ESKİŞEHİR TECHNICAL UNIVERSITY JOURNAL OF SCIENCE AND TECHNOLOGY
A- APPLIED SCIENCES AND ENGINEERING

2022, x(x), pp. xx-xx, DOI: xx.xxxxx/xxxxx.xxxx

WATER QUALITY PREDICTION USING MACHINE LEARNING MODELS

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ABSTRACT

Determining water quality and potability holds critical importance for human health. Water quality measurement is extremely vital and drinking water that does not comply with quality standards can directly negatively affect human health. This study focuses on assessing water potability through machine learning algorithms. Our analysis involved eight diverse machine learning models: Logistic Regression, Decision Tree, KNeighbours, AdaBoost, Gaussian Naive Bayes, XGBoost, Support Vector Machine (SVM), and Random Forest. The dataset consisted of 3276 records and 10 features that could affect water potability [1]. These features including pH levels, hardness, solids, chloramines, sulfate, conductivity, organic carbon, trihalomethanes, turbidity, and the potability status. We divided the dataset into 33% for testing and 66% for training. XGBoost achieved the highest accuracy rate of 66.08%, while the K-Nearest Neighbors (KNN) model reached the lowest accuracy rate of 57.56%. These results show the importance of using strong machine learning algorithms such as XGBoost for predicting water safety.

Keywords: Water quality, Potability prediction, Machine Learning, XGBoost, K-Nearest Neighbors (KNN)

1. INTRODUCTION

Ensuring safe water quality is vital to prevent health risks globally, with water-related issues accounting for a significant number of deaths annually. Employing early detection methods is crucial to mitigate these risks. Utilizing machine learning algorithms offers a promising avenue for early prediction of water quality issues.

In this research, we assessed the efficacy of eight diverse machine learning models to predict water quality parameters. The models encompassed Logistic Regression, Decision Tree, KNeighbours, AdaBoost, Gaussian Naive Bayes, XGBoost, Support Vector Machine (SVM), and Random Forest. The dataset consisted of 3276 records and 10 features such as pH levels, dissolved solids, turbidity, chlorine levels, conductivity, organic carbon, temperature, nitrates, phosphates, and water potability status.

Training and testing of these models were conducted using a 66/33 train/test split. The analysis revealed that the XGBoost model yielded the highest accuracy, reaching 66.08%. On the other hand, K-Nearest Neighbors displayed the lowest accuracy, achieving 57.56 %. These results suggest the potential of machine learning in forecasting water quality, XGBoost as a potentially optimal model for this purpose.

We would like to give information about the algorithms we use in our project.

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Recieving Date: ... Publishing Date: ...

1.1. Logistic Regression

Logistic regression is a supervised machine learning algorithm primarily employed for binary classification tasks. It utilizes a logistic function, or sigmoid function, to generate probability values between 0 and 1. For instance, in a scenario with two classes (Class 0 and Class 1), if the logistic function output exceeds a predefined threshold (typically 0.5), the instance is assigned to Class 1; otherwise, it belongs to Class 0. This method is an extension of linear regression tailored for classification problems.

One of its core functions is predicting a categorical dependent variable by leveraging independent variables. Consequently, the anticipated output must be discrete or categorical, such as Yes/No, 0/1, or true/false. However, instead of producing precise binary values, logistic regression yields probabilities ranging between 0 and 1, reflecting the likelihood of a data point belonging to a specific class.

Comparatively, logistic regression shares similarities with linear regression, yet their usage differs significantly. While linear regression tackles regression problems, logistic regression is geared towards solving classification challenges. Rather than fitting a linear regression line, logistic regression employs an "S"-shaped logistic function, which yields predictions predominantly as 0 or 1.

The sigmoid curve generated by the logistic function signifies the probability of an outcome, like determining if cells are cancerous or non-cancerous based on specific characteristics or whether a mouse is obese depending on its weight. Its significance in machine learning lies in its capability to furnish probabilities and classify new data, accommodating both continuous and discrete datasets.

Moreover, logistic regression proves versatile in classifying observations across diverse data types. It adeptly identifies the most influential variables crucial for effective classification, contributing to its widespread use in various domains [2].

