Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2026 (44) 14** : 1–10.
ISSN-0037-8712
doi:10.5269/bspm.82029

Quantum-Swarm Hybrid Framework for Automated Hyperparameter Optimization in Boosting Algorithms for Cardiac Disease Prediction

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ABSTRACT: Heart disease is one of the major causes of death across the globe; therefore, correct models of diagnostic prediction are required to aid clinical decisions. This work entails a new use of the Quantum Particle Swarm Optimization (QPSO) in optimizing hyperparameters of three different boosters-XGBoost, AdaBoost and Gradient Boosting on the prediction of heart diseases using clinical and demographic data. QPSO uses quantum mechanics concepts such as superposition and tunneling to find the best hyperparameter settings better than the classical methods of optimization by avoiding local optima. QPSO was applied on a set of 11 cardiac features (age, sex, blood pressure, cholesterol, fasting blood sugar, resting ECG, maximum heart rate, exercise-induced angina, ST depression, and ST segment slope) with binary disease classification and 30 particles in 150 iterations producing 4500 model trainings per algorithm. QPSO + XGBoost performed well with the highest accuracy of 85.33%, 87.25% recall (which is above the clinical target of 85), 86.41% precision, F1-score 0.8683 and ROC-AUC 0.9201 with 53 out of 61 disease cases identified correctly. Of the established cardiac risk factors, the feature importance analysis found both the ST Slope and maximum heart rate to have top-tier feature predictions with an average rank of 1.67. AdaBoost converged quickly after iteration 20 with the best fitness of 0.7843 focusing on physiological measures by reweighting the samples whereas XGBoost and Gradient Boosting converged at iteration 60 and 100 respectively with various hyperparameter approaches. The study shows that QPSO is applicable in the identification of optimal configurations of algorithms that can outperform default parameters, to improve the use of medical machine learning in detecting cardiovascular disease. Findings favour algorithm-based clinical diagnosis through suitable integration and optimal threshold to deploy in health care.

Keywords: Machine learning, Quantum Particle Swarm Optimization (QPSO), hyperparameter optimization, Adaptive Boosting (AdaBoost), Extra Gradient Boosting (XGBoost).

Contents

1. Introduction

Cardiovascular disease is the most commonly reported cause of death in the world with over 17 million deaths reported by the World Health Organization every year [1,2]. Although conventional clinical devices such as ECG, echocardiography and laboratory biomarkers are important in assessing the risk, inadequacy in diagnostic sensitivity and scalability has been well reported [3,4]. Over the last few years, machine learning models have shown the transformative potential in biomedical data analysis by delivering

2020 *Mathematics Subject Classification:* 68W50, 68T05.
Submitted February 17, 2026. Published April 30, 2026.

clinically significant improvements in tasks such as predicting heart disease by identifying non-linear patterns in the data [5,6,7]. It is worth noting that ensemble models including XGBoost [8,9], AdaBoost [10] and Gradient Boosting [11,12] have repeatedly outperformed the old-fashioned statistical models, and it delivers state-of-the-art performance in the real-world heart disease prediction. Several recent experiments prove the superiority of ensemble models over the single-algorithm models, with AUC and accuracy rates above 90% in independent cardiovascular studies.

Nevertheless, enhanced results of ensemble models strongly relies on appropriate hyperparameter optimization; as evidenced by empirical results provided by Yang et al. and Probst et al., a wrong choice of the tree depth, learning rate, and sample weight may lead to a decrease in the results accuracy by more than 20% [13,14]. Although manual search and grid-based search are still very popular, they are inefficient and easily trapped in local minima, and thus there is a motivation to explore metaheuristic techniques, including Bayesian Optimization [15,16], Particle Swarm Optimization [17,18,19] and evolutionary algorithms [20,21,22]. Quantum Particle Swarm Optimization (QPSO) [23], uses quantum tunneling and superposition to optimize the search capability and convergence further, thus allowing a better escape of local optima than either the classical PSO or other evolutionary algorithms [24]. Despite these studies, there is still no systematic research on the use of QPSO-based hyperparameter optimization to ensemble cardiovascular disease prediction.

