Personalized cancer diagnosis

1. Business Problem ¶

1.1. Description

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

Context:

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

Problem statement:

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

1.3. Real-world/Business objectives and constraints.

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

2. Machine Learning Problem Formulation

2.1. Data

2.1.1. Data Overview

- Source: https://www.kaggle.com/c/msk-redefining-cancer-treatment/data)
- 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)

2.1.2. Example Data Point

training_variants

ID,Gene,Variation,Class 0,FAM58A,Truncating Mutations,1 1,CBL,W802*,2 2,CBL,Q249E,2

•••

training text

ID, Text

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

2.2. Mapping the real-world problem to an ML problem

2.2.1. Type of Machine Learning Problem

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

2.2.2. Performance Metric

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

Metric(s):

- Multi class log-loss
- · Confusion matrix

2.2.3. 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.

2.3. Train, CV and Test Datasets

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

3. Exploratory Data Analysis

```
In [4]:
        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 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
```

3.1. Reading Data

3.1.1. Reading Gene and Variation Data

```
In [5]: data = pd.read_csv('training_variants')
    print('Number of data points : ', data.shape[0])
    print('Number of features : ', data.shape[1])
    print('Features : ', data.columns.values)
    data.head()
```

```
Number of data points : 3321
Number of features : 4
```

Features : ['ID' 'Gene' 'Variation' 'Class']

Out[5]:

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

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

Fields are

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

3.1.2. Reading Text Data

```
In [7]: # note the seprator in this file
         data_text =pd.read_csv("training_text",sep="\|\|",engine="python",names=["ID","TE
         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[7]:
             ID
                                                    TEXT
             0
                 Cyclin-dependent kinases (CDKs) regulate a var...
             1
                   Abstract Background Non-small cell lung canc...
          1
          2
             2
                   Abstract Background Non-small cell lung canc...
             3 Recent evidence has demonstrated that acquired...
```

3.1.3. Preprocessing of text

4 Oncogenic mutations in the monomeric Casitas B...

```
In [8]: # Loading stop words from nltk library
        stop words = set(stopwords.words('english'))
        def nlp_preprocessing(total_text, index, column):
            if type(total text) is not int:
                string = ""
                 # replace every special char with space
                total_text = re.sub('[^a-zA-Z0-9\n]', ' ', total_text)
                 # replace multiple spaces with single space
                total_text = re.sub('\s+',' ', total_text)
                # converting all the chars into lower-case.
                total text = total text.lower()
                for word in total text.split():
                 # if the word is a not a stop word then retain that word from the data
                     if not word in stop words:
                         string += word + " "
                data text[column][index] = string
```

```
In [9]: #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, "second
          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: 53.09783729893066 seconds
In [10]:
          #merging both gene variations and text data based on ID
          result = pd.merge(data, data text,on='ID', how='left')
          result.head()
Out[10]:
              ID
                    Gene
                                  Variation Class
                                                                                     TEXT
                 FAM58A Truncating Mutations
              0
                                                    cyclin dependent kinases cdks regulate variety...
                    CBL
                                    W802*
                                                    abstract background non small cell lung cancer...
           1
              1
                                               2
           2
              2
                    CBL
                                    Q249E
                                               2
                                                    abstract background non small cell lung cancer...
                                                  recent evidence demonstrated acquired uniparen...
           3
              3
                    CBL
                                    N454D
                    CBL
                                     L399V
                                                  oncogenic mutations monomeric casitas b lineag...
In [11]:
          result[result.isnull().any(axis=1)]
Out[11]:
                   ID
                                       Variation Class TEXT
                        Gene
                                        S1088F
           1109
                1109
                      FANCA
                                                    1
                                                        NaN
           1277 1277 ARID5B Truncating Mutations
                                                       NaN
           1407
                1407
                       FGFR3
                                         K508M
                                                       NaN
           1639
                1639
                        FLT1
                                    Amplification
                                                       NaN
           2755 2755
                        BRAF
                                         G596C
                                                    7
                                                       NaN
          result.loc[result['TEXT'].isnull(), 'TEXT'] = result['Gene'] +' '+result['Variatio
In [12]:
In [13]:
          result[result['ID']==1109]
Out[13]:
                       Gene Variation Class
                                                     TEXT
                  ID
           1109 1109
                      FANCA
                               S1088F
                                          1 FANCA S1088F
```

3.1.4. Test, Train and Cross Validation Split

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

```
In [14]: 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 verification, test_df, y_train, y_test = train_test_split(result, y_true, stratify=y_t # split the train data into train and cross validation by maintaining same distribution distribution of output verification.
```

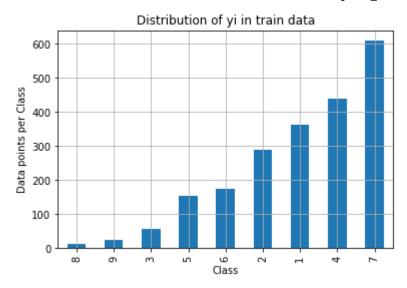
We split the data into train, test and cross validation data sets, preserving the ratio of class distribution in the original data set

```
In [15]: print('Number of data points in train data:', train_df.shape[0])
    print('Number of data points in test data:', test_df.shape[0])
    print('Number of data points in cross validation data:', cv_df.shape[0])

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

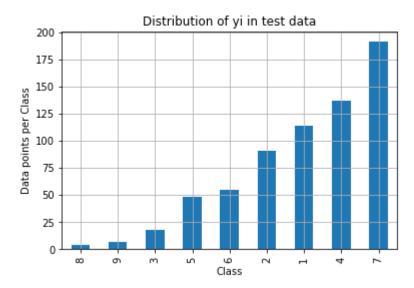
3.1.4.2. Distribution of y_i's in Train, Test and Cross Validation datasets

```
In [21]: # it returns a dict, keys as class labels and values as the number of data points
         train class distribution = train_df['Class'].value_counts().sort_values()
         test class distribution = test df['Class'].value counts().sort values()
         cv class distribution = cv df['Class'].value counts().sort values()
         my colors = 'rgbkymc'
         train class distribution.plot(kind='bar')
         plt.xlabel('Class')
         plt.ylabel('Data points per Class')
         plt.title('Distribution of yi in train data')
         plt.grid()
         plt.show()
         # ref: argsort https://docs.scipy.org/doc/numpy/reference/generated/numpy.argsort
         # -(train class distribution.values): the minus sign will give us in decreasing o
         sorted_yi = np.argsort(-train_class_distribution.values)
         for i in sorted vi:
             print('Number of data points in class', i+1, ':',train class distribution.val
         print('-'*80)
         my colors = 'rgbkymc'
         test class distribution.plot(kind='bar')
         plt.xlabel('Class')
         plt.ylabel('Data points per Class')
         plt.title('Distribution of yi in test data')
         plt.grid()
         plt.show()
         # ref: argsort https://docs.scipy.org/doc/numpy/reference/generated/numpy.argsort
         # -(train class distribution.values): the minus sign will give us in decreasing o
         sorted_yi = np.argsort(-test_class_distribution.values)
         for i in sorted vi:
             print('Number of data points in class', i+1, ':',test_class_distribution.valu
         print('-'*80)
         my colors = 'rgbkymc'
         cv class distribution.plot(kind='bar')
         plt.xlabel('Class')
         plt.ylabel('Data points per Class')
         plt.title('Distribution of yi in cross validation data')
         plt.grid()
         plt.show()
         # ref: argsort https://docs.scipy.org/doc/numpy/reference/generated/numpy.argsort
         # -(train class distribution.values): the minus sign will give us in decreasing o
         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
```



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

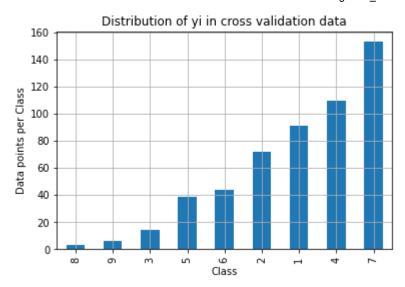
-



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

validation and points in class 1 . 4 (0.002 %)

_



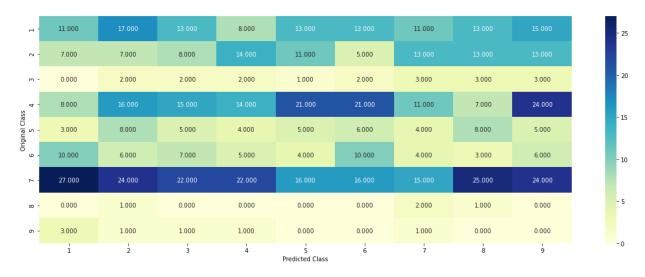
```
Number of data points in class 9: 153 ( 28.759 %)
Number of data points in class 8: 110 ( 20.677 %)
Number of data points in class 7: 91 ( 17.105 %)
Number of data points in class 6: 72 ( 13.534 %)
Number of data points in class 5: 44 ( 8.271 %)
Number of data points in class 4: 39 ( 7.331 %)
Number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

