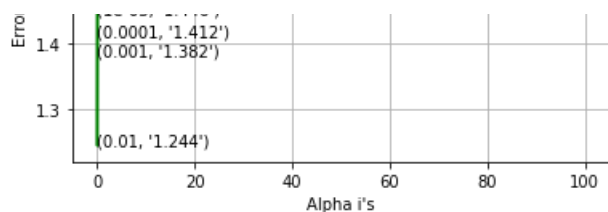
```
for C = 1e-05
Log Loss : 1.4456349250609233
for C = 0.0001
Log Loss : 1.4117883301099556
for C = 0.001
Log Loss : 1.3818342037841624
for C = 0.01
Log Loss : 1.2442964974823838
for C = 0.1
Log Loss : 1.5346828298587332
for C = 1
Log Loss : 1.722800653929441
for C = 10
Log Loss : 1.7286360420759161
for C = 100
Log Loss : 1.7286184454094997
```

```
(0.0001, '1.412')
(0.001, '1.382')

(0.01, '1.244')
```
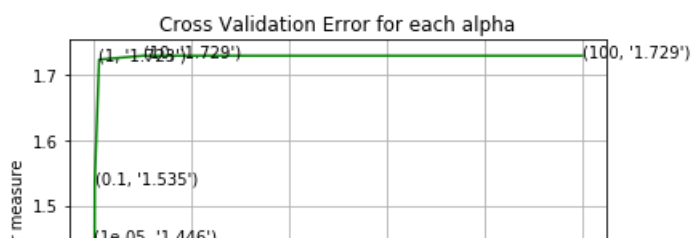
For values of best alpha = 0.01 The train log loss is: 0.7628309867716067
For values of best alpha = 0.01 The cross validation log loss is: 1.2442964974823838
For values of best alpha = 0.01 The test log loss is: 1.1541891969863685

