
Do we need more bikes?

Project in Statistical Machine Learning

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Abstract

In this project, we aim to create a classification model that can predict whether an increase in the number of bikes is needed in Washington D.C. on a specific temporal and meteorological conditions. We will compare various classification models which consists of Logistic Regression, Linear Discriminant Analysis (LDA), K-Nearest Neighbors (KNN), Random Forest, and Gradient Boosting. The models are evaluated using Accuracy, Precision, Recall, and F1-Score metrics with 10-Fold Cross Validation. The results indicate that the Random Forest model outperforms the other models in all evaluation metrics, with an accuracy of 94.44%, recall of 94.99%, precision of 94.00%, and F1-score of 94.47%. This suggests that Random Forest is the most effective model for predicting bike demand in this context.

Number of group member: 4

1 Problem Description

Capital Bikeshare is a 24-hour public bicycle-sharing system that serves Washington, D.C., and offers transportation for thousands of people throughout the city. The problem that arises is that there are certain occasions when, due to various circumstances, there are not as many bikes available as there are demands. In the long term, this situation will result in more people taking the car instead of the bicycle, increasing CO2 emissions in the city. To tackle this situation, the District Department of Transportation in the city wants to know if at certain hours an increase in the number of bikes available will be necessary.

In this Project, we aim to analyze whether the increase in the number of bikes is necessary or not based on the various temporal and meteorological data provided in the dataset.

2 Data Analysis

The Training Dataset training.csv consists of 1600 randomly selected observation over the period of three years in the city of Washington D.C. The dataset contains 16 features and 1 target variable. The features are: *hour_of_day*, *day_of_week*, *month*, *holiday*, *weekday*, *summertime*, *temp*, *dew*, *humidity*, *precip*, *snow*, *snow_depth*, *windspeed*, *cloudcover*, and *visibility*. And the target variable is *increase_stock*.

2.1 Variable Types and Processing

The target variable *increase_stock* indicates whether an increase in the number of bikes is needed at a particular hour. the value *'low_bike_demand'* indicates that no increase is needed, while *'high_bike_demand'* indicates that an increase is necessary. For the analysis, we will convert these categorical values into binary numerical values, where *'low_bike_demand'* is represented as 0 and

33 'high_bike_demand' as 1. Since the target variable is binary, this problem can be treated as a binary
 34 classification task.

35 For Binary features such as *holiday*, *weekday*, and *summertime*, they will be counted as categorical
 36 variables with values 0 and 1.

37 The Features *temp*, *dew*, *humidity*, *precip*, *snow*, *snow_depth*, *windspeed*, *cloudcover*, and *visibility*
 38 will be treated as numerical variables as they represent continuous measurements.

39 Regarding Ordinal features such as *hour_of_day*, *day_of_week*, and *month*, special attention is needed.
 40 For these features, we can't simply treat them as numerical values due to their cyclical nature. For
 41 example, after hour 23 comes hour 0 again. However, treating them as categorical variables may lead
 42 to loss of information regarding their order and cyclical patterns. Therefore, there are several possible
 43 approaches to handle them:

- 44 • One-Hot Encoding: Convert each of these features into multiple binary features, each
 45 representing a specific category. For example, *hour_of_day* would be converted into 24
 46 binary features.
- 47 • Cyclical Transformation: Transform these features using sine and cosine functions to capture
 48 their cyclical nature. For example, for *hour_of_day*, we can create two new features:

$$\text{hour_sin} = \sin\left(2\pi \cdot \frac{\text{hour_of_day}}{24}\right) [4]$$

49

$$\text{hour_cos} = \cos\left(2\pi \cdot \frac{\text{hour_of_day}}{24}\right) [4]$$

50 Since One-Hot Encoding wouldn't effectively capture the cyclical nature of these features and may
 51 lead to high dimensionality, for this analysis, we will use the Cyclical Transformation approach to
 52 handle these ordinal features. [4]

53 After processing, the dataset will consist of 18 features and 1 target variable. Those features are
 54 shown in Table 1.

Table 1: Processed Features in the Dataset

Feature	Type	Description
hour_sin	Numerical	Sine transformation of hour of the day
hour_cos	Numerical	Cosine transformation of hour of the day
day_sin	Numerical	Sine transformation of day of the week
day_cos	Numerical	Cosine transformation of day of the week
month_sin	Numerical	Sine transformation of month of the year
month_cos	Numerical	Cosine transformation of month of the year
holiday	Binary / Categorical	Whether the day is a holiday or not (0 or 1)
weekday	Binary / Categorical	Whether the day is a weekday or not (0 or 1)
summertime	Binary / Categorical	Whether the day is in the summer time period or not (0 or 1)
temp	Numerical	Temperature in Celsius
dew	Numerical	Dew point temperature in Celsius
humidity	Numerical	Relative Humidity in percentage
precip	Numerical	Precipitation in mm
snow	Numerical	Amount of snow in the last hour in cm
snow_depth	Numerical	Accumulated snow depth in cm
windspeed	Numerical	Wind speed in km/h
cloudcover	Numerical	Percentage of cloud cover
visibility	Numerical	Distance in km at which objects or landmarks can be clearly seen and identified
increase_stock (Target)	Binary / Categorical	Whether an increase in bike stock is needed (0 or 1)

55 2.2 Exploratory Data Analysis

56 For the initial stage, we will perform Exploratory Data Analysis (EDA) to understand the distribution
57 and trends that arises in the dataset. Including which features are more correlated with the target
58 variable *increase_stock*.