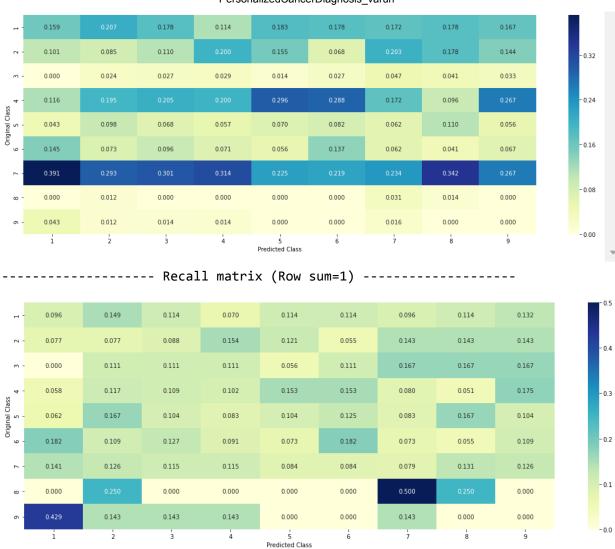
3.2 Prediction using a 'Random' Model

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

```
In [22]: # This function plots the confusion matrices given y_i, y_i_hat.
         def plot_confusion_matrix(test_y, predict_y):
             C = confusion_matrix(test_y, predict_y)
             A = (((C.T)/(C.sum(axis=1))).T)
             B = (C/C.sum(axis=0))
             labels = [1,2,3,4,5,6,7,8,9]
             # representing A in heatmap format
             print("-"*20, "Confusion matrix", "-"*20)
             plt.figure(figsize=(20,7))
             sns.heatmap(C, annot=True, cmap="YlGnBu", fmt=".3f", xticklabels=labels, ytic
             plt.xlabel('Predicted Class')
             plt.ylabel('Original Class')
             plt.show()
             print("-"*20, "Precision matrix (Columm Sum=1)", "-"*20)
             plt.figure(figsize=(20,7))
             sns.heatmap(B, annot=True, cmap="YlGnBu", fmt=".3f", xticklabels=labels, ytic
             plt.xlabel('Predicted Class')
             plt.ylabel('Original Class')
             plt.show()
             # representing B in heatmap format
             print("-"*20, "Recall matrix (Row sum=1)", "-"*20)
             plt.figure(figsize=(20,7))
             sns.heatmap(A, annot=True, cmap="YlGnBu", fmt=".3f", xticklabels=labels, ytic
             plt.xlabel('Predicted Class')
             plt.ylabel('Original Class')
             plt.show()
```

In [23]: # ref: https://stackoverflow.com/a/18662466/4084039 test data len = test df.shape[0] cv data len = cv df.shape[0] # we create a output array that has exactly same size as the CV data cv predicted y = np.zeros((cv data len,9)) for i in range(cv data len): rand probs = np.random.rand(1,9) cv_predicted_y[i] = ((rand_probs/sum(sum(rand_probs)))[0]) print("Log loss on Cross Validation Data using Random Model",log loss(y cv,cv pre # Test-Set error. #we create a output array that has exactly same as the test data test_predicted_y = np.zeros((test_data_len,9)) for i in range(test data len): rand_probs = np.random.rand(1,9) test_predicted_y[i] = ((rand_probs/sum(sum(rand_probs)))[0]) print("Log loss on Test Data using Random Model",log loss(y test,test predicted y predicted_y =np.argmax(test_predicted_y, axis=1) plot_confusion_matrix(y_test, predicted_y+1)





3.3 Univariate Analysis

```
In [24]:
         # get qv fea dict: Get Gene varaition Feature Dict
         def get_gv_fea_dict(alpha, feature, df):
             value count = train df[feature].value counts()
             # gv dict : Gene Variation Dict, which contains the probability array for each
             gv dict = dict()
             # denominator will contain the number of time that particular feature occured
             for i, denominator in value count.items():
                 # vec will contain (p(yi==1/Gi) probability of gene/variation belongs to
                 # vec is 9 diamensional vector
                 vec = []
                 for k in range(1,10):
                     cls_cnt = train_df.loc[(train_df['Class']==k) & (train_df[feature]==i
                     # cls_cnt.shape[0](numerator) will contain the number of time that pa
                     vec.append((cls_cnt.shape[0] + alpha*10)/ (denominator + 90*alpha))
                 # we are adding the gene/variation to the dict as key and vec as value
                 gv dict[i]=vec
             return gv_dict
         # Get Gene variation feature
         def get gv feature(alpha, feature, df):
             gv_dict = get_gv_fea_dict(alpha, feature, df)
             # value count is similar in get gv fea dict
             value count = train df[feature].value counts()
             # gv fea: Gene variation feature, it will contain the feature for each feature
             gv fea = []
             # for every feature values in the given data frame we will check if it is the
             # if not we will add [1/9,1/9,1/9,1/9,1/9,1/9,1/9,1/9] to gv_fea
             for index, row in df.iterrows():
                 if row[feature] in dict(value count).keys():
                     gv_fea.append(gv_dict[row[feature]])
                 else:
                     gv_fea.append([1/9,1/9,1/9,1/9,1/9,1/9,1/9,1/9])
             return gv fea
```

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

(numerator + 10*alpha) / (denominator + 90*alpha)

3.2.1 Univariate Analysis on Gene Feature

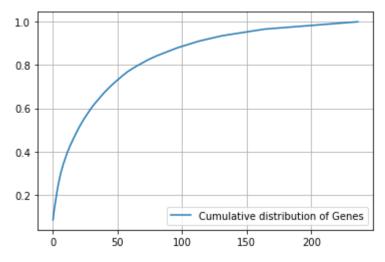
Q1. Gene, What type of feature it is?

Ans. Gene is a categorical variable

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

```
In [25]:
          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 : 237
          BRCA1
                     179
          TP53
                     103
                      82
          EGFR
          PTEN
                      82
          BRCA2
                      72
          KIT
                      63
          BRAF
                      56
          ERBB2
                      45
                      45
          ALK
          CDKN2A
                      37
          Name: Gene, dtype: int64
          print("Ans: There are", unique_genes.shape[0] ,"different categories of genes in
In [0]:
          Ans: There are 229 different categories of genes in the train data, and they ar
          e distibuted as follows
In [26]: | 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()
                                                 Histrogram of Genes
             0.08
          Number of Occurances
             0.06
             0.04
             0.02
             0.00
                            50
                                    100
                                             150
                                                       200
                                   Index of a Gene
```

```
In [27]: c = np.cumsum(h)
    plt.plot(c,label='Cumulative distribution of Genes')
    plt.grid()
    plt.legend()
    plt.show()
```



Q3. How to featurize this Gene feature?

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

```
In [29]: print("train_gene_feature_responseCoding is converted feature using respone coding)
```

train_gene_feature_responseCoding is converted feature using respone coding met hod. The shape of gene feature: (2124, 9)

```
In [30]: # 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'])
```

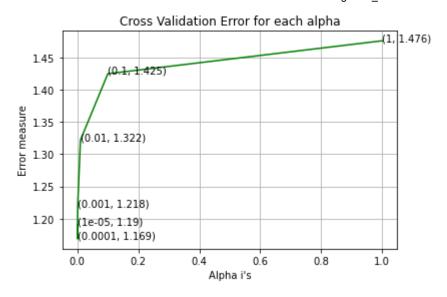
train_gene_feature_onehotCoding is converted feature using one-hot encoding met hod. The shape of gene feature: (2124, 237)

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

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

```
In [34]: 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='12', 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=
             print('For values of alpha = ', i, "The log loss is:",log_loss(y_cv, predict_
         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='12', loss='log', random_sta
         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:",
         predict_y = sig_clf.predict_proba(cv_gene_feature_onehotCoding)
         print('For values of best alpha = ', alpha[best alpha], "The cross validation log
         predict_y = sig_clf.predict_proba(test_gene_feature_onehotCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The test log loss is:",1
         For values of alpha = 1e-05 The log loss is: 1.1901198329691247
         For values of alpha = 0.0001 The log loss is: 1.1685824305462422
         For values of alpha = 0.001 The log loss is: 1.2184519609886837
         For values of alpha = 0.01 The log loss is: 1.3217444834733574
```

```
For values of alpha = 0.1 The log loss is: 1.4247488195515197
For values of alpha = 1 The log loss is: 1.4758292218934486
```



For values of best alpha = 0.0001 The train log loss is: 0.9812520083686037

For values of best alpha = 0.0001 The cross validation log loss is: 1.16858243
05462422

For values of best alpha = 0.0001 The test log loss is: 1.2027569957312394

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

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

```
In [35]: print("Q6. How many data points in Test and CV datasets are covered by the ", uni
    test_coverage=test_df[test_df['Gene'].isin(list(set(train_df['Gene'])))].shape[0]
    cv_coverage=cv_df[cv_df['Gene'].isin(list(set(train_df['Gene'])))].shape[0]
    print('Ans\n1. In test data',test_coverage, 'out of',test_df.shape[0], ":",(test_print('2. In cross validation data',cv_coverage, 'out of ',cv_df.shape[0],":",(cov_df.shape[0])
```

Q6. How many data points in Test and CV datasets are covered by the 237 genes in train dataset?

Ans

- 1. In test data 646 out of 665 : 97.14285714285714
- In cross validation data 515 out of 532 : 96.80451127819549

3.2.2 Univariate Analysis on Variation Feature

Q7. Variation, What type of feature is it?

Ans. Variation is a categorical variable

Q8. How many categories are there?

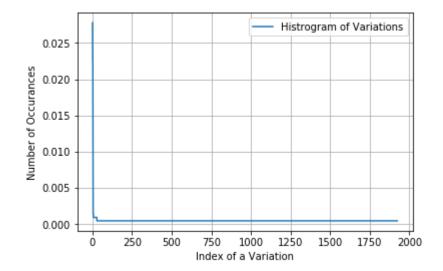
```
In [36]: unique_variations = train_df['Variation'].value_counts()
    print('Number of Unique Variations :', unique_variations.shape[0])
# the top 10 variations that occured most
    print(unique_variations.head(10))
```

Number of Unique Variations: 1928 Truncating_Mutations 60 Deletion 48 Amplification 43 **Fusions** 25 Overexpression 4 4 **G12V** Q61R 3 Q61H 3 061L 3 EWSR1-ETV1 Fusion Name: Variation, dtype: int64

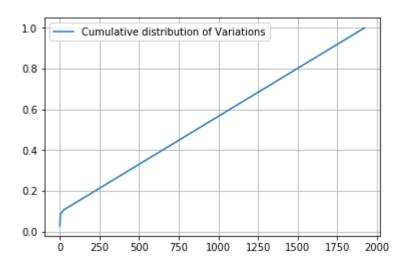
```
In [0]: print("Ans: There are", unique_variations.shape[0] ,"different categories of variations.shape[0] ,"di
```

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

```
In [0]: 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()
```



[0.02777778 0.05084746 0.07297552 ... 0.99905838 0.99952919 1.



