

COMPLEX ENGINEERING PROBLEM MACHINE LEARNING (CS-324)

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Course Code: CS-324
Course Title: Machine Learning
Complex Engineering Problem
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Grading Rubric
TERM PROJECT

Group Members:

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CRITERIA AND SCALES					Marks Obtained		
				S1	S2	S3	
Criterion 1: Does the applica	tion meet the desired spectrum (CPA-1, CPA-2, CPA	-	e the desired outputs?				
1	1 2 3 4						
The application does not meet the desired specifications and is producing incorrect outputs.	The application partially meets the desired specifications and is producing incorrect or partially correct outputs.	The application meets the desired specifications but is producing incorrect or partially correct outputs.	The application meets all the desired specifications and is producing correct outputs.				
Criterion	2: How well is the code	organization? [2 mark	s]				
1	2	3	4				
The code is poorly organized and very difficult to read.	The code is readable only to someone who knows what it is supposed to be doing.	Some part of the code is well organized, while some part is difficult to follow.	The code is well organized and very easy to follow.				
Criterion 3: Does the	report adhere to the give	n format and requireme	nts? [6 marks]				
1	2	3	4				
The report does not contain the required information and is formatted poorly.	The report contains the required information only partially but is formatted well.	The report contains all the required information but is formatted poorly.	The report contains all the required information and completely adheres to the given format.				
Criterion 4: How do	es the student performed (CPA-1, CPA-2, CPA	•	eam member?				
1	2	3	4				
The student did not work on the assigned task.	The student worked on the assigned task, and accomplished goals partially.	The student worked on the assigned task, and accomplished goals satisfactorily.	The student worked on the assigned task, and accomplished goals beyond expectations.				

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Introduction:

The problem given on hand is to explore and apply all the machine learning techniques from cleaning data to visualizing the results of multiple models for comparison of best models for the given dataset. The main key features of the dataset given are, the data has more than 30000 examples and the features are multiple also the output is supposed to be generated in multiclass. For this pupose we have applied all the techniques to preprocessed data, scale the data, model training and visualizing the models as following:

Preprocessing:

Preprocessing refers to the steps taken to clean, transform, and prepare raw data before it can be used for analysis or modeling. Here are some short steps for preprocessing data:

- 1. Identifying Features and Target
 - Import the necessary libraries: Start by importing the required libraries such as pandas, NumPy, or scikit-learn, which are commonly used for data preprocessing tasks.
 - Load the data: Read the raw data into programming environment using the appropriate functions or methods. The data was in CSV format.
 - Initially 9 features were identified including:
 - Summary was taken as target which consisted of 27 number of classes.
- 2. Handle missing values:
 - There are no missing values for except for 'Precip Type' which has 517 missing values.
 - As 'Precip Type' is a categorical variable, so we can't fill missing values with mean/med/mode but fill based on the assumption that adjacent observations are similar to one another using 'ffill' method.

- 3. Encoding categorical variables: Convert categorical variables into numerical representations that can be understood by machine learning algorithms.
 - This was done on 'PrecipType' categorical variable using label encoding.
 - Target was remained as categorical.
- 4. Feature engineering: Created new features or transformed existing ones to enhance the predictive power of the data.
 - Collinearity test was carried out on features which resulted in removing 'Apparent temperature' feature which was causing collinearity.
 - Grouping suitable classes; grouped classes into 4 namely, Partly Cloudy, Mostly Cloudy, Overcast, Non-Cloudy
 - Feature Scaling using standardization
- 5. Split the data: Split the preprocessed data into training and testing sets. The training set is used to build the model, while the testing set is used to evaluate its performance which ensures an unbiased evaluation of the model's capabilities.

Model Implementation:

The models selected for implementation includes:

- Knn (non-parametric)
- Logistic Regression (parametric)
- ANN

Best Model Selection:

As the model are implemented, their hyperparameter selection is not an easy task. For that k-fold cross validation is used to ensure that the best hyperparameters according to the chosen evaluation metric are selected.