59 The feature *snow* only contains zero values in all observations, therefore it will be removed from the
60 dataset as it doesn't provide any useful information for the analysis. Upon analyzing the dataset, we
61 found that there are no missing values in any of the features or the target variable. Therefore, no
62 handling is required.

63 Using Pearson correlation coefficient, we found correlation values between each feature and the target
64 variable as shown in Table 2.

Table 2: Ordered Correlation between Features and Target Variable

Feature	Correlation Coefficient
hour_of_day_cos	-0.339960
temp	0.336981
humidity	-0.308726
hour_of_day_sin	-0.308121
summertime	0.216052
month_cos	-0.169059
dew	0.132663
weekday	-0.116446
visibility	0.113443
windspeed	0.096011
month_sin	-0.092078
day_of_week_sin	-0.088152
precip	-0.059304
snowdepth	-0.047526
cloudcover	-0.045534
day_of_week_cos	-0.031473
holiday	-0.004909

65 As the table suggests, the feature *hour_of_day_cos* has the highest positive correlation with the target
66 variable *increase_stock*, indicating that the time of day plays a significant role in determining whether
67 an increase in bike stock is needed. On the other hand, the feature *holiday* has the lowest correlation
68 with the target variable, suggesting that whether a day is a holiday or not has minimal impact on bike
69 demand.

70 2.3 Imbalance in the Dataset

71 Upon analyzing the target variable *increase_stock*, we found that there is 1312 instances of class 0
72 (low bike demand) and 288 instances of class 1 (high bike demand). This indicates a significant class
73 imbalance in the dataset [2], with class 0 being the majority class.

74 To address this class imbalance, we will employ the use of Synthetic Minority Over-sampling
75 Technique (SMOTE). SMOTE works by generating synthetic samples for the minority class (class 1
76 in this case) by interpolating between existing minority class instances. This helps to balance the
77 class distribution and provides the model with more representative samples of the minority class
78 during training. [1]

79 The interpolation is done by selecting a minority class instance and finding its k-nearest neighbors.
80 A synthetic sample is then created by randomly selecting one of the neighbors and interpolating
81 between the two instances. This process is repeated until the desired balance between the classes is
82 achieved.

83 3 Models and Methods

84 In this experiment, we will compare various classification models to determine which one performs
85 best for predicting whether an increase in bike stock is needed using the provided dataset. The models
86 we will consider includes Logistic Regression, Linear Discriminant Analysis (LDA), K-Nearest
87 Neighbors (KNN), Random Forest, and Gradient Boosting.

88 For each model, we will perform hyperparameter tuning using techniques such as Grid Search or
89 Random Search combined with cross-validation to find the optimal set of hyperparameters that yield
90 the best performance on the validation set.

91 3.1 Benchmark Model

92 As the benchmark model, we will use a naive model that predict each instance using stratified random
93 sampling based on the training set's class distribution. This means that for each instance, the model
94 will randomly assign a class label (0 or 1) based on the proportion of each class in the training data
95 [3]. This will provide a baseline accuracy to compare the performance of more sophisticated models.

96 3.2 Evaluation Metrics

97 To evaluate the performance of each classification model, we will use several metrics including
98 Accuracy, Precision, Recall, and F1-Score. These metrics will provide a comprehensive understanding
99 of how well each model performs in predicting the target variable. [2]

100 We will also use K-Fold Cross Validation to ensure that our evaluation metrics are robust and not
101 overly dependent on a particular train-test split.

102 K-Fold Cross Validation involves dividing the dataset into K subsets, using one of the subsets as the
103 test set and the remaining K-1 subsets as the training set. This process is repeated K times, with each
104 subset used as the test set once. The final evaluation metrics are then averaged over all K iterations to
105 provide a more reliable estimate of model performance. For this experiment, we will use K=10. [2]

106 3.3 Logistic Regression

107 Logistic Regression is a linear model used for binary classification tasks. It models the probability of
108 the target variable being in a particular class using the logistic function. The model estimates the
109 coefficients for each feature, which represent the impact of each feature on the log-odds of the target
110 variable [2].