Q9. How to featurize this Variation feature?

Ans.There are two ways we can featurize this variable

- 1. One hot Encoding
- 2. Response coding

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

```
In [37]: # alpha is used for laplace smoothing
    alpha = 1
    # train gene feature
    train_variation_feature_responseCoding = np.array(get_gv_feature(alpha, "Variatio
    # test gene feature
    test_variation_feature_responseCoding = np.array(get_gv_feature(alpha, "Variation
    # cross validation gene feature
    cv_variation_feature_responseCoding = np.array(get_gv_feature(alpha, "Variation",
```

```
In [0]: print("train_variation_feature_responseCoding is a converted feature using the re
```

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

```
In [39]: # one-hot encoding of variation feature.
    variation_vectorizer = CountVectorizer()
    train_variation_feature_onehotCoding = variation_vectorizer.fit_transform(train_d)
    test_variation_feature_onehotCoding = variation_vectorizer.transform(test_df['Var
    cv_variation_feature_onehotCoding = variation_vectorizer.transform(cv_df['Variation_onehotCoding)]
```

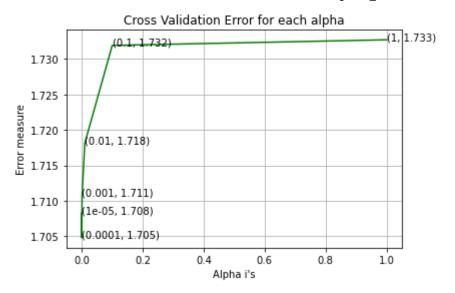
```
In [0]: print("train_variation_feature_onehotEncoded is converted feature using the onne-
```

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

Q10. How good is this Variation feature in predicting y i?

Let's build a model just like the earlier!

```
In [40]: | alpha = [10 ** x for x in range(-5, 1)]
         cv_log_error_array=[]
         for i in alpha:
             clf = SGDClassifier(alpha=i, penalty='12', 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=
             print('For values of alpha = ', i, "The log loss is:",log_loss(y_cv, predict_
         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='12', loss='log', random_sta
         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:",
         predict y = sig clf.predict proba(cv variation feature onehotCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The cross validation log
         predict y = sig clf.predict proba(test variation feature onehotCoding)
         print('For values of best alpha = ', alpha[best alpha], "The test log loss is:",l
         For values of alpha = 1e-05 The log loss is: 1.7082431858288039
         For values of alpha = 0.0001 The log loss is: 1.7047589176085123
         For values of alpha = 0.001 The log loss is: 1.7106904073827571
         For values of alpha = 0.01 The log loss is: 1.71812568029598
         For values of alpha = 0.1 The log loss is: 1.731925607343552
         For values of alpha = 1 The log loss is: 1.7327170913083907
```



For values of best alpha = 0.0001 The train log loss is: 0.6472958168887896 For values of best alpha = 0.0001 The cross validation log loss is: 1.70475891 76085123

For values of best alpha = 0.0001 The test log loss is: 1.709905394636484

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

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

```
In [41]: print("Q12. How many data points are covered by total ", unique_variations.shape[
    test_coverage=test_df[test_df['Variation'].isin(list(set(train_df['Variation'])))
    cv_coverage=cv_df[cv_df['Variation'].isin(list(set(train_df['Variation'])))].shap
    print('Ans\n1. In test data',test_coverage, 'out of',test_df.shape[0], ":",(test_
    print('2. In cross validation data',cv_coverage, 'out of ',cv_df.shape[0],":",(c)
```

Q12. How many data points are covered by total 1928 genes in test and cross validation data sets?

Ans

- 1. In test data 64 out of 665 : 9.624060150375941
- In cross validation data 57 out of 532 : 10.714285714285714

3.2.3 Univariate Analysis on Text Feature

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

```
In [48]: # building a CountVectorizer with all the words that occured minimum 3 times in to
    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 (...
    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 time
    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 : 53968

```
In [51]: dict list = []
         # dict list =[] contains 9 dictoinaries each corresponds to a class
         for i in range(1,10):
             cls text = train df[train df['Class']==i]
             # build a word dict based on the words in that class
             dict_list.append(extract_dictionary_paddle(cls_text))
             # append it to dict list
         # dict list[i] is build on i'th class text data
         # total dict is buid on whole training text data
         total dict = extract dictionary paddle(train df)
         confuse array = []
         for i in train text features:
             ratios = []
             max val = -1
             for j in range(0,9):
                 ratios.append((dict_list[j][i]+10 )/(total_dict[i]+90))
             confuse array.append(ratios)
         confuse array = np.array(confuse array)
```

- In [52]: #response coding of text features
 train_text_feature_responseCoding = get_text_responsecoding(train_df)
 test_text_feature_responseCoding = get_text_responsecoding(test_df)
 cv_text_feature_responseCoding = get_text_responsecoding(cv_df)
- In [54]: # normalizing every feature
 train_text_feature_onehotCoding = normalize(train_text_feature_onehotCoding, axis

 # we use the same vectorizer that was trained on train data
 test_text_feature_onehotCoding = text_vectorizer.transform(test_df['TEXT'])

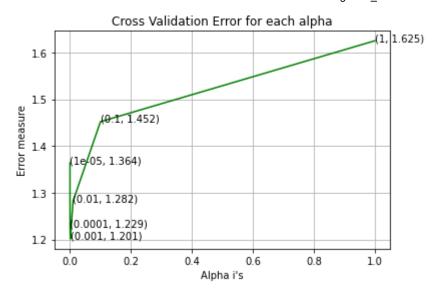
 # normalizing every feature
 test_text_feature_onehotCoding = normalize(test_text_feature_onehotCoding, axis=0)

 # we use the same vectorizer that was trained on train data
 cv_text_feature_onehotCoding = text_vectorizer.transform(cv_df['TEXT'])
 # normalizing every feature
 cv_text_feature_onehotCoding = normalize(cv_text_feature_onehotCoding, axis=0)
- In [76]: #https://stackoverflow.com/a/2258273/4084039
 sorted_text_fea_dict = dict(sorted(text_fea_dict.items(), key=lambda x: x[1] , resorted_text_occur = np.array(list(sorted_text_fea_dict.values()))

```
In [57]: # Number of words for a given frequency.
print(Counter(sorted text occur))
```

ט, סס. אט, בער איט, 6: 40, 109: 40, 127: 39, 124: 39, 123: 39, 156: 38, 136: 38, 151: 37, 130: 3 7, 122: 36, 160: 35, 132: 35, 142: 34, 138: 34, 106: 34, 155: 33, 149: 33, 14 1: 33, 125: 33, 118: 33, 200: 32, 169: 32, 137: 32, 134: 32, 126: 32, 129: 3 1, 174: 30, 145: 30, 168: 29, 139: 29, 187: 28, 164: 28, 161: 28, 159: 28, 15 4: 28, 131: 28, 128: 28, 180: 27, 163: 27, 158: 27, 234: 26, 208: 26, 197: 2 6, 194: 26, 181: 26, 166: 26, 152: 26, 146: 26, 143: 26, 266: 25, 186: 25, 17 8: 25, 150: 25, 144: 25, 222: 24, 204: 24, 175: 24, 223: 23, 218: 23, 211: 2 3, 201: 23, 195: 23, 192: 23, 189: 23, 177: 23, 173: 23, 162: 23, 203: 22, 19 6: 22, 171: 22, 165: 22, 213: 21, 198: 21, 176: 21, 167: 21, 267: 20, 231: 2 0, 228: 20, 216: 20, 207: 20, 191: 20, 184: 20, 182: 20, 170: 20, 236: 19, 22 5: 19, 212: 19, 210: 19, 206: 19, 270: 18, 246: 18, 230: 18, 229: 18, 221: 1 8, 209: 18, 205: 18, 157: 18, 287: 17, 272: 17, 258: 17, 248: 17, 243: 17, 22 0: 17, 214: 17, 309: 16, 245: 16, 232: 16, 217: 16, 190: 16, 188: 16, 183: 1 6, 341: 15, 294: 15, 291: 15, 282: 15, 280: 15, 279: 15, 276: 15, 264: 15, 26 3: 15, 261: 15, 254: 15, 250: 15, 227: 15, 199: 15, 179: 15, 172: 15, 330: 1 4, 300: 14, 289: 14, 284: 14, 268: 14, 259: 14, 249: 14, 215: 14, 370: 13, 35 9: 13, 316: 13, 315: 13, 312: 13, 307: 13, 298: 13, 295: 13, 273: 13, 251: 1 3, 247: 13, 244: 13, 202: 13, 469: 12, 412: 12, 361: 12, 353: 12, 351: 12, 30 5: 12, 303: 12, 299: 12, 269: 12, 265: 12, 257: 12, 252: 12, 242: 12, 241: 1

```
In [58]: # Train a Logistic regression+Calibration model using text features which are on-
         alpha = [10 ** x for x in range(-5, 1)]
         cv_log_error_array=[]
         for i in alpha:
             clf = SGDClassifier(alpha=i, penalty='12', 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=
             print('For values of alpha = ', i, "The log loss is:",log_loss(y_cv, predict_
         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='12', loss='log', random sta
         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:",
         predict_y = sig_clf.predict_proba(cv_text_feature_onehotCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The cross validation log
         predict_y = sig_clf.predict_proba(test_text_feature_onehotCoding)
         print('For values of best alpha = ', alpha[best alpha], "The test log loss is:",1
         For values of alpha = 1e-05 The log loss is: 1.36361870374097
         For values of alpha = 0.0001 The log loss is: 1.2285895647516927
         For values of alpha = 0.001 The log loss is: 1.2014457912100782
         For values of alpha = 0.01 The log loss is: 1.281986991738801
         For values of alpha = 0.1 The log loss is: 1.451908981735228
         For values of alpha = 1 The log loss is: 1.6247969033234715
```



```
For values of best alpha = 0.001 The train log loss is: 0.625889574286602

For values of best alpha = 0.001 The cross validation log loss is: 1.201445791
2100782

For values of best alpha = 0.001 The test log loss is: 1.177458263252274
```

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

Ans. Yes, it seems like!

