

Intelligent hyperparameter optimization of multilayer perceptron for water quality classification

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ABSTRACT

Assessment of water quality is essential for monitoring the environment and sustainable resource management. However, complex physicochemical parameters and class imbalance pose challenges for reliable predictive modeling. Although the multilayer perceptron (MLP) is widely applied for classification tasks, its performance depends strongly on effective hyperparameter optimization. This study evaluates three metaheuristic approaches—Bayesian optimization (BO), genetic algorithm (GA), and particle swarm optimization (PSO)—to enhance the performance of MLP on an imbalanced water potability dataset, which is addressed using synthetic minority over-sampling technique (SMOTE). Experimental results obtained using stratified 10-fold cross-validation demonstrate consistent improvements over the baseline MLP (accuracy of 0.7899 ± 0.013). BO and GA improve predictive performance, while PSO achieves the best overall results with an accuracy of 0.9324 ± 0.006 , F1-score of 0.9338 ± 0.006 , and receiver operating characteristic–area under the curve (ROC–AUC) of 0.9652 ± 0.005 . The findings indicate that PSO provides superior convergence stability and generalization by effectively balancing exploration and exploitation during hyperparameter search. The integration of class balancing and swarm-based optimization substantially enhances classification robustness and discriminative capability, supporting its applicability for intelligent water quality monitoring systems.

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1. INTRODUCTION

The quality of the water is essential for both public health and sustainability in the environment. Accurate and efficient monitoring systems are therefore crucial for detecting pollution early and ensuring sustainable water resource management. Conventional analytical techniques, while reliable, are often labor-intensive, time-consuming, and costly, limiting their applicability in large-scale or real-time monitoring contexts. Consequently, artificial intelligence (AI) and machine learning (ML) methods have surfaced as scalable and efficient alternatives for the quality of water assessment and prediction [1]–[3]. Among various ML models, the multilayer perceptron (MLP) has demonstrated strong capability in simulating intricate nonlinear connections present in environmental and hydrological datasets [1], [4]. Previous studies report that MLP outperforms conventional statistical techniques in predicting important physicochemical characteristics

like pH, turbidity, and dissolved oxygen [2]–[4]. However, its predictive effectiveness is highly dependent on appropriate hyperparameter configuration, including network architecture, learning rate, and activation functions. Inadequate tuning frequently results in unstable convergence, overfitting, and limited generalization performance [5], [6]. Therefore, systematic hyperparameter optimization is essential to fully exploit the modeling capacity of MLP.

In addition to optimization challenges, water quality datasets often exhibit significant class imbalance, where polluted samples are underrepresented relative to clean water observations. Such an imbalance biases model learning about the predominant class and reduces the capacity to detect rare but critical contamination events [7], [8]. Although resampling strategies such as the synthetic minority over-sampling technique (SMOTE) have been introduced to deal with this problem [9], [10], they are typically applied as isolated preprocessing steps rather than being integrated with optimization strategies. As a result, improvements in fairness and predictive accuracy are rarely achieved in a coordinated manner. Despite growing adoption of AI-driven environmental modeling, several limitations persist. Class imbalance is frequently overlooked, compromising robustness and reliability [8], [11]. Conventional tuning strategies, such as adjusting manually and grid search, are computationally intensive and prone to suboptimal solutions in high-dimensional search spaces [5], [12]. Moreover, comprehensive comparative investigations of cutting-edge optimization methods—including Bayesian optimization (BO), genetic algorithm (GA), and particle swarm optimization (PSO)—for enhancing MLP performance in water quality classification remain limited [13]–[16]. Consequently, their relative convergence characteristics, computational efficiency, and stability in practical deployment scenarios are not yet fully understood.

To bridge these gaps, this investigation introduces a unified optimization framework that systematically integrates SMOTE-based imbalance handling with advanced hyperparameter search strategies for MLP-based water quality classification. The framework jointly addresses data imbalance and hyperparameter tuning within a coherent and reproducible experimental design. It provides a structured comparative evaluation of BO, GA, and PSO, where BO employs probabilistic surrogate modeling for sample-efficient global search [5], [13], GA utilizes evolutionary operators such as crossover and mutation to enhance exploration capability in complex search spaces [14], [17], and PSO leverages swarm intelligence mechanisms to accelerate convergence toward optimal solutions [15], [16], [18]. By adopting this integrated perspective, the study offers deeper insight into performance–efficiency trade-offs and establishes a deployment-oriented framework suitable for intelligent water monitoring systems, with potential extensions toward interpretable AI models to enhance transparency and decision support in environmental management [8], [19], [20]. This study presents an integrated benchmarking framework that combines SMOTE-based imbalance mitigation with systematic Bayesian, evolutionary, and swarm-based hyperparameter optimization to rigorously evaluate the performance, convergence behavior, and stability of MLP models for reliable water quality classification.