1.2. Decision Tree

A decision tree represents a hierarchical tree-like structure in which each internal node signifies a feature or attribute, branches illustrate the decision rules based on those features, and the leaf nodes convey the output or prediction of the algorithm. Its versatility makes it a valuable tool in supervised machine learning, catering to both classification and regression problems. Due to its intuitive representation and ability to handle complex datasets, the decision tree algorithm holds significant prominence in various applications within the field of machine learning.

During the training phase, the decision tree algorithm operates by recursively segmenting the training data into subsets based on attribute values. This segmentation occurs through selecting the optimal attribute that maximizes information gain or minimizes impurity, measured using metrics like entropy or Gini impurity. The goal is to effectively partition the data, reducing randomness or impurity within each subset. This process continues until a stopping criterion is met, which could be reaching a defined maximum depth for the tree, or a minimum number of samples required to split a node.

The strength of decision trees lies in their ability to handle non-linear relationships between features and target variables. Furthermore, decision trees are fundamental components of ensemble methods like Random Forest. In Random Forest, multiple decision trees are constructed using different subsets of the training data and features. The combination of predictions from these trees through a voting or averaging mechanism results in improved accuracy and robustness, making Random Forest one of the most powerful and widely used algorithms in machine learning [3].

1.3.K-Nearest Neighbors (KNN)

The K-Nearest Neighbors (KNN) algorithm is a fundamental method used in machine learning for both classification and regression tasks. It predicts the label or value of a new data point by considering its K closest neighbors in the training dataset. This supervised learning algorithm finds extensive application in pattern recognition, data mining, and intrusion detection.

One of the key advantages of KNN is its non-parametric nature, which means it does not assume any specific distribution of the data. Unlike some other algorithms like Gaussian Mixture Models (GMM), KNN does not impose constraints based on data distribution. Instead, it relies on prior training data to classify coordinates into groups based on attributes, making it applicable in various real-life scenarios.

KNN's popularity lies in its simplicity and ease of implementation in machine learning. It can handle both numerical and categorical data without requiring assumptions about the underlying data distribution, offering flexibility across different types of datasets. Additionally, its non-parametric approach makes it less sensitive to outliers compared to other algorithms, enhancing its robustness in practical applications.

The algorithm operates by identifying the K nearest neighbors to a given data point using distance metrics like Euclidean distance. Subsequently, the classification or value of the data point is determined by the majority vote or average of these K neighbors. This adaptability to different patterns and reliance on local data structure for predictions highlight the significance of KNN in various machine learning applications [4].

1.4.AdaBoost

AdaBoost, also known as Adaptive Boosting, operates as an Ensemble Method in Machine Learning. Its primary choice for an estimator is decision trees with minimal complexity, often referred to as Decision Stumps due to their structure of just one split.

The algorithm's mechanism involves constructing a model initially, assigning equal weights to all data points, and subsequently focusing more on misclassified points by assigning them larger weights. With each iteration, AdaBoost aims to iteratively improve the model's performance by prioritizing those data points that were incorrectly classified in the previous iterations. This iterative process continues until a better model with reduced error is achieved.

In essence, AdaBoost sequentially trains models, emphasizing the significance of misclassified data points in subsequent iterations to refine the overall predictive capability of the ensemble [5].

1.5.Gaussian Naïve Bayes

Gaussian Naive Bayes stands as a machine learning classification technique rooted in a probabilistic approach. It assumes a normal distribution (also termed Gaussian distribution) for each class. This assumption means that the parameters associated with the classes follow a bell-shaped curve, emphasizing independence among parameters in predicting the output variable.

The model's underlying principle assumes that each parameter possesses an independent capability to predict the output variable, facilitating the prediction of the probability of a dependent variable being classified into each group.

During the prediction phase, Gaussian Naive Bayes combines the predictions for all parameters, ultimately yielding a probability for the dependent variable to belong to each group. The final classification is then assigned to the group with the higher probability.

