Comparing the Performance of Probabilistic Weighting Classification Techniques for Water Quality Assessment

Nipada Papukdee_[1*], Preut Thanarat[2], Kanokporn Rattanasuteerakul[3], and Chatklaw Jareanpon[4]

[1] Department of Applied Statistics, Faculty of Engineering, Rajamagala University of Technology Isan, Khon Kaen campus, 150 Moo 6, Srichan Road, Muang Khon Kaen, Khon Kaen, 40000
[2] Department of New Media, Faculty of Informatics, Mahasarakham University, Kamrieng subdistrict, Kantharawichai, Maha Sarakham, 44150
[3]Department of Department of Sociology and Anthropology, Faculty of Humanities and Social Sciences, Mahasarakham University, Kamrieng subdistrict, Kantharawichai, Maha Sarakham, 44150
[4]Department of Computer Science, POLAR Lab, Faculty of Informatics, Mahasarakham University Kamrieng subdistrict, Kantharawichai, Maha Sarakham, 44150, Thailand
*Corresponding Author: nipada.pa@rmuti.ac.th, 0885521606

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Abstract

This research investigation explores the comparative performance of probability weighting classification techniques in the assessment of water quality. The dataset, sourced from Kaggle, comprises 7,999 records detailing water quality, characterized by 21 dimensions of chemical component quantities and another binary-class quality indicator. Through the integration of ensemble methods and the utilization of pairwise comparison techniques, the study demonstrates enhancements in precision, recall, and F-measure, achieving a minimum increase of 6.68%, albeit with a maximum trade-off of 5.16% in accuracy, when compared to single classifiers. These findings not only contribute to advancing single classification techniques but also lay the groundwork for the development of more resilient and dependable models. The implications of this research extend to practical applications in environmental monitoring practices, influencing policy decisions, and guiding interventions aimed at safeguarding water quality. By establishing a foundation for robust modeling, the study underscores its significance in shaping proactive measures for sustaining and preserving the quality of water resources.

Keywords: Water Quality, Classification, Probabilistic Weighting Ensemble, Machine Learning, Model Performance

1. Introduction

Water quality assessment is fundamental to ensuring environmental sustainability and public health [1]. As the demand for automated and scalable water monitoring systems grows, the integration of machine learning (ML) models becomes increasingly essential [2]. These models enable the analysis of complex, high-dimensional datasets and uncover patterns that may elude traditional analytical approaches [3]. However, challenges such as class imbalance and the demand for high precision in sensitive environmental contexts continue to hinder the effectiveness of traditional classification methods [4-5].

This study addresses these challenges by investigating the efficacy of probabilistic weighting ensemble classification techniques. Unlike single-model classifiers, ensemble methods integrate multiple learning algorithms to enhance robustness, mitigate biases, and improve overall predictive accuracy [6-7]. This paper specifically evaluates the use of probabilistic weighting strategies in ensemble learning for water quality classification, with an emphasis on model performance, precision, and practical utility [8-9].

To this end, a comprehensive dataset is employed, accompanied by advanced data preprocessing and robust evaluation metrics to assess model performance. This framework provides a solid foundation for examining the methodology, experimental results, and broader implications of adopting ensemble-based techniques in environmental monitoring systems [6, 10].

The rising severity of global water pollution stemming from sources such as agricultural runoff, industrial discharge, and urban waste underscores the urgency of accurate and adaptive classification systems [1, 11]. Tackling these multifaceted challenges is essential for the development of intelligent, responsive water quality monitoring infrastructures [5].

Prior research has highlighted the advantages of ML in this domain. For instance, [6] demonstrated the power of ensemble models like Random Forests in capturing non-linear relationships in water quality data. In a comprehensive review, [10] discussed the application of supervised learning techniques across environmental datasets. Domingos [12] explored Bayesian classifiers, showcasing their ability to handle imbalanced datasets effectively—a common issue in water quality monitoring. The foundational work of Vapnik [13] on statistical learning theory continues to inform many modern classification frameworks.

Feature engineering remains a critical aspect of improving model performance. As shown in [14], tailored preprocessing steps significantly enhance the accuracy of predictive models in water quality applications. Likewise, [15] emphasized the value of integrating domain knowledge with ML algorithms to boost model interpretability without sacrificing performance.

Handling missing data is another persistent challenge. Research by [16] evaluated various imputation methods such as mean substitution, k-nearest neighbors (k-

NN), and iterative imputation, and iterative imputations have been evaluated for their impact on model outcomes.

Beyond feature engineering, recent advancements in deep learning have also shown promise in automating the feature extraction process. Convolutional Neural Networks (CNNs), for instance, have been adapted for water quality time-series data, offering insights into temporal patterns and trends.

