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# Do we need more bikes?

## Project in Machine Learning

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### Abstract

A binary classification problem of bike demand tendency is the focus of this paper, which compares different machine learning methods for solving it. These methods are discriminant analysis, nearest neighbors, tree-based methods, and deep neural networks. The paper uses accuracy, precision, and recall to measure the performance of these methods. The results indicate that the deep neural network has the best performance on this tendency prediction task. There are 4 people in this group.

## 1 Introduction

The bike demand in Washington is affected by several factors, such as weather conditions and time of the day, among others. Accurate and reliable predictions of the bike demand are a crucial step in distributing resources more efficiently.

In this study, we have been given a tabular dataset with 1600 samples of 15 features, that may be related to low and high bike demand, see table 1. In addition to the 15 input features in the dataset, we are also given the corresponding labels, zeros, and ones, that correspond to low and high bike demand respectively. The problem is therefore formulated as a binary classification problem.

Our goal is to compare several machine-learning models that are capable of classifying the conditions where low or high demand occurs. The comparison involves Linear Discriminant Analysis, Quadratic Discriminant Analysis, k-nearest neighbors, tree-based methods such as the Random Forest Classifier, Boosting methods like Adaboost and XGBoost, and finally, an ensemble of Deep Neural Networks.

## 2 Data Analysis

In our data analysis, key findings emerged regarding the impact of time, weather, and day type on shared bicycle demand. Numerical and certain dual-character (numerical and categorical) features, detailed in table 1, are pivotal in understanding these trends.

Seasonal patterns in Washington D.C. show higher bicycle demand during warmer months and daytime hours, with a noticeable decrease during colder months like January- February and November-December. Weekdays experience higher demand compared to weekends, likely due to different travel habits and choices, with weekends being more leisure-oriented.

Weather conditions also significantly influence bicycle usage. Demand drops on colder or wetter days, indicating a direct correlation between less favorable weather and decreased bicycle sharing.

In summary, our analysis reveals that time, weather, and day type are crucial determinants of shared bicycle usage patterns.

We scale each of the features with the min-max scaling for our dataset:

$$X_{\text{scaled}} = \frac{X - X_{\min}}{X_{\max} - X_{\min}}, \quad (1)$$

our motivation is that this removes the units of the features of the dataset, making them comparable to our machine-learning models.

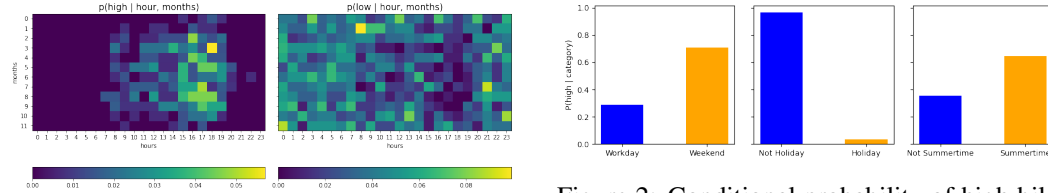


Figure 1: Given the hour of the day and the month of the year, we plot the probability of observing high and low bike demand respectively.

Figure 2: Conditional probability of high bike demand given some categorical feature. Note that there are many more cases where the days are not holidays.

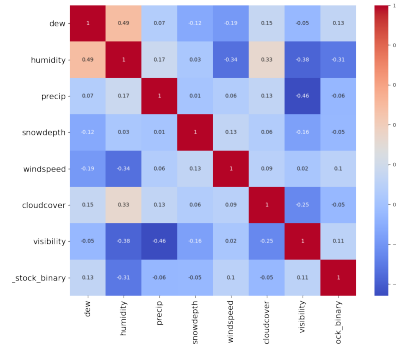


Figure 3: Correlation between weather features and bike demand.

Table 1: Data Type Table

Data Type	Features
Numerical Data	temp, dew, humidity, precip, snow, snowdepth, windspeed, cloudcover, visibility
Categorical Data	hour of day, day of week, month, holiday, weekday, summertime

### 3 Discriminant Analysis

Linear Discriminant Analysis (LDA) and Quadratic Discriminant Analysis (QDA) are statistical approaches used in machine learning for classifying a set of observations into different classes. These methods project input data onto a linear subspace, which maximizes the separation between classes (1). In LDA the decision surface is linear, while in QDA, it has the quadratic decision surfaces. The choice between LDA and QDA depends on the underlying distribution of the data and the complexity of the classification problem.

### 3.1 Mathematical Formulation

Both LDA and QDA model(1) the class conditional distribution  $P(y|x)$  as a multivariate Gaussian distribution.

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)} = \frac{P(x|y)P(y)}{\sum_i P(x|y_i)P(y_i)} \quad (2)$$

$$P(x|y) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_y)^T \Sigma^{-1}(x - \mu_y)\right), \quad (3)$$

Where  $n$  is the number of features,  $\mu_y$  is the mean vector of the features that belong to class  $y$ , and  $\Sigma$  is the covariance matrix of the Gaussian for class  $y$  respectively.

**QDA** Log-posterior of QDA is given by:

$$\begin{aligned} \log P(y|x) &= \log P(x|y = k) + \log P(y = k) + C \\ &= -\frac{1}{2} \log |\Sigma_y| - \frac{1}{2}(x - \mu_y)^T \Sigma_y^{-1}(x - \mu_y) + \log P(y) + C, \end{aligned} \quad (4)$$

where  $C$  is a constant that is related to  $P(x)$  and all other terms in the log-posterior that do not depend on the class  $y$ . The outcomes predicted class from QDA is the one that maximizes this log-posterior.

**LDA** LDA is simply a special case of QDA with the assumption that covariance *Sigma* is the same for all classes. Hence the log-posterior for LDA simplifies to:

$$\log P(y|x) = -\frac{1}{2}(x - \mu_y)^T \Sigma^{-1}(x - \mu_y) + \log P(y) + C. \quad (5)$$

Since covariance *Sigma* are the same for all classes, the LDA method can be seen as finding the class with mean vector that is "closest" to a given data point, with "closeness" measured by the Mahalanobis distance.

## 4 Nearest Neighbors

Nearest Neighbors(2) is one of the simplest machine learning algorithms that can be used for both classification and regression. It is a supervised learning algorithm. Upon analysis, it is determined that the problem is a classification task, for which the k-Nearest Neighbors (k-NN) algorithm is aptly suited. Employing grid search and 5-fold cross-validation, we optimize the model, selecting  $k=13$  as the ideal parameter. This optimized model achieves an accuracy of 86%(see table 2 for details), demonstrating the effectiveness of k-NN in classification scenarios and the importance of targeted parameter tuning.

### 4.1 k-Nearest Neighbor

In k-NN, the prediction of a sample's label is based on the labels of its  $K$  nearest neighbors. The term "nearest" is usually determined based on a distance metric, such as the Euclidean distance.

We define the training data  $\{\mathbf{x}_i, y_i\}_{i=1}^n$ , test input  $\mathbf{x}_*$  and the set  $\mathcal{N}_* = \{i\}$ ,  $\mathbf{x}_i$  is one of the  $k$  training data points closest to  $\mathbf{x}_*$ . The weight function:

$$\omega(\mathbf{x}, \mathbf{x}_i; k) = \begin{cases} 1, & \text{if } \mathbf{x}_i \text{ is } k \text{ nearest neighbour to } \mathbf{x} \\ 0, & \text{else} \end{cases} \quad (6)$$

A simple classifier based on the k-Nearest Neighbors (k-NN) algorithm can be described by the following general formula:

$$f(\mathbf{x}; k, \mathcal{T}) = \arg \max_y \sum_{i=1}^n \omega(\mathbf{x}, \mathbf{x}_i; k) \mathbb{I}_{\{y_i=y\}} \quad (7)$$

Depending on the purpose, k-NN prediction can be divided into regression and classification problems.

$$\hat{y}(\mathbf{x}_*) = \begin{cases} \text{Average}\{y_j : j \in \mathcal{N}_*\} & \text{(Regression problems)} \\ \text{Majority Vote}\{y_j : j \in \mathcal{N}_*\} & \text{(Classification problems)} \end{cases} \quad (8)$$

## 5 Tree-based Methods

### 5.1 Decision Trees

Decision trees are interpretable, simple machine learning algorithms effective for both categorical and numerical data. Their efficiency with tabular datasets enables the construction of powerful ensemble models using Bagging, see section 5.2 and Boosting, see section 6. The DT functions by creating a tree-like structure, consisting of root nodes (RNs), internal decision nodes (DNs), and leaf nodes (LNs). The DT starts from the RN and finds a decision boundary that minimizes a certain criterion. We choose to minimize the entropy:

$$S = - \sum_{a \in \mathcal{A}} \pi(y|a) \log \pi(y|a). \quad (9)$$

In this formula,  $\mathcal{A}$  represents the space of possible split actions, and  $\pi(y|a)$  represents the proportion of samples belonging to a class  $y$  in a DN, relative to the total number of samples at that node, given the split action  $a$ .