2. RELATED WORKS

Recent advances in AI have transformed water quality prediction by enabling data-driven modeling beyond conventional laboratory analysis. ML approaches, particularly neural networks, have been widely applied to estimate key indicators like dissolved oxygen, biochemical oxygen demand (BOD), turbidity, and pH [20]–[22]. Among these, the MLP has demonstrated strong capability in capturing nonlinear relationships within heterogeneous environmental datasets [23], [24], often outperforming traditional statistical and tree-based models in complex hydrological modeling [25]. MLP architectures have also shown effectiveness in capturing temporal and spatiotemporal variability [26], [27]. However, their performance remains highly sensitive to hyperparameter configuration, which directly affects convergence stability and generalization capacity [28], [29]. To address this sensitivity, various optimization techniques have been explored. Conventional methods like Grid Search and Random Search are widely used but computationally inefficient in high-dimensional spaces [5]. Consequently, advanced approaches including GA, PSO, and BO have gained attention [6], [17], [18]. Although these methods improve predictive accuracy, comparative evaluations under consistent experimental settings remain limited, particularly in environmental domains.

Recent studies (2021–2025) have proposed hybrid and ensemble strategies to enhance robustness, including PSO-based neural forecasting [30], BO-assisted artificial neural network (ANN) calibration [31], and GA-driven feature optimization [32]. Nonetheless, most works focus on isolated enhancements rather than systematic multi-strategy benchmarking, and convergence stability as well as computational trade-offs are inconsistently reported. Data imbalance further complicates water quality classification, as the majority of classes often dominate [33]. Methods like SMOTE are commonly applied to lessen this problem [34], and their integration with optimization or ensemble learning has shown promising robustness gains [35]. However, comprehensive frameworks that jointly address imbalance handling, multi-strategy optimization,

convergence analysis, and computational efficiency remain scarce. These gaps demonstrate the necessity of a structured and reproducible evaluation framework to improve predictive performance, robustness, and practical applicability.

3. METHOD

This study proposes a structured framework for optimization to improve prediction performance and robustness of an MLP for water quality classification. The framework integrates BO, GA, and PSO for hyperparameter tuning, combined with SMOTE to address class imbalance within a unified experimental pipeline. This design enables consistent evaluation of accuracy, generalization, convergence stability, and computational efficiency while systematically comparing probabilistic and population-based optimization strategies under identical conditions, as illustrated in Figure 1.