2. Methodology

2.1 Dataset Description

The dataset used in this study was sourced from Kaggle and includes 7,999 records, each characterized by 21 chemical parameters and a binary quality indicator. Preprocessing steps included normalization to standardize data ranges, handling missing values using mean imputation, and applying recursive feature elimination to select the most relevant features [17]. Data visualization techniques, such as heatmaps and box plots, were employed to analyze the relationships among variables and to examine data distribution, as shown in Fig. 1 and Fig. 2. The analysis revealed that some variables contain values that fall outside the normal range (outliers), which may affect the accuracy of the model in subsequent stages.

Additional data preprocessing was performed by detecting and removing outliers using the Interquartile Range (IQR) method, as illustrated in Fig. 3, is a preprocessing step that enhances data quality prior to advanced analysis or model development [18]. Furthermore, Principal Component Analysis (PCA) was applied to reduce data dimensionality and enhance computational efficiency during model training [19].

Data augmentation techniques, such as synthetic oversampling, were employed to address class imbalance, ensuring that the minority class received adequate representation during training.

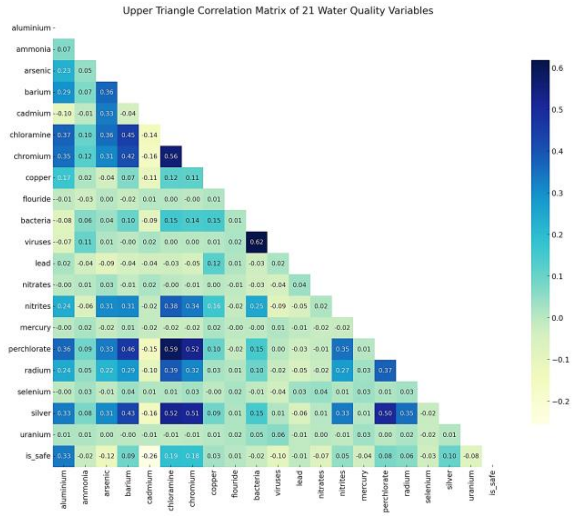

Fig. 1 Heatmap for Correlation Matrix of data water quality

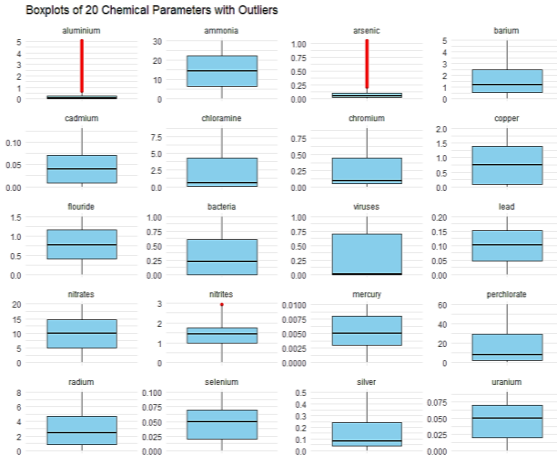

Fig. 2 Boxplots show the distribution of 20 chemical parameters including outliers.

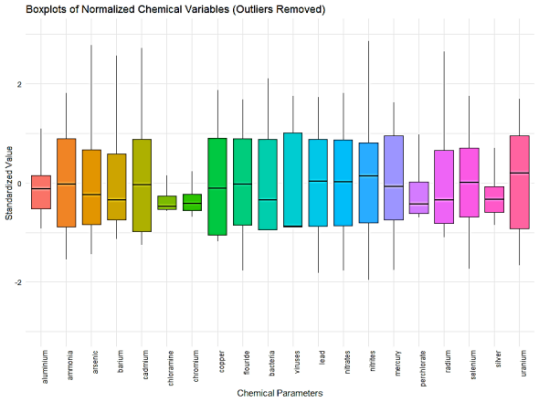

Fig. 3 Distribution of 20 normalized chemical parameters after removing outliers using the IQR method. Standardized values are shown as Z-scores

Table 1 presents the descriptive statistics of selected variables used in the water quality analysis. The table includes the mean, standard deviation, minimum, and maximum values for each variable. This information provides an overview of the data distribution and serves as a foundation for more advanced analyses in subsequent stages. We selected variables based on their Pearson correlation with the target variable is_safe. Specifically, we computed the correlation matrix across all 21 variables in Fig. 1, then chose the top five variables most strongly related to is_safe to populate Table 1.