4.4.2. Testing model with best hyper parameters

In [86]:

```python
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,cv_x_onehotCoding,cv_y, clf)
```
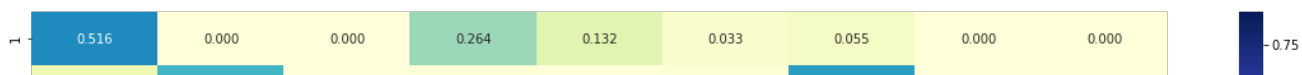
Log loss : 1.2442964974823838
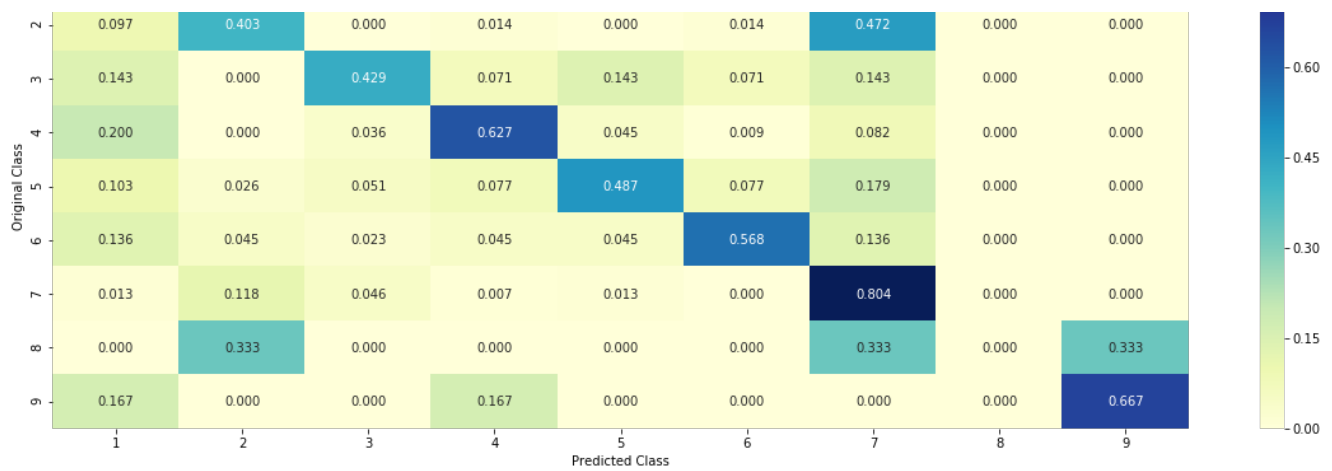Number of mis-classified points : 0.39473684210526316
-------------------- Confusion matrix --------------------
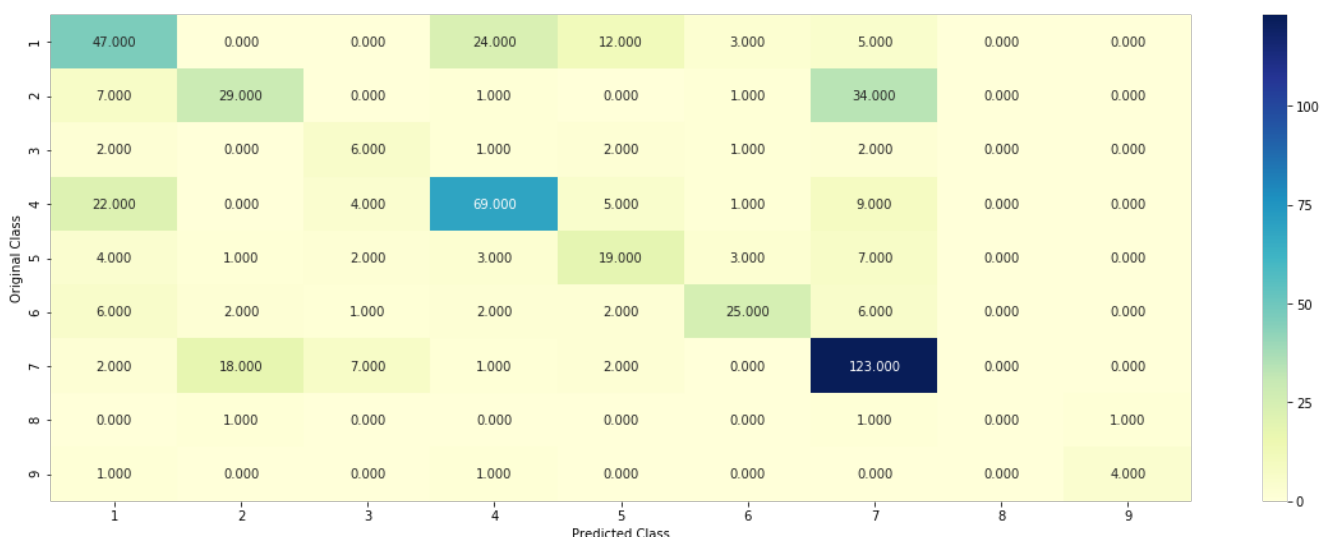
-------------------- Precision matrix (Columm Sum=1) --------------------

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

Feature Importance

For Correctly classified point

```python
clf = SGDClassifier(alpha=alpha[best_alpha], penalty='l2', loss='hinge', random_state=42)
clf.fit(train_x_onehotCoding,train_y)
test_point_index = 1
# test_point_index = 100
no_feature = 500
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 : 7
Predicted Class Probabilities: [[0.0153 0.1199 0.0029 0.0151 0.0121 0.0075 0.8104 0.0129 0.0039]]
Actual Class : 7
--------------------------------------------------
28 Text feature [constitutively] present in test data point [True]
29 Text feature [cysteine] present in test data point [True]
49 Text feature [cdnas] present in test data point [True]
76 Text feature [flt1] present in test data point [True]
79 Text feature [concentrations] present in test data point [True]
82 Text feature [gaiix] present in test data point [True]
96 Text feature [technology] present in test data point [True]
101 Text feature [inhibited] present in test data point [True]
104 Text feature [activating] present in test data point [True]
114 Text feature [oncogenes] present in test data point [True]
147 Text feature [expressing] present in test data point [True]
150 Text feature [mapk] present in test data point [True]
151 Text feature [oncogene] present in test data point [True]
169 Text feature [thyroid] present in test data point [True]
171 Text feature [inhibitor] present in test data point [True]
205 Text feature [transduced] present in test data point [True]
211 Text feature [seeded] present in test data point [True]
230 Text feature [ligand] present in test data point [True]
255 Text feature [activation] present in test data point [True]
279 Text feature [downstream] present in test data point [True]
314 Text feature [doses] present in test data point [True]
351 Text feature [subcutaneous] present in test data point [True]
366 Text feature [atcc] present in test data point [True]
405 Text feature [melanocyte] present in test data point [True]
436 Text feature [hours] present in test data point [True]
445 Text feature [selleck] present in test data point [True]
446 Text feature [dramatic] present in test data point [True]
454 Text feature [chemiluminescence] present in test data point [True]
487 Text feature [viability] present in test data point [True]
489 Text feature [ser473] present in test data point [True]
```