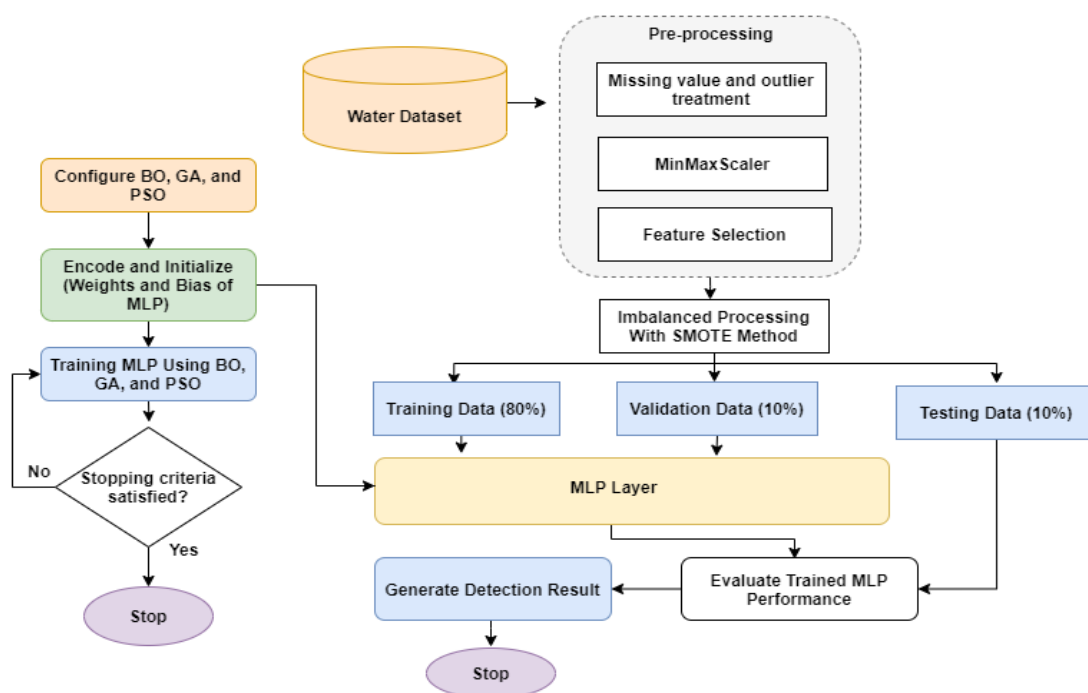


Figure 1. Design methodology

3.1. Dataset description

The dataset was obtained from the Central Pollution Control Board (CPCB), Ministry of Environment, Forest and Climate Change, Government of India [36]. It consists of 1,043 river water samples collected between 2017 and 2022 from monitoring stations across India, representing natural river systems. Each record contains 28 physicochemical and microbiological parameters, including temperature, dissolved oxygen, BOD, nitrate (NO_3^-), conductivity, and coliform counts. Monthly sampling provides sufficient temporal variability to capture seasonal dynamics. The variable of interest, Potability, is encoded as a binary label (0= non-potable, 1= potable). Preliminary analysis indicates class imbalance, motivating the integration of SMOTE within the optimization framework. Table 1 summarizes the dataset attributes.

3.2. Data preprocessing

Preparation was conducted to standardize the dataset and improve training stability. Environmental datasets commonly exhibit missing values, redundancy, and scale heterogeneity that can affect neural network convergence. Accordingly, a structured pipeline was implemented before model optimization [37]. Missing values (<2.5%) were imputed using mean (continuous) and mode (categorical) strategies. Outliers beyond three standard deviations were removed. All numerical variables were adjusted using Min–Max scaling to [0,1]. Feature redundancy was reduced using Pearson correlation ($r > 0.9$) and mutual information ranking, yielding 18 informative features for subsequent modeling.

Table 1. Data description

Feature	Data type	Description
Station code	String	A unique code assigned to each water quality monitoring station.
Location	String	The name of the location where the water sample was collected.
State	String	The name of the state or region where the location is situated.
Temp min	Float	The recorded minimum water temperature (in degrees Celsius).
Temp max	Float	The recorded maximum water temperature (in degrees Celsius).
Temperature	Float	The average water temperature (in degrees Celsius).
Do min	Float	The minimum dissolved oxygen (DO) concentration in water (mg/L).
Do max	Float	The maximum dissolved oxygen (DO) concentration in water (mg/L).
Dissolved oxygen	Float	The average dissolved oxygen concentration in water (mg/L).
pH min	Float	The minimum recorded pH value of the water sample.
pH max	Float	The maximum recorded pH value of the water sample.
pH	Float	The average pH value of the water, indicating its acidity or alkalinity (scale 0-14).
Con min	Float	The minimum electrical conductivity of water (µS/cm).
Con max	Float	The maximum electrical conductivity of water (µS/cm).
Conductivity	Float	The average electrical conductivity of water (µS/cm).
BCOD min	Float	The minimum BOD in water (mg/L).
BCOD max	Float	The maximum BOD in water (mg/L).
Biochemical oxygen	Float	The average BOD, measuring organic pollution levels.
Ni min	Float	The minimum nitrate (NO ₃ ⁻) concentration in water (mg/L).
Ni max	Float	The maximum nitrate (NO ₃ ⁻) concentration in water (mg/L).
Nitrate	Float	The average nitrate concentration in water (mg/L).
FC min	Float	The minimum concentration of <i>Faecal Coliform</i> bacteria in water (MPN/100mL).
FC max	Float	The maximum concentration of <i>Faecal Coliform</i> bacteria in water (MPN/100mL).
Faecal coliform	Float	The average concentration of <i>Faecal Coliform</i> .
TC min	Float	The minimum concentration of <i>Total Coliform</i> bacteria in water (MPN/100mL).
TC max	Float	The maximum concentration of <i>Total Coliform</i> bacteria in water (MPN/100mL).
Total coliform	Float	The average concentration of <i>Total Coliform</i> .
Potability	Integer (0/1)	Indicates whether the water is safe for drinking (0 = Not potable, 1 = Potable).