```
In [59]: def get_intersec_text(df):
    df_text_vec = CountVectorizer(min_df=3)
    df_text_fea = df_text_vec.fit_transform(df['TEXT'])
    df_text_features = df_text_vec.get_feature_names()

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

```
In [60]: len1,len2 = get_intersec_text(test_df)
print(np.round((len2/len1)*100, 3), "% of word of test data appeared in train data
len1,len2 = get_intersec_text(cv_df)
print(np.round((len2/len1)*100, 3), "% of word of Cross Validation appeared in train
```

97.738 % of word of test data appeared in train data 98.281 % of word of Cross Validation appeared in train data

4. Machine Learning Models

```
In [61]: #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 will provide the array of probabilities belong:
    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))
    plot_confusion_matrix(test_y, pred_y)
```

```
In [62]: 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 [85]: # 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):</pre>
                      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 [{}]".form
                 elif (v < fea1 len+fea2 len):</pre>
                     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 [{}]"
                  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 [{}]".form
             print("Out of the top ",no_features," features ", word_present, "are present
```

Stacking the three types of features

```
In [64]: # merging gene, variance and text features
         train gene var onehotCoding = hstack((train gene feature onehotCoding,train varia
         test_gene_var_onehotCoding = hstack((test_gene_feature_onehotCoding,test_variatio)
         cv gene var onehotCoding = hstack((cv gene feature onehotCoding,cv variation feat
         train x onehotCoding = hstack((train gene var onehotCoding, train text feature on
         train_y = np.array(list(train_df['Class']))
         test_x_onehotCoding = hstack((test_gene_var_onehotCoding, test_text_feature_onehot
         test_y = np.array(list(test_df['Class']))
         cv x onehotCoding = hstack((cv gene var onehotCoding, cv text feature onehotCoding
         cv_y = np.array(list(cv_df['Class']))
         train_gene_var_responseCoding = np.hstack((train_gene_feature_responseCoding,trai
         test gene var responseCoding = np.hstack((test gene feature responseCoding,test v
         cv gene var responseCoding = np.hstack((cv gene feature responseCoding,cv variati
         train x responseCoding = np.hstack((train gene var responseCoding, train text fea
         test_x_responseCoding = np.hstack((test_gene_var_responseCoding, test_text_feature)
         cv_x_responseCoding = np.hstack((cv_gene_var_responseCoding, cv_text_feature_resp
In [65]:
         print("One hot encoding features :")
         print("(number of data points * number of features) in train data = ", train x on
         print("(number of data points * number of features) in test data = ", test_x_oneh
         print("(number of data points * number of features) in cross validation data =",
         One hot encoding features :
         (number of data points * number of features) in train data = (2124, 56155)
         (number of data points * number of features) in test data = (665, 56155)
         (number of data points * number of features) in cross validation data = (532, 5
         6155)
In [66]:
         print(" Response encoding features :")
         print("(number of data points * number of features) in train data = ", train x re
         print("(number of data points * number of features) in test data = ", test_x_resp
         print("(number of data points * number of features) in cross validation data =",
          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, 2
         7)
```

4.1. Base Line Model

4.1.1. Naive Bayes

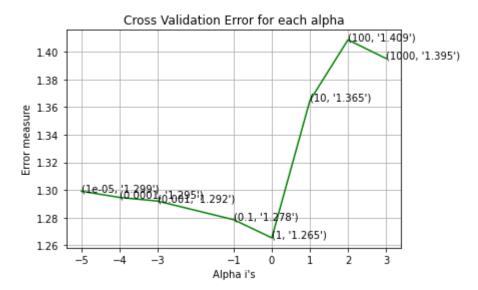
4.1.1.1. Hyper parameter tuning

```
In [67]:
         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_,
             # to avoid rounding error while multiplying probabilites we use log-probabili
             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:",
         predict y = sig clf.predict proba(cv x onehotCoding)
         print('For values of best alpha = ', alpha[best alpha], "The cross validation log
         predict y = sig clf.predict proba(test x onehotCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The test log loss is:",1
         for alpha = 1e-05
         Log Loss: 1.299124812093323
         for alpha = 0.0001
         Log Loss: 1.2946307612790837
         for alpha = 0.001
         Log Loss: 1.291985139550523
         for alpha = 0.1
         Log Loss: 1.2784862241644395
         for alpha = 1
         Log Loss: 1.2653570618225016
         for alpha = 10
         Log Loss: 1.3648165427218035
         for alpha = 100
```

Log Loss: 1.4087839749711353

for alpha = 1000

Log Loss: 1.3952182404724107



For values of best alpha = 1 The train log loss is: 0.8857842350022214

For values of best alpha = 1 The cross validation log loss is: 1.2653570618225

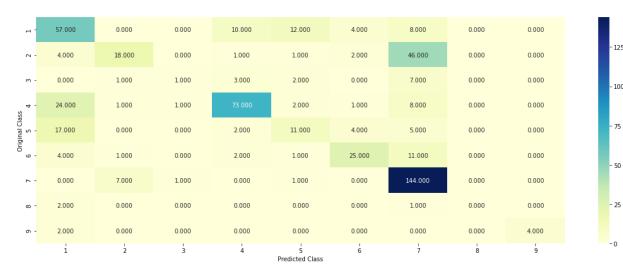
016

For values of best alpha = 1 The test log loss is: 1.3288125990526927

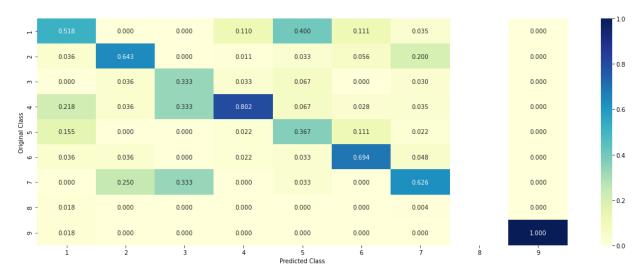
4.1.1.2. Testing the model with best hyper paramters

In [68]:

```
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 e.
print("Log Loss :",log_loss(cv_y, sig_clf_probs))
print("Number of missclassified point :", np.count_nonzero((sig_clf.predict(cv_x_oplot_confusion_matrix(cv_y, sig_clf.predict(cv_x_onehotCoding.toarray()))
```



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



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



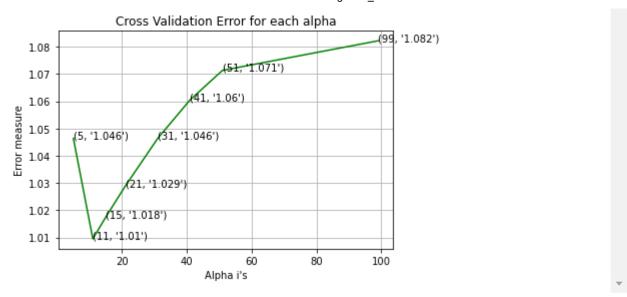
4.1.1.3. Feature Importance, Correctly classified point

4.1.1.4. Feature Importance, Incorrectly classified point

4.2. K Nearest Neighbour Classification

4.2.1. Hyper parameter tuning

```
In [79]:
         alpha = [5, 11, 15, 21, 31, 41, 51, 99]
         cv log error array = []
         for i in alpha:
             print("for alpha =", i)
             clf = KNeighborsClassifier(n_neighbors=i)
             clf.fit(train x responseCoding, train y)
             sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
             sig clf.fit(train x responseCoding, train y)
             sig_clf_probs = sig_clf.predict_proba(cv_x_responseCoding)
             cv_log_error_array.append(log_loss(cv_y, sig_clf_probs, labels=clf.classes_,
             # to avoid rounding error while multiplying probabilites we use log-probabili
             print("Log Loss :",log_loss(cv_y, sig_clf_probs))
         fig, ax = plt.subplots()
         ax.plot(alpha, cv_log_error_array,c='g')
         for i, txt in enumerate(np.round(cv log error array,3)):
             ax.annotate((alpha[i],str(txt)), (alpha[i],cv_log_error_array[i]))
         plt.grid()
         plt.title("Cross Validation Error for each alpha")
         plt.xlabel("Alpha i's")
         plt.ylabel("Error measure")
         plt.show()
         best alpha = np.argmin(cv log error array)
         clf = KNeighborsClassifier(n neighbors=alpha[best alpha])
         clf.fit(train_x_responseCoding, train_y)
         sig clf = CalibratedClassifierCV(clf, method="sigmoid")
         sig_clf.fit(train_x_responseCoding, train_y)
         predict y = sig clf.predict proba(train x responseCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The train log loss is:",
         predict_y = sig_clf.predict_proba(cv_x_responseCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The cross validation log
         predict_y = sig_clf.predict_proba(test_x_responseCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The test log loss is:",1
         for alpha = 5
         Log Loss: 1.0463826255378885
         for alpha = 11
         Log Loss: 1.009521670795516
         for alpha = 15
         Log Loss: 1.017500535784801
         for alpha = 21
         Log Loss: 1.0288543571290953
         for alpha = 31
         Log Loss: 1.046346343428731
         for alpha = 41
         Log Loss: 1.0604966469127457
         for alpha = 51
         Log Loss: 1.0713145794669074
         for alpha = 99
         Log Loss: 1.0821611734429417
```