Gaussian distribution, synonymous with normal distribution, is a statistical model characterizing the distributions of continuous random variables. Its defining trait is the bell-shaped curve, showcasing the probability density function. The crucial characteristics of the normal distribution include the mean (μ) and standard deviation (σ). The mean represents the average value within the distribution, while the standard deviation indicates the "width" or dispersion of the distribution around the mean, signifying how much the values deviate from the mean value [6].

1.6. XGBoost

XGBoost stands as an optimized distributed gradient boosting library meticulously crafted for efficient and scalable machine learning model training. Functioning as an ensemble learning method, it amalgamates predictions from numerous weak models to generate a robust prediction. The term "XGBoost" itself represents "Extreme Gradient Boosting" and has gained immense popularity in the machine learning realm for its prowess in handling large datasets and achieving top-notch performance in tasks like classification and regression.

A key hallmark of XGBoost lies in its adeptness at managing missing values within datasets, streamlining real-world data handling without the need for extensive preprocessing. Furthermore, it boasts inherent support for parallel processing, enabling the training of models on massive datasets within reasonable time frames.

The versatility of XGBoost spans various domains, finding applications in Kaggle competitions, recommendation systems, click-through rate prediction, and more. Notably, its high level of customization allows practitioners to fine-tune a multitude of model parameters, optimizing performance based on specific requirements.

Originally proposed by researchers at the University of Washington, XGBoost operates as a C++ library tailored to optimize Gradient Boosting training, emphasizing efficiency and performance in machine learning tasks [7].

1.7. Support Vector Machines (SVM)

Support Vector Machines (SVM) represent a supervised learning algorithm used in machine learning to address classification and regression tasks, excelling particularly in binary classification problems where data elements are grouped into two categories.

The fundamental goal of an SVM is to identify the optimal line, known as the decision boundary or hyperplane in high-dimensional feature spaces, that effectively separates data points belonging to different classes. This separation aims to maximize the margin, which signifies the distance between the hyperplane and the closest data points of each category, enabling clear distinction between classes.

SVMs are instrumental in analyzing intricate data that cannot be linearly separated. Nonlinear SVMs achieve this by employing a mathematical technique that transforms data into higher-dimensional space, facilitating boundary identification.

The working principle of SVMs revolves around transforming input data into a higher-dimensional feature space, enhancing the ability to ascertain a linear separation or classify the dataset more accurately. To achieve this transformation, SVMs utilize a kernel function. Instead of explicitly calculating transformed space coordinates, the kernel function enables implicit computation of dot products between transformed feature vectors, bypassing costly computations for extreme cases.

SVMs accommodate both linearly separable and non-linearly separable data through various kernel functions like linear, polynomial, or radial basis function (RBF) kernels. These kernels empower SVMs to capture intricate data relationships and patterns effectively.

During training, SVMs employ a mathematical formulation to pinpoint the optimal hyperplane in the higher-dimensional kernel space. This hyperplane's significance lies in maximizing the margin between different class data points while minimizing classification errors.

The choice of kernel function significantly influences SVM performance by mapping data from the original feature space to the kernel space. Optimal kernel function selection depends on data characteristics, emphasizing the critical role of the chosen kernel in SVM algorithm performance [8].

1.8.Random Forest

The Random Forest Algorithm has garnered immense popularity due to its ease of use and versatility in addressing classification and regression challenges within machine learning. Its robustness lies in the capability to effectively manage intricate datasets while mitigating the risk of overfitting, rendering it an invaluable tool across various predictive tasks.

A standout feature of the Random Forest Algorithm is its proficiency in handling diverse types of data, including both continuous variables (common in regression problems) and categorical variables (typical in classification tasks). This versatility contributes to its effectiveness in performing well across both classification and regression tasks, making it a preferred choice in diverse applications.

This tutorial aims to delve into the inner workings of the Random Forest Algorithm, offering insights into its functionality and implementation in a classification task. By understanding how Random Forest operates, users can harness its strengths to effectively address classification challenges and leverage its adaptability for robust predictive modeling [9].

