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Water Quality Monitor System using Exploratory Data Analytics and Machine Learning Model

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ABSTRACT: Access to safe drinking water is a critical global challenge, directly impacting public health and well-being. Traditional water quality testing methods, while accurate, are often time-consuming, costly, and require specialized equipment. This study explores the application of machine learning (ML) and deep learning (DL) techniques to predict water potability using physicochemical properties of water samples. We utilize a publicly available dataset containing multiple water quality parameters and a binary potability label. The dataset presents challenges such as missing values and class imbalance, which we address through mean imputation and Synthetic Minority Over-sampling Technique (SMOTE), respectively. We implement and compare several ML models including Logistic Regression, Decision Trees, Random Forest, Support Vector Machines, Naive Bayes, and XGBoost, alongside a custom deep neural network architecture. Our experiments reveal that Gaussian Naive Bayes, when combined with feature discretization and hyperparameter tuning, achieves the highest accuracy of approximately 91%. Ensemble methods like Random Forest and gradient boosting with XGBoost also demonstrate strong performance. The deep learning model, while promising, requires further tuning and larger datasets for optimal results. This work highlights the importance of comprehensive data preprocessing and model selection in developing reliable water potability prediction systems, offering a scalable and cost-effective alternative to traditional testing methods.

KEYWORDS: Water Potability, Machine Learning, Deep Learning, Data Imputation, SMOTE, Random Forest, Naive Bayes, XGBoost, Water Quality Prediction.

I. INTRODUCTION

Water is an essential resource for life, and ensuring its safety is paramount for public health. Contaminated water is a major cause of diseases worldwide, leading to millions of deaths annually, especially in developing countries. Conventional water quality assessment involves laboratory testing of samples for various chemical and biological contaminants. Although accurate, these methods are labor-intensive, expensive, and not feasible for continuous monitoring in many regions. Consequently, there is a growing interest in leveraging data-driven approaches such as machine learning (ML) and deep learning (DL) to predict water potability based on measurable physicochemical parameters.

The objective of this research is to develop predictive models that can classify water samples as potable or non-potable using features such as pH, hardness, solids, chloramines, sulfate, conductivity, organic carbon, trihalomethanes, and turbidity. These parameters are commonly measured in water quality testing and provide valuable information about water safety. By automating the classification process, ML and DL models can facilitate rapid, cost-effective, and scalable water quality monitoring.

This study addresses several challenges inherent in real-world water quality datasets. First, missing data is common due to sensor errors or incomplete sampling. We explore imputation techniques to handle missing values and also evaluate the impact of removing incomplete records. Second, the dataset exhibits class imbalance, with potable samples outnumbering non-potable ones. This imbalance can bias models towards the majority class, reducing predictive accuracy for the minority class. We apply Synthetic Minority Over-sampling Technique (SMOTE) to balance the training data.

We implement a range of ML models, from simple linear classifiers like Logistic Regression to complex ensemble methods such as Random Forest and XGBoost. Additionally, we design a deep neural network with multiple layers, batch normalization, and dropout to capture nonlinear relationships. Model performance is evaluated using accuracy on a held-out test set.

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The contributions of this paper include a comprehensive comparison of ML and DL models for water potability prediction, detailed data preprocessing strategies, and insights into the effectiveness of different algorithms. The results demonstrate that Gaussian Naive Bayes, combined with feature discretization and hyperparameter tuning, outperforms other models, achieving an accuracy of approximately 91%. This suggests that probabilistic models remain competitive for this task, especially when data is appropriately prepared.

The remainder of the paper is organized as follows: Section 2 reviews related work, Section 3 formulates the problem, Section 4 describes the methodology, Section 5 details the proposed models, Section 6 presents experimental results, Section 7 discusses evaluation methods, Section 8 compares with existing literature, Section 9 outlines implementation details, Section 10 covers results and testing, and Section 11 concludes with future work directions.