The action of reducing the entropy can be interpreted as reducing the disorder  $\pi(y|a)$  creates when a node split has occurred. Given the optimal split, the algorithm follows the path to the next node. This branching continues until a leaf node is reached, which signifies the final decision or classification outcome.

This approach aims to create subsets of data that are as homogeneous as possible, thereby enhancing the clarity and accuracy of decisions made by the tree. The decision-making process is iterative and may stop when the maximum depth of the tree is reached. We provide a diagram visualizing DT on our dataset shown in figure 6. One of the most important hyper-parameters that controls the trade-off between bias and variance is the maximal tree depth. A deep DT will in general also contain many DNs. A complex DT may thus have low bias but high variance.

### 5.2 Bagging

Bagging stands for *Bootstrap AGGREGatING*, an ensemble method used in machine learning. The term bootstrapping refers to sampling with replacement, in the context of our work, the training dataset is sampled such that each subset is independently identically distributed (IID). Furthermore, since we sample with replacement, each of the subsets likely has some overlapping elements.

With the new bootstrapped dataset, we may train a set of independent classifiers for each of the subsets of training data. Each of the classifiers is thus weakly correlated. After the completion, an aggregation step is performed. One type of aggregation operation, hard voting, works by counting the predicted label of each classifier, and the final prediction is made by picking the most frequent prediction. Another type of aggregation operation, soft voting, is performing an average of the probability of each classifier.

The Random Forest Classifier (RFC) (3) is a type of ensemble algorithm that uses bagging. Specifically, the RFC fits a set of DTs that is trained on a bootstrapped dataset, both in terms of samples, but also features. Each DT in a RFC is thus made as uncorrelated as possible. As a result, the combined effect of each DT contributes to reduced variance without increasing the bias.

### 5.3 Soft-voting ensemble

A general technique that we deploy in multiple models that is capable of predicting probability distribution is retraining the same model on the same training set using bagging, where each of the models is initialized with  $s$  different seeds:

$$H(x) = \frac{1}{s \cdot N_{cv}} \sum_{t=1}^s \sum_{j=1}^{N_{cv}} h_t(x; x_{cv,j}), \quad (10)$$

where  $x_{cv,j}$  is the inputs corresponding to the  $j$ :th cross validation fold,  $h_t$  is a single model that is trained on  $x_{cv,j}$ ,  $H(x)$  is the ensemble model, and  $N_{cv} = 5$  is the number of cross validation folds.

For RFC in 2, the performance is measured for  $s = 50$ , e.g., an ensemble of  $5 \cdot 50 = 250$  RFCs.

## 6 Boosting Methods

Bike-sharing usage depends on numerous factors that interact in a nonlinear fashion across different time horizons. Individual variables may carry limited signals on their own. Boosting overcomes this by allowing many simple base models, each capturing one aspect, to collectively build a sophisticated overall representation. The best hyperparameters for AdaBoost found via grid search were: learning\_rate = 0.1, max\_depth = 7, n\_estimators = 100, while the best parameters for XGBoost were: learning\_rate = 0.2, n\_estimators = 50.

### 6.1 AdaBoost Algorithm

AdaBoost (Adaptive Boosting) is an ensemble learning method that combines weak learners to create a strong classifier. It was introduced by Yoav Freund and Robert Schapire in 1996(4). The basic idea behind AdaBoost is to focus on the mistakes made by weak learners and give more weight to misclassified samples, allowing subsequent weak learners to correct these mistakes.

The following is the basic algorithm flow of Adaboost. The description of mathematical symbols is in Appendix 3:

**Input:** Training dataset  $D = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$ , where  $x_i$  is the feature vector and  $y_i$  is the label; Weak learner algorithm; Number of iterations  $T$ .

**Output:** Ensemble strong classifier  $H(x)$ .

1. **Initialize Weights:** Assign equal weights to each sample, i.e.,  $w_i = \frac{1}{N}$ .
2. **Iterative Training:**
  - (a) For each round  $t = 1, 2, \dots, T$ :
    - i. Select the weak classifier with the lowest current error rate as the t-th base classifier  $h_t$ .
    - ii. Compute the classifier  $h_t$  error rate and compute the weight for classifier  $h_t$ :

$$\varepsilon_t = \sum_{i=1}^N w_i^{(t)} \cdot \mathbf{I}(h_t(x_i) \neq y_i), \alpha_t = \frac{1}{2} \ln \left( \frac{1 - \varepsilon_t}{\varepsilon_t} \right). \quad (11)$$

- iii. Update sample weights, where  $Z_t$  is the normalization factor:

$$w_i^{(t+1)} = \frac{w_i^{(t)} \cdot \exp(-\alpha_t \cdot y_i \cdot h_t(x_i))}{Z_t}, Z_t = \sum_{i=1}^N w_i^{(t)} \cdot \exp(-\alpha_t \cdot y_i \cdot h_t(x_i)). \quad (12)$$

3. **Build Strong Classifier:**

Construct the final strong classifier:  $H(x) = \frac{1}{2} \left( \text{sign} \left( \sum_{t=1}^T \alpha_t \cdot h_t(x) \right) + 1 \right)$ .

### 6.2 XGBoost Algorithm

XGBoost(Extreme Gradient Boosting) is a gradient-boosting algorithm designed for regression and classification problems. Proposed by Tianqi Chen in 2016 (5).

XGBoost is an ensemble learning algorithm based on decision tree models. It employs the gradient boosting approach, iteratively training a series of weak learners. Each iteration adjusts the data based on the previous round's predictions to minimize the prediction error.

Combining the loss function and regularization term, the XGBoost objective function is represented below, the description of mathematical symbols and the derivation of the equation are shown in Appendix 4:

$$\text{Obj} = \sum_{i=1}^n \frac{1}{2} (y_i - \hat{y}_i)^2 + \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2 \quad (13)$$

The goal is to minimize this objective function. XGBoost utilizes optimization algorithms such as gradient descent to achieve this objective.

## Decision Tree Structure

XGBoost uses CART (Classification and Regression Trees) as the base learner. Each decision tree consists of nodes and leaves. Each node has a conditional statement dividing the data to left or right child.

## Training Process of Weak Learners

In each iteration, XGBoost calculates residuals, representing the difference between the true values and the current predictions. A new tree is fit to the residuals to correct the model's errors. Model parameters are updated through gradient descent to minimize the objective function.

## 7 Deep Neural Network

We choose to implement a Deep Neural Network (DNN) for predicting bike demand due to its ability to learn complex, non-linear feature interactions, which allows it to produce a non-linear decision boundary. Furthermore, DNNs handle high-dimensional data efficiently, a key advantage when limited feature engineering is performed.

### 7.1 Logistic Regression

Generalized Linear Models (GLMs) extend traditional linear regression for an arbitrary number of parameters  $\theta \in \Theta$

$$z = z(x; \theta) = x^T \theta. \quad (14)$$

We can modify the GLM to perform a binary classification task by applying the logistic function

$$\mathbb{P}(y|x; \theta) = \frac{1}{1 + e^{-z}}. \quad (15)$$

The optimal parameters  $\theta^*$  are estimated using Maximum Likelihood Estimation (MLE), which involves numerically minimizing the expected negative log-likelihood function

$$\theta^* = \arg \min_{\theta \in \Theta} \mathbb{E} [-\log \mathbb{P}(y|x; \theta)]. \quad (16)$$

The empirical expectation value above can be written as the binary cross-entropy (BCE) loss

$$\mathcal{L}(\theta) = -\frac{1}{n} \sum_{i=1}^n y_i \log \mathbb{P}(y_i|x_i; \theta) + (1 - y_i) \log \mathbb{P}(1 - y_i|x_i; \theta). \quad (17)$$

The method of minimizing the BCE to find the optimal parameters given a GLM is known as logistic regression and is capable of producing a linear decision boundary that separates the label classes.