2. MATERIALS AND METHODS (or EXPERIMENTAL)

The dataset utilized in this study comprises records gathered from various sources, encompassing information on water quality parameters and potability status. It includes 3276 entries with 10 features known to influence water potability, such as pH levels, hardness, solids, chloramines, sulfate, conductivity, organic carbon, trihalomethanes, turbidity, and the status of water potability. The dataset was preprocessed to handle missing values and outliers before the modeling phase.

This study assessed the performance of eight diverse machine learning models to predict water potability. The models considered were Logistic Regression, Decision Tree, K-Nearest Neighbors, AdaBoost, Gaussian Naive Bayes, XGBoost, Support Vector Machine (SVM), and Random Forest. Each model was implemented using widely adopted libraries in Python, such as Scikit-learn [10] and XGBoost.

Before training the models, the dataset underwent preprocessing steps, including feature scaling, and splitting the dataset into training and testing subsets. Feature scaling involved standardizing numerical attributes to ensure uniform scales across all features. The dataset split into 33% for testing and 66% for training purposes using a stratified sampling technique.

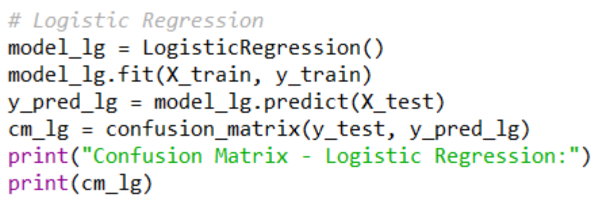
The machine learning models were trained on the training dataset and evaluated using the test dataset. Performance metrics such as accuracy, precision, recall, and F1-score were computed to assess each model's predictive capability. Hyperparameter tuning was performed using cross-validation to optimize model performance.

Statistical analyses were conducted using Python libraries to derive insights into feature importance and correlation among variables. Visualization techniques including histograms, correlation matrices, and feature importance plots were employed to enhance the understanding of the dataset's characteristics and the models' behavior.

Models	**Accuracy Score**	**Codes**	**Confusion Matrix**
Logistic Regression	60.11%	*Figure 1*	*Figure 2*
Decision Tree	62.62%	*Figure 3*	*Figure 4*
K-Nearest Neighbors	57.56%	*Figure 5*	*Figure 6*
AdaBoost	60.98%	*Figure 7*	*Figure 8*
Gaussian Naive Bayes	61.39%	*Figure 9*	*Figure 10*
XGBoost	66.08%	*Figure 11*	*Figure 12*
Support Vector Machine (SVM)	62.84%	*Figure 13*	*Figure 14*
Random Forest	62.84%	*Figure 15*	*Figure 16*

Tablo 1: Models used in predicting water quality, their accuracy rates, confusion matrix codes, and visuals.

2.9.Figures



```
# Logistic Regression
model_lg = LogisticRegression()
model_lg.fit(X_train, y_train)
y_pred_lg = model_lg.predict(X_test)
cm_lg = confusion_matrix(y_test, y_pred_lg)
print("Confusion Matrix - Logistic Regression:")
print(cm_lg)
```

Figure 1

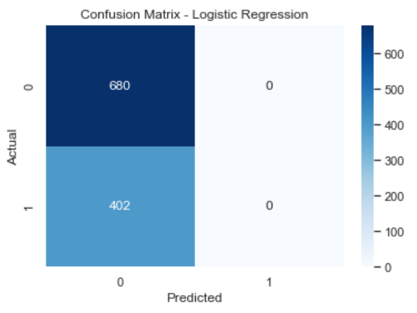
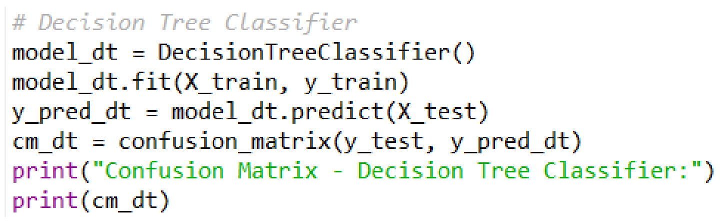