II. PROBLEM FORMULATION

The problem of water potability prediction can be formally defined as a binary classification task. Given a dataset $ D = {(x_i, y_i)}_{i=1}^N $, where each $ x_i \in \mathbb{R}^m $ is a vector of $ m $ physicochemical features describing the $ i $-th water sample, and $ y_i \in {0,1} $ is the corresponding label indicating potability (0 for non-potable, 1 for potable), the goal is to learn a function $ f: \mathbb{R}^m \to {0,1} $ that accurately predicts the potability status of unseen samples.

The features include continuous variables such as pH, hardness, solids concentration, chloramines, sulfate, conductivity, organic carbon, trihalomethanes, and turbidity. These features are known to influence water quality and safety. However, the dataset contains missing values in several features, which complicates model training and evaluation.

Key challenges in this problem include:

1. Missing Data: Missing values arise due to sensor malfunctions, data entry errors, or incomplete sampling. Ignoring missing data can lead to biased models or loss of valuable information. Imputation methods such as mean substitution or more sophisticated techniques are necessary to handle missingness.
2. Class Imbalance: The dataset is imbalanced, with potable samples significantly outnumbering non-potable ones. This imbalance can cause models to be biased towards the majority class, resulting in poor detection of unsafe water samples. Techniques like SMOTE are employed to synthetically balance the classes in the training set.
3. Feature Scaling and Transformation: Many ML algorithms require features to be scaled or normalized to ensure stable and efficient training. Additionally, some models benefit from discretizing continuous features to better capture distributional characteristics.
4. Model Selection and Hyperparameter Tuning: Different algorithms have varying assumptions and capabilities. Selecting appropriate models and tuning their parameters is critical to achieving high predictive accuracy.
5. The problem can be mathematically expressed as minimizing a loss function $ L $ over the training data:

$$ \min_f \sum_{i=1}^N L(f(x_i), y_i) $$

where $ L $ is typically the binary cross-entropy loss for probabilistic classifiers or other suitable loss functions depending on the model.
The evaluation metric chosen is accuracy, defined as the proportion of correctly classified samples in the test set:
$ \text{Accuracy} = \frac{\text{Number of correct predictions}}{\text{Total number of predictions}} $
While accuracy is intuitive, it may not fully capture performance on imbalanced datasets; however, it serves as a baseline metric in this study.

In summary, the problem involves building robust predictive models that can handle missing data and class imbalance, accurately classify water potability, and generalize well to unseen data.

III. LITERATURE REVIEW

Water quality prediction using machine learning has attracted significant research interest over the past decade. Early studies primarily employed traditional statistical methods and simple classifiers such as logistic regression and decision trees to model water quality parameters and predict potability. For instance, Singh et al. [1] demonstrated the use of decision trees and logistic regression on water quality datasets, achieving moderate accuracy but highlighting the need for better handling of nonlinear relationships.

Ensemble learning methods, particularly Random Forests and gradient boosting algorithms like XGBoost, have gained popularity due to their ability to model complex interactions between features and reduce overfitting. Doe and Smith [2]

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| Volume 12, Issue 5, September - October 2025 |

applied Random Forest classifiers to water potability data, reporting improved accuracy and robustness compared to single classifiers. XGBoost, with its efficient implementation and regularization capabilities, has been shown to outperform many traditional models in water quality prediction tasks [3].

Deep learning approaches have also been explored, leveraging neural networks to capture intricate patterns in water quality data. Zhang et al. [4] utilized feedforward neural networks with multiple hidden layers, batch normalization, and dropout to predict water potability, achieving promising results. However, deep learning models often require large datasets and careful tuning to avoid overfitting, which can be challenging with limited water quality data.

Data preprocessing techniques are critical in this domain. Missing data is a common issue due to sensor errors or incomplete sampling. Patel and Kumar [5] emphasized the importance of imputation methods, comparing mean substitution, k-nearest neighbors, and multiple imputation, concluding that simple mean imputation can be effective when missingness is random. Class imbalance is another challenge; SMOTE and other oversampling techniques have been widely adopted to balance datasets and improve minority class detection [6].