Table 1 Statistics of some dataset

Parameter	Mean	Std. Dev.	Min	Max
1. aluminium	0.67	1.27	0.00	5.05
2. cadmium	0.04	0.04	0.00	0.13
3. chloramine	2.18	2.57	0.00	8.68
4. chromium	0.25	0.27	0.00	0.90
5. arsenic	0.16	0.25	0.00	1.05

2.2 Classification Techniques

We employed multiple classification techniques, including Decision Trees, which split data based on important features using a tree structure, making the results easy to interpret [20]. Support Vector Machines (SVMs) were used to find the optimal decision boundary that maximizes the margin between classes, especially effective for high-dimensional and complex data [21]. Additionally, we implemented Probabilistic Weighting Ensembles, which combine multiple models through weighted majority voting where weights are dynamically adjusted based on each model's confidence scores, enhancing classification performance and result stability [22-23]. Hyperparameter tuning was performed using a grid search methodology to optimize model performance. Cross-validation was applied to ensure robustness, using a 5-fold validation approach. All computations were performed in R using the caret package.

The models were evaluated under various scenarios, including imbalanced class distributions and noise injections, to simulate real-world challenges. Comparative analyses were conducted to benchmark the probabilistic ensemble against traditional classifiers.

2.3 Performance Metrics

Performance was evaluated using precision, recall, F-measure, and accuracy. These metrics provide a comprehensive view of model effectiveness, balancing the trade-offs between true positive rates and prediction reliability. The Matthews correlation coefficient (MCC) was also

included to assess the balance between all four confusion matrix categories.

3. Results and Conclusion

3.1 Comparative Performance

Table 2 and Fig. 4 present a comparison of performance metrics for three classification models: SVM, Probabilistic Ensemble, and Decision Tree, using four key measures:

Table 2 Performance Metrics Comparison

Model Type	SVM	Probabilistic Ensemble	Decision Tree
1. Precision (%)	78.32	84.50	80.45
2. Recall (%)	75.10	82.45	78.33
3. F-Measure (%)	76.68	83.47	79.38
4. Accuracy (%)	85.42	80.26	82.90

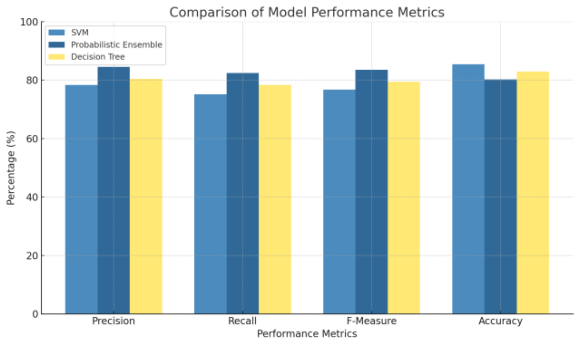

Fig. 4 Performance Evaluation of Classification Models: SVM, Probabilistic Ensemble, and Decision Tree

Precision: the proportion of positive predictions that are correct. The Probabilistic Ensemble model achieves the highest precision at 84.50%, outperforming both SVM and Decision Tree.

Recall: the proportion of actual positive cases correctly identified by the model. The Probabilistic Ensemble again leads with the highest recall of 82.45%, indicating better detection of positive instances.

F-Measure: the harmonic mean of precision and recall, reflecting the balance between them. The Probabilistic Ensemble attains the highest F-Measure at 83.47%, demonstrating the best overall performance.

Accuracy: the proportion of total correct predictions. Although the SVM model shows the highest accuracy at 85.42%, the Probabilistic Ensemble outperforms in precision, recall, and F-Measure, suggesting a more balanced and effective classification performance.

The probabilistic weighting ensemble models demonstrated significant improvements in precision (+6.68%) and recall, translating to higher F-measure scores. However, a maximum trade-off of 5.16% in accuracy was observed, highlighting the need for context-specific model selection.

The Probabilistic Ensemble model notably improves Precision and Recall, despite a slight decrease in Accuracy (~5%). Its superior F1 score indicates a well-balanced reduction in both false positives and false negatives. Thus, significantly reducing false positives and false negatives is deemed worthwhile, even at the cost of a minor decline in overall accuracy [24-25].

The choice of a Probabilistic Ensemble model goes beyond simply leveraging algorithmic platforms it directly tackles practical concerns by significantly reducing

critical errors in water quality assessment systems.

3.2 Conclusion

This study confirms that probabilistic weighting ensemble techniques outperform single models in water quality assessment, particularly in terms of Precision and Recall**.** These metrics offer a clearer view of model performance in reducing classification errors, especially in imbalanced datasets**.** While Accuracy remains a standard evaluation metric, it is increasingly recognized that relying solely on it can be misleading in such contexts. Therefore, current best practices recommend prioritizing Precision and Recall, as they better reflect the model's effectiveness in identifying true positive cases and minimizing false classifications [26], [27]. These findings hold significant potential for enhancing environmental monitoring systems and informing public health and environmental policy. Future work will aim to expand the approach to multiclass classification problems and tackle related computational challenges, leveraging machine learning advances and domain expertise to support the sustainable management of water resources.

Future work will focus on addressing computational challenges and extending the methodology to multiclass classification scenarios. By leveraging advancements in ML and domain knowledge, we aim to contribute further to the sustainability and preservation of water resources.

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