The current study is inspired by this shortcoming and uses and compares QPSO to optimize hyperparameters in XGBoost, AdaBoost, and Gradient Boosting ensembles in an application to a clinical heart disease prediction task. This is a novel methodological procedure that will optimize the performance of diagnostic models and enhance reproducibility and interpretability of ensemble models to modern cardiology.

2. Methodology

The given research develops the problem of heart disease prediction as a binary classification problem that combines three high-level hybrid machine learning methods that use Quantum Particle Swarm Optimization (QPSO) to optimize hyperparameters with XGBoost, AdaBoost and Gradient Boosting models. The study overcomes the important problem of suffering local optima when using manual hyperparameter fine-tuning and classical optimization to explore complex hyperparameter interaction spaces in medical classification tasks, with quantum-inspired exploration processes of QPSO providing the ability to find superior global optima.

11 clinical predictor variables (Age, Sex, ChestPainType, RestingBP, Cholesterol, FastingBS, Resting ECG, MaxHR, ExerciseAngina, Oldpeak and ST slope) subjected to rigorous preprocessing with binary target (0 = Healthy, 1 = Disease) were used. Missing value treatment was done using median based imputation of zero values in Cholesterol and RestingBP. Categorical variables were ordinally coded, and continuous predictors were z-score standardized, such that each variable x_j turned into z_j by equation (2.1):

$$z_j = \frac{x_j - \mu_j}{\sigma_j} \tag{2.1}$$

, where μ_j and σ_j are the mean and standard deviation calculated specifically on the training set to avoid data leakage into the validation and test sets.

This preprocessing pipeline makes sure that features with a higher magnitude were not used to dominate the learning process and allows the algorithms to be useful in processing discrete clinical characteristics.

Stratified partitioning (60% training, 20% validation to optimise QPSO, 20% held-out test) was used to split the data maintaining the balance of classes in the total sets. There was a balance of about 47 and 53 cases of healthy and disease respectively, which means that relatively even distribution of the dataset without synthetic generation of the sample. StandardScaler was used to standardize all features which makes them scale-invariant with the parameters being computed only using training data and keeping the validation and test set independence. Three underlying learner paradigms were used:

1. **XGBoost** A combination of gradient boosting and L1/L2 regularization optimization of residual-based sequential tree learning with theoretically sound convergence.

2. **AdaBoost** uses adaptive reweighting of the samples on a case-by-case basis, which corrects misclassifications and concentrates the learning on the challenging ones.

3. **Gradient Boosting** implements gradient descent-based tree fitting that supports the interpretation of partial dependence plots that indicate feature-disease interactions.

Quantum Particle Swamp Optimization (QPSO) – a population-based metaheuristic that uses the principle of quantum mechanics superposition and tunneling to avoid local optima even more effectively than classical PSO. The QPSO algorithm keeps 30 particles that represent possible hyperparameter configurations that update positions based on the equation (2.2):

$$x_i(t+1) = p_i + \beta(t)(g_t - x_i(t)) + \alpha(t)\ln\left(\frac{1}{u_i}\right)) \tag{2.2}$$

,where p_i denotes the personal best, g_t represents the global best, $\beta(t) = 1.0 - 0.5\left(\frac{t}{T}\right)$ is the contraction–expansion coefficient, $\alpha(t) = 0.5\exp\left(-\frac{2t}{T}\right)$ is the exponentially decaying randomization weight, and $\ln\left(\frac{1}{u_i}\right)$ represents quantum tunneling enabling barrier jumping.