### 7.2 Non-linear Classification

The logistic regression is limited to producing linear decision boundaries by the GLM. Therefore, for a more complex dataset, we consider a natural non-linear generalization of the logistic regression, namely, Deep Neural Network (DNN). Instead of the GLM in 14, we consider a non-linear model with a weight matrix  $\mathbf{W}$  and a offset vector  $\mathbf{b}$  in the form

$$x_{l+1} = \sigma(x_l^T \mathbf{W}_l + \mathbf{b}_l), \quad (18)$$

where  $1 \leq l \leq L$  denotes the number of layers of the DNN,  $\mathbf{W}_l \in \mathbb{R}^{h \times h}$ ,  $\mathbf{b}_l \in \mathbb{R}^h$ , with  $h$  being the number of hidden units, and  $\sigma(\cdot)$  represents a non-linear activation function. Note that we have:

$$x_0^T = x^T \mathbf{W}_{\text{in}} + \mathbf{b}_{\text{in}}, \quad (19)$$

where  $\mathbf{W}_{\text{in}} \in \mathbb{R}^{\# \text{input features} \times h}$  and  $\mathbf{b}_{\text{in}} \in \mathbb{R}^h$ .

We use the Rectified Linear Unit (RELU) activation function, defined as

$$\sigma(\cdot) = \max(0, \cdot). \quad (20)$$

Since the relation between  $x_{l+1}$  and  $x_l$  is non-linear, we can construct an arbitrary complex regression model by considering some large value of  $L$ . Furthermore, we consider additional techniques such as residual connections (6)

$$x_{l+1} = \sigma(x_l^T \mathbf{W}_l + \mathbf{b}_l) + x_l, \quad (21)$$

to improve the training process. In addition, we also perform batch normalization (7), defined as

$$\text{BN}_{\gamma_l, \beta_l}(x_l) = \gamma_l \cdot \frac{x_l - \mathbb{E}[x_l]}{\sqrt{\text{Var}[x_l] + \varepsilon}} + \beta_l \quad (22)$$

with some trainable parameter  $\gamma_l$  and  $\beta_l$  and  $\varepsilon > 0$  for numerical stability, before applying the non-linear function. The final non-linear regression model is thus

$$x_{l+1} = \sigma(\text{BN}_{\gamma_l, \beta_l}(x_l^T \mathbf{W}_l + \mathbf{b}_l)) + x_l. \quad (23)$$

Since our goal is to perform non-linear binary classification, we can replace the GLM with the DNN such that

$$z(x_{l+1}; \theta) = x_{l+1}^T \theta + b, \quad (24)$$

where  $\theta \in \mathbb{R}^{h \times 1}$  and  $b \in \mathbb{R}$ . Finally, the logistic function in equation 15 is applied to get the probability of predicting  $y$ , conditioned on  $x$ . The DNN in our case can thus be interpreted as a non-linear generalization of the logistic regression that is capable of producing non-linear decision boundaries.

The performance presented in table 2 is based on the same technique discussed in 5.3 with  $s = 10$ . We also over-parameterize the DNNs with  $h = 200$ ,  $L = 2$ , trained with  $l_2$ -regularization, this method is inspired by the deep double descent phenomena (8). Figure 5 demonstrates that the ensemble is capable of achieving higher accuracy than the individual model.

## 8 Evaluation

To evaluate our models, we split the shuffled dataset into two parts, a larger part consisting of 75% of the original dataset. This part performs a 5-fold stratified cross-validation to find the desired hyperparameters. The models are then evaluated on the hold-out dataset with the remaining 25%. The results are shown in table 2.

The data analysis suggests that there are 82% of low bike demands (label 0). Our baseline model is thus only predicting 0, independent from the inputs.

Table 2: Comparison of model performance with low bike demand having label 0 and high bike demand with label 1.

Model	Accuracy	Precision (0)	Precision (1)	Recall (0)	Recall (1)
Baseline Model	0.81	0.81	0.00	<b>1.00</b>	0.00
LDA	0.85	0.89	0.56	0.95	0.37
QDA	0.88	0.92	0.71	0.94	0.66
Nearest Neighbours	0.86	<b>0.93</b>	0.64	0.90	<b>0.71</b>
Random Forest	0.88	0.91	0.72	0.95	0.58
AdaBoost	0.85	0.92	0.59	0.91	0.62
XGBoost	0.88	0.91	0.70	0.94	0.60
Deep Neural Network	<b>0.90</b>	<b>0.93</b>	<b>0.74</b>	0.94	<b>0.71</b>

## 9 Conclusions

We evaluated five classification models for predicting the demand for bikes. The best overall methodology was to construct an ensemble of 50 over-parameterized DNNs, which shows the best performance on most metrics, with no significant weaknesses.

## References

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## 10 Appendix

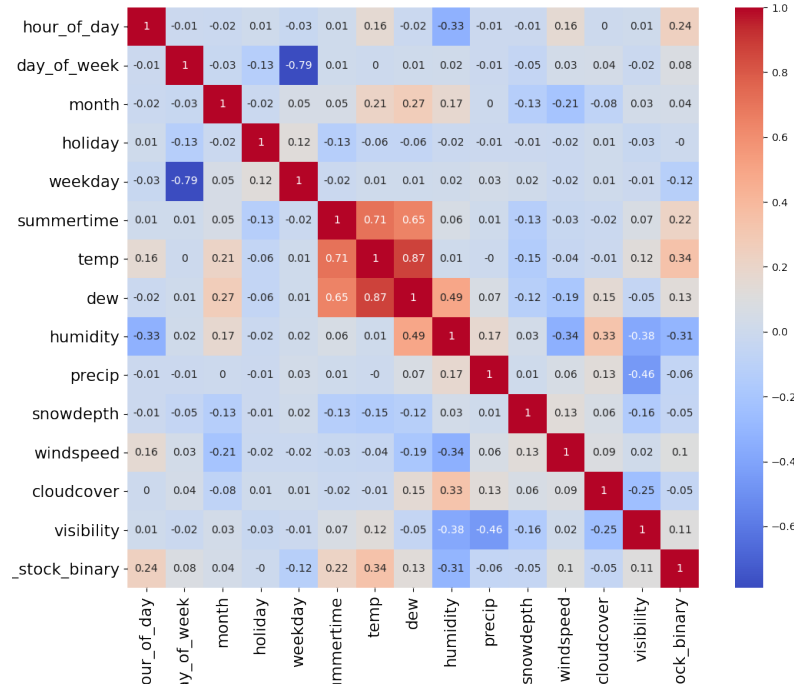


Figure 4: Correlation matrix of the features.

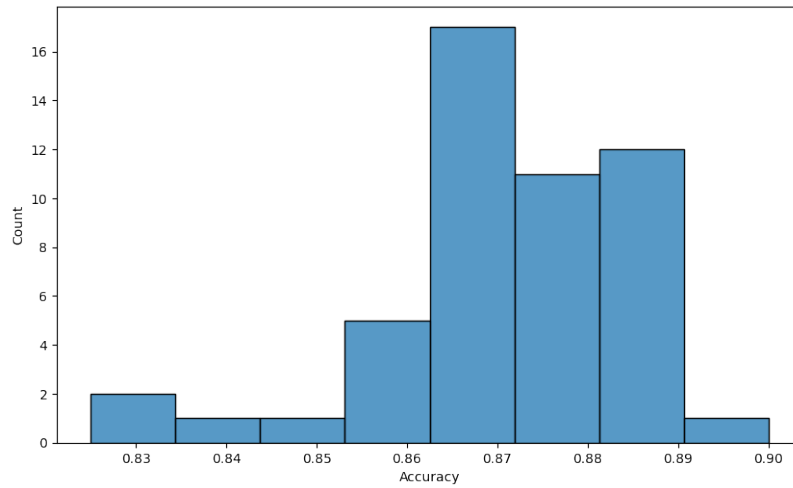


Figure 5: We show the accuracy for the 50 DNNs that form the DNN ensemble in table 2. From the accuracy distribution, we see that despite there being poor models in the ensemble, they still helped to increase the overall accuracy.