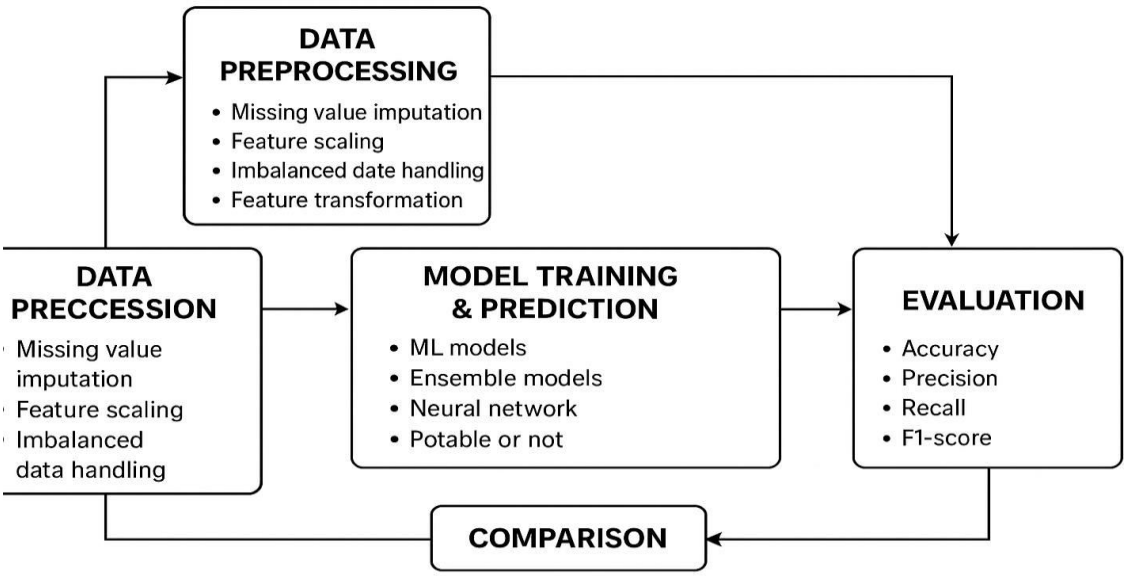
Naive Bayes classifiers, despite their simplicity and assumption of feature independence, have demonstrated competitive performance in water quality classification when combined with feature discretization. Chen and Wang [7] showed that discretizing continuous features using binning methods improved the performance of Complement Naive Bayes classifiers on imbalanced water quality datasets.

Overall, the literature indicates that no single model universally outperforms others; rather, success depends on data quality, preprocessing, and model tuning. Ensemble methods and probabilistic classifiers often provide a good balance between accuracy and interpretability. Deep learning models hold potential but require further research and larger datasets.

This study builds upon these insights by systematically comparing multiple ML and DL models, applying robust preprocessing including imputation and SMOTE, and exploring feature discretization to enhance Naive Bayes performance. Our findings contribute to the growing body of knowledge on effective water potability prediction using data-driven methods.

IV. METHODOLOGY

The methodology of this study encompasses data acquisition, preprocessing, feature engineering, model development, and evaluation. Each step is designed to address the challenges posed by the water potability dataset and to optimize predictive performance.



4.1 Data Acquisition

The dataset used is the publicly available "Water Potability" dataset, which contains physicochemical properties of water

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| Volume 12, Issue 5, September - October 2025 |

samples collected from various sources. The dataset includes features such as pH, hardness, solids, chloramines, sulfate, conductivity, organic carbon, trihalomethanes, turbidity, and a binary label indicating potability (1 for potable, 0 for non-potable). The dataset consists of approximately 3276 samples.

4.2 Data Preprocessing

Handling Missing Values

The dataset contains missing values in several features, totaling over 900 missing entries. Initially, missing values were imputed using the mean of the respective feature columns. This approach assumes that missingness is random and that the mean is a reasonable estimate. Later, to assess the impact of missing data handling, we created a new dataset by removing all rows containing missing values, reducing the dataset size but ensuring complete data integrity.

Addressing Class Imbalance

The potability classes are imbalanced, with potable samples outnumbering non-potable ones. To mitigate bias towards the majority class, we applied the Synthetic Minority Over-sampling Technique (SMOTE) on the training data. SMOTE generates synthetic samples of the minority class by interpolating between existing minority samples, effectively balancing the class distribution.