111 In Logistic Regression, we use the sigmoid function to map the linear combination of features to a
112 probability value between 0 and 1. With the formulation:

$$P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n)}} [3]$$

113 Where $P(Y = 1|X)$ is the probability of the target variable being in class 1 given the features X , β_0
114 is the intercept, and $\beta_1, \beta_2, \dots, \beta_n$ are the coefficients for each feature X_1, X_2, \dots, X_n .

115 The parameters of the model are estimated using Maximum Likelihood Estimation (MLE), which
116 finds the set of coefficients that maximize the likelihood of the observed data given the model.

117 3.4 Linear Discriminant Analysis (LDA)

118 Linear Discriminant Analysis (LDA) is a classification method that finds a linear combination of
119 features that best separates the classes. [2].

120 LDA is derived from the probabilistic model which models the class-conditional distributions of the
121 data $P(X|y=k)$ for each class k [3]. Predictions are made by applying Bayes theorem for each training
122 sample $x \in \mathbb{R}^d$:

$$P(y = k|x) = \frac{P(x|y = k)P(y = k)}{P(x)} [3]$$

123 Then we select the class with the highest posterior probability. For LDA, $P(X|y=k)$ is modeled as a
 124 multivariate Gaussian distribution with density function as follows:

$$P(x|y = k) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k)\right) [3]$$

125 where μ_k is the mean vector of class k , and Σ is the shared covariance matrix across all classes, and d
 126 is the number of features.

127 In LDA, we assume that the covariance matrices of all classes are equal, i.e., $\Sigma_k = \Sigma$ for all k . This
 128 reduces the log posterior to:

$$\log P(y = k|x) = -\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k) + \log P(y = k) + Constant [3]$$

129 which can be simplified to:

$$\log P(y = k|x) = w_k^T x + w_{k0} + Constant [3]$$

130 where $w_k = \Sigma^{-1} \mu_k$ and $w_{k0} = -\frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log P(y = k)$. [3]

131 3.5 K-Nearest Neighbors (KNN)

132 K-Nearest Neighbors (KNN) is a non-parametric classification method that classifies new instances
 133 based on the majority class of their K nearest neighbors in the feature space. The distance metric used
 134 to determine the nearest neighbors can be Euclidean distance, Manhattan distance, or other distance
 135 measures. [3]

136 KNN algorithm are usually used for unsupervised learning tasks such as clustering. However, it can
 137 also be adapted for supervised learning tasks by using the labels of the nearest neighbors to make
 138 predictions.

139 For Supervised learning tasks, KNN works using these following steps:

- 140 • Choose the number of neighbors K .
- 141 • For each new instance to be classified, calculate the distance between the new instance and
 142 all instances in the training dataset.
- 143 • Identify the K nearest neighbors based on the calculated distances.
- 144 • Determine the majority class among the K nearest neighbors.
- 145 • Assign the majority class as the predicted class for the new instance.

146 For the distance metric, we will use Manhattan distance, which is defined as:

$$d(p, q) = \sum_{i=1}^n |p_i - q_i| [3]$$

147 where p and q are two instances in the feature space, and n is the number of features.

148 3.6 Random Forest

149 Random Forest is an ensemble learning method that consists of multiple decision trees. Each tree is
 150 trained on a random subset of the training data and a random subset of features. The final prediction
 151 is made by aggregating the predictions from all trees. The method to aggregate the results in this
 152 experiment will use majority voting. [3]

153 Decision trees in principle work by recursively splitting the data based on feature values to create
 154 branches that lead to leaf nodes representing class labels. The splits are chosen based on the feature
 155 that maximizes the information gain or minimizes the impurity at each node. For the metric to
 156 measure impurity, we will use Entropy, which is defined as:

$$H(X) = - \sum_{i=1}^c p_i \log_2(p_i) [3]$$

157 where p_i is the proportion of instances belonging to class i in the node, and c is the number of classes.
158 Decision trees can be prone to overfitting, especially when they are deep and complex. To mitigate
159 this, we can use Random Forest.

160 Random Forest Algorithm, works using these following steps:

- 161 • For each tree in the forest:
 - 162 – Randomly sample the training data with replacement (bootstrap sampling).
 - 163 – Randomly select a subset of features to consider for splitting at each node.
 - 164 – Train a decision tree on the sampled data using the selected features.
- 165 • For making predictions:
 - 166 – For each new instance, pass it through each tree in the forest to obtain the predicted
167 class.
 - 168 – Aggregate the predictions from all trees using majority voting to determine the final
169 predicted class.