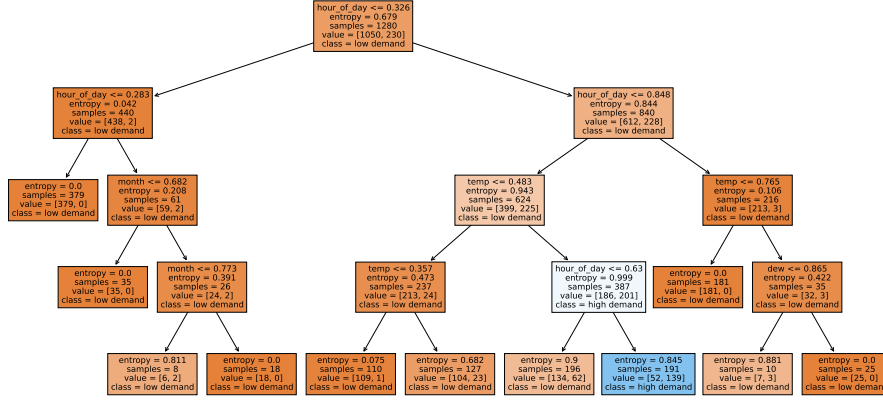


Figure 6: Visualization of a decision tree of depth 4. The RN first checks if the hour of the day (normalized) is below 0.326, if not, it creates a new DN to the right, checking for a later time in the day. If yes, it creates a DN to the left, this time it checks for the temperature of the day if it is below 0.483. This procedure is repeated until the max depth of the DT is reached. The resulting LNs contain the entropy of each prediction.

### Objective Function

The XGBoost objective function consists of a loss function and a regularization term. The objective function is formulated as:

$$\text{Obj} = \sum_{i=1}^n \ell(y_i, \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (25)$$

The loss function measures the model's prediction error with respect to the true values. In XGBoost, the loss function can be the logistic loss for classification problems, squared loss for regression problems, and so on, depending on the problem at hand. For regression problems, the squared loss function is commonly used and takes the following form:

$$\ell(y_i, \hat{y}_i) = \frac{1}{2}(y_i - \hat{y}_i)^2 \quad (26)$$

The regularization term is employed to control the model's complexity and prevent overfitting. The XGBoost regularization term consists of two parts: the number of leaf nodes and the sum of the squares of leaf node weights. The regularization term is expressed as:

$$\Omega(f) = \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2 \quad (27)$$

### Mathematical Symbol Description

Table 3: Description of Symbols in AdaBoost

Symbol	Description
$D$	Training dataset, where $x_i$ is the feature vector and $y_i$ is the label.
$w_i$	Weight assigned to each sample. Initialized as $\frac{1}{N}$ .
$T, t$	Number of iterations (rounds).
$h_t$	Weak classifier selected at the $t$ -th round.
$\varepsilon_t$	Error rate of the $t$ -th base classifier $h_t$ .
$\alpha_t$	Weight assigned to the $t$ -th classifier.
$Z_t$	Normalization factor for sample weights at the $t$ -th iteration.
$H(x)$	Final strong classifier.
$I(\cdot)$	Indicator function. Returns 1 if the condition is true, 0 otherwise.
$\text{sign}(\cdot)$	Sign function. Returns -1 for negative values, 0 for zero, and 1 for positive values.

Table 4: Description of Symbols in XGBoost

Symbol	Description
$\text{Obj}$	Objective function
$\ell(y_i, \hat{y}_i)$	Loss function
$\Omega(f_k)$	Regularization term
$n$	Number of samples
$K$	Number of trees
$T$	Number of leaf nodes
$w_j$	Weight of a leaf node
$\gamma$	Regularization parameter
$\lambda$	Regularization parameter

## Code

### LDA

```

1 import numpy as np
2 import pandas as pd
3 from sklearn.model_selection import train_test_split
4 from sklearn.metrics import classification_report, confusion_matrix,
  accuracy_score
5 from sklearn.preprocessing import StandardScaler
6 from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
  as LDA
7 from sklearn.discriminant_analysis import
  QuadraticDiscriminantAnalysis as QDA
8 from sklearn.utils import shuffle
9 from sklearn.model_selection import cross_val_score
10
11 # Load the dataset
12 file_path = 'training_data.csv'
13 data = pd.read_csv(file_path)
14 data['increase_stock_binary'] = data['increase_stock'].apply(lambda x:
  1 if x == 'high_bike_demand' else 0)
15
16 # Manually combining weather data with only numerical values
17
18 # Creating a "Feels-Like" Temperature feature
19 def calculate_feels_like_temp(temp, humidity, wind_speed):
20     # Constants for the formula

```

```

21 c1 = -8.78469475556
22 c2 = 1.61139411
23 c3 = 2.33854883889
24 c4 = -0.14611605
25 c5 = -0.012308094
26 c6 = -0.0164248277778
27 c7 = 0.002211732
28 c8 = 0.00072546
29 c9 = -0.000003582
30
31 apparent_temp = (c1 + (c2 * temp) + (c3 * humidity) + (c4 * temp *
    humidity) +
32                 (c5 * temp**2) + (c6 * humidity**2) + (c7 * temp
    **2 * humidity) +
33                 (c8 * temp * humidity**2) + (c9 * temp**2 *
    humidity**2))
34
35 # Adjusting for wind speed (only if temperature is below 10
    degrees Celsius)
36 if temp < 10:
37     wind_chill = 13.12 + 0.6215 * temp - 11.37 * wind_speed**0.16
    + 0.3965 * temp * wind_speed**0.16
38     return min(apparent_temp, wind_chill)
39 else:
40     return apparent_temp
41
42 # Apply the function to the dataset
43 data['feels_like_temp'] = data.apply(lambda x:
    calculate_feels_like_temp(x['temp'], x['humidity'], x['windspeed'
    ]), axis=1)
44
45
46 # Creating "workday" feature
47 data['workday'] = data.apply(lambda row: 1 if row['day_of_week'] < 5
    and row['holiday'] == 0 else 0, axis=1)
48
49 # Daytime: day 7-18: 1, night 19 - 6: 0
50 data['daytime'] = data['hour_of_day'].apply(lambda x: 1 if x in np.
    arange(7, 19) else 0)
51
52 # Dropping original features used in composition
53 data = data.drop(['temp', 'humidity', 'windspeed', 'snow', 'dew', '
    increase_stock', 'holiday', 'weekday',
54
55                 'day_of_week', 'summertime', 'month', 'hour_of_day',
    'cloudcover', 'month'], axis=1)
56
57
58
59 # Displaying the modified DataFrame
60 data.head()
61
62
63 # Shuffle train data
64 data = shuffle(data, random_state=0)
65
66 # Preparing the dataset
67 X = data.drop(['increase_stock_binary'], axis=1)
68 y = data['increase_stock_binary']
69
70 # Standardizing the features
71 scaler = StandardScaler()
72 X_scaled = scaler.fit_transform(X)
73
74 # split train and test data set

```

```

75 X_train, X_test, y_train, y_test = train_test_split(X_scaled, y,
76             test_size=0.2, random_state=0)
77 # Creating the classifier to the data
78 qda = QDA()
79
80 # Fitting the classifier with the training data
81 qda.fit(X_scaled, y)
82
83 # Prediction on test data
84 y_predic = qda.predict(X_test)
85
86 # Apply k-fold cross-validation
87 # Set the number of folds in 'cv'; for example, 5 folds
88 cv_scores = cross_val_score(qda, X_scaled, y, cv=10, scoring='accuracy
89                             ',)
90
91 # Print the accuracy for each fold
92 print("Accuracy scores for each fold:", cv_scores)
93
94 # Print the average accuracy across all folds
95 print("Average accuracy E_holdout:", np.mean(cv_scores))
96
97 # Evaluation
98 print("Confusion Matrix:\n", confusion_matrix(y_test, y_predic))
99 print("\nClassification Report:\n", classification_report(y_test,
100 y_predic))
101 print("Accuracy Score E_train:", accuracy_score(y_test, y_predic))