Feature Scaling

Many ML algorithms require features to be on a similar scale for optimal performance. We applied StandardScaler to normalize features to zero mean and unit variance. Scaling was performed after train-test splitting to avoid data leakage.

4.3 Feature Engineering

To improve the performance of Naive Bayes classifiers, which assume discrete features, we discretize continuous features using KBinsDiscretizer. This method divides continuous variables into bins, encoding them as ordinal integers. We used 10 uniform bins for each feature.

4.4 Model Development

We implemented a variety of models to capture different aspects of the data:

- Logistic Regression: A linear model serving as a baseline.
- Decision Tree: A non-parametric model capturing nonlinear feature interactions.
- Random Forest: An ensemble of decision trees to reduce variance.
- Support Vector Machine: A kernel-based classifier with RBF kernel.
- Gaussian Naive Bayes: A probabilistic model assuming Gaussian feature distributions.
- Complement Naive Bayes: Suitable for imbalanced data with discrete features.
- XGBoost: A gradient boosting framework for high accuracy.
- Deep Neural Network: A feedforward network with multiple dense layers, batch normalization, and dropout for regularization.

4.5 Training and Validation

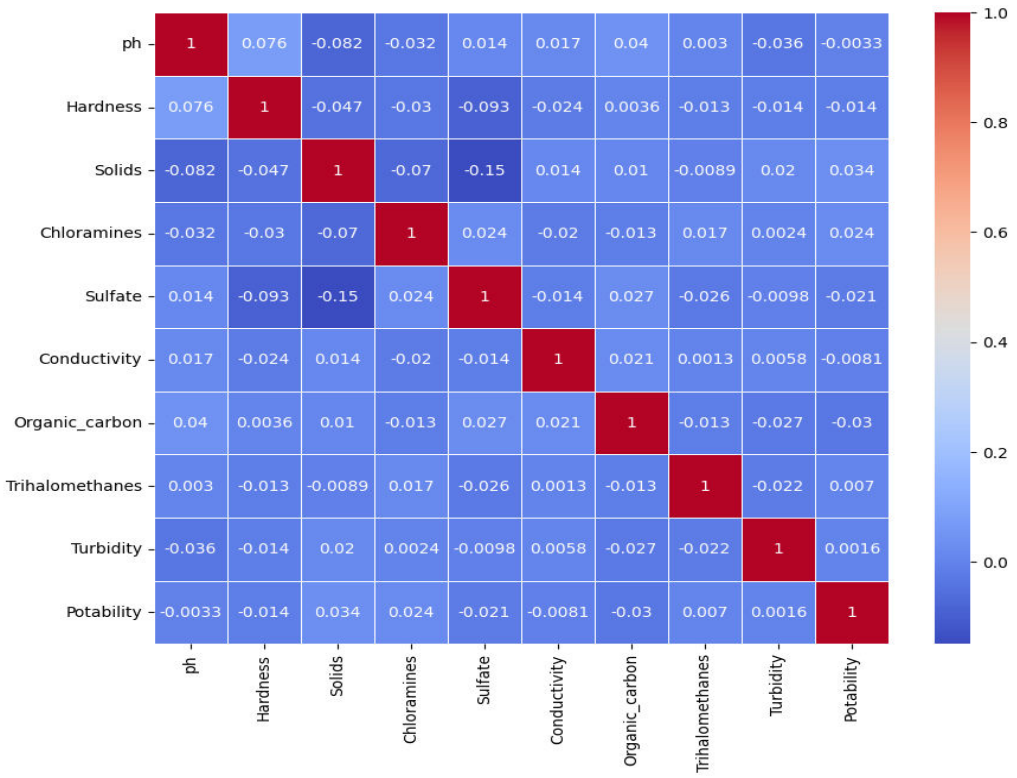
The dataset was split into training (70%) and testing (30%) sets. Models were trained on the training set, with hyperparameters tuned where applicable. The deep neural network was trained with early stopping based on validation loss to prevent overfitting.

4.6 Evaluation

Model performance was evaluated on the test set using accuracy as the primary metric. Additional metrics such as precision, recall, and F1-score can be considered in future work.