Figure 2



```
# Decision Tree Classifier
model_dt = DecisionTreeClassifier()
model_dt.fit(X_train, y_train)
y_pred_dt = model_dt.predict(X_test)
cm_dt = confusion_matrix(y_test, y_pred_dt)
print("Confusion Matrix - Decision Tree Classifier:")
print(cm_dt)
```

Figure 3

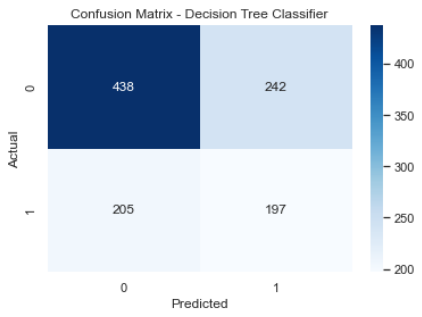
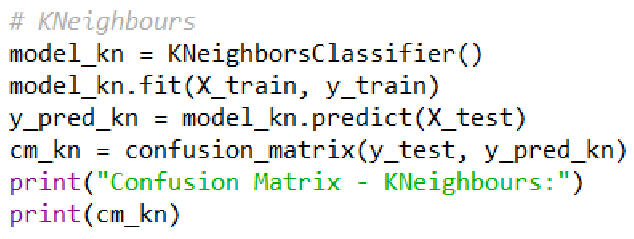


Figure 4



```
# KNeighbours
model_kn = KNeighborsClassifier()
model_kn.fit(X_train, y_train)
y_pred_kn = model_kn.predict(X_test)
cm_kn = confusion_matrix(y_test, y_pred_kn)
print("Confusion Matrix - KNeighbours:")
print(cm_kn)
```

Figure 5

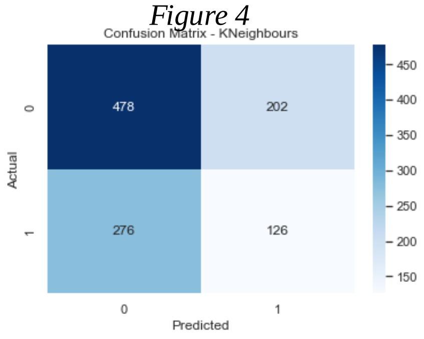
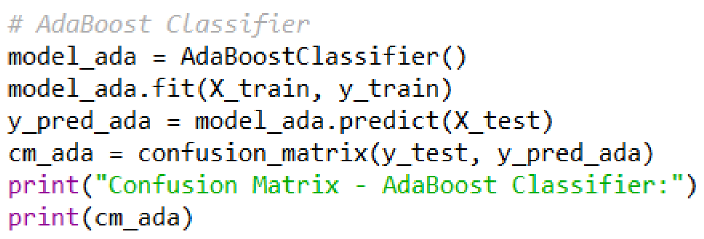


Figure 6



```
# AdaBoost Classifier
model_ada = AdaBoostClassifier()
model_ada.fit(X_train, y_train)
y_pred_ada = model_ada.predict(X_test)
cm_ada = confusion_matrix(y_test, y_pred_ada)
print("Confusion Matrix - AdaBoost Classifier:")
print(cm_ada)
```

Figure 7

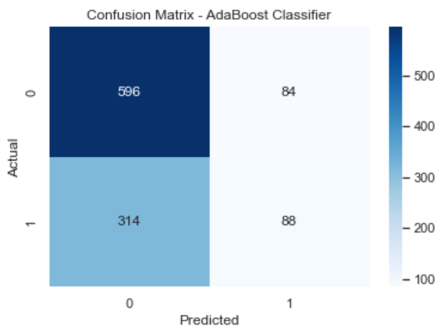
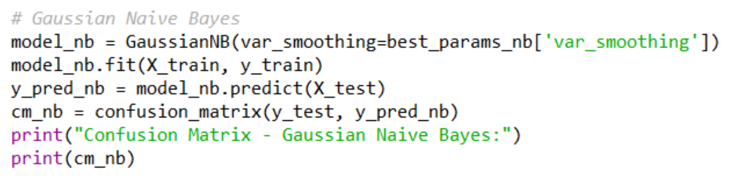