```

## QDA

```

1 # Load the dataset
2 file_path = 'training_data.csv'
3 data = pd.read_csv(file_path)
4 data['increase_stock_binary'] = data['increase_stock'].apply(lambda x:
5     1 if x == 'high_bike_demand' else 0)
6
7 # Manually combining weather data with only numerical values
8
9 # Creating a "Feels-Like" Temperature feature
10 def calculate_feels_like_temp(temp, humidity, wind_speed):
11     # Constants for the formula
12     c1 = -8.78469475556
13     c2 = 1.61139411
14     c3 = 2.33854883889
15     c4 = -0.14611605
16     c5 = -0.012308094
17     c6 = -0.0164248277778
18     c7 = 0.002211732
19     c8 = 0.00072546
20     c9 = -0.000003582
21
22     apparent_temp = (c1 + (c2 * temp) + (c3 * humidity) + (c4 * temp *
23         humidity) +
24         (c5 * temp**2) + (c6 * humidity**2) + (c7 * temp
25         **2 * humidity) +
26         (c8 * temp * humidity**2) + (c9 * temp**2 *
27         humidity**2))
28
29     # Adjusting for wind speed (only if temperature is below 10
30     degrees Celsius)
31     if temp < 10:
32         wind_chill = 13.12 + 0.6215 * temp - 11.37 * wind_speed**0.16
33         + 0.3965 * temp * wind_speed**0.16

```

```

28         return min(apparent_temp, wind_chill)
29     else:
30         return apparent_temp
31
32 # Apply the function to the dataset
33 data['feels_like_temp'] = data.apply(lambda x:
    calculate_feels_like_temp(x['temp'], x['humidity'], x['windspeed']
    ), axis=1)
34
35 # Creating "workday" feature
36 data['workday'] = data.apply(lambda row: 1 if row['day_of_week'] < 5
    and row['holiday'] == 0 else 0, axis=1)
37
38
39
40
41 data = data.drop(['temp', 'humidity', 'windspeed', 'dew', 'snow', '
    increase_stock', 'cloudcover', 'visibility', 'summertime',
42     'month', 'holiday', 'weekday', 'day_of_week', '
    precip', 'snowdepth'], axis=1)
43 data.head()
44
45 #Shuffle train data
46 data = shuffle(data, random_state=0)
47
48 # Preparing the dataset
49 X = data.drop(['increase_stock_binary'], axis=1)
50 y = data['increase_stock_binary']
51
52 # Standardizing the features
53 scaler = StandardScaler()
54 X_scaled = scaler.fit_transform(X)
55
56 # split train and test data set
57 X_train, X_test, y_train, y_test = train_test_split(X_scaled, y,
    test_size=0.2, random_state=0)
58
59 # Creating the classifier to the data
60 qda = QDA()
61
62 # Fitting the classifier with the training data
63 qda.fit(X_scaled, y)
64
65 # Prediction on test data
66 y_predic = qda.predict(X_test)
67
68 # Apply k-fold cross-validation
69 # Set the number of folds in 'cv'; for example, 5 folds
70 cv_scores = cross_val_score(qda, X_scaled, y, cv=10, scoring='accuracy
    ')
71
72 # Print the accuracy for each fold
73 print("Accuracy scores for each fold:", cv_scores)
74
75 # Print the average accuracy across all folds
76 print("Average accuracy E_holdout:", np.mean(cv_scores))
77
78 # Evaluation
79 print("Confusion Matrix:\n", confusion_matrix(y_test, y_predic))
80 print("\nClassification Report:\n", classification_report(y_test,
    y_predic))
81 print("Accuracy Score E_train:", accuracy_score(y_test, y_predic))

```

## k-NN

```

1 import numpy as np
2 import pandas as pd
3 from sklearn.model_selection import train_test_split
4 from sklearn.neighbors import KNeighborsClassifier
5 from sklearn.metrics import classification_report, confusion_matrix,
  accuracy_score
6 from sklearn.preprocessing import StandardScaler
7 from sklearn.pipeline import make_pipeline
8 from sklearn.preprocessing import MinMaxScaler
9 from sklearn.model_selection import cross_val_score
10 from sklearn.decomposition import PCA
11 import matplotlib.pyplot as plt
12 from sklearn.model_selection import StratifiedKFold
13 # Load the dataset
14 file_path = 'training_data.csv'
15 data = pd.read_csv(file_path)
16 data['increase_stock_binary'] = data['increase_stock'].apply(lambda x:
  1 if x == 'high_bike_demand' else 0)
17 # Separating features and the target variable
18 # split daytime into 3 values 0, 0.5, 1 depending on the hour of the
  day
19 data['daytime'] = data['hour_of_day'].apply(lambda x: 1 if 15 <= x <=
  19 else 0.5 if 8 <= x <= 14 else 0)
20 #identify this day is weekday or not?
21 def is_workday(row):
22     if row['day_of_week'] >= 5: # If the day is Saturday (5) or
  Sunday (6), it's not a workday
23         return 0
24     if row['holiday'] == 1: # If it's a holiday, it's not a workday
25         return 0
26     return 1 # Otherwise, it's a workday
27
28 # Apply the function to the dataset
29 data['is_workday'] = data.apply(is_workday, axis=1)
30 #http://www.qxkp.net/qxbk/qxsy/202103/t20210301_2787280.html
31 def categorize_precipitation(mm):
32     if mm < 10:
33         return 1
34     elif 10 <= mm < 25:
35         return 2
36     elif 25 <= mm < 50:
37         return 3
38     elif 50 <= mm < 100:
39         return 4
40     elif 100 <= mm < 250:
41         return 5
42     elif mm >= 250:
43         return 6
44     else:
45         return 0
46
47 # Snowfall: Categorizing based on the description
48 def categorize_snow(snowfall, snowdepth):
49     if snowfall == 0 and snowdepth == 0:
50         return 0
51     elif snowfall == 0 and snowdepth > 0:
52         return 1
53     elif snowfall > 0 and snowdepth == 0:
54         return 2
55     elif snowfall > 0 and snowdepth > 0:
56         return 3
57     else:
58         return 4
59
60 # Apply the function to the rows of the dataframe

```

```

61 data['snow_condition'] = data.apply(lambda row: categorize_snow(row['
    snow'], row['snowdepth']), axis=1)
62
63 # Now let's drop the original 'snow' and 'snowdepth' columns
64
65 # Atmospheric pressure: No categories needed, it's a continuous
    variable
66
67 # Wind speed: The description is related to the Beaufort scale which
    is different from the wind speed.
68 # Hence, no categorization is needed. However, if there is a specific
    request to categorize wind speed based on
69 # a given scale, that could be done.
70
71 # Applying the categorization functions to the precipitation and
    snowfall columns
72 data['precip_category'] = data['precip'].apply(
    categorize_precipitation)
73 # # Apply the function to the 'windspeed' column
74 # data['wind_level'] = data['windspeed'].apply(categorize_wind_speed)
75 apparent_temp = 1.07 * data['temp'] + 0.2 * data['dew'] - 0.65 * data[
    'windspeed'] - 2.7
76
77 # Add the calculated apparent temperatures to the dataframe
78 data['apparent_temp'] = apparent_temp
79 #season spring, summer, fall, winter
80 # Function to categorize months into seasons
81 def categorize_season(month):
82     if month in [12, 1, 2]:
83         return 0
84     elif month in [3, 4, 5]:
85         return 1
86     elif month in [6, 7, 8]:
87         return 2
88     else: # months 9, 10, 11
89         return 3
90
91 # Apply the function to categorize seasons
92 data['season'] = data['month'].apply(categorize_season)
93
94 # Merge 'season' and 'summertime' into a single column
95 # If summertime is 1, then it overrides the season to 'Summer'
96 data['season_summertime'] = data.apply(lambda row: 2 if row['
    summertime'] == 1 else row['season'], axis=1)
97 #drop some features.
98 data = data.drop(columns=['hour_of_day', 'day_of_week', 'holiday', '
    weekday', 'snow', 'month', 'summertime', 'season', 'temp', 'dew']) #
    windspeed fearture is very important.
99 # X = data.drop(['increase_stock', 'increase_stock_binary'], axis=1)
100 # y = data['increase_stock_binary']
101 # X_train, X_test, y_train, y_test = train_test_split(X, y, test_size
    =0.2, random_state=1)
102 # split feature and target
103 X = data.drop(['increase_stock', 'increase_stock_binary'], axis=1)
104 y = data['increase_stock_binary']
105
106 # split train and test data set
107 X_train, X_test, y_train, y_test = train_test_split(X, y, train_size
    =0.75, random_state=0)
108 from sklearn.model_selection import GridSearchCV
109 from sklearn.pipeline import make_pipeline
110 from sklearn.preprocessing import StandardScaler
111 from sklearn.preprocessing import MinMaxScaler
112 from sklearn.neighbors import KNeighborsClassifier