KNeighborsClassifier (KNN):

The K-Nearest Neighbors (KNN) algorithm is a non-parametric and instance-based classification algorithm. It does not involve explicit model training but instead stores the entire training dataset in memory for prediction. KNN makes predictions based on the similarity or proximity between instances in the feature space.

KNN classifier with its possible parameters is defined below:

Although, there are many hyperparameters, we choose to tune the following: n_neighbors, p, weights.

```
KNeighborsClassifier(n\_neighbors=5, *, weights='uniform', algorithm='auto', leaf\_size=30, p=2, metric='minkowski', metric\_params=None, n\_jobs=None)
```

GridSearch on KNN:

```
# Define the hyperparameters and their possible values
hyperparameters = {
    'n_neighbors': np.arange(1,30,2) ,
    'weights': ['uniform', 'distance'],
    'p': [1, 2]
}
```

In order to choose the best value for the hyperparameters, we applied the Grid search technique.

Values of the hyperparameters are defined below:

n_neigbors:

It is a hyperparameter that determines the number of neighbors to consider when making predictions for a new instance. Its default value is 5.

By hit-and-trial, we take range as (1,30,2)

weights:

It specifies how the neighbor's contributions are weighted when making predictions.

Its possible values are: 'distance' and 'uniform'.

- ✓ <u>distance</u>: weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- ✓ <u>uniform:</u> uniform weights. All points in each neighborhood are weighted equally.

p:

Power parameter for the Minkowski metric.

Its possible values are: 1 and 2 ✓ p=1: Manhattan distance

✓ p=2: Euclidean distance

This Grid Search selects the following values as the best values for the hyperparameters mentioned above:

```
Best Hyperparameters:{'n_neighbors': 29, 'p': 1, 'weights': 'distance'}
```

Implementing the model as Function:

A function is defined as 'knn_classifier', in which KNN model is defined and trained.

This function calculates the roc_auc_curves value for one-vs-rest and one-vs-one techniques.

This also gives us the confusion matrix, precision and recall values for the model.

KNN Model 1 (Best model):

In KNN model 1, we use the best values of the hyperparameters obtained by Grid

ROC AUC score: Train Set:	Search.						
ovr: 0.81 ovo: 0.82	precision_score: [0.44 0.81 0.54 0.51] recall_score: [0.44 0.52 0.48 0.66]						
ROC AUC score:							
Test Set:	precision recall f1-score	support					
ovr: 0.79 ovo: 0.8	Mostly Cloudy 0.44 0.44 0.44	5837					
	Other 0.81 0.52 0.63	3647					
confusion_matrix:	Overcast 0.54 0.48 0.50	3382					
[[2553 125 849 2310]	Partly Cloudy 0.51 0.66 0.58	6425					
[397 1896 203 1151]	accuracy 0.53	19291					
[1197 53 1609 523]	macro avg 0.58 0.52 0.54	19291					
[1591 266 346 4222]]	weighted avg 0.55 0.53 0.53	19291					
	<pre>accuracy 0.53 classificationscore(testset): 0.53 classificationscore(trainset): 0.56</pre>						

KNN Model 2:

In this the combination of other values for the hyperparameters is used:

```
ROC AUC score:
                                                                   precision score: [0.48 0.71 0.61 0.55]
Train Set:
                                                                  recall_score: [0.5 0.58 0.46 0.66]
                                                                             precision recall f1-score support
ovr: 0.86 ovo: 0.87
ROC AUC score:
                                                                                                       5677
                                                                  Mostly Cloudy
                                                                                 0.48 0.50
                                                                                 0.71
0.61
                                                                                        0.58
0.46
Test Set:
                                                                                                       3653
ovr: 0.81 ovo: 0.81
                                                                  Partly Cloudy
                                                                                        0.66
                                                                                                0.60
                                                                                                       6487
confusion_matrix:
                                                                      accuracy
                                                                                                0.56
                                                                                                       19291
 [[2899 270 635 1873]
                                                                   weighted avg
                                                                                 0.57
                                                                                        0.56
                                                                                                0.56
   411 2103 189 950]
 [1227 234 1621 392]
                                                                  classificationscore(testset): 0.56
[1698 472 294 4023]]
```