170 Due to the randomness introduced in the training process, Random Forests are less prone to overfitting
171 compared to individual decision trees and often achieve better generalization performance. [3]

172 3.7 Gradient Boosting

173 Gradient Boosting is an ensemble learning method that builds a series of weak learners in a sequential
174 manner. Each weak learner is trained to correct the errors made by the previous learners. The final
175 prediction is made by combining the predictions from all weak learners. [3]

176 Gradient Boosting Algorithm works using these following steps:

- 177 • Initialize the model with a constant value, typically the mean of the target variable.
- 178 • For each iteration $m = 1$ to M :
 - 179 – Compute the pseudo-residuals, which are the negative gradients of the loss function
180 with respect to the current model's predictions.
 - 181 – Train a weak learner (e.g., decision tree, logistic regression) on the pseudo-residuals.
 - 182 – Compute the optimal step size (learning rate) for the weak learner.
 - 183 – Update the model by adding the weighted predictions of the weak learner to the current
184 model.
- 185 • For making predictions:
 - 186 – For each new instance, pass it through all weak learners and sum their weighted
187 predictions to obtain the final predicted value.

188 Since the problem we're working on is a binary classification task, we will use logistic loss as the
189 loss function for Gradient Boosting. The logistic loss is defined as:

$$L(y, \hat{y}) = -\frac{1}{N} \sum_{i=1}^N [y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)] [3]$$

190 where y_i is the true label, \hat{y}_i is the predicted probability, and N is the number of instances. For the
191 weak learners, we will use decision trees with a maximum depth of 5.

192 3.8 Hyperparameter Tuning

193 For each classification model, we will perform hyperparameter tuning using Grid Search com-
194 bined with 10-Fold Cross Validation to find the optimal set of hyperparameters that yield the best
195 performance on the validation set. The hyperparameters to be tuned for each model are as follows:

196 Grid Search works by exhaustively searching through a specified subset of hyperparameters for
197 each model. For each combination of hyperparameters, the model is trained and evaluated using
198 cross-validation. The combination that yields the best average performance across the folds is selected
199 as the optimal set of hyperparameters. [2]

4 Experiment and Results

After performing the experiments using the described models and methods. We obtained the results as shown in Table 3.

Table 3: Results of Classification Models (rounded to 4 decimal places)

Model	Accuracy	Precision	Recall	F1-Score
Random Forest	0.9037	0.9065	0.9037	0.9043
Gradient Boosting	0.8994	0.9015	0.8994	0.8999
Logistic Regression	0.8100	0.8696	0.8100	0.8271
LDA	0.7956	0.8676	0.7956	0.8155
K-Nearest Neighbors	0.7675	0.8233	0.7675	0.7863
Benchmark Model	0.4781	0.6889	0.4781	0.5375

Using Grid Search with 10-Fold Cross Validation, we found the optimal hyperparameters for each model is as follows:

- **Logistic Regression:** Regularization strength $C = 1.0$, Solver type using Liblinear, and Penalty type using Ridge Regularization (L2).
- **LDA:** Solver Type using SVD (Singular Value Decomposition)
- **K-Nearest Neighbors:** Number of neighbors $K = 3$, Distance metric using Manhattan distance, and Weighting type using the inverse of their distance.
- **Random Forest:** Number of trees $n_estimators = 250$, Maximum depth of each tree $max_depth = 15$, Minimum samples per leaf $min_samples_leaf = 1$, Minimum samples per split $min_samples_split = 2$, and Criterion using Entropy.
- **Gradient Boosting:** Number of estimators $n_estimators = 100$, Learning rate = 0.1, Maximum Depth for each estimator = 10, and Subsample = 0.6

Based on the results, we can see that the more complex models such as Random Forest and Gradient Boosting outperformed the simpler models like Logistic Regression, LDA, and KNN.

Random Forest achieved an accuracy of 90.37%, indicating that it correctly classified a high percentage of instances in the dataset. The F1-Score of 90.43% also suggests that the model has a good balance between precision and recall, suggesting that it is effective in identifying both positive and negative instances. Gradient Boosting also performed comparably well, achieving an accuracy and F1-Score of 89.94% and 89.99% respectively, which is slightly lower than Random Forest but still significantly better than the other models.

If we compare the simpler models such as Logistic Regression, LDA, and KNN, we can see that they achieved lower accuracy and F1-scores. Logistic Regression achieved an accuracy of 81.00%, LDA achieved 79.56%, and KNN achieved 76.75%. This indicates that these models may not be as effective in capturing the complex relationships in the dataset compared to the ensemble methods.

Due to its superior performance, for production deployment, we recommend using either the Random Forest or Gradient Boosting model for predicting whether an increase in bike stock is needed.

5 Conclusion

Based on the analysis and experiments conducted in this project, we can conclude that the Random Forest is the most effective model for predicting whether an increase in bike stock is needed in Washington D.C. The model achieved the highest accuracy, recall, precision, and F1-score among all the models evaluated.