```



```

113 from sklearn.metrics import classification_report, confusion_matrix,
    accuracy_score
114
115 # Assuming X_train, X_test, y_train, y_test are already defined
116
117 # Creating a pipeline with a standard scaler and a KNN classifier
118 pipeline = make_pipeline(MinMaxScaler(), KNeighborsClassifier())
119
120 # Defining the parameter grid: testing different values for
    n_neighbors
121 param_grid = {'kneighborsclassifier__n_neighbors': range(1, 31)}
122
123 # Creating a GridSearchCV object
124 grid_search = GridSearchCV(pipeline, param_grid, cv=5)
125
126 # Fitting grid_search on the training data
127 grid_search.fit(X_train, y_train)
128
129 # Best parameters found by grid search
130 print("Best parameters:", grid_search.best_params_)
131
132 # Using the best model to make predictions
133 y_pred = grid_search.predict(X_test)
134
135 # Generating a classification report, confusion matrix, and accuracy
    score
136 classification_report_result = classification_report(y_test, y_pred)
137 confusion_matrix_result = confusion_matrix(y_test, y_pred)
138 accuracy_score_data = accuracy_score(y_test, y_pred)
139
140 # Printing the results
141 print("Classification Report:\n", classification_report_result)
142 print("Confusion Matrix:\n", confusion_matrix_result)
143 print("Accuracy Score:\n", accuracy_score_data)
144
145 # The cross-validation scores for the best model can also be accessed
146 print("Best Model Cross-Validation Scores:", grid_search.best_score_)

```

## Boosting

```

1 import pandas as pd
2 import numpy as np
3 from sklearn.model_selection import train_test_split
4 import matplotlib.pyplot as plt
5 import seaborn as sns
6 from sklearn.ensemble import AdaBoostClassifier
7 from sklearn.metrics import accuracy_score
8
9 # Load the dataset
10 file_path = r"Algorithms/training_data.csv"
11 data = pd.read_csv(file_path)
12 data1 = data.copy()
13 headers = list(data.columns)
14 # Display the first few rows of the dataframe
15 data.head()
16 import sklearn.preprocessing as preprocessing
17 from sklearn.preprocessing import MinMaxScaler
18
19 minmax = MinMaxScaler()
20 data_ = data.iloc[:, :-1]
21 minmax.fit(data_)
22 data = pd.DataFrame(minmax.transform(data_), columns=headers[:-1])

```

```

23 data["increase_stock"] = data1["increase_stock"]
24 data["increase_stock_binary"] = data["increase_stock"].apply(
25     lambda x: 1 if x == "high_bike_demand" else 0
26 )
27 data.head()
28 from sklearn.ensemble import GradientBoostingClassifier
29
30 from sklearn.model_selection import train_test_split
31
32 # set test set 20% of the original data, set random_state to ensure that
33     ↳ the training set and test set obtained each time are the same,
34     ↳ random_state can be set to any integer,
35 # as long as the value used for each training is the same
36 X_train, X_test, y_train, y_test = train_test_split(
37     data.iloc[:, :-1], data.iloc[:, -1], test_size=0.25, random_state=0
38 )
39
40 gb = GradientBoostingClassifier(n_estimators=100, learning_rate=0.1,
41     ↳ random_state=42)
42 gb.fit(X_train, y_train)
43
44 # output feature importance score
45 print("Feature importance scores:", gb.feature_importances_)
46
47 # select features with the top 9 feature importance scores
48 selected_features = np.array(data.columns)[
49     np.argsort(gb.feature_importances_)[:-1][:9]
50 ]
51 print("Selected features:", selected_features)
52
53 select_columns = [
54     "hour_of_day",
55     "temp",
56     "humidity",
57     "dew",
58     "day_of_week",
59     "weekday",
60     "windspeed",
61     "month",
62     "cloudcover",
63     "increase_stock_binary",
64 ]
65 data = data[select_columns]
66
67 ada = AdaBoostClassifier(random_state=0)
68 ada.fit(X_train, y_train)
69
70 from sklearn.model_selection import GridSearchCV
71 from sklearn.ensemble import AdaBoostClassifier
72
73 # create an AdaBoostClassifier
74 ada = AdaBoostClassifier(random_state=0)
75
76 # define the hyperparameter space to be tuned
77 param_grid = {"n_estimators": [50, 100, 200], "learning_rate": [0.01, 0.1,
78     ↳ 0.2]}

```

```

78 # use GridSearchCV for grid search
79 grid_search = GridSearchCV(
80     estimator=ada, param_grid=param_grid, scoring="accuracy", cv=3
81 )
82 grid_search.fit(X_train, y_train)
83
84 # output the best parameters and corresponding performance
85 print("Best Parameters:", grid_search.best_params_)
86 print("Best Accuracy:", grid_search.best_score_)
87
88
89 from xgboost.sklearn import XGBClassifier
90
91
92 xgb = XGBClassifier(random_state=0)
93
94 xgb.fit(X_train, y_train)
95
96 from sklearn.model_selection import GridSearchCV
97 from xgboost.sklearn import XGBClassifier
98
99 # create XGBoost classifier
100 xgb = XGBClassifier(random_state=0)
101
102 # define the hyperparameter space to optimize
103 param_grid = {
104     "n_estimators": [50, 100, 200],
105     "max_depth": [3, 5, 7],
106     "learning_rate": [0.01, 0.1, 0.2],
107 }
108
109 # use GridSearchCV for grid search
110 grid_search = GridSearchCV(
111     estimator=xgb, param_grid=param_grid, scoring="accuracy", cv=4
112 )
113 grid_search.fit(X_train, y_train)
114
115 # output the best parameters and the corresponding performance
116 print("Best Parameters:", grid_search.best_params_)
117 print("Best Accuracy:", grid_search.best_score_)
118
119
120 from sklearn.model_selection import StratifiedKFold
121
122 kf = StratifiedKFold(5, shuffle=True, random_state=0)
123 ac = []
124 model = ada
125 for train_index, test_index in kf.split(X_train, y_train):
126     X_train_kf, X_test_kf = X_train.iloc[train_index], X_train.iloc[
127         ↪ test_index]
128     y_train_kf, y_test_kf = y_train.iloc[train_index], y_train.iloc[
129         ↪ test_index]
130     model.fit(X_train_kf, y_train_kf)
131     ac.append(accuracy_score(y_test_kf, model.predict(X_test_kf)))
132 print(np.mean(ac))
133 print("as", accuracy_score(y_test, model.predict(X_test)))
134 print(ac)
135
136 from sklearn.metrics import mean_squared_error
137 from sklearn.metrics import mean_absolute_error

```

```

135 from sklearn.metrics import r2_score
136 from math import sqrt
137
138 print("RMSE:", sqrt(mean_squared_error(y_test, model.predict(X_test))))
139 print("MAE:", mean_absolute_error(y_test, model.predict(X_test)))
140 print("R2:", r2_score(y_test, model.predict(X_test)))
141 from sklearn.metrics import classification_report
142
143 print(classification_report(y_test, model.predict(X_test)))
144
145
146 from sklearn.model_selection import StratifiedKFold
147
148 kf = StratifiedKFold(5, shuffle=True, random_state=0)
149 ac = []
150 model = xgb
151 for train_index, test_index in kf.split(X_train, y_train):
152     X_train_kf, X_test_kf = X_train.iloc[train_index], X_train.iloc[
153         ↪ test_index]
154     y_train_kf, y_test_kf = y_train.iloc[train_index], y_train.iloc[
155         ↪ test_index]
156     model.fit(X_train_kf, y_train_kf)
157     ac.append(accuracy_score(y_test_kf, model.predict(X_test_kf)))
158 print(np.mean(ac))
159 print("as", accuracy_score(y_test, model.predict(X_test)))
160 from sklearn.metrics import mean_squared_error
161 from sklearn.metrics import mean_absolute_error
162 from sklearn.metrics import r2_score
163 from math import sqrt
164
165 print("RMSE:", sqrt(mean_squared_error(y_test, model.predict(X_test))))
166 print("MAE:", mean_absolute_error(y_test, model.predict(X_test)))
167 print("R2:", r2_score(y_test, model.predict(X_test)))
168
169 from sklearn.metrics import classification_report
170
171 print(classification_report(y_test, model.predict(X_test)))
172 # stratifiedfrom sklearn.model_selection import StratifiedKFold
173 kf = StratifiedKFold(5, shuffle=True, random_state=0)
174 ac = []
175 model = xgb
176 for train_index, test_index in kf.split(X_train, y_train):
177     X_train_kf, X_test_kf = X_train.iloc[train_index], X_train.iloc[
178         ↪ test_index]
179     y_train_kf, y_test_kf = y_train.iloc[train_index], y_train.iloc[
180         ↪ test_index]
181     model.fit(X_train_kf, y_train_kf)
182     ac.append(accuracy_score(y_test_kf, model.predict(X_test_kf)))
183 print(np.mean(ac))
184 print("as", accuracy_score(y_test, model.predict(X_test)))
185 from sklearn.metrics import mean_squared_error
186 from sklearn.metrics import mean_absolute_error
187 from sklearn.metrics import r2_score
188 from math import sqrt
189
190 print("RMSE:", sqrt(mean_squared_error(y_test, model.predict(X_test))))
191 print("MAE:", mean_absolute_error(y_test, model.predict(X_test)))
192 print("R2:", r2_score(y_test, model.predict(X_test)))
193 # recall precise