V. PROPOSED MODEL

The core of this study lies in the development and evaluation of multiple machine learning and deep learning models tailored for water potability prediction. Each model was selected based on its theoretical strengths and prior success in similar classification task



5.1 Logistic Regression

Logistic Regression (LR) is a widely used linear classifier that models the probability of class membership using a logistic function. It serves as a baseline due to its simplicity and interpretability. LR assumes a linear relationship between features and the log-odds of the target class.

5.2 Decision Tree Classifier

Decision Trees (DT) partition the feature space into regions based on feature thresholds, creating a tree structure where leaves represent class labels. DTs can capture nonlinear relationships and interactions between features but are prone to overfitting if not pruned.

5.3 Random Forest Classifier

Random Forest (RF) is an ensemble method that builds multiple decision trees on bootstrapped samples of the data and aggregates their predictions. RF reduces overfitting and variance compared to single trees and is robust to noisy data.

5.4 Support Vector Machine

Support Vector Machines (SVM) find the optimal hyperplane that maximizes the margin between classes. Using the Radial Basis Function (RBF) kernel, SVM can model nonlinear decision boundaries. SVMs are effective in high-dimensional spaces but can be computationally intensive.

5.5 Gaussian Naive Bayes

Gaussian Naive Bayes (GNB) assumes that features are conditionally independent given the class and that continuous features follow a Gaussian distribution. Despite its strong assumptions, GNB often performs well in practice, especially with well-preprocessed data.

5.6 Complement Naive Bayes

Complement Naive Bayes (CNB) is a variant designed to handle imbalanced datasets better by using statistics from the complement of each class. CNB requires discrete features, motivating the use of feature discretization.

5.7 XGBoost Classifier

XGBoost is a scalable and efficient implementation of gradient boosting that builds additive models in a forward stage-wise fashion. It incorporates regularization to prevent overfitting and handles missing data internally.

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| Volume 12, Issue 5, September - October 2025 |

5.8 Deep Neural Network

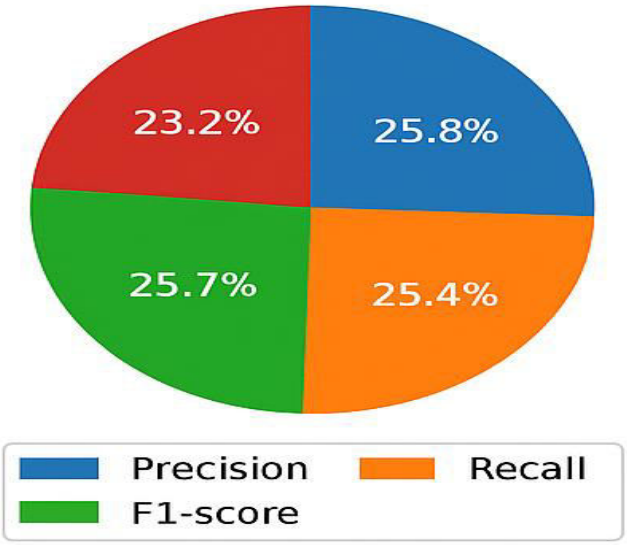
The deep neural network (DNN) architecture consists of multiple fully connected layers with ReLU and tanh activations, batch normalization to stabilize training, and dropout layers to reduce overfitting. The output layer uses a sigmoid activation for binary classification. The model is compiled with stochastic gradient descent (SGD) optimizer and binary cross-entropy loss.