KNN Model 3:

In this the combination of other values for the hyperparameters is used:

```
ROC AUC score:
                                                   precision_score: [0.48 0.71 0.61 0.55]
 Train Set:
                                                   recall score: [0.5 0.58 0.46 0.66]
ovr: 0.85 ovo: 0.86
ROC AUC score:
                                                   Mostly Cloudy
 Test Set:
                                                         Other
                                                                 0.71
                                                                        0.58
                                                                               0.64
                                                                                       3653
                                                       Overcast
ovr: 0.81 ovo: 0.82
                                                   Partly Cloudy
                                                                 0.55
                                                                        0.66
                                                                               0.60
                                                                                       6487
                                                       accuracy
                                                                                      19291
confusion_matrix:
                                                      macro avg
                                                                                0.56
                                                                                      19291
 [[2823 244 602 2008]
                                                    weighted avg
  [ 347 2125 170 1011]
 [1196 225 1613 440]
                                                   classificationscore(testset): 0.56
 [1556 415 263 4253]]
                                                   classificationscore(trainset): 0.61
```

Decision Tree:

Decision Trees (DTs) are a non-parametric supervised learning method used for classification and Regression. The goal is to create a model that predicts the value of a target variable by learning simple decision rules inferred from the data features. A tree can be seen as a piecewise constant approximation.

DecisionTree Classifier with its possible hyperparameters is defined below:

 $\label{local_problem} \textbf{DecisionTreeClassifier}(*, criterion='gini', splitter='best', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None, random_state=None, max_leaf_nodes=None, min_impurity_decrease=0.0, class_weight=None, ccp_alpha=0.0)$

Although, there are many hyperparameters, we choose to tune the following: max_depth, min_samples_split, min_samples_leaf, criterion.

GridSearch on Decision Tree Classifier

```
# Define the hyperparameters to tune
param_grid = {
    'max_depth': [None, 5, 10],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 4],
    'criterion': ['gini', 'entropy']
}
```

In order to choose the best value for the hyperparameters, we applied the Grid search technique.

Values of the hyperparameters are defined below:

- max_depth:
 - The maximum depth of the tree. It limits the number of nodes and splits in the tree, helping to control overfitting. Options include are: None, 5 and 10
- min_samples_split:
 - The minimum number of samples required to split an internal node. Options include are: [2,5,10]
- min_samples_leaf:
 - The minimum number of samples required to be at a leaf node. Options include are: [1,2,4]
- criterion

The function used to measure the quality of a split. Common criteria are "gini" for Gini impurity and "entropy" for information gain.

DecisionTreeClassifier Model 1 (Best model):

In model 1, we use the best values of the hyperparameters obtained by Grid Search.

DecisionTreeClassifier Model 2:

In this the combination of other values for the hyperparameters is used:

```
ROC AUC score:
Train Set:
ovr: 0.81 ovo:
ROC AUC score:
Test Set:
ovr: 0.79 ovo:
                      ovo: 0.8
confusion matrix:
  [[2533 145 655 2344]
[ 352 1962 170 1169]
[1300 49 1524 601]
[1574 306 312 4295]]
precision_score: [0.44 0.8 0.57 0.51]
recall_score: [0.45 0.54 0.44 0.66]
precision recall f1-score
                                                                                       support
Mostly Cloudy
Other
                                                       0.45
                                                                         0.44
                                                                                            5677
                                    0.80
0.57
0.51
                                                       0.54
0.44
0.66
                                                                         0.64
                                                                                             3653
         accuracy
                                                                          0.53
                                                                                           19291
  macro avg
weighted avg
                                                                          0.54
                                                                                           19291
                                                                                           19291
accuracy 0.53 classificationscore(testset):
classificationscore(testset): 0.53
classificationscore(trainset): 0.56
```