References

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- [2] A. Lindholm, N. Wahlström, F. Lindsten, and T. B. Schön. *Machine Learning - A First Course for Engineers and Scientists*. Cambridge University Press, 2022. URL <https://smlbook.org>.
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247 A Appendix

```
248 1 # %% [markdown]
249 2 # # Appendix A
250 3
251 4 # %%
252 5 import pandas as pd
253 6 import pycaret
254 7 import numpy as np
255 8 import copy
256 9
257 10 # %% [markdown]
258 11 # ## Read Raw Data
259 12
260 13 # %%
261 14 df_raw = pd.read_csv('training_data_ht2025.csv')
262 15
263 16 # %%
264 17 df_raw
265 18
266 19 # %% [markdown]
267 20 # ### Check Data Contents
268 21
269 22 # %%
270 23 df_raw['increase_stock'].value_counts()
271 24
272 25 # %% [markdown]
273 26 # Based on above code that shows the values on the target variable *
274     increase_stock*, there's a problem of Imbalance Dataset, where the
275     records with low bike demand are much more compared to records
276     with high bike demands.
277 27
278 28 # %%
279 29 df_raw['holiday'].value_counts()
280 30
281 31 # %%
282 32 df_raw['weekday'].value_counts()
283 33
284 34 # %%
285 35 df_raw['summertime'].value_counts()
286 36
287 37 # %%
288 38 df_raw['increase_stock'].value_counts()
289 39
290 40 # %%
291 41 df_raw['hour_of_day'].value_counts()
292 42
293 43 # %%
294 44 df_raw['day_of_week'].value_counts()
295 45
296 46 # %%
297 47 df_raw['month'].value_counts()
298 48
299 49 # %%
300 50 df_raw['snow'].value_counts()
301 51
302 52 # %% [markdown]
303 53 # Note: The Snow Features only have one value: 0, and therefore isn't
304     really useful for this dataset. And In Feature selection we can
305     drop them.
306 54
307 55 # %%
308 56 df_raw.isnull().sum()
309 57
310 58 # %% [markdown]
```

```

31159 # Based on the checking results, there're no NaN values, so we can
312     proceed with feature processing.
31360
31461 # %% [markdown]
31562 # ##### Cyclical Encoding
31663
31764 # %% [markdown]
31865 # Function to encode Ordinal Variables into Cyclical encoding using
319     Sine and Cosine
32066
32167 # %%
32268 def cyclical_encode(x, max_val, start_val=0):
32369     x_arr = np.asarray(x, dtype=float)
32470
32571     # If values are 1..period (e.g. months 1..12), shift to 0..period
326     -1
32772     if not start_val:
32873         x_arr = x_arr - 1
32974
33075     angle = 2 * np.pi * x_arr / max_val
33176     sin_x = np.sin(angle)
33277     cos_x = np.cos(angle)
33378
33479     if np.isscalar(x):
33580         return float(sin_x), float(cos_x)
33681
33782     return sin_x, cos_x
33883
33984 # %%
34085
34186
34287 # %%
34388 # Transform Cyclical Values for hour_of_day
34489
34590 # Transform Cyclical Values for hour_of_day
34691 # Hour of day ranges from 0 to 23
34792 df_hour_feat = pd.DataFrame(df_raw['hour_of_day'].apply(lambda x:
348     cyclical_encode(x, max(df_raw['hour_of_day']), min(df_raw['
349     hour_of_day']))) .to_list())
35093 df_hour_feat.columns = ['hour_of_day_sin', 'hour_of_day_cos']
35194 df_hour_feat
35295
35396
35497 # Transform Cyclical Values for day_of_week
35598 # Day of week ranges from 0 (Monday) to 6 (Sunday)
35699 df_day_feat = pd.DataFrame(df_raw['day_of_week'].apply(lambda x:
357     cyclical_encode(x, 6, 0)) .to_list())
35800 df_day_feat.columns = ['day_of_week_sin', 'day_of_week_cos']
35901 df_day_feat
36002
36103 # Transform Cyclical Values for month
36204 # Month ranges from 1 to 12
36305 df_month_feat = pd.DataFrame(df_raw['month'].apply(lambda x:
364     cyclical_encode(x, 12, 1)) .to_list())
36506 df_month_feat.columns = ['month_sin', 'month_cos']
36607 df_month_feat
36708
36809 # Concat Cyclical Features
36910 df_cyclical = pd.concat([df_hour_feat, df_day_feat, df_month_feat],
370     axis=1)
37111 df_cyclical
37212
37313 # %%
37414 # Creating Final Feature and Target DataFrames
37515 df_features = copy.deepcopy(df_raw)