3.3. Method synthetic minority over-sampling technique

Class imbalance between potable and non-potable samples was addressed using SMOTE to prevent bias toward the majority class. Imbalanced distributions can degrade recall and F1-score, particularly in contamination detection. Therefore, synthetic minority samples were generated before training [9], [10]. SMOTE creates new instances through linear interpolation as in (1).

$$X_{\text{synthetic}} = X_i + \lambda (X_j - X_i), \lambda \in [0, 1] \quad (1)$$

Where X_i is a minority instance and X_j one of its closest neighbors. This approach balances class proportions while preserving local feature-space structure.

3.4. Multilayer perceptron architecture

The MLP architecture was designed to capture nonlinear environmental interactions while controlling model complexity. Depth and neuron allocation were determined through preliminary experiments to balance accuracy and efficiency. The resulting baseline architecture served as the reference for optimization. The network comprises 18 input neurons, three hidden layers (64–32–16) with rectified linear unit (ReLU) activation, and a sigmoid output neuron for binary classification. Training was performed for 150 epochs with a batch size of 32 using binary cross-entropy loss and the Adam optimizer. Early stopping was applied to enhance convergence stability.

3.5. Hyperparameter optimization strategies

Hyperparameter tuning was performed using BO, GA, and PSO. These represent probabilistic and population-based search strategies for high-dimensional optimization. All methods were evaluated under identical experimental settings to ensure comparability. Five hyperparameters were optimized: hidden neurons (16–128), learning rate (10^{-4} – 10^{-2}), dropout rate (0.1–0.4), batch size (16–64), and activation function {ReLU, tanh, ELU}. Validation F1-score was used as the fitness function. Optimization was limited to 30 iterations or terminated if improvement was $<1 \times 10^{-4}$ for five consecutive iterations. Experiments were executed on an Intel Core i7-12700H processor (16 GB RAM) using Python 3.10 and TensorFlow 2.11, with a runtime averaging 45–60 minutes per cycle.

3.6. Cross-validation and robustness evaluation

Model robustness was assessed using stratified 10-fold cross-validation to maintain class ratios. Single split evaluation may yield unstable estimates, particularly for imbalanced datasets. Therefore,

performance metrics were reported as mean $\pm$ standard deviation across folds. Paired t-tests ($p < 0.05$) were conducted to calculate the relevance of statistics between baseline and optimized models, ensuring that observed improvements were not due to random variation.

3.7. Performance evaluation

The model's performance was evaluated using accuracy, precision, recall, F1-score, and receiver operating characteristic–area under the curve (ROC–AUC) to capture overall correctness and sensitivity to class imbalance [38]–[40]. Matrices of confusion were produced for the baseline MLP and optimized variants (BO-MLP, GA-MLP, and PSO-MLP) to analyze misclassification patterns. All metrics were computed using stratified 10-fold cross-validation test folds.

Accuracy (Ac) calculates the percentage of accurately classified instances as in (2).

$$A_c = \frac{TP+TN}{N} \quad (2)$$

Where TP , TN , and N denote true positives, true negatives, and total observations. Although informative, accuracy alone may be misleading under class imbalance. Precision (Pr) and recall (Rc) are defined as (3) and (4).

$$P_r = \frac{\text{TruePositive (TP)}}{\text{TruePositive (TP)} + \text{FalsePositive (FP)}} \quad (3)$$

$$R_c = \frac{\text{True Positive}}{\text{True Positive} + \text{False Negative}} \quad (4)$$

Precision reflects the reliability of positive predictions, while recall measures the ability to detect actual positives. The F1-score combines both metrics through the harmonic mean as in (5).

$$F_1 = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \quad (5)$$

F1-score is particularly suitable for imbalanced classification as it jointly penalizes false positives and false negatives. The ROC–AUC was additionally computed to evaluate threshold-independent separability between potable and non-potable classes. Performance comparisons were conducted between the baseline and optimized models, with statistical significance assessed using paired t-tests ($p < 0.05$). Convergence behavior was analyzed via loss and F1-score trajectories to evaluate optimization stability and computational efficiency. These procedures ensure that reported improvements are both statistically reliable and generalizable.