Figure 8



```
# Gaussian Naive Bayes
model_nb = GaussianNB(var_smoothing=best_params_nb['var_smoothing'])
model_nb.fit(X_train, y_train)
y_pred_nb = model_nb.predict(X_test)
cm_nb = confusion_matrix(y_test, y_pred_nb)
print("Confusion Matrix - Gaussian Naive Bayes:")
print(cm_nb)
```

Figure 9

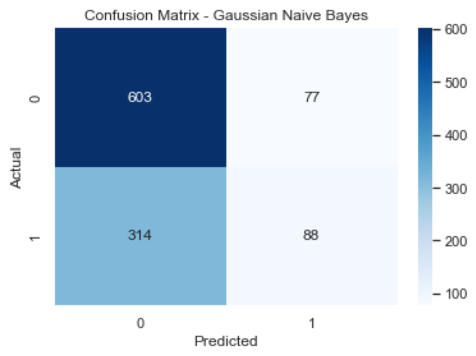
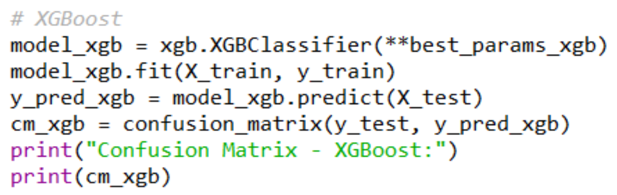


Figure 10



```
# XGBoost
model_xgb = xgb.XGBClassifier(**best_params_xgb)
model_xgb.fit(X_train, y_train)
y_pred_xgb = model_xgb.predict(X_test)
cm_xgb = confusion_matrix(y_test, y_pred_xgb)
print("Confusion Matrix - XGBoost:")
print(cm_xgb)
```

Figure 11

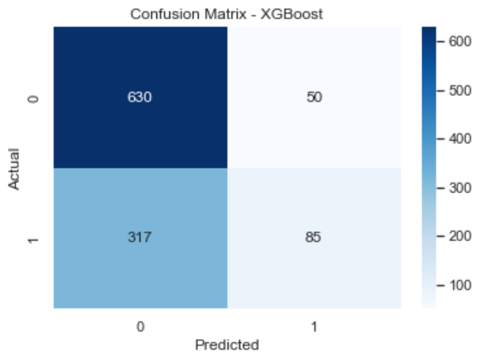
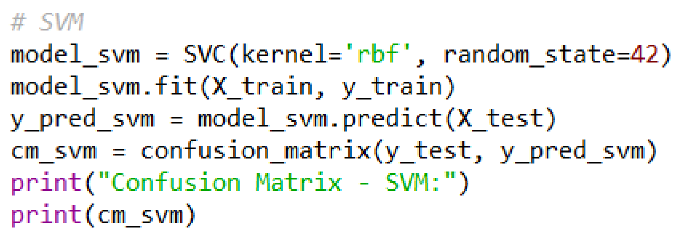


Figure 12



```
# SVM
model_svm = SVC(kernel='rbf', random_state=42)
model_svm.fit(X_train, y_train)
y_pred_svm = model_svm.predict(X_test)
cm_svm = confusion_matrix(y_test, y_pred_svm)
print("Confusion Matrix - SVM:")
print(cm_svm)
```

Figure 13

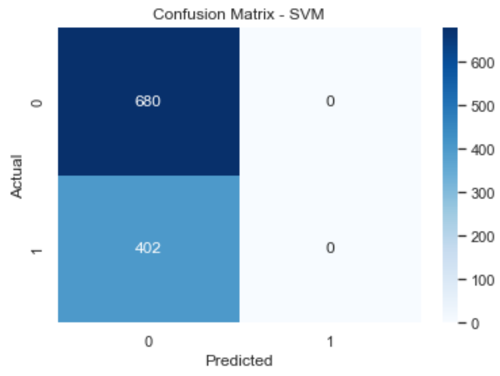
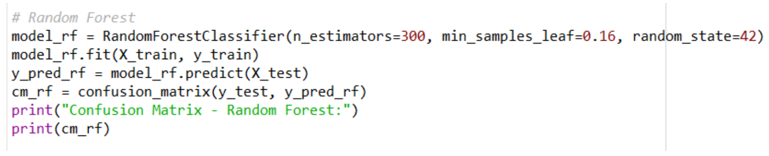