Out of the top 500 features 30 are present in query point

For Incorrectly classified point

In [88]:

```
test_point_index = 100
no_feature = 500
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 : 7
Predicted Class Probabilities: [[0.0786 0.1516 0.0146 0.1064 0.1105 0.0323 0.4839 0.0128 0.0094]]
Actual Class : 7
--------------------------------------------------
28 Text feature [constitutively] present in test data point [True]
40 Text feature [constitutive] present in test data point [True]
73 Text feature [activated] present in test data point [True]
75 Text feature [transforming] present in test data point [True]
94 Text feature [receptors] present in test data point [True]
97 Text feature [exchange] present in test data point [True]
101 Text feature [inhibited] present in test data point [True]
104 Text feature [activating] present in test data point [True]
151 Text feature [oncogene] present in test data point [True]
231 Text feature [transform] present in test data point [True]
255 Text feature [activation] present in test data point [True]
279 Text feature [downstream] present in test data point [True]
440 Text feature [doubled] present in test data point [True]
470 Text feature [substituting] present in test data point [True]
Out of the top  500  features  14 are present in query point
```

Random Forest Classifier

Hyper paramter tuning

In [89]:

```
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))


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 : 1.2572535683354957
for n_estimators = 100 and max depth =  10
Log Loss : 1.1868414223711878
for n_estimators = 200 and max depth =  5
Log Loss : 1.2378734502517341
for n_estimators = 200 and max depth =  10
Log Loss : 1.1811031780258958
for n_estimators = 500 and max depth =  5
Log Loss : 1.2368241894319212
for n_estimators = 500 and max depth =  10
Log Loss : 1.176754594516683
for n_estimators = 1000 and max depth =  5
Log Loss : 1.2357829533963691
for n_estimators = 1000 and max depth =  10
Log Loss : 1.174993079576866
for n_estimators = 2000 and max depth =  5
Log Loss : 1.236042392554891
for n_estimators = 2000 and max depth =  10
Log Loss : 1.1759745074379755
For values of best estimator =  1000 The train log loss is: 0.7095396732082752
For values of best estimator =  1000 The cross validation log loss is: 1.174993079576866
For values of best estimator =  1000 The test log loss is: 1.1630923149103904
```