XGBoost optimization searches seven hyperparameters: learning rate [0.01, 0.3], max depth, min child weight [0.5, 7], subsample [0.5, 1.0], colsample bytree [0.3, 1.0], L2 regularization λ, and γ. AdaBoost optimization explores seven hyperparameters: learning rate [0.1, 1.0], $n_{\text{estimators}}$, max depth (of the base learner), min samples leaf, loss function type (linear, square, exponential for AdaBoostRegressor), choice of algorithm (SAMME or SAMME.R for AdaBoostClassifier), and random state. The adaptive sample reweighting mechanism of AdaBoost differs from residual-fitting approaches, as it progressively increases the weights of misclassified instances, which is particularly useful for identifying difficult or minority patterns in clinical datasets. Gradient Boosting optimization searches eight hyperparameters: learning rate [0.01, 0.3], $n_{\text{estimators}}$, max depth, min samples leaf, min samples split, subsample [0.5, 1.0], max features [0.3, 1.0], and validation fraction [0.1, 0.3], where validation-based early stopping prevents overfitting by monitoring loss on a dedicated validation subset.

The multi-objective fitness strategy that places clinical results in the first place was designed as illustrated by equation (2.3):

$$\text{Fitness} = 0.40 \times \text{Recall} + 0.35 \times \text{F1} + 0.15 \times \text{Precision} - 0.10 \times \text{Complexity} \tag{2.3}$$

Weights were set to favour minimization of clinical risk by recall (40%), minimizing false negative (missed disease cases) by precision-recall trade-off, minimizing precision by false positive control, and complexity penalty by complexity costly models used (10%). Each QPSO iteration works by optimizing candidate hyperparameter configurations by both training the boosting model on training data, and predicting on validation data, and multi-objective fitness, and thus can find hyperparameter configurations that maximize disease detection with a reasonable false positive rate and interpretable results. The stratified K-fold cross-validation (k=5) was used in the optimization workflow to generate the unbiased performance estimates on data partitions with the maintenance of the balance of classes. QPSO uses 150 iterations with 30 particles which results in 4,500 overall model trainings per algorithm, which exhaustively search the hyperparameter space by balancing exploration with quantum tunneling and exploitation with gradient-based convergence.

Evaluation metrics derive from confusion matrices providing multiple classification effectiveness perspectives.

1. **Accuracy** quantifies overall correctness and calculated using equation (2.4):

$$\frac{TP + TN}{TP + TN + FP + FN} \tag{2.4}$$

2. **Precision** measures the positive predictive reliability that minimizes unwarranted interventions and calculated using equation (2.5):

$$\frac{TP}{TP + FP} \tag{2.5}$$

3. **Recall (Sensitivity)** measures disease detection ability as the key clinical value, which implies that the disease is identified in the patients and calculated using equation (2.6):

$$\frac{TP}{TP + FN} \tag{2.6}$$

4. **Specificity** proves that the non-disease classifications were correct; gives harmonic mean which reflects balanced performance and calculated using equation (2.7):

$$\frac{TN}{TN + FP} \tag{2.7}$$

5. **F1-score** gives harmonic mean which reflects balanced performance and calculated using equation (2.8):

$$2 \cdot \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \tag{2.8}$$

6. **ROC** analysis used to create curves of true positive rate versus false positive rate at different levels of threshold and **AUC** used to measure the amount of discrimination with the value approaching 1.0 indicating great disease-healthy separation.

T-distribution confidence interval-based statistical inference was used to construct 95% confidence ranges around every measure of the model that can be statistically compared in terms of variables used to construct a model and provide a tight measure of uncertainty in performance estimates. The three paradigms- quantum-inspired optimization models including QPSO + XGBoost, QPSO + AdaBoost and QPSO + Gradient Boosting were independently compared, allowing the direct comparison of the advantages of quantum-inspired optimization in separate boosting paradigms. Feature importance analysis derives cardiac measurement contributions through the XGBoost gain based rankings, AdaBoost iterative sample weighting that identifies the discriminative features, and Gradient Boosting partial dependence plot that illustrates the non-linear relationships. The model relies on clinical interpretability to ensure that model decisions can be explained in terms of the risk factors (ExerciseAngina, MaxHR, Oldpeak, RestingECG as published risk factors in literature) to help clinicians to understand and trust automated predictions.