For values of best alpha = 11 The train log loss is: 0.6038224111225744

For values of best alpha = 11 The cross validation log loss is: 1.009521670795

516

For values of best alpha = 11 The test log loss is: 1.1057287985411093

4.2.2. Testing the model with best hyper paramters

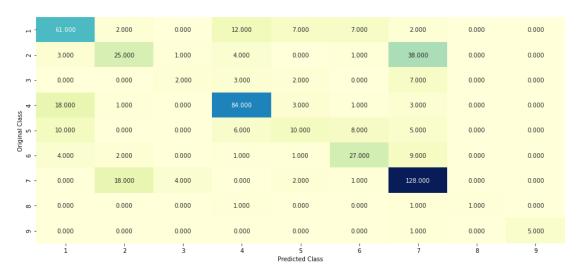
In [80]:

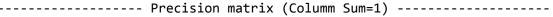
clf = KNeighborsClassifier(n_neighbors=alpha[best_alpha])
predict_and_plot_confusion_matrix(train_x_responseCoding, train_y, cv_x_responseCoding)

Log loss: 1.009521670795516

Number of mis-classified points : 0.35526315789473684

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







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



- 25

- 0.6

-04

- 0.2

- 0.0

0.75

- 0.60

0.45

- 0.30

-0.15

-0.00

4.2.3. Sample Query point -1

```
In [81]: | clf = KNeighborsClassifier(n_neighbors=alpha[best_alpha])
         clf.fit(train_x_responseCoding, train_y)
         sig_clf = CalibratedClassifierCV(clf, method="sigmoid")
         sig clf.fit(train x responseCoding, train y)
         test point index = 1
         predicted_cls = sig_clf.predict(test_x_responseCoding[0].reshape(1,-1))
         print("Predicted Class :", predicted_cls[0])
         print("Actual Class :", test_y[test_point_index])
         neighbors = clf.kneighbors(test_x_responseCoding[test_point_index].reshape(1, -1)
         print("The ",alpha[best_alpha]," nearest neighbours of the test points belongs to
         print("Fequency of nearest points :",Counter(train y[neighbors[1][0]]))
         Predicted Class : 1
         Actual Class : 6
         The 11 nearest neighbours of the test points belongs to classes [6 6 6 6 6
         6 6 6 6 6 1
         Fequency of nearest points : Counter({6: 11})
```

4.2.4. Sample Query Point-2

```
In [82]:
         clf = KNeighborsClassifier(n neighbors=alpha[best alpha])
         clf.fit(train x responseCoding, train y)
         sig clf = CalibratedClassifierCV(clf, method="sigmoid")
         sig clf.fit(train x responseCoding, train y)
         test_point_index = 100
         predicted cls = sig clf.predict(test x responseCoding[test point index].reshape(1
         print("Predicted Class :", predicted_cls[0])
         print("Actual Class :", test y[test point index])
         neighbors = clf.kneighbors(test_x_responseCoding[test_point_index].reshape(1, -1)
         print("the k value for knn is",alpha[best_alpha],"and the nearest neighbours of t
         print("Fequency of nearest points :",Counter(train_y[neighbors[1][0]]))
         Predicted Class: 4
         Actual Class: 4
         the k value for knn is 11 and the nearest neighbours of the test points belongs
         to classes [4 4 4 4 4 4 4 4 4 7 4]
         Fequency of nearest points : Counter({4: 10, 7: 1})
```

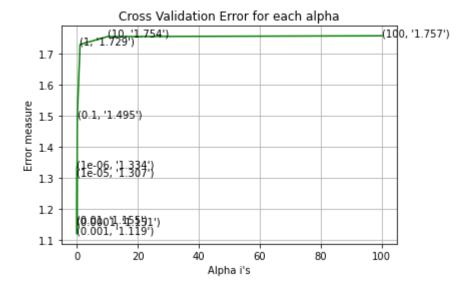
4.3. Logistic Regression

- 4.3.1. With Class balancing
- 4.3.1.1. Hyper paramter tuning

```
In [83]:
         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='12', loss='log
             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_,
             # to avoid rounding error while multiplying probabilites we use log-probabili
             print("Log Loss :",log loss(cv y, sig clf probs))
         fig, ax = plt.subplots()
         ax.plot(alpha, cv_log_error_array,c='g')
         for i, txt in enumerate(np.round(cv_log_error_array,3)):
             ax.annotate((alpha[i],str(txt)), (alpha[i],cv log error array[i]))
         plt.grid()
         plt.title("Cross Validation Error for each alpha")
         plt.xlabel("Alpha i's")
         plt.ylabel("Error measure")
         plt.show()
         best_alpha = np.argmin(cv_log_error_array)
         clf = SGDClassifier(class weight='balanced', alpha=alpha[best alpha], penalty='12
         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:",
         predict y = sig clf.predict proba(cv x onehotCoding)
         print('For values of best alpha = ', alpha[best_alpha], "The cross validation log
         predict y = sig clf.predict proba(test x onehotCoding)
         print('For values of best alpha = ', alpha[best alpha], "The test log loss is:",1
         for alpha = 1e-06
         Log Loss: 1.3335476221684441
         for alpha = 1e-05
         Log Loss: 1.3065902646122092
         for alpha = 0.0001
         Log Loss: 1.150678356021762
         for alpha = 0.001
         Log Loss: 1.1192692412260004
         for alpha = 0.01
         Log Loss: 1.1554949895981694
         for alpha = 0.1
         Log Loss: 1.4951787419953513
         for alpha = 1
         Log Loss: 1.7289437212722742
         for alpha = 10
         Log Loss: 1.7542144930759165
```

for alpha = 100

Log Loss: 1.7567948772379163



For values of best alpha = 0.001 The train log loss is: 0.49521010275728744 For values of best alpha = 0.001 The cross validation log loss is: 1.119269241 2260004

For values of best alpha = 0.001 The test log loss is: 1.0926946004956906

4.3.1.2. Testing the model with best hyper paramters

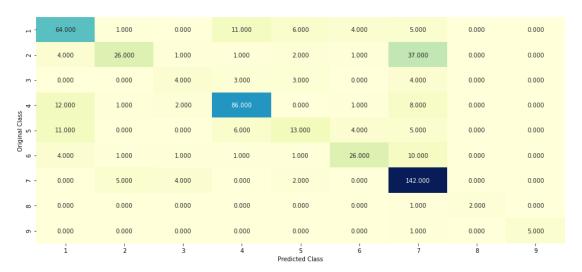
In [87]:

clf = SGDClassifier(class_weight='balanced', alpha=alpha[best_alpha], penalty='12
predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y, cv_x_onehotCoding)

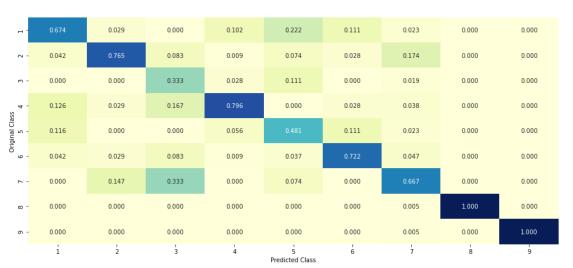
Log loss: 1.1192692412260004

Number of mis-classified points: 0.3082706766917293

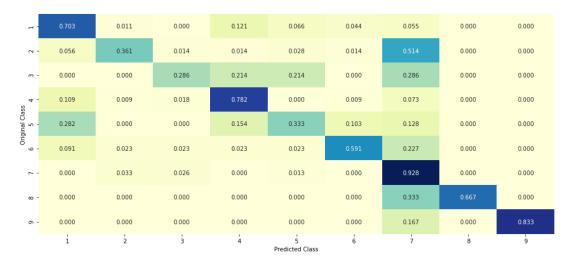
----- Confusion matrix -----







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



125

50

- 25

- 0.6

-04

- 0.2

- 0.0

- 0.6

- 0.4

- 0.2

-0.0

4.3.1.3. Feature Importance

```
In [88]: 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]:</pre>
                     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_n
                  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 No
```

4.3.1.3.1. Correctly Classified point

```
In [89]: # from tabulate import tabulate
         clf = SGDClassifier(class weight='balanced', alpha=alpha[best alpha], penalty='12
         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 one
         print("Actual Class :", test_y[test_point_index])
         indices = np.argsort(-1*abs(clf.coef_))[predicted_cls-1][:,:no_feature]
         print("-"*50)
         get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_df['
         Predicted Class: 6
         Predicted Class Probabilities: [[0.0011 0.0037 0.0022 0.153 0.0015 0.8317 0.00
         12 0.0044 0.0013]]
         Actual Class: 6
         112 Text feature [simplex] present in test data point [True]
         232 Text feature [encoding] present in test data point [True]
         316 Text feature [2b] present in test data point [True]
         323 Text feature [hospitals] present in test data point [True]
         328 Text feature [3b] present in test data point [True]
         336 Text feature [author] present in test data point [True]
         387 Text feature [3a] present in test data point [True]
         400 Text feature [nih] present in test data point [True]
         437 Text feature [mutants] present in test data point [True]
         438 Text feature [2c] present in test data point [True]
         466 Text feature [previously] present in test data point [True]
         469 Text feature [constructs] present in test data point [True]
         475 Text feature [weakened] present in test data point [True]
         483 Text feature [tagged] present in test data point [True]
         487 Text feature [ccdc98] present in test data point [True]
         Out of the top 500 features 15 are present in query point
```