DecisionTreeClassifier Model 3:

In this the combination of other values for the hyperparameters is used:

```
ROC AUC score:
 Train Set:
ovr: 0.97
ovr: 0.97 or
ROC AUC score:
              ovo: 0.97
 Test Set:
ovr: 0.74
              ovo: 0.75
confusion_matrix:
 [[2819 389 874 1595]
[ 480 2316 160 697]
[1108 167 1781 418]
[1935 828 501 3223]]
precision_score: [0.44 0.63 0.54 0.54]
recall_score: [0.5 0.63 0.51 0.5 ]

precision recall f1-score
                                                      support
Mostly Cloudy
                        0.44
                                   0.50
                                               0.47
                                                           5677
        Other
                        0.63
                                   0.63
                                               0.63
                                                           3653
     Overcast
                        0.54
                                   0.51
                                               0.52
                                                           3474
Partly Cloudy
                       0.54
                                   0.50
                                                           6487
                                               0.52
                                               0.53
                                                          19291
     accuracy
                                   0.54
                                               0.54
 weighted avg
                      0.53
                                   0.53
                                               0.53
                                                          19291
classificationscore(testset): 0.53
classificationscore(trainset): 0.83
```

Logistic Regression:

Logistic regression is a statistical model used for binary classification problems, where the dependent variable takes two possible values. Logistic regression can be extended to handle multiclass classification problems through various strategies, such as one-vs-rest (also known as one-vs-all).

The goal of logistic regression is to estimate the probability of the dependent variable belonging to a specific class based on the values of the independent variables.

Logistic Regression with its possible hyperparameters is defined below:

Although, there are many hyperparameters, we choose to tune the following: C, penalty, solver.

```
\textbf{LogisticRegression}(penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit\_intercept=True, intercept\_scaling=1, class\_weight=None, random\_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm\_start=100, multi_class='auto', verbose=100, warm\_start=100, multi_class='auto', verbose=100, warm\_start=100, warm\_start=100,
```

GridSearch on Logistic Regression:

In order to choose the best value for the hyperparameters, we applied the Grid search technique.

Values of the hyperparameters are defined below:

```
# Define the hyperparameters to tune
param_grid = {
    'penalty': ['12'],
    'C': [0.1,0.001, 0.01],
    'solver': ['lbfgs', 'newton-cg']
}
```

• C:

This is Inverse of regularization strength; must be a positive float and smaller values specify stronger regularization. By some research and hit-and-trial, we select 0.1, 1.0 and 10.0 as the options.

penalty:

The penalty hyperparameter specifies the type of regularization used in multiclass logistic regression. Options include":

- ✓ '11' (L1 regularization)
- ✓ '12' (L2 regularization)
- ✓ 'elasticnet' (combination of L1 and L2 regularization)
- ✓ 'none' (no regularization).

But because of the compatibility issue we select only '12'

• solver:

The solver algorithm determines the optimization algorithm used to estimate the coefficients in multinomial logistic regression. Common choices include 'newton-cg', 'lbfgs', 'sag', and 'saga'.

Because 12 is only compatible with 'lbfgs' and 'newton-cg', we select these as the options.

This Grid Search selects the following values as the best values for the hyperparameters mentioned above: In addition to these hyperparameters, we set:

```
Best Hyperparameters:{ {'C': 10.0, 'penalty': '12', 'solver': 'newton-cg'}

multi-class = auto and max-iter = 1000
```

Logistic Regression Model 1 (Best model):