Figure 14



```
# Random Forest
model_rf = RandomForestClassifier(n_estimators=300, min_samples_leaf=0.16, random_state=42)
model_rf.fit(X_train, y_train)
y_pred_rf = model_rf.predict(X_test)
cm_rf = confusion_matrix(y_test, y_pred_rf)
print("Confusion Matrix - Random Forest:")
print(cm_rf)
```

Figure 15

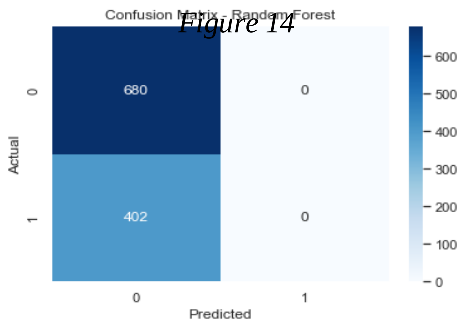


Figure 16

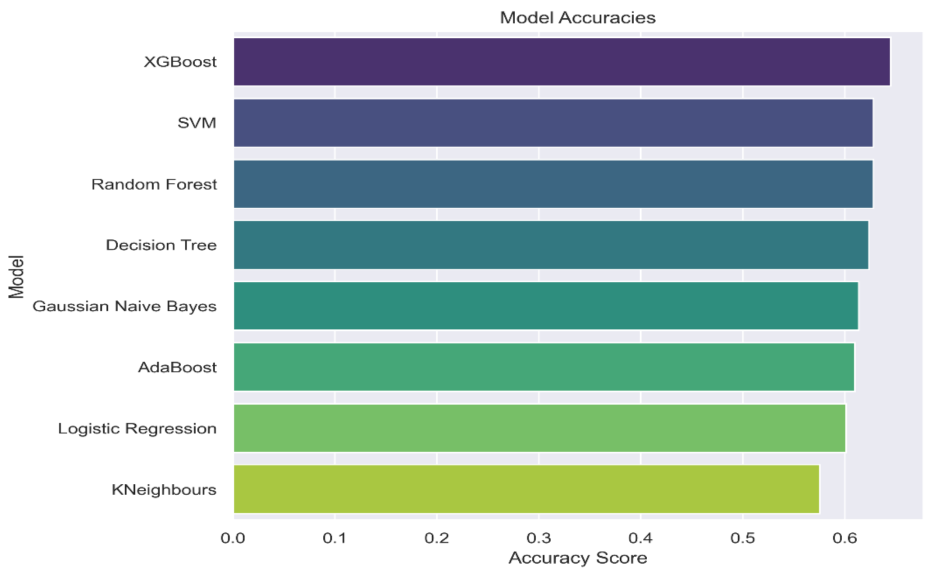


Figure 17

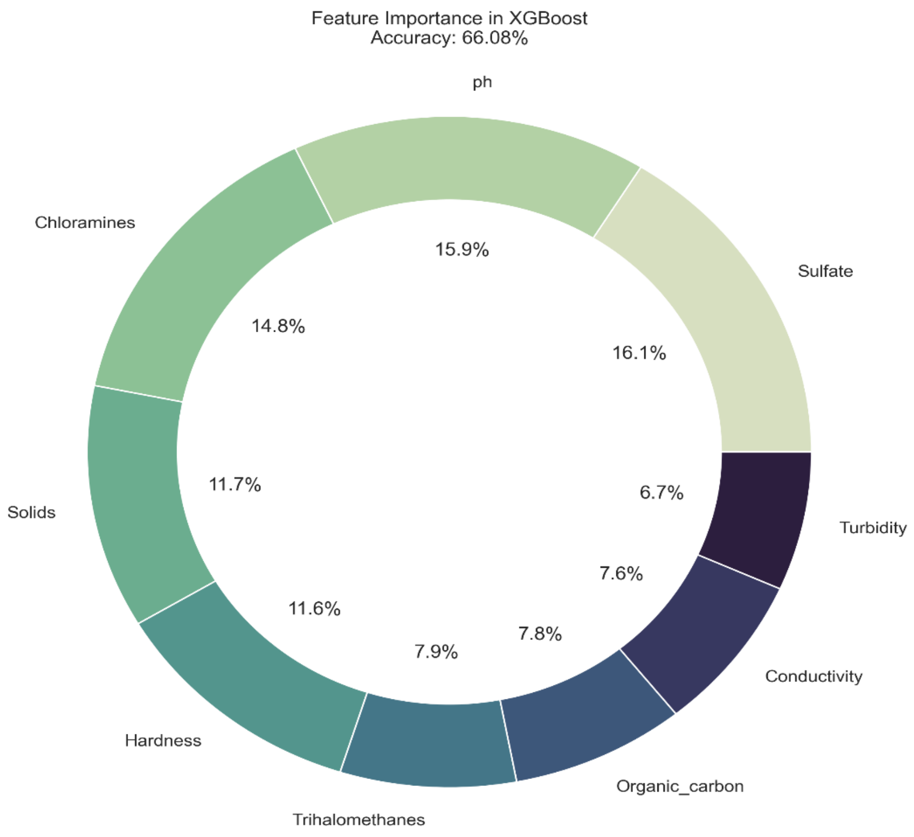


Figure 18

3.RESULTS

The Logistic Regression model has an accuracy of 60.11%, the Decision Tree model has an accuracy of 62.62%, the K-Nearest Neighbors (KNN) model has an accuracy of 57.56%, the AdaBoost model has an accuracy of 60.98%, the Gaussian Naïve Bayes model has an accuracy of 61.39%, the XGBoost model has an accuracy of 66.08%, the Support Vector Machines (SVM) model has an accuracy of 62.84%, the Random Forest model has an accuracy of 62.84%. So, the XGBoost model has the highest accuracy, with a score of 66.08% in *Figure 17*. The weight ratios of the features in the XGBoost model with the highest accuracy rate are illustrated in *Figure 18*.

4. DISCUSSION

The results of this study suggest that machine learning models may be useful in predicting whether water is drinkable. Among the eight models tested, the XGBoost model had the highest accuracy with a score of 66.08%. This suggests that the XGBoost model may be the most suitable model for predicting water quality. However, considering that our world is rich in water resources, we can infer that the dataset used is relatively small and cannot represent the entire population. Therefore, it is important to note that the results of this study should be interpreted with caution. Further studies with larger and more diverse data sets are needed to confirm these findings.