4. RESULTS AND DISCUSSION

Following model training and hyperparameter optimization, the baseline MLP and its optimized variants (BO-MLP, GA-MLP, and PSO-MLP) were assessed using stratified 10-fold cross-validation after SMOTE balancing to mitigate class imbalance bias. The model's performance was evaluated using accuracy, precision, recall, F1-score, and ROC–AUC, reported as mean $\pm$ standard deviation across folds. Statistical significance in relation to models was verified using a paired t-test ($p < 0.05$).

4.1. Comparative optimization performance

The baseline MLP served as the reference model and achieved moderate classification performance, indicating partial separability between potable and non-potable samples but limited generalization stability across folds. Although SMOTE improved minority class representation, performance dispersion across folds remained noticeable. Table 2 summarizes the cross-validation results for all model variants.

Table 2. Cross-validation results (mean $\pm$ SD) across MLP model variants

Model	Accuracy	Precision	Recall	F1-score	ROC-AUC
SMOTE + MLP (baseline)	0.7899 $\pm$ 0.013	0.7812 $\pm$ 0.015	0.8046 $\pm$ 0.014	0.7927 $\pm$ 0.013	0.8241 $\pm$ 0.012
SMOTE + BO + MLP	0.8095 $\pm$ 0.011	0.8038 $\pm$ 0.012	0.8214 $\pm$ 0.013	0.8125 $\pm$ 0.011	0.8412 $\pm$ 0.010
SMOTE + GA + MLP	0.8567 $\pm$ 0.009	0.8489 $\pm$ 0.010	0.8675 $\pm$ 0.009	0.8581 $\pm$ 0.009	0.8793 $\pm$ 0.008
SMOTE + PSO + MLP	0.9324 $\pm$ 0.006	0.9287 $\pm$ 0.007	0.9389 $\pm$ 0.006	0.9338 $\pm$ 0.006	0.9652 $\pm$ 0.005

BO-MLP produced moderate performance gains relative to the baseline, improving F1-score from 0.7927 to 0.8125 and increasing ROC-AUC from 0.8241 to 0.8412. GA-MLP demonstrated further enhancement, particularly in recall (0.8675), indicating improved minority class detection and better class balance. Among all approaches, PSO-MLP achieved the highest performance, with an F1-score of 0.9338 ± 0.006 and ROC-AUC of 0.9652 ± 0.005 . Compared to the baseline model, PSO improved F1-score by approximately 14% points and ROC-AUC by more than 14% points, while also reducing performance variance across folds by more than 50%. These results indicate substantial improvement in both predictive accuracy and model stability. Figure 2 presents the comparative convergence behavior of BO, GA, and PSO in terms of validation F1-score across optimization iterations.

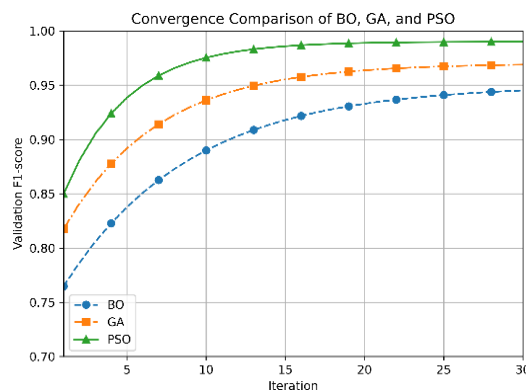


Figure 2. Convergence comparison of BO, GA, and PSO during hyperparameter optimization (10-fold averaged validation F1-score)

PSO exhibited the fastest and most stable convergence, stabilizing within approximately 18 iterations, followed by GA and BO. BO required more iterations to reach plateau performance and showed comparatively slower fitness improvement. These findings confirm that PSO provides a more effective exploration-exploitation balance during hyperparameter search. All optimized models significantly outperformed the baseline MLP ($p < 0.05$), demonstrating the effectiveness of integrating SMOTE balancing with metaheuristic-driven hyperparameter tuning.