In model 1, we use the best values of the hyperparameters obtained by Grid Search.

```
ROC AUC score:
Train Set:
ovr: 0.86 ovo: 0.8
ROC AUC score:
Test Set:
ovr: 0.8 ovo: 0.81
confusion_matrix:

[[2861 257 642 1958]

[430 2127 185 917]

[1137 210 1650 437]
precision_score: [0.47 0.69 0.6 0.
recall_score: [0.5 0.58 0.48 0.62]
                              precision
                                                                           f1-score
                                                         recall
                                                                                                  support
Mostly Cloudy
Other
Overcast
Partly Cloudy
                                                              0.50
0.58
0.48
0.62
                                                                                                        5718
          accuracy
                                                                                                      19291
  macro avg
weighted avg
                                         0.56
                                                                                   0.55
                                                                                                      19291
accuracy 0.55
classificationscore(testset): 0.55
classificationscore(trainset): 0.62
```

Logistic Regression Model 2:

In this the combination of other values for the hyperparameters is used:

Logistic Regression Model 3:

In this the combination of other values for the hyperparameters is used:

```
ROC AUC score:
Train Set:
ovr: 0.72 o
ROC AUC score:
Test Set:
ovr: 0.72 o
                          ovo: 0.72
confusion_matrix:
[[2071 570 572 2464]
[ 363 1712 346 1232]
[1174 694 1112 494]
[1475 504 282 4226]]
precision_score: [0.41 0.49 0.48 0.5 ]
recall_score: [0.36 0.47 0.32 0.65]
precision recall f1-
Mostly Cloudy
Other
                                             0.49
0.48
                                                                                          0.48
           Overcast
Partly Cloudy
                                           0.50
                                                                                          0.57
                                                                                                                 6487
                                                                                                               19291
19291
19291
          accuracy
  macro avg
weighted avg
accuracy 0.47 classificationscore(testset): 0.47 classificationscore(trainset): 0.47
```

Multiple Layer Perceptron (MLP):

The Multilayer Perceptron (MLP) is a feedforward artificial neural network that consists of multiple layers of interconnected neurons. It is a versatile model widely used for both regression and classification tasks.

MLP with its possible hyperparameters is defined below:

As we can see there are many hyperparameters, we choose to tune the following: 'hidden_layer', 'activation', 'solver', 'alpha', 'learning_rate'

GridSearch on MLP Classifier:

```
# Define the parameter grid for GridSearchCV
param_grid = {
    'hidden_layer_sizes': [(100,), (100, 50), (50, 50)],
    'activation': ['relu', 'tanh'],
    'solver': ['adam', 'sgd'],
    'alpha': [0.0001, 0.001, 0.01],
    'learning_rate': ['constant', 'invscaling', 'adaptive']
}
```

In order to choose the best value for the hyperparameters, we applied the Grid search technique.

Values of the hyperparameters are defined below:

hidden layer:

MLP can have one or more hidden layers between the input and output layers. Each hidden layer consists of multiple neurons that perform nonlinear transformations on the input data.

Here we added two hidden layers, and by hit-and-trial method take the options for the values as:

```
(100,), (100,50), (50,50)
```

activation:

Activation functions introduce nonlinearity to the MLP, enabling it to learn complex patterns and relationships in the data. Following activation functions are taken for the model

- ✓ relu: the rectified linear unit function, returns f(x) = max(0, x)
- ✓ tanh: the hyperbolic tan function, returns $f(x) = \tanh(x)$.
- solver:

This hyperparameter refers to the optimization algorithm used to train the neural network by minimizing the loss function. The solver determines how the weights are updated during the learning process.

The solver hyperparameter options we used are:

- ✓ sgd (Stochastic Gradient Descent): This solver performs updates to the model's weights based on a randomly selected subset of training samples (mini-batches).
- ✓ Adam (Adaptive Moment Estimation): It adapts the learning rates for each parameter based on estimates of the first and second moments of the gradients.
- alpha:

It controls the regularization strength applied to the neural network model.

Values selected are: [0.0001, 0.001, 0.01]

All these values are selected by some research and hit-and-trial method.

learning_rate:

It determines the step size taken during the optimization process to update the weights of the neural network.

The different options are as follows:

- ✓ constant: this is a constant learning rate given by 'learning rate init'.
- ✓ invscaling: It gradually decreases the learning rate at each time step 't' using an inverse scaling exponent of 'power_t'.

 effective_learning_rate = learning_rate_init / pow(t, power_t)
- ✓ adaptive: It keeps the learning rate constant to 'learning rate init' as long as training loss keeps decreasing.