4.3.1.3.2. Incorrectly Classified point

```
In [91]: | test point index = 105
         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 one
         print("Actual Class :", test_y[test_point_index])
         indices = np.argsort(-1*abs(clf.coef ))[predicted cls-1][:,:no feature]
         print("-"*50)
         get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_df['
         Predicted Class: 6
         Predicted Class Probabilities: [[0.0184 0.0052 0.0016 0.0051 0.4195 0.5409 0.00
         15 0.0066 0.0012]]
         Actual Class : 5
         182 Text feature [v1804d] present in test data point [True]
         400 Text feature [nih] present in test data point [True]
         424 Text feature [assays] present in test data point [True]
         466 Text feature [previously] present in test data point [True]
         468 Text feature [e2663v] present in test data point [True]
         474 Text feature [similarly] present in test data point [True]
         476 Text feature [res] present in test data point [True]
         489 Text feature [mayo] present in test data point [True]
         493 Text feature [analyzed] present in test data point [True]
         Out of the top 500 features 9 are present in query point
```

4.3.2. Without Class balancing

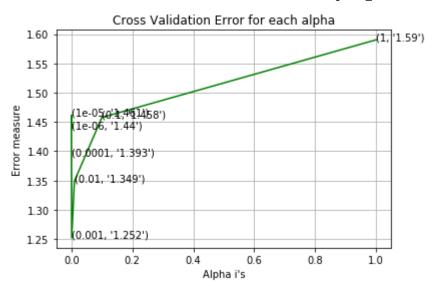
4.3.2.1. Hyper paramter tuning

```
In [0]:
        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='12', loss='log', random_state=42)
            clf.fit(train x onehotCoding, train y)
            sig clf = CalibratedClassifierCV(clf, method="sigmoid")
            sig clf.fit(train x onehotCoding, train y)
            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 ,
            print("Log Loss :",log_loss(cv_y, sig_clf_probs))
        fig, ax = plt.subplots()
        ax.plot(alpha, cv log error array,c='g')
        for i, txt in enumerate(np.round(cv_log_error_array,3)):
            ax.annotate((alpha[i],str(txt)), (alpha[i],cv_log_error_array[i]))
        plt.grid()
        plt.title("Cross Validation Error for each alpha")
        plt.xlabel("Alpha i's")
        plt.ylabel("Error measure")
        plt.show()
        best alpha = np.argmin(cv log error array)
        clf = SGDClassifier(alpha=alpha[best alpha], penalty='12', loss='log', random sta
        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:",
        predict y = sig clf.predict proba(cv x onehotCoding)
        print('For values of best alpha = ', alpha[best_alpha], "The cross validation log
        predict_y = sig_clf.predict_proba(test_x_onehotCoding)
        print('For values of best alpha = ', alpha[best alpha], "The test log loss is:",1
        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 : 1.457591708320943 for alpha = 1 Log Loss : 1.5902258764770603

Log Loss: 1.349151219922669

for alpha = 0.1



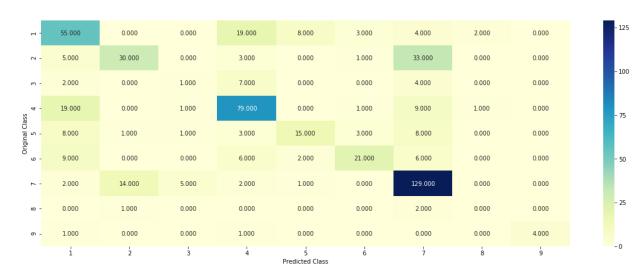
For values of best alpha = 0.001 The train log loss is: 0.6257422677412771

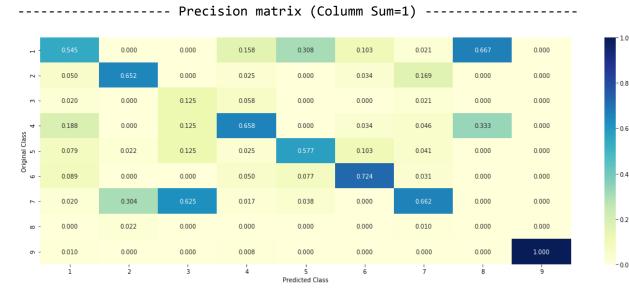
For values of best alpha = 0.001 The cross validation log loss is: 1.252181162

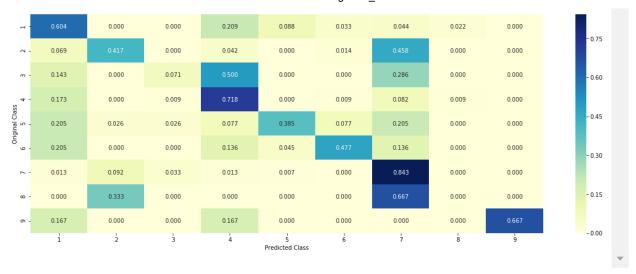
8755943

For values of best alpha = 0.001 The test log loss is: 1.1306020069615057

4.3.2.2. Testing model with best hyper parameters







4.3.2.3. Feature Importance, Correctly Classified point

```
In [0]: clf = SGDClassifier(alpha=alpha[best alpha], penalty='12', loss='log', random sta
        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 one
        print("Actual Class :", test y[test point index])
        indices = np.argsort(-1*abs(clf.coef_))[predicted_cls-1][:,:no_feature]
        print("-"*50)
        get impfeature names(indices[0], test df['TEXT'].iloc[test point index],test df['
        Predicted Class : 7
        Predicted Class Probabilities: [[5.100e-03 1.255e-01 2.000e-04 1.300e-03 2.300e
        -03 1.400e-03 8.556e-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]
```

4.3.2.4. Feature Importance, Inorrectly Classified point

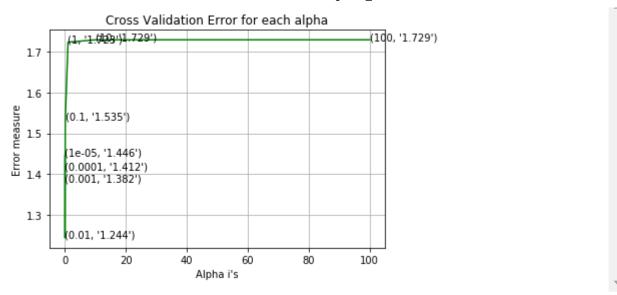
Out of the top 500 features 23 are present in query point

```
In [0]: | 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 one
        print("Actual Class :", test_y[test_point_index])
        indices = np.argsort(-1*abs(clf.coef ))[predicted cls-1][:,:no feature]
        print("-"*50)
        get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_df['
        Predicted Class : 7
        Predicted Class Probabilities: [[0.0485 0.1851 0.0052 0.0442 0.0617 0.0143 0.63
        17 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
```

4.4. Linear Support Vector Machines

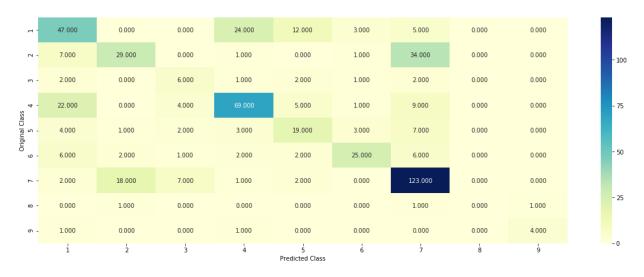
4.4.1. Hyper paramter tuning

```
In [0]:
        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='12', loss='hi
            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_,
            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='12
        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:",
        predict_y = sig_clf.predict_proba(cv_x_onehotCoding)
        print('For values of best alpha = ', alpha[best_alpha], "The cross validation log
        predict y = sig clf.predict proba(test x onehotCoding)
        print('For values of best alpha = ', alpha[best_alpha], "The test log loss is:",1
        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
```

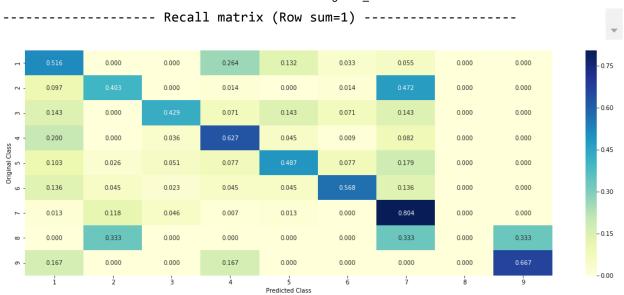


For values of best alpha = 0.01 The train log loss is: 0.7628309867716067
For values of best alpha = 0.01 The cross validation log loss is: 1.2442964974
823838
For values of best alpha = 0.01 The test log loss is: 1.1541891969863685

4.4.2. Testing model with best hyper parameters







4.3.3. Feature Importance

4.3.3.1. For Correctly classified point

```
In [0]: clf = SGDClassifier(alpha=alpha[best alpha], penalty='12', loss='hinge', random s
        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 one
        print("Actual Class :", test_y[test_point_index])
        indices = np.argsort(-1*abs(clf.coef_))[predicted_cls-1][:,:no_feature]
        print("-"*50)
        get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_df['
        Predicted Class : 7
        Predicted Class Probabilities: [[0.0153 0.1199 0.0029 0.0151 0.0121 0.0075 0.81
        04 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
```

4.3.3.2. For Incorrectly classified point