5. CONCLUSION

To sum up, this study demonstrated the potential of machine learning algorithms to help predict whether water is drinkable by measuring water quality. Eight different models were evaluated on a dataset containing 3276 records and 10 features. The results showed that the XGBoost model had the highest accuracy with a score of 66.08%, while K-Nearest Neighbors has the lowest accuracy with a score of 57.56%. These findings suggest that machine learning models may be useful in predicting whether water is drinkable and that the XGBoost model may be the most suitable model for this purpose. Further research is needed to confirm these results and determine the most effective ways to apply these models in the clinical setting.

ACKNOWLEDGEMENTS

We would like to thank to Associate Professor Doctor Mehmet KOÇ. We are grateful for the education given to us.

CONFLICT OF INTEREST

The authors (Duygu HALİSYAMA, Furkan DÖNMEZ) declare that they have no conflict of interest.

AI DECLERATION

In this project, we used ChatGPT [11] to correct and improve the errors in our code. Additionally, we utilized this artificial intelligence to check the academic language suitability in the project report that we wrote.

Contributors and Responsibilities in the Project

The project progressed collaboratively at every step. A dataset was obtained, exploratory data analysis was conducted, various models were built, and project reports were prepared together.

ETHICAL STATEMENT

While preparing the project, we did not take any action that could be considered as plagiarism.

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