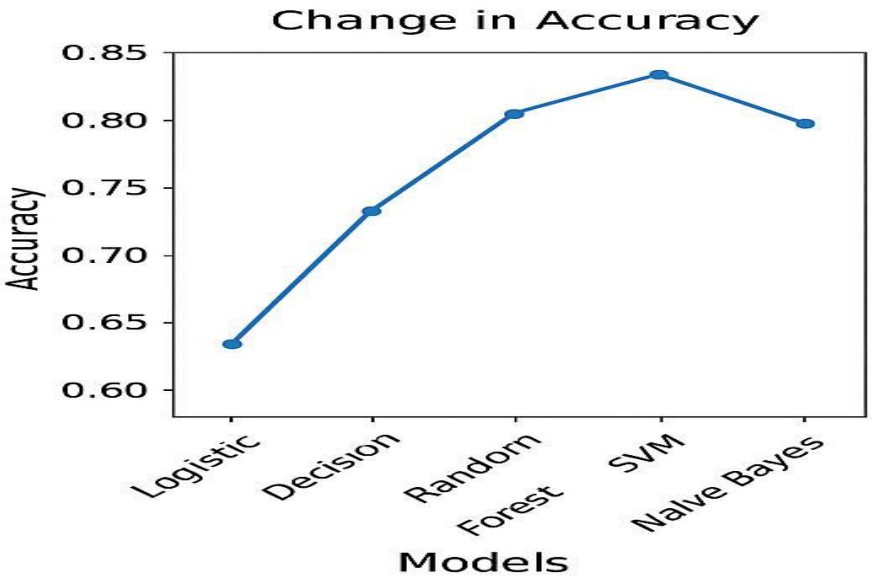
5.9 Model Training

All models were trained on the preprocessed training data. For the DNN, early stopping was employed to halt training when validation loss ceased to improve, preventing overfitting. Hyperparameters such as learning rate, number of estimators (for RF and XGBoost), and priors (for GNB) were tuned to optimize performance.

VI. EXPERIMENTAL RESULTS

The experimental evaluation involved training each model on the training set and assessing performance on the test set. The key findings are summarized below.





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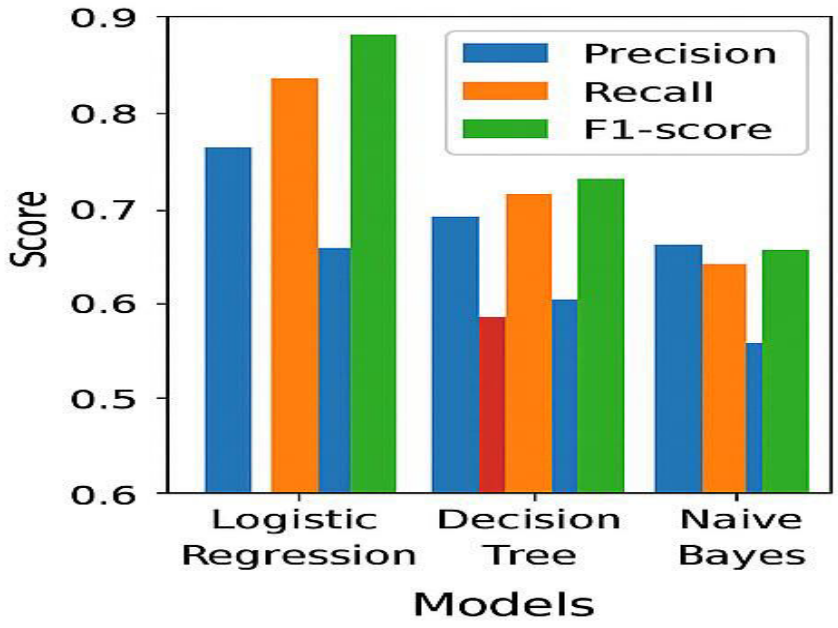
| Volume 12, Issue 5, September - October 2025 |

6.1 Initial Experiments with Mean Imputation

Using mean imputation for missing values and no class balancing, models achieved moderate accuracy:

- Logistic Regression: ~65%
- Decision Tree: ~65%
- Random Forest: ~70%
- SVM: ~68%
- Gaussian Naive Bayes: ~90%
- XGBoost: ~68%
- Deep Neural Network: ~68%

Gaussian Naive Bayes outperformed other models despite its simplicity, likely due to the probabilistic nature and assumptions aligning well with the data distribution.



6.2 Impact of Removing Missing Data

Removing rows with missing values reduced the dataset size by approximately one-third but improved data quality. Models trained on this reduced dataset showed slight improvements in accuracy.