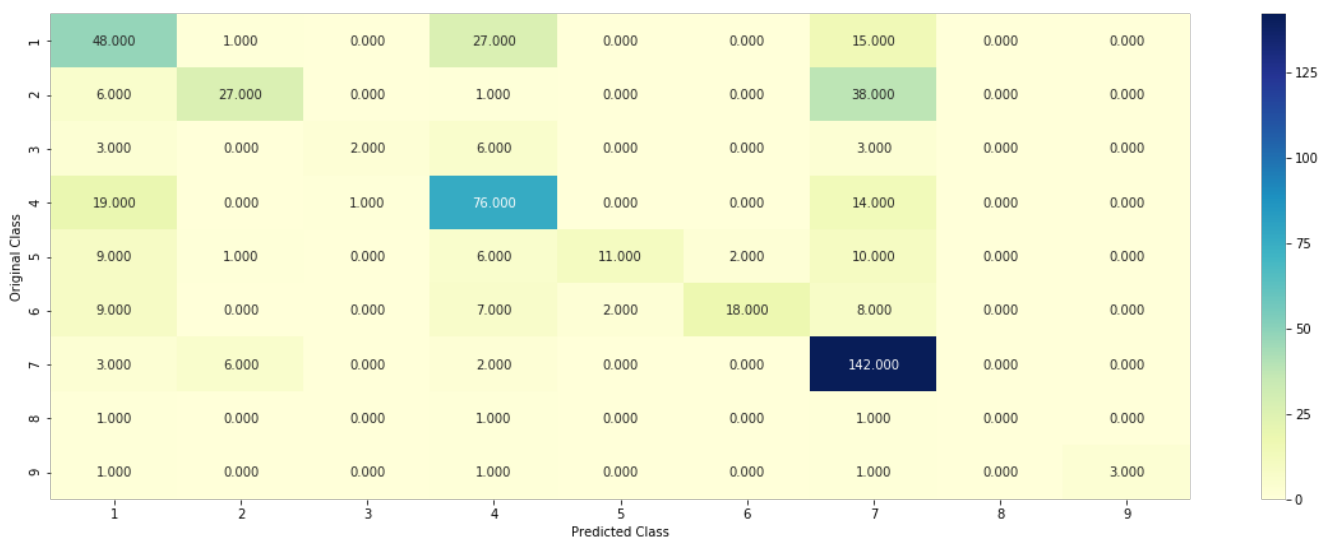## Testing model with best hyper parameters

```
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,cv_x_onehotCoding,cv_y, clf)
```

```
Log loss : 1.174993079576866
Number of mis-classified points : 0.38533834586466165
------------------- Confusion matrix --------------------
```
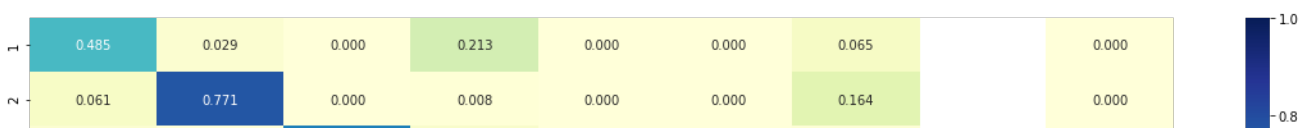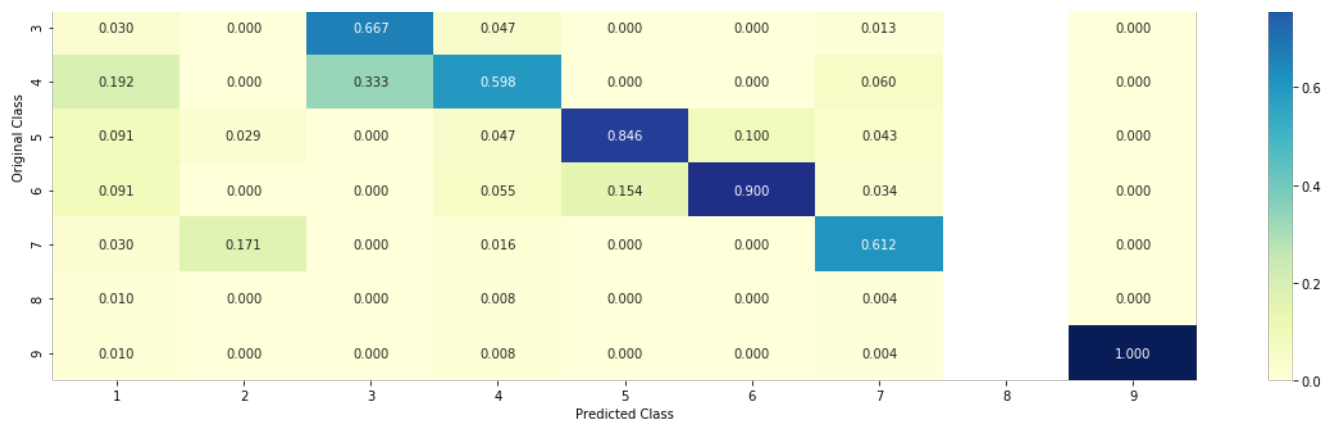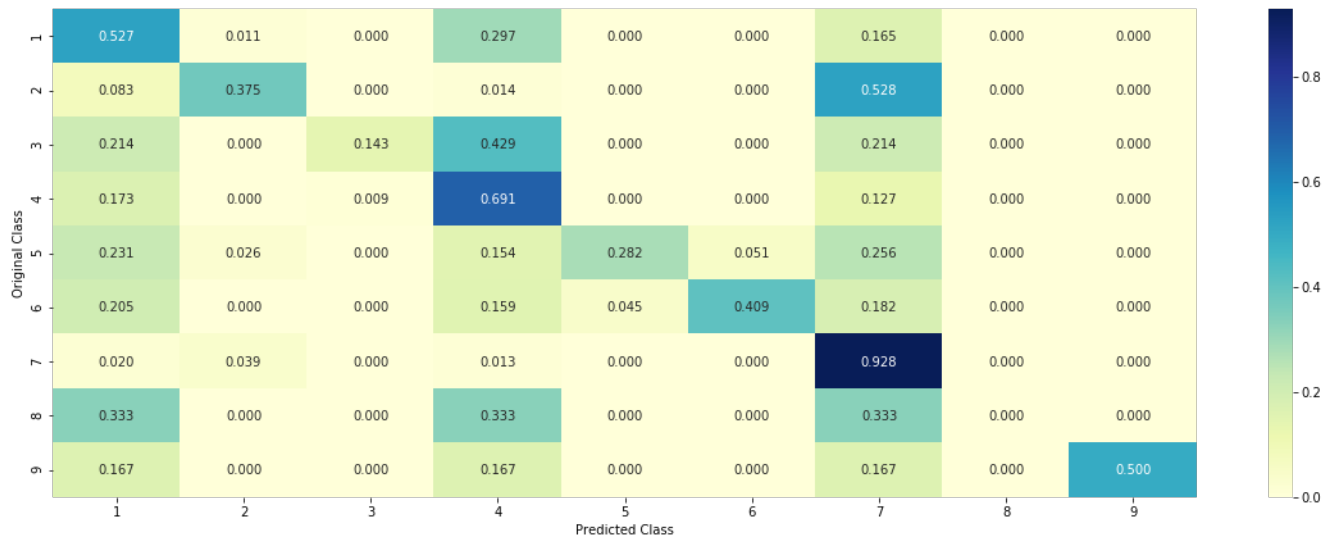


```
------------------- Precision matrix (Columm Sum=1) --------------------
```