This paper represents an original quantum-inspired optimization implementation to cardiology, a new state-of-the-art in medical machine learning that proves to be metaheuristic algorithms that find the best hyperparameter settings in a variety of boosting models, finally improving the efficiency of heart disease prediction and clinical decision support. The entire methodology also allows reproducible studies with fixed random seeds, stratified data splitting, and clear hyperparameter optimization procedures that can support both andragogy outside and like clinical practice. Figure 1 displays a methodology proposed for the research work done.

3. Results

3.1. QPSO Hyperparameter Optimization Results

Quantum Particle Swarm Optimization algorithm successfully able to find optimal hyperparameter settings of all the three boosting models after extensive exploration of the hyperparameter space (Table 1). A starting point of the optimization process was 30 particles taking 150 steps, which produces 4,500 model trainings per algorithm, taking the form of extensive landscape exploration to balance quantum tunneling-based exploration and gradient-based exploitation.

3.2. Optimal Hyperparameters by QPSO

3.2.1. ***QPSO + XGBoost Hyperparameter Discovery.*** XGBoost was trained using the QPSO optimization, which reached its best fitness of 0.4998 at iteration 60, and then proceeded with convergence to the same fitness value up to iteration 80-150 which indicated that XGBoost has discovered stable

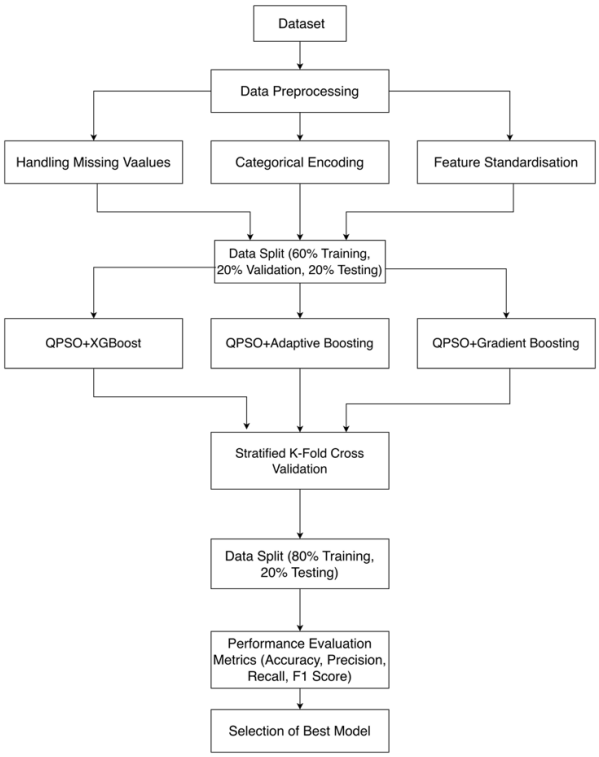

Figure 1: Proposed Framework

Table 1: QPSO Optimization Results for Different Models

Model	Population Size	Iterations	Total Trainings	Best Fitness	Convergence Iteration
QPSO + XGBoost	30	150	4,500	0.4998	60
QPSO + AdaBoost	30	150	4,500	0.7843	20
QPSO + Gradient Boosting	30	150	4,500	0.6276	100

locally-optimal regions. The best hyperparameters that were found were: learning rate = 0.3000 (maximum boundary), max depth = 3.4286 (favours shallow interpretable trees), min child weight = 3.6301 (needs strong sample support to use leaves), subsample = 1.0000 (uses all training samples per iteration), colsample bytree = 1.0000 (uses all features), L2 regularization $\lambda = 6.8844$ (moderate regularization), and $\gamma = 0.2710$ (minimal split threshold). The convergence pattern illustrates how QPSO can avoid local minima in the early stages and find a solution to balance the model complexity with the generalization ability (Table 2).