MLP Classifier Model 1 (Best model):

In model 1, we use the best values of the hyperparameters obtained by Grid Search.

```
ROC AUC score:
Train Set:
ovr: 0.85 ovo:
ROC AUC score:
Test Set:
ovr: 0.83 ovo:
confusion_matrix:
[[2539 165 996 2018]
[ 246 2122 211 1080]
[ 873 77 2079 405]
[1379 425 420 4256]]
precision_score: [0.5 0.76 0.56 0.55] recall_score: [0.44 0.58 0.61 0.66]
                                                                                 f1-score
                                 precision
                                                              recall
                                                                                                         support
Mostly Cloudy
Other
Overcast
Partly Cloudy
                                                                                                                5718
                                                                  0.58
0.61
0.66
                                            0.56
0.55
                                                                                          0.58
0.60
                                                                                                                6480
           accuracy
                                                                                                              19291
  macro avg
weighted avg
                                                                                          0.58
0.57
                                                                                                               19291
                                                                                                              19291
accuracy 0.57
classificationscore(testset): 0.57
classificationscore(trainset): 0.6
```

MLP Classifier Model 2:

In this the combination of other values for the hyperparameters is used:

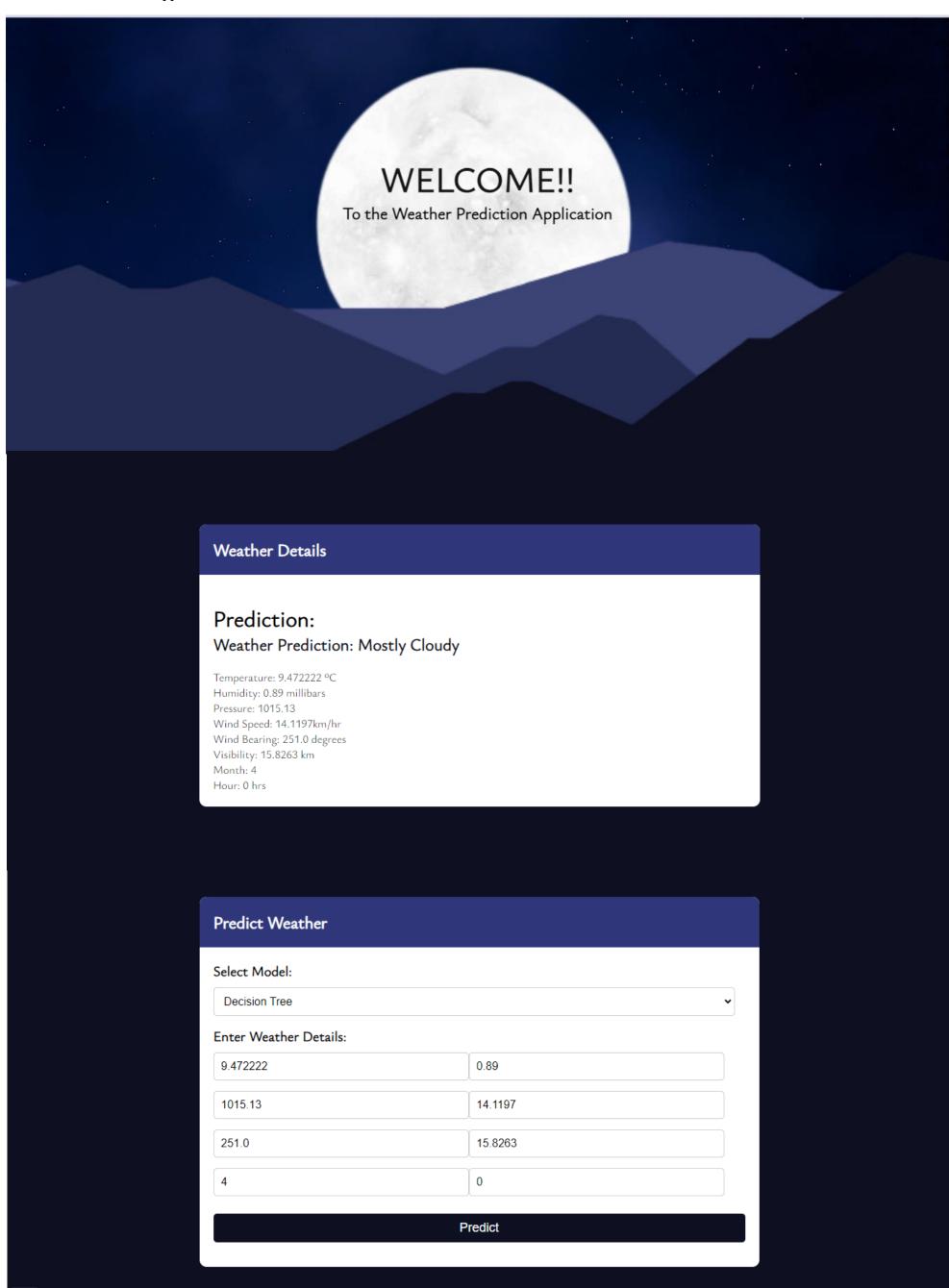
MLP Classifier Model 3:

In this the combination of other values for the hyperparameters is used:

```
ROC AUC score:
Train Set:
ovr: 0.85 or
ROC AUC score:
Test Set:
                      ovo: 0.86
ovr: 0.83 ovo: 0.84
precision_score: [0.5 0.76 0.56 0.55]
recall_score: [0.44 0.58 0.61 0.66]
precision recall f1-score
                                                                                  support
Mostly Cloudy
Other
                                  0.50
                                                    0.44
                                                                     0.47
                                                                                       5718
                                                                                       3659
3434
Otner
Overcast
Partly Cloudy
                                                                                       6480
 accuracy
macro avg
weighted avg
                                                                                     19291
 accuracy 0.57
classificationscore(testset): 0.57
classificationscore(trainset): 0.6
```

User Interface:

For user interface, flask app is used to show the results



Tabular Comparison:

	Knn_	Knn_mo	Knn_mod	DecisonTree_	DecisonTree_	DecisonTree_m	MLP_Classifier_	MLP_Classifier	MLP_Classifier
	model 1	del2	el3	model1	model2	odel3	model1	_model2	_model3
Train roc_auc score	0.82	0.87	0.86	0.82	0.82	0.97	0.86	.86	0.86
Test roc_auc score	0.82	0.81	0.82	0.82	0.80	0.75	0.84	0.84	0.84
Precision score	[0.45, 0.83, 0.57, 0.54]	[0.47, 0.69, 0.6, 0.55]	[0.48, 0.71, 0.61, 0.55]	[0.45, 0.83, 0.57, 0.54]	[0.44,0.8, 0.57, 0.51]	[0.44, 0.63, 0.54, 0.54]	[0.5, 0.76, 0.56, 0.55]	[0.5, 0.76, 0.56, 0.55]	[0.5, 0.76, 0.56, 0.55]
Recall_score	[0.5 0.54 0.5 0.63]	[0.47 0.69 0.6 0.55]	[0.5 0.58 0.46 0.66]	[0.5 0.54 0.5 0.63]	[0.45 0.54 0.44 0.66]	[0.5, 0.63, 0.51, 0.5]	[0.44, 0.58, 0.61, 0.66]	[0.44, 0.58, 0.61, 0.66]	[0.44, 0.58, 0.61, 0.66]
Accuracy	0.55	0.55	0.56	0.55	0.53	0.53	0.57	0.57	0.57
Test classification score	0.55	0.55	0.56	0.55	0.53	0.53	0.57	0.57	0.57
Train classification score	0.55	0.62	0.67	0.55	0.56	0.83	0.60	0.60	0.60