```

```

37616
37717 # Creating Target Variable and Mapping text to binary
37818 df_target = df_features['increase_stock'].map({'low_bike_demand': 0, '
379         high_bike_demand': 1})
38019
38120 # Dropping original cyclical columns and target from features
38221 df_features = df_features.drop(['hour_of_day', 'day_of_week', 'month',
383         'increase_stock'], axis=1)
38422
38523 # Concatenating Cyclical Features to Features DataFrame
38624 df_features = pd.concat([df_cyclical, df_features], axis=1)
38725
38826 df_features
38927
39028 # %%
39129 df_target
39230
39331 # %%
39432 # Correlation Analysis between Features and Target
39533 df_corr = pd.concat([df_features, df_target], axis=1).corr()
39634 df_corr['increase_stock'].sort_values(key=abs, ascending=False)
39735
39836 # %% [markdown]
39937 # Based on above result, The variables hour_of_day_cos, temp, humidity
400         , hour_of_day_sin, and summertime held the biggest correlation to
401         the target variable. Because of this, we could check the trends
402         more based on those attributes
40338
40439 # %%
40540 from imblearn.over_sampling import SMOTE
40641
40742 # Applying SMOTE to Balance the Dataset
40843 smote = SMOTE(sampling_strategy='minority')
40944
41045 print("Before SMOTE:\n", df_target.value_counts())
41146
41247 print()
41348
41449 X_resampled, y_resampled = smote.fit_resample(df_features, df_target)
41550
41651 print("After SMOTE:\n", y_resampled.value_counts())
41752
41853 # Note: Don't use SMOTE outside training data to avoid data leakage,
419         this block is just for experimentation purposes. In practice,
420         SMOTE should only be applied to the training set within each cross
421         -validation folds.
42254
42355
42456 # %% [markdown]
42557 # ## Model Experiment
42658
42759 # %%
42860 from sklearn.metrics import accuracy_score, precision_score,
429         recall_score, f1_score, roc_auc_score, classification_report
43061 from sklearn.model_selection import KFold, train_test_split
43162 from sklearn.model_selection import GridSearchCV
43263
43364 # %% [markdown]
43465 # #### K-Fold Classification Report
43566
43667 # %%
43768 ## Function to do K-Fold Cross Validation and return the
438         classification report
43969 def kfold_classification_reports(clf, X, y, n_splits=10, shuffle=True,
440         random_state=42):

```

```

44170 kf = KFold(n_splits=n_splits, shuffle=shuffle, random_state=
442 random_state)
44371 reports = []
44472
44573 for train_index, test_index in kf.split(X):
44674     # Applying SMOTE to Balance the Dataset
44775     smote = SMOTE(sampling_strategy='minority')
44876
44977     X_train, X_test = X.iloc[train_index], X.iloc[test_index]
45078     y_train, y_test = y.iloc[train_index], y.iloc[test_index]
45179
45280     X_resampled, y_resampled = smote.fit_resample(X_train, y_train
45381 )
454
45582     clf.fit(X_resampled, y_resampled)
45683     y_pred = clf.predict(X_test)
45784
45885     report = classification_report(y_test, y_pred, output_dict=
45986 True)
460
46187     reports += [report]
46288
46389     detailed = []
46490     for i, rep in enumerate(reports):
46591         fold_result = {
46692             "fold": i + 1,
46793             "accuracy": rep["accuracy"],
46894             "precision": rep["weighted avg"]["precision"],
46995             "recall": rep["weighted avg"]["recall"],
47096             "f1": rep["weighted avg"]["f1-score"],
47197         }
47298         detailed.append(fold_result)
47399
47400     # compute averaged (generalized) metrics
47501     accuracies = [d["accuracy"] for d in detailed]
47602     precisions = [d["precision"] for d in detailed]
47703     recalls = [d["recall"] for d in detailed]
47804     f1s = [d["f1"] for d in detailed]
47905
48006     report_dict = {
48107         "general": {
48208             "accuracy_mean": float(np.mean(accuracies)),
48309             "accuracy_std": float(np.std(accuracies)),
48410             "precision_mean": float(np.mean(precisions)),
48511             "precision_std": float(np.std(precisions)),
48612             "recall_mean": float(np.mean(recalls)),
48713             "recall_std": float(np.std(recalls)),
48814             "f1_mean": float(np.mean(f1s)),
48915             "f1_std": float(np.std(f1s)),
49016         },
49117         "detailed": detailed
49218     }
49319
49420     return report_dict
49521
49622 # %% [markdown]
49723 # ## Benchmark Model
49824
49925 # %% [markdown]
50026 # For the benchmark model, we use a naive model that predict each
501 instance as the majority class in the training dataset. This will
502 provide a baseline accuracy to compare the performance of more
503 sophisticated models.
50427
50528 # %%