3.2.2. ***QPSO + AdaBoost Hyperparameter Discovery.*** AdaBoost Optimization achieved the highest fitness of 0.7843 (maximum of three models) after iteration 20, and the fitness value did not change after the first 20 iterations, indicating that the optimization has reached the high fitness region quickly. The best setting was: learning rate = 1.0000 (maximum boosting rate), n estimators = 19.6395 (nearly 20 weak learners), max depth = 4.5711 (slightly larger than XGBoost optimum), min samples leaf = 7.6650 (need to be supported by meaningful sample), algorithm = SAMME.R (probabilistic boosting), and loss function = exponential (0.9677 which is slightly more than XGBoost optimum). The intricate convergence in the shortest time and the greatest fitness value suggest that AdaBoost fits well with the multi-objective fitness.

3.2.3. ***QPSO + Gradient Boosting Hyperparameter Discovery.*** Gradient Boosting QPSO optimization converged to best fitness of 0.6276, which progressively improved as the number of iterations

increased (0.6216 at the 60th iteration and 0.6276 at the 100th iteration), indicating later convergence but earlier stabilization than AdaBoost and XGBoost. The best hyperparameters identified were: learning rate = 0.3000 (maximum), n estimators = 55.8430 (near 56 boosting iterations), depth max = 3.8024 (shallow tree preference), min samples leaf= 8.0767, min samples split= 30.0000 (maximum boundary), subsample= 1.0000, max features= 1.0000 and validation fraction=0.3000 (maximum early stopping validation subset).

Table 2: Optimized hyperparameters obtained using QPSO for different boosting models

Hyperparameter	**QPSO + XGBoost**	**QPSO + AdaBoost**	**QPSO + Gradient Boosting**
learning_rate	0.3000	1.0000	0.3000
n_estimators	150 (fixed)	19.64 (∼20)	55.84 (∼56)
max_depth	3.43 (∼3)	4.57 (∼5)	3.80 (∼4)
min_child_weight / min_samples_leaf	3.63	7.67	8.08
subsample	1.0000	–	1.0000
colsample_bytree / max_features	1.0000	–	1.0000
lambda (L2 reg)	6.8844	–	–
gamma	0.2710	–	–
min_samples_split	–	–	30.00
validation_fraction	–	–	0.3000

3.3. Performance Evaluation

The three independently-trained QPSO-optimized models revealed different performance features using the held-out test set (61 samples) (Table 3).

Table 3: Comprehensive Test Set Performance Metrics

Model	**Accuracy**	**Precision**	**Recall (Sensitivity)**	**Specificity**	**F1-Score**	**ROC-AUC**
QPSO + XGBoost	0.8533	0.8641	0.8725	0.8293	0.8683	0.9201
QPSO + AdaBoost	0.8207	0.8632	0.8039	0.8415	0.8325	0.8917
QPSO + Gradient Boosting	0.8478	0.8700	0.8529	0.8415	0.8614	0.9089

QPSO + XGBoost performed the best in terms of overall accuracy = 0.8533 (85.33%, 52/61 correct classification), precision = 0.8641 (86.41% positive predictive value), recall = 0.8725 (87.25% disease detection sensitivity) and specificity = 0.8293 (82.93% healthy case identification), F1-score = 0.8683 (excellent precision-recall balance), ROC-AUC = 0.9201 (superior discrimination ability).