```

```

190 from sklearn.metrics import classification_report
191
192 print(classification_report(y_test, model.predict(X_test)))
193 # stratified
194
195
196 from sklearn.model_selection import StratifiedKFold
197 from sklearn.model_selection import cross_val_score
198
199 kf = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)
200
201 # cross_val_results = cross_val_score(model, X_train, y_train, cv=kf,
202   ↪ scoring='accuracy', fit_params={'sample_weight': None})
203 # use cross validation to evaluate the trained model
204 cross_val_results = cross_val_score(
205     model, X_test, y_test, cv=kf, scoring="accuracy", fit_params={
206         ↪ sample_weight": None}
207 )
208
209 # output performance indicators
210 print("Cross-Validation Results:", cross_val_results)
211 print("Mean Accuracy:", cross_val_results.mean())

```

## DNN

```

1 # !pip install optuna -q
2 import pandas as pd
3 import numpy as np
4 import optuna
5 from sklearn.model_selection import train_test_split
6 from sklearn.preprocessing import MinMaxScaler
7 from sklearn.model_selection import StratifiedKFold
8 from tqdm import tqdm
9
10 import torch
11 import torch.nn as nn
12 import torch.nn.functional as F
13
14 import matplotlib.pyplot as plt
15 import seaborn as sns
16
17 plt.rcParams["figure.figsize"] = (10, 7)
18 plt.rcParams["figure.dpi"] = 100
19
20 file_path = 'training_data.csv'
21 data = pd.read_csv(file_path)
22 data['increase_stock_binary'] = data['increase_stock'].map(lambda x: 0 if x
23   ↪ == 'low_bike_demand' else 1)
24 data = data.drop(['snow', 'increase_stock'], axis=1)
25
26 # pick out the labels
27 y = data['increase_stock_binary'].to_numpy().astype(np.float32)
28 y = torch.tensor(y).unsqueeze(-1)
29 data = data.drop(['increase_stock_binary'], axis=1)
30
31 # Separating the numerical and categorical data to handle them separately
32 onehot = True
33 if onehot:

```

```

33 cat_data = pd.DataFrame({key:data[key] for key in data.keys() if data[
    ↪ key].dtype == int})
34 num_data = pd.DataFrame({key:data[key] for key in data.keys() if data[
    ↪ key].dtype == float})
35
36 # performing onehot encoding on the categorical data
37 cat_data = torch.from_numpy(cat_data.to_numpy())
38 cat_onehot = torch.cat([F.one_hot(x, num_classes=24) for x in cat_data
    ↪ ]).view(cat_data.shape[0], -1)
39
40 # constructing the complete input dataset
41 data = np.concatenate([num_data.to_numpy(), cat_onehot.numpy()], axis
    ↪ =-1).astype(np.float32)
42
43 # scaling
44 X = MinMaxScaler().fit_transform(data)
45 X = torch.Tensor(X)
46
47 X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.75,
    ↪ shuffle=True, random_state=0)
48
49 print(X_train.shape, X_test.shape, y_train.shape, y_test.shape)
50
51 class DNN(nn.Module):
52     def __init__(self, hidden_size, input_size, layers=2, seed=0, submodule
    ↪ =False):
53         super().__init__()
54         torch.manual_seed(seed)
55
56         self.hidden_size = hidden_size
57         self.input_size = input_size
58         self.submodule = submodule
59
60         self.activation = nn.ReLU()
61         self.input_layer = nn.Linear(input_size, hidden_size)
62         self.batch_norm_input = nn.BatchNorm1d(hidden_size) # BatchNorm
    ↪ for input layer
63         self.linear_layers = nn.ModuleList()
64         self.batch_norm_layers = nn.ModuleList() # BatchNorm for other
    ↪ layers
65
66         for _ in range(layers):
67             self.linear_layers.append(nn.Linear(hidden_size, hidden_size))
68             self.batch_norm_layers.append(nn.BatchNorm1d(hidden_size))
69
70         self.output_layer = nn.Linear(hidden_size, 1)
71
72     def forward(self, x):
73         x = self.input_layer(x)
74         x = self.batch_norm_input(x)
75         x = self.activation(x)
76
77         for layer, batch_norm in zip(self.linear_layers, self.
    ↪ batch_norm_layers):
78             residual = x
79             x = layer(x)
80             x = batch_norm(x)
81             x = self.activation(x + residual)
82

```

```

83         if not self.submodule:
84             x = self.output_layer(x)
85             x = torch.sigmoid(x)
86         return x
87
88 epochs = 100
89 metric = lambda prediction, label: (prediction.round() == label).numpy().
    ↪ mean()
90 loss_fn = torch.nn.BCELoss()
91
92 model = DNN(17, X_train.shape[-1], 2)
93 optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
94
95 train_loss_history = []
96 test_loss_history = []
97 test_metric_history = []
98
99 for epoch in tqdm(range(epochs)):
100     optimizer.zero_grad()
101     model.train()
102     y_pred = model(X_train)
103     loss = loss_fn(y_pred, y_train)
104     loss.backward()
105     optimizer.step()
106
107     model.eval()
108     train_loss_history.append(loss.item())
109     with torch.no_grad():
110         y_pred_test = model(X_test)
111         test_loss = loss_fn(y_pred_test, y_test)
112         test_loss_history.append(test_loss.item())
113         accuracy = metric(y_pred_test, y_test)
114         if len(test_metric_history) > 0 and accuracy > max(
    ↪ test_metric_history):
115             optimal_epoch = epoch
116             test_metric_history.append(accuracy)
117
118
119 plt.figure(figsize=(10, 5), dpi=100)
120 plt.plot(test_metric_history, label="test accuracy")
121 plt.axvline(
122     optimal_epoch,
123     color="red",
124     label=f"best accuracy {test_metric_history[optimal_epoch]:.3f} occurred
    ↪ at epoch {optimal_epoch}")
125 plt.ylim(0.8, 0.95)
126 plt.legend(), plt.grid()
127 plt.show()
128
129
130 epochs = 100
131 loss_fn = nn.BCELoss()
132 n_ensembles = 10 # checking the performance for different weight
    ↪ initialization
133 kf = StratifiedKFold(n_splits=5, random_state=0, shuffle=True)
134 optimal_models = []
135
136 for n in range(n_ensembles):
137     fold_performance = []