```

```

50629 from sklearn.dummy import DummyClassifier
50730
50831 clf_dummy = DummyClassifier(strategy="stratified")
50932
51033 # %%
51134 reports = kfold_classification_reports(clf_dummy, df_features,
512      df_target)
51335 reports['general']
51436
51537 # %% [markdown]
51638 # ## Logistic Regression
51739
51840 # %% [markdown]
51941 # For Logistic Regression, we will do hyperparameter tuning on
520      Regularization Strength (*C*), Penalty type (*penalty*), and
521      Solver type (*solver*)
52242
52343 # %%
52444
52545 # %%
52646
52747
52848 from sklearn.linear_model import LogisticRegression
52949
53050 clf = LogisticRegression()
53151
53252 #Grid Search to find the best hyperparameters for Logistic Regression
53353 grid_search = GridSearchCV(
53454     estimator=clf,
53555     param_grid={
53656         'C': [0.01, 0.1, 1, 10, 100],
53757         'penalty': ['l1', 'l2'],
53858         'solver': ['liblinear', 'lbfgs', 'saga', 'newton-cg']
53959     },
54060     scoring='f1',
54161     cv=10,
54262     n_jobs=-1,
54363     verbose=1
54464 )
54565 clf_grid_lg = grid_search.fit(df_features, df_target)
54666
54767 # %%
54868 clf_grid_lg.best_params_
54969
55070 # %%
55171 clf_lg = LogisticRegression(**clf_grid_lg.best_params_)
55272
55373 # %%
55474 reports = kfold_classification_reports(clf_lg, df_features, df_target)
55575 reports['general']
55676
55777 # %% [markdown]
55878 # ## Linear Discriminant Analysis (LDA)
55979
56080 # %% [markdown]
56181 # For LDA, we us Hyperparameter tuning for Solver Type (*solver*)
56282
56383 # %%
56484 from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
56585
56686 clf = LinearDiscriminantAnalysis()
56787
56888 # Grid Search to find the best hyperparameters for LDA
56989 grid_search = GridSearchCV(
57090     estimator=clf,

```

```

57191     param_grid={
57292         'solver': ['svd', 'lsqr', 'eigen']
57393     },
57494     scoring='f1',
57595     cv=10,
57696     n_jobs=-1,
57797     verbose=1
57898 )
57999 clf_grid_lda = grid_search.fit(df_features, df_target)
58000
58101
58202 # %%
58303 clf_grid_lda.best_params_
58404
58505 # %%
58606 clf_lda = LinearDiscriminantAnalysis(**clf_grid_lda.best_params_)
58707 clf_lda
58808
58909 # %%
59010 reports = kfold_classification_reports(clf_lda, df_features, df_target
59111 )
59212 reports['general']
59313
59414 # %% [markdown]
59515 # ## K Nearest Neighbor (KNN)
59616
59717 # %% [markdown]
59818 # For K Nearest Neighbor, we use Hyperparameter tuning for selecting
59919 the number of neighbors (*n_neighbors*), weight function used in
60020 prediction (*weights*), and the metric used for distance
60121 computation (*metric*)
60222
60323 # %%
60424 from sklearn.neighbors import KNeighborsClassifier
60525
60626 clf = KNeighborsClassifier()
60727
60828 #Grid Search to find the best hyperparameters for KNN
60929 grid_search = GridSearchCV(
61030     estimator=clf,
61131     param_grid={
61232         'n_neighbors': range(3, 21, 2),
61333         'weights': ['uniform', 'distance'],
61434         'metric': ['euclidean', 'manhattan', 'minkowski']
61535     },
61636     scoring='f1',
61737     cv=10,
61838     n_jobs=-1,
61939     verbose=1
62040 )
62141 clf_grid_knn = grid_search.fit(df_features, df_target)
62242
62343 # %%
62444 clf_grid_knn.best_params_
62545
62646 # %%
62747 clf_knn = KNeighborsClassifier(**clf_grid_knn.best_params_)
62848 clf_knn
62949
63050 # %%
63151 reports = kfold_classification_reports(clf_knn, df_features, df_target
63252 )
63353 reports['general']
63454
63555 # %% [markdown]