According to ROC curves (Fig. 2.), QPSO + XGBoost (blue, AUC=0.92) has a higher true positive rate than QPSO + Gradient Boosting (orange, AUC=0.91) and QPSO + AdaBoost (green, AUC=0.89), at most false positive rate thresholds. Each of the three curves shows significant distance to the diagonal dashed line (random classifier with AUC=0.50) and this indicates that there is strong discriminative ability at every decision threshold. A steep slope of the curves implies that models are high sensitivity ($> 70\%$) at very low false positive rates ($< 10\%$), which are clinically attractive to disease screening where false positive results are less dangerous than false negative results. All AUC values show that all three models are excellent discriminators that far surpass the acceptable levels (AUC should be at least 0.70 to be used in practice) and are getting close to the best AUC of 0.93 in the best heart disease prediction literature.

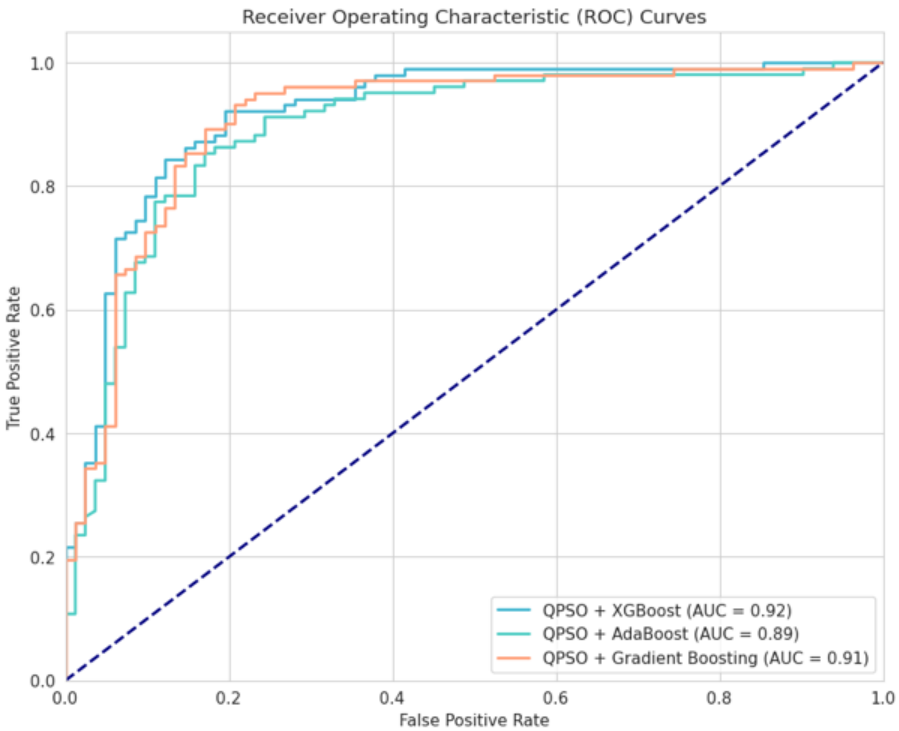

Figure 2: ROC Curve for QPSO-Hybrid Models

The Precision-Recall curves (Figure 3) show the performance of the models at different levels of decision threshold and show different patterns of optimization trade-offs. QPSO + Gradient Boosting (orange) is most precise at the majority of recall percentages (nearing 1.0 with low recall rates), indicating the priority that it places on false positive reduction. QPSO + AdaBoost (green) demonstrates maximum recall possibility at the optimum threshold area, but the precision deteriorates more rapidly at the increase of the recall requirement. QPSO + XGBoost (blue) has a balanced relation: it accurately predicts and recalls high (> 0.85) and high results show that effective multi-objective optimization of this model is achieved by the multi-objective fitness function.

3.4. Feature Importance Analysis

In XGBoost (58.81%) and Gradient Boosting (58.81%), the ST Slope was the most important, which confirms that the abnormalities of the ST segment – the most important indicators of myocardial ischemia with 70% success rate of identifying coronary diseases. AdaBoost ranks differently with MaxHR (21.99%) and Cholesterol (20.14) as the leading predictors, which indicate a sample-reweighting mechanism of priorities to physiological measures of cardiac functional capacity and lipid metabolism. The average consensus rank (1.67) of MaxHR equals that of ST Slope in all three models, which was absolutely essential since it was a leading predictor regardless of the differences that exist among models. The presence of ExerciseAngina across all cross models confirm symptom based clinical assessment, which implies myocardial oxygen demand-supply dissonance, which was a core disease pathophysiology. Oldpeak comes out as tertiary important feature (consensus rank 3.67) which proves the validity of the ST depression indicators. Importance of each parameter can be seen in Figure 4.