```
In [0]: | 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 one
        print("Actual Class :", test_y[test_point_index])
        indices = np.argsort(-1*abs(clf.coef ))[predicted cls-1][:,:no feature]
        print("-"*50)
        get_impfeature_names(indices[0], test_df['TEXT'].iloc[test_point_index],test_df['
        Predicted Class : 7
        Predicted Class Probabilities: [[0.0786 0.1516 0.0146 0.1064 0.1105 0.0323 0.48
        39 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
```

4.5 Random Forest Classifier

4.5.1. Hyper paramter tuning (With One hot Encoding)

```
In [0]:
        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='
                 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.classe
                 print("Log Loss :",log loss(cv y, sig clf probs))
        '''fig, ax = plt.subplots()
        features = np.dot(np.array(alpha)[:,None],np.array(max_depth)[None]).ravel()
        ax.plot(features, cv_log_error_array,c='g')
        for i, txt in enumerate(np.round(cv log error array,3)):
            ax.annotate((alpha[int(i/2)],max depth[int(i%2)],str(txt)), (features[i],cv l
        plt.grid()
        plt.title("Cross Validation Error for each alpha")
        plt.xlabel("Alpha i's")
        plt.ylabel("Error measure")
        plt.show()
        best alpha = np.argmin(cv log error array)
        clf = RandomForestClassifier(n estimators=alpha[int(best alpha/2)], criterion='gi
        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
        predict_y = sig_clf.predict_proba(cv_x_onehotCoding)
        print('For values of best estimator = ', alpha[int(best_alpha/2)], "The cross val
        predict y = sig clf.predict proba(test x onehotCoding)
        print('For values of best estimator = ', alpha[int(best_alpha/2)], "The test log
        for n_estimators = 100 and max depth =
        Log Loss: 1.2572535683354957
        for n estimators = 100 and max depth =
                                                10
        Log Loss: 1.1868414223711878
        for n estimators = 200 and max depth =
        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
```

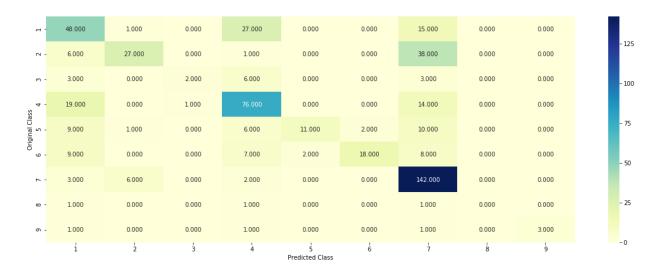
Log Loss: 1.2357829533963691

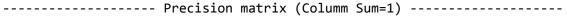
```
for n_estimators = 1000 and max depth = 10
Log Loss : 1.174993079576866
for n_estimators = 2000 and max depth = 5
Log Loss : 1.236042392554891
for n_estimators = 2000 and max depth = 10
Log Loss : 1.1759745074379755
For values of best estimator = 1000 The train log loss is: 0.709539673208275
2
For values of best estimator = 1000 The cross validation log loss is: 1.1749
93079576866
For values of best estimator = 1000 The test log loss is: 1.1630923149103904
```

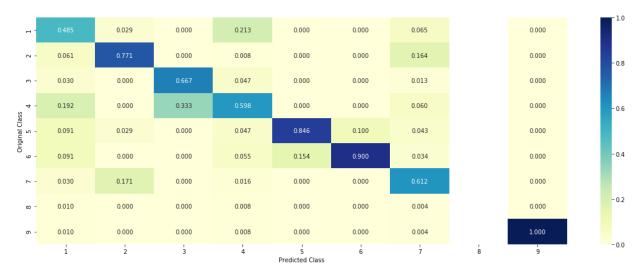
4.5.2. Testing model with best hyper parameters (One Hot Encoding)

In [0]:

clf = RandomForestClassifier(n_estimators=alpha[int(best_alpha/2)], criterion='gi
predict_and_plot_confusion_matrix(train_x_onehotCoding, train_y,cv_x_onehotCoding









4.5.3. Feature Importance

4.5.3.1. Correctly Classified point

```
In [0]: | # test_point_index = 10
        clf = RandomForestClassifier(n estimators=alpha[int(best alpha/2)], criterion='gi
        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_one
        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]
        Predicted Class: 7
        Predicted Class Probabilities: [[0.0454 0.1404 0.0133 0.029 0.036 0.0294 0.69
        77 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
```

4.5.3.2. Inorrectly Classified point

```
In [0]: | 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 one
        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]
        Predicted Class : 7
        Predicted Class Probabilities: [[0.1337 0.116 0.0224 0.1773 0.0674 0.0545 0.41
        56 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
```

4.5.3. Hyper paramter tuning (With Response Coding)

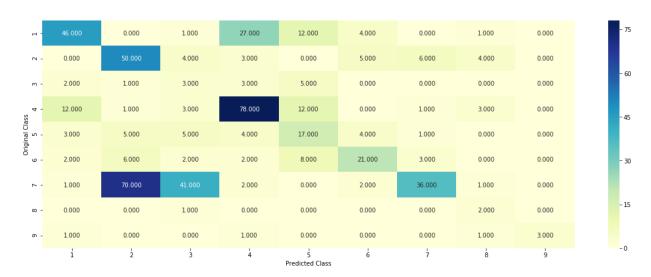
```
In [0]:
        alpha = [10,50,100,200,500,1000]
        max depth = [2,3,5,10]
        cv log error array = []
        for i in alpha:
            for j in max_depth:
                 print("for n estimators =", i,"and max depth = ", j)
                 clf = RandomForestClassifier(n estimators=i, criterion='gini', max depth='
                 clf.fit(train_x_responseCoding, train_y)
                 sig clf = CalibratedClassifierCV(clf, method="sigmoid")
                 sig_clf.fit(train_x_responseCoding, train_y)
                 sig_clf_probs = sig_clf.predict_proba(cv_x_responseCoding)
                 cv log error array.append(log loss(cv y, sig clf probs, labels=clf.classe
                 print("Log Loss :",log_loss(cv_y, sig_clf_probs))
        1.1.1
        fig, ax = plt.subplots()
        features = np.dot(np.array(alpha)[:,None],np.array(max_depth)[None]).ravel()
        ax.plot(features, cv_log_error_array,c='g')
        for i, txt in enumerate(np.round(cv log error array,3)):
            ax.annotate((alpha[int(i/4)],max depth[int(i%4)],str(txt)), (features[i],cv l
        plt.grid()
        plt.title("Cross Validation Error for each alpha")
        plt.xlabel("Alpha i's")
        plt.ylabel("Error measure")
        plt.show()
        best alpha = np.argmin(cv log error array)
        clf = RandomForestClassifier(n estimators=alpha[int(best alpha/4)], criterion='gi
        clf.fit(train x responseCoding, train y)
        sig clf = CalibratedClassifierCV(clf, method="sigmoid")
        sig clf.fit(train x responseCoding, train y)
        predict_y = sig_clf.predict_proba(train_x_responseCoding)
        print('For values of best alpha = ', alpha[int(best_alpha/4)], "The train log los
        predict_y = sig_clf.predict_proba(cv_x_responseCoding)
        print('For values of best alpha = ', alpha[int(best_alpha/4)], "The cross validat
        predict y = sig clf.predict proba(test x responseCoding)
        print('For values of best alpha = ', alpha[int(best_alpha/4)], "The test log loss
        for n estimators = 10 and max depth = 2
        Log Loss: 2.2657048897349608
        for n_estimators = 10 and max depth =
        Log Loss : 1.7459205010556096
        for n estimators = 10 and max depth =
        Log Loss: 1.4368353925512503
        for n estimators = 10 and max depth =
                                               10
        Log Loss: 1.904597809032912
        for n estimators = 50 and max depth = 2
        Log Loss: 1.7221951095007484
        for n estimators = 50 and max depth =
        Log Loss: 1.4984825877845531
        for n estimators = 50 and max depth =
        Log Loss: 1.4593628982873716
        for n estimators = 50 and max depth = 10
```

```
Log Loss: 1.8434939703555409
for n_{estimators} = 100 and max depth = 2
Log Loss: 1.6182209245331227
for n estimators = 100 and max depth =
Log Loss: 1.5199297988828253
for n_estimators = 100 and max depth =
Log Loss: 1.4177501184246677
for n_estimators = 100 and max depth =
Log Loss: 1.8227504417195126
for n estimators = 200 and max depth =
Log Loss: 1.6622571648074496
for n_estimators = 200 and max depth = 3
Log Loss: 1.4800771339141767
for n_estimators = 200 and max depth =
Log Loss: 1.4412060242341358
for n estimators = 200 and max depth =
Log Loss: 1.7892406351442258
for n_estimators = 500 and max depth =
Log Loss: 1.715950314170445
for n_estimators = 500 and max depth =
Log Loss: 1.5658682738699774
for n estimators = 500 and max depth = 5
Log Loss: 1.4445360301518217
for n_estimators = 500 and max depth = 10
Log Loss: 1.8421097596928397
for n estimators = 1000 and max depth = 2
Log Loss: 1.6834927870864949
for n estimators = 1000 and max depth =
Log Loss: 1.5631973035931377
for n_{estimators} = 1000 and max depth = 5
Log Loss: 1.4449980792724129
for n estimators = 1000 and max depth = 10
Log Loss: 1.85233132619749
For values of best alpha =  100 The train log loss is: 0.060702709444608406
For values of best alpha = 100 The cross validation log loss is: 1.417750118
424668
For values of best alpha = 100 The test log loss is: 1.3806278998341923
```

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

In [0]:

clf = RandomForestClassifier(max_depth=max_depth[int(best_alpha%4)], n_estimators
predict_and_plot_confusion_matrix(train_x_responseCoding, train_y,cv_x_responseCo



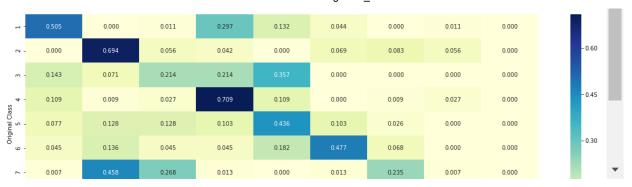


----- Recall matrix (Row sum=1)

- 0.6

0.4

0.2



4.5.5. Feature Importance

4.5.5.1. Correctly Classified point