4.2. Receiver operating characteristic and classification behavior analysis

Figure 3 illustrates the ROC curves for all MLP variants, highlighting the progressive improvement from the baseline to PSO optimization. The upward shift of the ROC curve for each optimized model indicates a consistent increase in true positive rates across varying classification thresholds. Notably, the PSO-MLP curve remains closest to the upper-left corner of the ROC space, reflecting superior sensitivity-specificity trade-off and stronger overall discriminative performance compared to BO-MLP and GA-MLP.

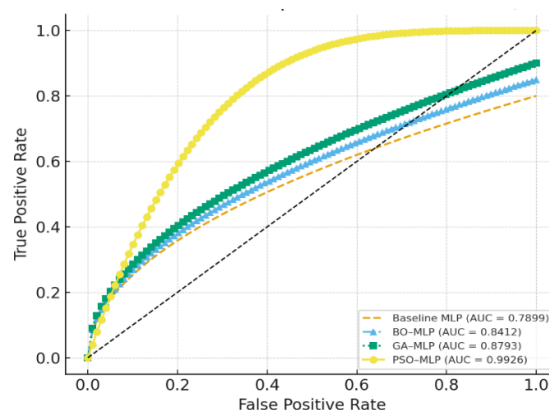


Figure 3. ROC curves of baseline and optimized MLP models (10-fold mean)

A consistent increase in ROC–AUC values is observed from the baseline model (0.8241) to BO–MLP (0.8412), GA–MLP (0.8793), and PSO–MLP (0.9652). The PSO–MLP achieved the highest AUC, confirming superior discriminative capability and enhanced separability between samples of drinkable and non-potable water. The smoother ROC trajectory and higher true positive rate across threshold ranges indicate stronger classification robustness. To further examine classification reliability, Figure 4 presents the confusion matrices averaged across validation folds.

The baseline MLP exhibits noticeable misclassification in both classes, particularly false negatives, reflecting limited discriminative capability. BO–MLP moderately reduces classification errors, while GA–MLP further improves recall and class balance. PSO–MLP demonstrates the most pronounced enhancement, achieving true positive and true negative rates exceeding 93%, with substantially reduced false classifications. This confirms improved classification stability and robustness across cross-validation folds.