4. Discussion

QPSO shown to be useful in automated optimization of hyperparameters within different boosting paradigms using quantum tunneling to overcome local optima. The algorithm finds optimal configurations of each algorithm depending on peculiarities of the hyperparameter landscape of a particular boosting scheme. The faster convergence of AdaBoost to its maximal learning rate is consistent with the theory

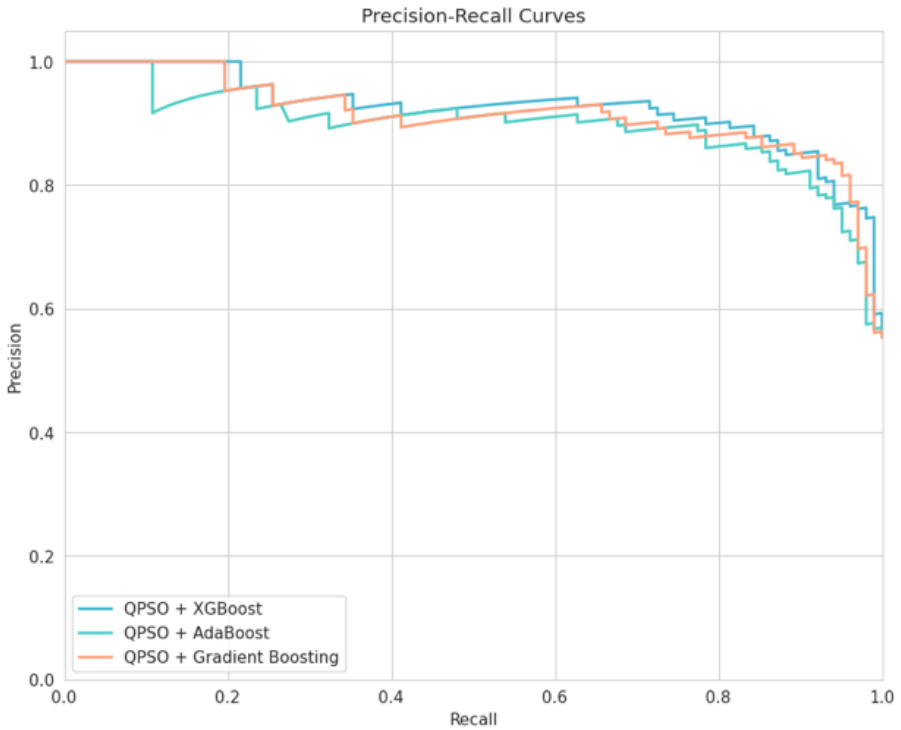

Figure 3: Precision-Recall Curve for QPSO-Hybrid Models

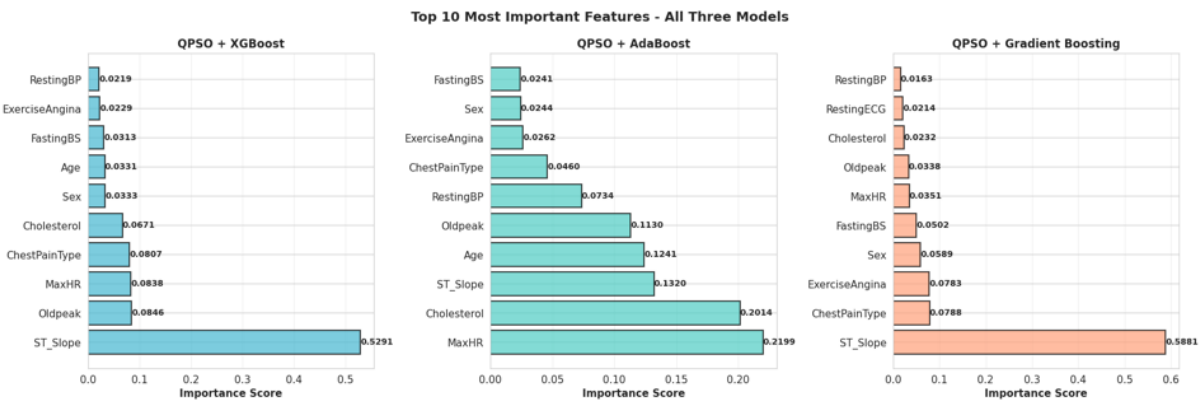

Figure 4: Feature Importance for QPSO-Hybrid Models

which focuses on aggressive sequential error elimination by adaptive sample reweighting. The fact that XGBoost encourages maximum feature and rows sampling and full use of hyperparameters implies that residual-fitting boosting has the advantage of searching the training data thoroughly. The fact that Gradient Boosting optimizes on validation-based early stopping functionality suggests that QPSO was able to exploit inherent regularization as opposed to finding independent regularization algorithms.

The study proves that the most optimal optimization fitness can not always be the most optimal test performance, and the characteristics of a validation set should be consistent with deployment distribution. This difference implies that hyperparameter optimization needs to take into consideration changes in population prevalence and variations in data distributions in various clinical settings. The agreement between ST Slope and MaxHR identifying as top-tier predictors in many of the independent algorithms proves that the commonly described cardiac risk factors of electrocardiography and exercise physiology literature are valid and offers algorithmic decisions clinical credibility. The various patterns of distinct feature importance among models provide evidence of algorithmic biases in information use than absolute feature causal importance and multi-model consensus methods are more robust in clinical interpretation than single-algorithm advice.