```

```

138     for cv, (train_index, test_index) in enumerate(kf.split(X_train,
139         ↪ y_train)):
140         model = DNN(200, X.shape[-1], 2, seed=n)
141         optimizer = torch.optim.Adam(model.parameters(), lr=1e-3,
142         ↪ weight_decay=1)
143
144         train_loss_history = []
145         test_loss_history = []
146         test_metric_history = []
147         optimal_weights = 0
148
149         for epoch in tqdm(range(epochs)):
150             optimizer.zero_grad()
151             model.train()
152             y_pred = model(X_train[train_index])
153             loss = loss_fn(y_pred, y_train[train_index])
154             loss.backward()
155             optimizer.step()
156
157             with torch.no_grad():
158                 model.eval()
159                 y_pred_test = model(X_train[test_index])
160                 test_loss = loss_fn(y_pred_test, y_train[test_index])
161                 test_loss_history.append(test_loss.item())
162                 accuracy = metric(y_pred_test, y_train[test_index])
163
164                 if len(test_metric_history) > 0 and accuracy > max(
165                 ↪ test_metric_history):
166                     optimal_epoch = epoch
167                     optimal_weights = model.state_dict()
168                     test_metric_history.append(accuracy)
169
170             train_loss_history.append(loss.item())
171             optimal_models.append(optimal_weights)
172             fold_performance.append(test_metric_history[optimal_epoch])
173
174     mean_performance = np.mean(fold_performance)
175     print(f"{optimal_epoch}")
176     print(f"Mean performance for ensemble {n}: {mean_performance:.3f} $\pm$
177     ↪ {np.std(fold_performance).round(3)}")
178     print(f"{np.round(fold_performance, 3)}")
179
180     def compute_precision(predictions, labels, positive_label=1):
181         TP = ((predictions == positive_label) & (labels == positive_label)).sum
182         ↪ ().item()
183         FP = ((predictions == positive_label) & (labels != positive_label)).sum
184         ↪ ().item()
185         return TP / (TP + FP) if (TP + FP) > 0 else 0
186
187     def compute_recall(predictions, labels, positive_label=1):
188         TP = ((predictions == positive_label) & (labels == positive_label)).sum
189         ↪ ().item()
190         FN = ((predictions != positive_label) & (labels == positive_label)).sum
191         ↪ ().item()
192         return TP / (TP + FN) if (TP + FN) > 0 else 0
193
194     def DeepNeuralNetworkEnsemble(optimal_models, test_data):
195         DNN_ensemble = []

```



```

189     for weights in optimal_models:
190         model = DNN(200, X.shape[-1], 2)
191         model.load_state_dict(weights)
192         y_pred = model(test_data)
193         DNN_ensemble.append(y_pred.detach().numpy())
194     return torch.Tensor(DNN_ensemble).mean(0).round()
195
196 prediction = DeepNeuralNetworkEnsemble(optimal_models, X_test)
197 accuracy = metric(prediction, y_test)
198
199 print(round(accuracy, 2))
200 for positive_label in [0, 1]:
201     recall = compute_recall(prediction, y_test, positive_label)
202     precision = compute_precision(prediction, y_test, positive_label)
203     print(round(precision, 2), round(recall, 2))
204
205 single_DNN_performance = []
206 for weights in optimal_models:
207     model = DNN(200, X.shape[-1], 2)
208     model.load_state_dict(weights)
209     y_pred = model(X_test)
210     single_DNN_performance.append(metric(y_pred, y_test))
211
212 plt.figure(figsize=(10, 6), dpi=100)
213 sns.histplot(single_DNN_performance)
214 plt.xlabel("Accuracy")
215 #plt.savefig("Accuracy distribution for DNN ensemble", bbox_inches="tight")

```

## Random Forest

```

1 import pandas as pd
2 import numpy as np
3 from sklearn.model_selection import train_test_split
4 from sklearn.ensemble import RandomForestClassifier
5 from sklearn.datasets import make_classification
6 from sklearn.preprocessing import MinMaxScaler
7 from sklearn.model_selection import KFold, StratifiedKFold
8 from tqdm import tqdm
9
10 import matplotlib.pyplot as plt
11 import seaborn as sns
12
13 plt.rcParams["figure.figsize"] = (10, 7)
14 plt.rcParams["figure.dpi"] = 100
15
16 # Load the dataset
17 file_path = 'training_data.csv'
18 data = pd.read_csv(file_path)
19 data['increase_stock_binary'] = data['increase_stock'].apply(lambda x: 1 if
20     ↪ x == 'high_bike_demand' else 0)
21 data = data.drop(["increase_stock"], axis=1)
22
23 X = data.to_numpy()
24 scaler = MinMaxScaler()
25 X = scaler.fit_transform(X)
26
27 y = X[:, -1].astype(np.float32)
28 X = X[:, :-1].astype(np.float32)

```

```

29 metric = lambda a, b: (a == b).mean()
30
31 def RandomForestEnsemble(x, models):
32     predictions = [model.predict_proba(x) for model in models]
33     proba1 = np.mean(predictions, axis=0)[: , 1] # probability of predicting
    ↪ label 1
34     return proba1.round() # [0,0,0,1,0,1,0,0,0,...]
35
36 def compute_precision(predictions, labels, positive_label=1):
37     TP = ((predictions == positive_label) & (labels == positive_label)).sum
    ↪ ().item()
38     FP = ((predictions == positive_label) & (labels != positive_label)).sum
    ↪ ().item()
39     return TP / (TP + FP) if (TP + FP) > 0 else 0
40
41 def compute_recall(predictions, labels, positive_label=1):
42     TP = ((predictions == positive_label) & (labels == positive_label)).sum
    ↪ ().item()
43     FN = ((predictions != positive_label) & (labels == positive_label)).sum
    ↪ ().item()
44     return TP / (TP + FN) if (TP + FN) > 0 else 0
45
46 X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.75,
    ↪ random_state=0, shuffle=True)
47
48 seeds = range(50)
49 scores = []
50 models = []
51 kf = StratifiedKFold(n_splits=5, shuffle=True, random_state=0)
52
53 for s in seeds:
54     # Note how the indices between the validation set and train set are
    ↪ flipped.
55     # This means that the classifier will be trained on less than 50% of
    ↪ the data.
56     for i, (train_index, test_index) in enumerate(kf.split(X_train, y_train
    ↪ )):
57         clf = RandomForestClassifier(
58             n_estimators=200, max_depth=100, criterion="entropy",
59             random_state=s, n_jobs=-1
60         )
61         clf.fit(X_train[train_index], y_train[train_index])
62         # accuracy = clf.score(X_train[test_index], y_train[test_index])
63         accuracy = clf.score(X_test, y_test)
64         scores.append(accuracy)
65         models.append(clf)
66
67 print("average accuracy", np.mean(scores))
68
69 X_pred = RandomForestEnsemble(X_test, models)
70 metric(X_pred, y_test)
71
72 X_pred = np.zeros(len(y_test))
73 print(metric(X_pred, y_test))
74 for positive_label in [0, 1]:
75     recall = compute_recall(X_pred, y_test, positive_label)
76     precision = compute_precision(X_pred, y_test, positive_label)
77     print(round(precision, 2), round(recall, 2))
78

```

```

79 X_pred = RandomForestEnsemble(X_test, models)
80 print(metric(X_pred, y_test))
81 for positive_label in [0, 1]:
82     recall = compute_recall(X_pred, y_test, positive_label)
83     precision = compute_precision(X_pred, y_test, positive_label)
84     print(round(precision, 2), round(recall, 2))
85
86 X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.75,
87     ↪ random_state=0, shuffle=True)
88
89 clf = RandomForestClassifier(
90     n_estimators=200, max_depth=100, criterion="entropy", oob_score=True,
91     random_state=0, n_jobs=-1
92 )
93 clf.fit(X_train, y_train)
94
95 seeds = range(10)
96 # kf = StrKFold(5, random_state=0, shuffle=True)
97
98 for i, (train_index, test_index) in tqdm(enumerate(kf.split(X_train,
99     ↪ y_train)))):
100     X_, X_test = X[train_index], X[test_index]
101     y_, y_test = y[train_index], y[test_index]
102     models = []
103
104     # This loop creates a list of 3 * seeds classifiers using Bagging,
105     # by splitting the training set into 3 sets.
106     for s in seeds:
107         # Note how the indices between the validation set and train set are
108         ↪ flipped.
109         # This means that the classifier will be trained on less than 50%
110         ↪ of the data.
111         for i, (train_index_, _) in enumerate(KFold(n_splits=3).split(X_)):
112             X_train = X_[train_index_]
113             y_train = y_[train_index_]
114             clf = RandomForestClassifier(
115                 n_estimators=200, max_depth=100, criterion="entropy",
116                 random_state=s, n_jobs=-1
117             )
118             clf.fit(X_train, y_train)
119             models.append(clf)
120
121     X_pred = RandomForestEnsemble(X_test, models)
122     print("ensemble accuracy", metric(X_pred, y_test))
123
124 plt.hist(scores)

```