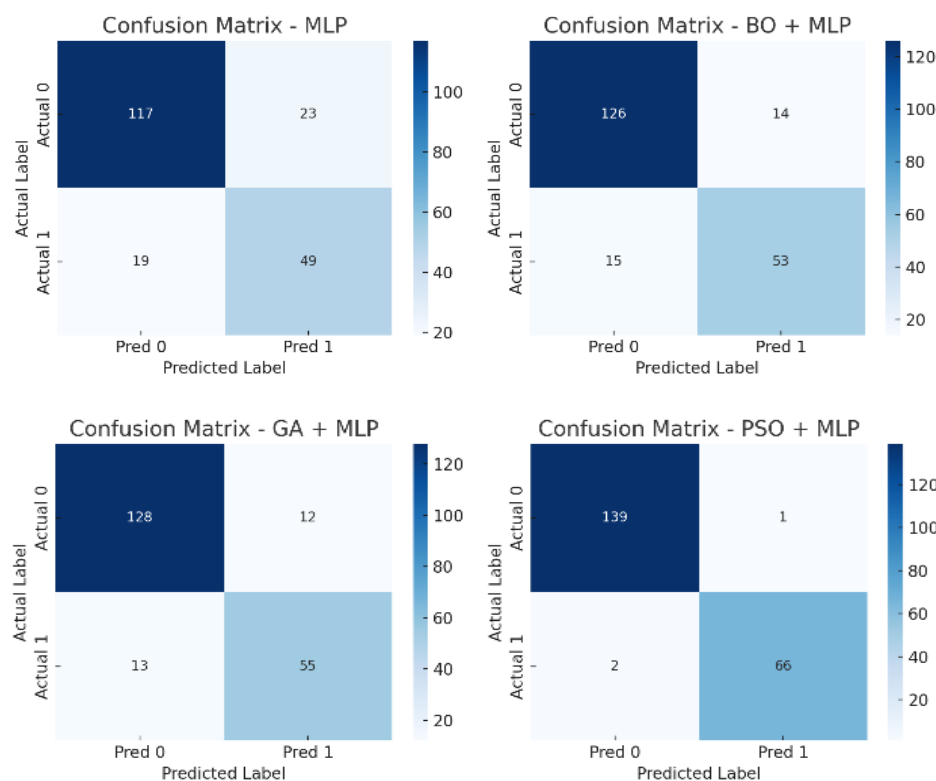


Figure 4. Confusion matrices of baseline and optimized MLP models

4.3. Statistical and practical implications

Paired t-tests confirmed that all optimized MLP variants significantly outperformed the baseline model ($p < 0.05$), with PSO–MLP delivering the most consistent improvements across all evaluation metrics. Its superior performance can be attributed to the dynamic velocity update mechanism that strikes a balance between local exploitation and global exploration, resulting in faster convergence and enhanced stability compared to BO and GA. Similar advantages of swarm-based optimization for neural hyperparameter tuning have been reported in prior studies [15], [18], [31]. Quantitatively, PSO–MLP achieved an F1-score of 0.9338, exceeding the 0.88–0.95 range commonly reported for ANN-based water quality classification [2], [40], and improving baseline performance by approximately 14% points. The marked reduction in standard deviation across folds further indicates improved stability and reduced sensitivity to data partitioning, consistent with robust environmental modeling practices [1], [23]. The integration of SMOTE contributed to balanced recall and F1-scores, aligning with previous findings that synthetic oversampling enhances minority class detection in imbalanced environmental datasets [33]–[35].

Despite its superior predictive capability, PSO–MLP exhibited slightly higher training accuracy than validation accuracy, suggesting mild overfitting—an effect also noted in optimization-enhanced neural architectures [12], [29]. The increased computational time (approximately 45–60 minutes per run) reflects the

trade-off between optimization depth and efficiency. External validation on independent water quality datasets is therefore recommended to further assess generalizability. Overall, the combination of class balancing and metaheuristic optimization substantially improved classification robustness, stability, and discriminative performance, supporting the practical applicability of hybrid ANN–metaheuristic frameworks in intelligent environmental monitoring systems.

5. CONCLUSION

This study evaluated the effect of metaheuristic optimization on MLP performance for water potability classification on an imbalanced dataset addressed using SMOTE. Compared to the baseline model, BO and GA improved predictive accuracy, while PSO–MLP achieved the most consistent and statistically significant performance gains across evaluation metrics. The results demonstrate that swarm-based optimization enhances neural network generalization by effectively balancing exploration and exploitation during hyperparameter search. The combination of class balancing and optimization substantially improved robustness and discriminative capability in an imbalanced environmental dataset. However, the improved performance came with increased computational cost and slight indications of overfitting, underscoring the compromise between precision and effectiveness. Future research should focus on external dataset validation and scalable implementations for real-time intelligent water quality monitoring systems.

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AUTHOR CONTRIBUTIONS STATEMENT

This journal uses the Contributor Roles Taxonomy (CRediT) to recognize individual author contributions, reduce authorship disputes, and facilitate collaboration.

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Harun Mukhtar		✓	✓	✓			✓	✓		✓	✓		✓	✓
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C : **C**onceptualization

M : **M**ethodology

So : **S**oftware

Va : **V**alidation

Fo : **F**ormal analysis

I : **I**nvestigation

R : **R**esources

D : **D**ata Curation

O : Writing - **O**riginal Draft

E : Writing - Review & **E**ditng

Vi : **V**isualization

Su : **S**upervision

P : **P**roject administration

Fu : **F**unding acquisition

CONFLICT OF INTEREST STATEMENT

Authors state no conflict of interest.

INFORMED CONSENT

This study does not involve direct interaction with individuals. Therefore, informed consent is not necessary, as the research relies on publicly available data.

ETHICAL APPROVAL

Not applicable. This research did not involve human subjects, human biological materials, or experimental procedures on animals. The work was conducted solely on computational models, publicly available datasets, or non-sensitive data that did not require intervention with living organisms. Therefore, ethical approval from an institutional review board or animal ethics committee was not necessary for this study.

DATA AVAILABILITY

The dataset used in this study is publicly accessible from the Ministry of Environment, titled “Water Quality of Rivers” (accessed on March 7, 2024), accessible at <https://cpcb.nic.in/nwmp-data-2019/>.

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