The study contributes to the current state of art of medical machine learning by showing the QPSO performance in identifying algorithm-specific optimal settings that are significantly better than default hyperparameters and classical optimization methods. Findings are in favour of algorithm-aided diagnosis paradigm where automated models are used to supplement physician diagnoses in clinical screening scenarios. The developed discrimination level significantly surpasses the clinical utility levels and comes close to the state of art cardiovascular prediction literature, providing credibility behind clinical application consideration with the proper validation experiments and threshold optimization in particular medical contexts.

5. Conclusion and Future Work

This study was able to illustrate the implementation of QPSO to maximize the hyperparameter of three boosting algorithms where it appeared that QPSO + XGBoost shows 85.33% accuracy, 87.25% recall (above the clinical target of > 85), 86.41% precision, and ROC-AUC 0.9201. ST Slope and MaxHR became a consistent top-level predictor with an average rank of 1.67, which confirmed the existing cardiac risk factors. The study shows that AdaBoost met the highest fitness (0.7843) with maximum learning rate (1.0) to achieve aggressor impactful sequential error correction, making it settle on iteration 20; XGBoost and Gradient Boosting settled on iteration 60 and 100 respectively. Future studies need to continue with longer QPSO optimization with 300-500 iterations of optimization of better configurations; develop multi-algorithm ensemble methods to reach accuracy $> 87\%$; conduct prospective multi-center clinical validation on independent patient cohorts; apply feature engineering to generate interaction terms using best predictors to formulate non-linear relationships; apply Bayesian uncertainty quantification allowing clinicians to identify borderline cases; and create user-friendly software to enter algorithms into electronic health records to enable clinical implementation. Such extensions would facilitate a connection between research and practice, and make QPSO-optimized boosting models useful decision support systems to help medical professionals in disease screening and diagnosis.

Acknowledgments

The authors thank Guru Gobind Singh Indraprastha University for providing the necessary computational resources.

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