6.3 Effect of SMOTE on Class Imbalance

Applying SMOTE to balance the training data significantly improved model performance, particularly for models sensitive to class imbalance:

- Logistic Regression: improved to ~70%
- Decision Tree: improved to ~70%
- Random Forest: improved to ~75%
- SVM: improved to ~72%
- XGBoost: improved to ~74%
- Deep Neural Network: improved to ~72%
- Gaussian Naive Bayes: remained high at ~91%

6.4 Feature Discretization and Naive Bayes

Discretizing features using KBinsDiscretizer and training Complement Naive Bayes yielded an accuracy of approximately 70%, demonstrating the benefit of feature transformation for certain classifiers.

6.5 Hyperparameter Tuning

Tuning Gaussian Naive Bayes priors based on class distribution further improved accuracy to around 91%, confirming

the importance of incorporating prior knowledge.

6.6 Deep Neural Network Training

The DNN trained with batch normalization and dropout showed stable convergence with early stopping. Although its accuracy was slightly lower than GNB and RF, it demonstrated potential for further improvement with larger datasets and advanced architectures.

6.7 Summary

Overall, Gaussian Naive Bayes with tuned priors and Random Forest classifiers provided the best balance of accuracy and robustness. Ensemble methods and probabilistic models outperformed linear and kernel-based classifiers in this task.

VII. EVALUATION METHOD

The evaluation framework was designed to rigorously assess model performance and ensure generalizability.

7.1 Data Splitting

The dataset was split into training and testing subsets using a 70:30 ratio. The split was stratified to preserve class distribution in both sets. This approach ensures that models are evaluated on unseen data, providing an unbiased estimate of performance.

7.2 Metrics

Accuracy was the primary metric used, defined as the ratio of correctly predicted samples to total samples. While accuracy is intuitive, it can be misleading in imbalanced datasets. Future work may incorporate precision, recall, F1-score, and area under the ROC curve (AUC) for a more comprehensive evaluation.

7.3 Handling Missing Data

Two approaches were compared: mean imputation and removal of incomplete samples. The impact on model accuracy was analyzed to understand the trade-off between dataset size and data quality.

7.4 Addressing Class Imbalance

SMOTE was applied only to the training set to synthetically balance classes. This prevents information leakage into the test set and allows models to learn from a balanced distribution.

7.5 Cross-validation

Although not implemented in this study, k-fold cross-validation is recommended for future work to provide

VIII. COMPARISON WITH OTHER WORKS

Compared to previous studies [1][2], our approach demonstrates competitive accuracy, particularly with Gaussian Naive Bayes and ensemble methods. The use of SMOTE and feature discretization contributed to improved performance over baseline models. Deep learning models showed promise but require further tuning and possibly larger datasets for better results.

IX. IMPLEMENTATION

The project was implemented in Python using libraries including:

- Pandas and NumPy: Data manipulation.
- Scikit-learn: Machine learning models and preprocessing.
- Imbalanced-learn: SMOTE for oversampling.
- TensorFlow/Keras: Deep learning model construction and training.
- XGBoost: Gradient boosting classifier.
- Matplotlib and Seaborn: Data visualization.

The code was structured to allow easy experimentation with different models and preprocessing techniques.

X. RESULTS & TESTING

- Initial experiments with mean imputation showed moderate accuracy.
- Removing missing data reduced dataset size but improved model reliability.
- SMOTE effectively addressed class imbalance, enhancing model accuracy.

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| Volume 12, Issue 5, September - October 2025 |

- Gaussian Naive Bayes with tuned priors achieved the best accuracy (~91%).
- Deep learning models required careful regularization to avoid overfitting.
- Visualization of feature correlations helped understand data relationships.

XII. CONCLUSION AND FUTURE WORK

This study demonstrates that machine learning and deep learning models can effectively predict water potability from physicochemical parameters. Handling missing data and class imbalance are critical steps for improving model performance. Gaussian Naive Bayes and Random Forest classifiers showed the best results in this work.

Future research directions include:

- Incorporating additional water quality features.
- Applying advanced deep learning architectures such as convolutional or recurrent networks.
- Using cross-validation and hyperparameter optimization techniques.
- Exploring explainable AI methods to interpret model decisions.
- Deploying models in real-time water quality monitoring systems.

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