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

Feature Importance

Correctly Classified point

```python
# 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 = 1
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_index],test_df['Gene'].
iloc[test_point_index],test_df['Variation'].iloc[test_point_index], no_feature)
```

```
Predicted Class : 7
Predicted Class Probabilities: [[0.0454 0.1404 0.0133 0.029  0.036  0.0294 0.6977 0.005  0.004 ]]
Actual Class : 7
--------------------------------------------------
0 Text feature [inhibitors] present in test data point [True]
1 Text feature [kinase] present in test data point [True]
2 Text feature [activating] present in test data point [True]
3 Text feature [tyrosine] present in test data point [True]
4 Text feature [missense] present in test data point [True]
```

```
5  Text feature [inhibitor] present in test data point [True]
7  Text feature [treatment] present in test data point [True]
8  Text feature [oncogenic] present in test data point [True]
9  Text feature [suppressor] present in test data point [True]
10 Text feature [activation] present in test data point [True]
11 Text feature [phosphorylation] present in test data point [True]
12 Text feature [kinases] present in test data point [True]
13 Text feature [nonsense] present in test data point [True]
14 Text feature [akt] present in test data point [True]
15 Text feature [function] present in test data point [True]
17 Text feature [erk] present in test data point [True]
19 Text feature [growth] present in test data point [True]
20 Text feature [variants] present in test data point [True]
22 Text feature [frameshift] present in test data point [True]
24 Text feature [therapeutic] present in test data point [True]
25 Text feature [functional] present in test data point [True]
28 Text feature [signaling] present in test data point [True]
30 Text feature [patients] present in test data point [True]
31 Text feature [cells] present in test data point [True]
32 Text feature [constitutively] present in test data point [True]
34 Text feature [trials] present in test data point [True]
35 Text feature [therapy] present in test data point [True]
37 Text feature [erk1] present in test data point [True]
38 Text feature [activate] present in test data point [True]
39 Text feature [downstream] present in test data point [True]
41 Text feature [efficacy] present in test data point [True]
42 Text feature [protein] present in test data point [True]
43 Text feature [loss] present in test data point [True]
44 Text feature [inhibited] present in test data point [True]
45 Text feature [expressing] present in test data point [True]
46 Text feature [pten] present in test data point [True]
48 Text feature [lines] present in test data point [True]
49 Text feature [treated] present in test data point [True]
50 Text feature [proliferation] present in test data point [True]
51 Text feature [drug] present in test data point [True]
57 Text feature [mek] present in test data point [True]
59 Text feature [inhibition] present in test data point [True]
61 Text feature [repair] present in test data point [True]
62 Text feature [sensitivity] present in test data point [True]
64 Text feature [receptor] present in test data point [True]
66 Text feature [assays] present in test data point [True]
68 Text feature [survival] present in test data point [True]
69 Text feature [cell] present in test data point [True]
71 Text feature [ligand] present in test data point [True]
73 Text feature [expression] present in test data point [True]
74 Text feature [variant] present in test data point [True]
75 Text feature [oncogene] present in test data point [True]
78 Text feature [extracellular] present in test data point [True]
79 Text feature [doses] present in test data point [True]
80 Text feature [mapk] present in test data point [True]
81 Text feature [hours] present in test data point [True]
84 Text feature [information] present in test data point [True]
86 Text feature [harboring] present in test data point [True]
90 Text feature [dna] present in test data point [True]
91 Text feature [concentrations] present in test data point [True]
92 Text feature [likelihood] present in test data point [True]
93 Text feature [months] present in test data point [True]
94 Text feature [binding] present in test data point [True]
96 Text feature [imatinib] present in test data point [True]
98 Text feature [preclinical] present in test data point [True]
Out of the top  100  features  65 are present in query point
```