```
In [0]: clf = RandomForestClassifier(n estimators=alpha[int(best alpha/4)], criterion='gi
        clf.fit(train x responseCoding, train y)
        sig clf = CalibratedClassifierCV(clf, method="sigmoid")
        sig clf.fit(train x responseCoding, train y)
        test point index = 1
        no feature = 27
        predicted cls = sig clf.predict(test x responseCoding[test point index].reshape(1
        print("Predicted Class :", predicted_cls[0])
        print("Predicted Class Probabilities:", np.round(sig_clf.predict_proba(test_x_res
        print("Actual Class :", test_y[test_point_index])
        indices = np.argsort(-clf.feature importances )
        print("-"*50)
        for i in indices:
            if i<9:
                print("Gene is important feature")
            elif i<18:
                print("Variation is important feature")
            else:
                print("Text is important feature")
        Predicted Class: 2
        Predicted Class Probabilities: [[0.0143 0.5044 0.1471 0.0191 0.0245 0.065 0.17
        24 0.039 0.0142]]
        Actual Class : 7
        Variation is important feature
        Variation is important feature
        Variation is important feature
        Variation is important feature
        Text is important feature
        Variation is important feature
        Gene is important feature
        Variation is important feature
        Text is important feature
        Text is important feature
        Text is important feature
        Gene is important feature
        Text is important feature
        Gene is important feature
        Variation is important feature
        Text is important feature
        Gene is important feature
        Gene is important feature
        Gene is important feature
        Variation is important feature
        Variation is important feature
        Text is important feature
        Text is important feature
        Gene is important feature
        Text is important feature
        Gene is important feature
        Gene is important feature
```

4.5.5.2. Incorrectly Classified point

```
In [0]: | test point index = 100
        predicted_cls = sig_clf.predict(test_x_responseCoding[test_point_index].reshape(1
        print("Predicted Class :", predicted_cls[0])
        print("Predicted Class Probabilities:", np.round(sig clf.predict proba(test x res
        print("Actual Class :", test_y[test_point_index])
        indices = np.argsort(-clf.feature importances )
        print("-"*50)
        for i in indices:
            if i<9:
                 print("Gene is important feature")
            elif i<18:
                 print("Variation is important feature")
            else:
                print("Text is important feature")
        Predicted Class: 7
        Predicted Class Probabilities: [[0.0281 0.2006 0.203 0.0857 0.0626 0.0906 0.22
        49 0.0676 0.0369]]
        Actual Class: 7
        Variation is important feature
        Variation is important feature
        Variation is important feature
        Variation is important feature
        Text is important feature
        Variation is important feature
        Gene is important feature
        Variation is important feature
        Text is important feature
        Text is important feature
        Text is important feature
        Gene is important feature
        Text is important feature
        Gene is important feature
        Variation is important feature
        Text is important feature
        Gene is important feature
        Gene is important feature
        Gene is important feature
        Variation is important feature
        Variation is important feature
        Text is important feature
        Text is important feature
        Gene is important feature
        Text is important feature
        Gene is important feature
        Gene is important feature
```

4.7 Stack the models

4.7.1 testing with hyper parameter tuning

```
In [0]:
        clf1 = SGDClassifier(alpha=0.001, penalty='12', loss='log', class_weight='balance
        clf1.fit(train x onehotCoding, train y)
        sig clf1 = CalibratedClassifierCV(clf1, method="sigmoid")
        clf2 = SGDClassifier(alpha=1, penalty='12', loss='hinge', class_weight='balanced'
        clf2.fit(train x onehotCoding, train y)
        sig clf2 = CalibratedClassifierCV(clf2, method="sigmoid")
        clf3 = MultinomialNB(alpha=0.001)
        clf3.fit(train x onehotCoding, train y)
        sig clf3 = CalibratedClassifierCV(clf3, method="sigmoid")
        sig_clf1.fit(train_x_onehotCoding, train_y)
        print("Logistic Regression : Log Loss: %0.2f" % (log loss(cv y, sig clf1.predict
        sig clf2.fit(train x onehotCoding, train y)
        print("Support vector machines : Log Loss: %0.2f" % (log_loss(cv_y, sig_clf2.pred
        sig clf3.fit(train x onehotCoding, train y)
        print("Naive Bayes : Log Loss: %0.2f" % (log_loss(cv_y, sig_clf3.predict_proba(cv)
        print("-"*50)
        alpha = [0.0001, 0.001, 0.01, 0.1, 1, 10]
        best alpha = 999
        for i in alpha:
            lr = LogisticRegression(C=i)
            sclf = StackingClassifier(classifiers=[sig clf1, sig clf2, sig clf3], meta cl
            sclf.fit(train x onehotCoding, train y)
            print("Stacking Classifer : for the value of alpha: %f Log Loss: %0.3f" % (i,
            log error =log loss(cv y, sclf.predict proba(cv x onehotCoding))
            if best alpha > log error:
                best alpha = log error
        Logistic Regression: Log Loss: 1.24
        Support vector machines : Log Loss: 1.72
        Naive Bayes : Log Loss: 1.37
        Stacking Classifer: for the value of alpha: 0.000100 Log Loss: 2.179
        Stacking Classifer: for the value of alpha: 0.001000 Log Loss: 2.049
        Stacking Classifer : for the value of alpha: 0.010000 Log Loss: 1.577
        Stacking Classifer: for the value of alpha: 0.100000 Log Loss: 1.224
        Stacking Classifer: for the value of alpha: 1.000000 Log Loss: 1.366
        Stacking Classifer: for the value of alpha: 10.000000 Log Loss: 1.690
```

4.7.2 testing the model with the best hyper parameters

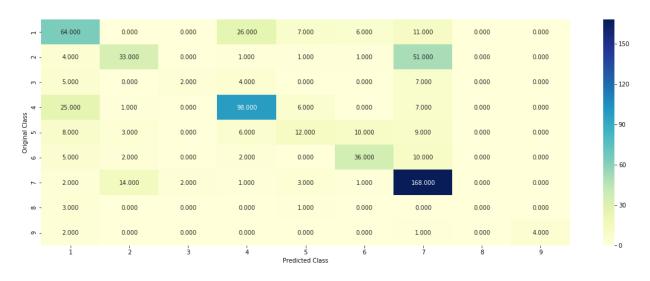
```
In [0]: lr = LogisticRegression(C=0.1)
sclf = StackingClassifier(classifiers=[sig_clf1, sig_clf2, sig_clf3], meta_classis.
sclf.fit(train_x_onehotCoding, train_y)

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

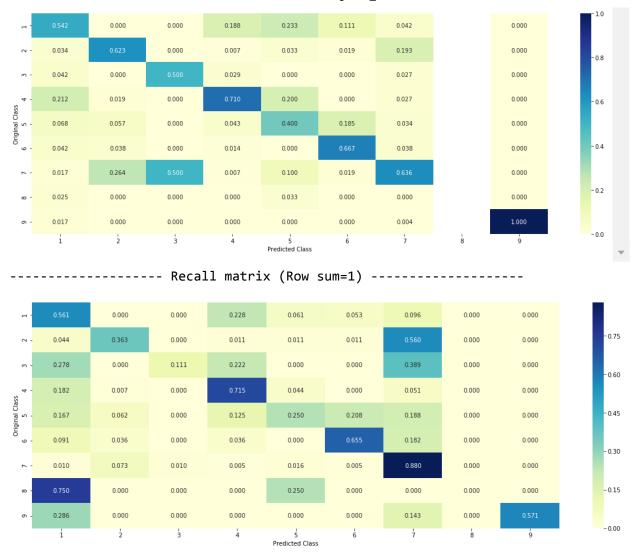
log_error = log_loss(cv_y, sclf.predict_proba(cv_x_onehotCoding))
print("Log loss (CV) on the stacking classifier:",log_error)

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

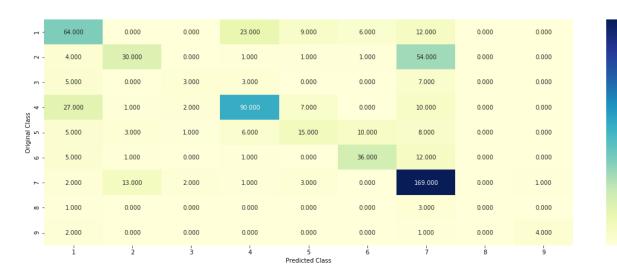
print("Number of missclassified point:", np.count_nonzero((sclf.predict(test_x_oplot_confusion_matrix(test_y=test_y, predict_y=sclf.predict(test_x_onehotCoding)))
```

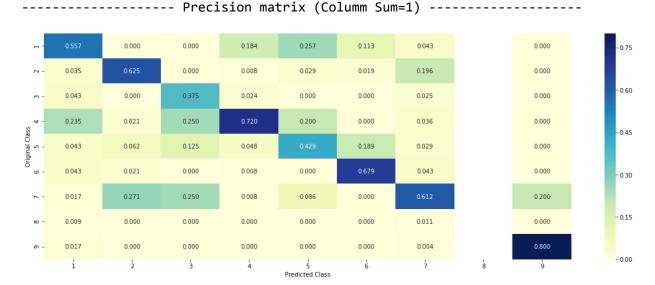






4.7.3 Maximum Voting classifier





- 120

60