```

```

63651 # ## Random Forest Classifier
63752
63853 # %% [markdown]
63954 # For Random Forest Classifier, we use Hyperparameter tuning for
640     selecting number of trees (*n_estimator*), maximum depth of each
641     trees (*max_depth*), minimum number of samples required to split
642     (*min_samples_split*), and minimum samples required to be a leaf
643     node (*min_samples_leaf*)
64455
64556 # %%
64657 from sklearn.ensemble import RandomForestClassifier
64758 clf = RandomForestClassifier()
64859 grid_search = GridSearchCV(
64960     estimator=clf,
65061     param_grid={
65162         'n_estimators': [20, 50, 100, 200, 250],
65263         'max_depth': [3, 5, 8, 10, 15, 20],
65364         'min_samples_split': [2, 5, 10],
65465         'min_samples_leaf': [1, 2, 4],
65566         'criterion': ['gini', 'entropy']
65667     },
65768     scoring='f1',
65869     cv=10,
65970     n_jobs=-1,
66071     verbose=1
66172 )
66273 clf_grid_rf = grid_search.fit(df_features, df_target)
66374
66475 # %%
66576 clf_grid_rf.best_params_
66677
66778 # %%
66879 clf_rf = RandomForestClassifier(**clf_grid_rf.best_params_)
66980 clf_rf
67081
67182 # %%
67283 reports = kfold_classification_reports(clf_rf, df_features, df_target)
67384 reports['general']
67485
67586 # %% [markdown]
67687 # ## Gradient Boosting
67788
67889 # %% [markdown]
67990 # For Gradient Boosting, we use Hyperparameter tuning to determine,
680     the number of sequential estimator (*n_estimators*), the learning
681     rate (*learning_rate*), Maximum depth of the individual regression
682     estimators (*max_depth*), and the fraction of samples to be used
683     for fitting the individual estimators (*subsample*).
68491
68592 # %%
68693 from sklearn.ensemble import GradientBoostingClassifier
68794 clf = GradientBoostingClassifier()
68895 grid_search = GridSearchCV(
68996     estimator=clf,
69097     param_grid={
69198         'n_estimators': [50, 100, 200],
69299         'learning_rate': [0.01, 0.05, 0.1, 0.2, 0.5],
69300         'max_depth': [3, 5, 8, 10],
69401         'subsample': [0.6, 0.8, 1.0]
69502     },
69603     scoring='f1',
69704     cv=10,
69805     n_jobs=-1,
69906     verbose=1
70007 )

```

```

70108 clf_grid_gb = grid_search.fit(df_features, df_target)
70209
70310 # %%
70411 clf_grid_gb.best_params_
70512
70613 # %%
70714 clf_gb = GradientBoostingClassifier(**clf_grid_gb.best_params_)
70815 clf_gb
70916
71017 # %%
71118 reports = kfold_classification_reports(clf_gb, df_features, df_target)
71219 reports['general']
71320
71421 # %% [markdown]
71522 # ### Saving Model
71623
71724 # %% [markdown]
71825 # Saving all model so we can use it later
71926
72027 # %%
72128 # Applying SMOTE to Balance the Full Training Dataset
72229 smote = SMOTE(sampling_strategy='minority')
72330
72431 print("Before SMOTE:\n", df_target.value_counts())
72532
72633 print()
72734
72835 X_resampled, y_resampled = smote.fit_resample(df_features, df_target)
72936
73037 print("After SMOTE:\n", y_resampled.value_counts())
73138
73239 # %%
73340 import pickle
73441
73542 # Save the Dummy Classifier model used as benchmark
73643 with open('clf_dummy.pkl', 'wb') as f:
73744     pickle.dump(clf_dummy, f)
73845
73946 # %%
74047
74148 # Train the Logistic Regression model on the full training dataset
74249 clf_lg = LogisticRegression(**clf_grid_lg.best_params_)
74350 clf_lg.fit(X_resampled, y_resampled)
74451
74552 # Save the trained Logistic Regression model
74653 with open('clf_lg.pkl', 'wb') as f:
74754     pickle.dump(clf_lg, f)
74855
74956 # %%
75057 # Train the LDA model on the full training dataset
75158 clf_lda = LinearDiscriminantAnalysis(**clf_grid_lda.best_params_)
75259 clf_lda.fit(X_resampled, y_resampled)
75360
75461 # Save the trained LDA model
75562 with open('clf_lda.pkl', 'wb') as f:
75663     pickle.dump(clf_lda, f)
75764
75865 # %%
75966 # Train the KNN model on the full training dataset
76067 clf_knn = KNeighborsClassifier(**clf_grid_knn.best_params_)
76168 clf_knn.fit(X_resampled, y_resampled)
76269
76370 # Save the trained KNN model
76471 with open('clf_knn.pkl', 'wb') as f:
76572

```



```

76673     pickle.dump(clf_knn, f)
76774
76875 # %%
76976 # Train the Random Forest Classifier model on the full training
77077     dataset
77178 clf_rf = RandomForestClassifier(**clf_grid_rf.best_params_)
77279 clf_rf.fit(X_resampled, y_resampled)
77380
77481 # Save the trained Random Forest Classifier model
77582 with open('clf_rf.pkl', 'wb') as f:
77683     pickle.dump(clf_rf, f)
77784
77885 # %%
77986 # Train the Gradient Boosting Classifier model on the full training
78087     dataset
78188 clf_gb = GradientBoostingClassifier(**clf_grid_gb.best_params_)
78289 clf_gb.fit(X_resampled, y_resampled)
78390
78491 # Save the trained Gradient Boosting Classifier model
78592 with open('clf_gb.pkl', 'wb') as f:
78693     pickle.dump(clf_gb, f)
78794
78895 # %%

```