Inorrectly Classified point

In [92]:

```
test_point_index = 100
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("Actuall 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_index],test_df['Gene'].
iloc[test_point_index],test_df['Variation'].iloc[test_point_index], no_feature)
```

Predicted Class : 7
Predicted Class Probabilities: [[0.1337 0.116 0.0224 0.1773 0.0674 0.0545 0.4156 0.0071 0.0059]]
Actuall Class : 7
----
0 Text feature [inhibitors] present in test data point [True]
1 Text feature [kinase] present in test data point [True]
2 Text feature [activating] present in test data point [True]
3 Text feature [tyrosine] present in test data point [True]
6 Text feature [activated] present in test data point [True]
8 Text feature [oncogenic] present in test data point [True]
10 Text feature [activation] present in test data point [True]
11 Text feature [phosphorylation] present in test data point [True]
12 Text feature [kinases] present in test data point [True]
14 Text feature [akt] present in test data point [True]
15 Text feature [function] present in test data point [True]
19 Text feature [growth] present in test data point [True]
21 Text feature [constitutive] present in test data point [True]
25 Text feature [functional] present in test data point [True]
28 Text feature [signaling] present in test data point [True]
31 Text feature [cells] present in test data point [True]
32 Text feature [constitutively] present in test data point [True]
38 Text feature [activate] present in test data point [True]
39 Text feature [downstream] present in test data point [True]
42 Text feature [protein] present in test data point [True]
43 Text feature [loss] present in test data point [True]
44 Text feature [inhibited] present in test data point [True]
46 Text feature [pten] present in test data point [True]
47 Text feature [transforming] present in test data point [True]
48 Text feature [lines] present in test data point [True]
50 Text feature [proliferation] present in test data point [True]
53 Text feature [neutral] present in test data point [True]
55 Text feature [transform] present in test data point [True]
56 Text feature [stability] present in test data point [True]
58 Text feature [transformation] present in test data point [True]
59 Text feature [inhibition] present in test data point [True]
62 Text feature [sensitivity] present in test data point [True]
64 Text feature [receptor] present in test data point [True]
66 Text feature [assays] present in test data point [True]
69 Text feature [cell] present in test data point [True]
75 Text feature [oncogene] present in test data point [True]
84 Text feature [information] present in test data point [True]
90 Text feature [dna] present in test data point [True]
94 Text feature [binding] present in test data point [True]
Out of the top 100 features 39 are present in query point
```