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Auto ML For Adaptive Model Selection And Hyperparameter Optimization

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Abstract
Automated Machine Learning (AutoML) improves predictive systems by reducing manual intervention in model configuration and parameter tuning. Existing frameworks often face unstable convergence and limited adaptability in complex hyperparameter search spaces. This research develops an intelligent AutoML framework for adaptive hyperparameter optimization (HPO) and model selection, employing Convolutional Neural Networks (CNN) and Graph Neural Networks (GNN) with a Hybrid Whale-Aquila Optimization (HWAO) algorithm. In HWAO, Whale Optimization performs global exploration to maintain diversity, while Aquila Optimization enhances local exploitation and accelerates convergence toward optimal parameters. This hybrid approach balances exploration and exploitation, reduces premature convergence, and strengthens adaptive learning. Performance evaluation compares standalone Whale and Aquila optimization with the hybrid method. CNN-HWAO achieved an error rate of 11.0%, convergence in 30 iterations, a model size of 115 MB, HPO score of 92.1, and prediction accuracy of 89.0%. GNN-HWAO reached an error rate of 10.2%, convergence in 32 iterations, model size of 125 MB, HPO score of 93.4, and prediction accuracy of 90.1%. The system is trained using Keras 2.2.4 and evaluated with TensorFlow on Python 3.9, demonstrating superior accuracy, efficiency, and generalization.

Keywords: AutoML, Adaptive Hyperparameter Optimization, Intelligent Model Selection, Evolutionary Computing, Hybrid Optimization Strategies, Computational Intelligence.

1. Introduction

Automated Machine Learning (AutoML) is a process that automates the entire Machine Learning (ML) pipeline, from selecting the appropriate ML model to adjusting hyperparameters and even deploying the models in production [1]. Adaptive modeling, involving the selection of algorithms, parameter tuning, and preprocessing methods, is becoming increasingly important for ML applications. Adaptive optimization of modeling processes improve performance and increase efficiency, as well as allow the model adjustments across different tasks and inputs [2]. AutoML make modeling easy, efficient, and more widely available to those without expertise in the field. Using AutoML across various fields and situations has made the application of algorithms much more convenient [3]. The feature selection, model selection, and HPO processes are some examples of complex tasks that fall under the scope of ML. The AutoML approach streamlines such complicated procedures, making ML quicker, simpler, and more convenient for users who have no prior training in the field [4]. The ML pipeline is very dependent on experts' knowledge, so the model, preprocessor, and hyperparameters need to be selected with care. The optimization process requires significant time due to its complexity and the interdependence of the hyperparameters. Contemporary AutoML techniques have low flexibility and speed since they create static models [5]. Class imbalance, heterogeneity in industrial data, and the challenge of fine-tuning hyperparameters pose difficulties when deploying ML in predictive maintenance operations. At present, existing approaches usually focus on performing basic optimizations; do not incorporate considerations regarding model selection and tuning as a holistic process, adaptive modeling according to various operational states, and ensemble techniques, resulting in poor performance in the above aspects [6]. Model optimization is a time-consuming process, lacks reproducibility, and cannot handle high-dimensional space parameter optimization since ML techniques are highly dependent on human skills in fine-tuning hyperparameters. This problem can be partially addressed using traditional AutoML, although it favors supervised learning over unsupervised learning approaches like outlier detection [7]. Designing ML pipelines, feature selection, and optimization of hyperparameters through a manual approach is challenging and ineffective. Though there are existing approaches to automating ML project processes, these methods have limitations in terms of flexibility and effectiveness as they focus on only one objective, assume sparsity implicitly, and often produce few different Pareto optimal models [8].

Research Aim: This research proposes an adaptive approach for joint learning of model selection and hyperparameter tuning to address AutoML challenges. The proposed method leverages the Hybrid Whale-Aquila Optimization (HWAO) algorithm to predict promising configurations based on learned latent space representations, leading to improved prediction accuracy, faster convergence, and efficient, high-performing ML.

This research is organized as follows: The introduction is given in Section 1, the associated work is discussed in Section 2, the methodology is described in Section 3, the findings and performance evaluation are detailed in Section 4, and the conclusion is given in Section 5.

2. Related Works

In smart manufacturing, intelligent fault diagnosis of time-series data was conducted by implementation of Convolutional Neural Networks (CNNs), AutoML, and data fusion with image images. Results showed that the framework provided highly accurate classification for two case studies, combined with automatic HPO and with an efficient deployment on cloud and edge devices. However, only certain datasets and fault diagnosis scenarios were used for validation [9]. AutoML systems, including Artificial Intelligence (AI) and Tree-based Pipeline Optimization Tool (TPOT), were applied to vibration-signal analysis for gearbox fault diagnosis and feature selection. Findings indicated ensembles of XGBoost and stacked models achieved accuracy up to 90% using 10 common features across failure modes. Nevertheless, the analysis was limited to three gearbox fault conditions and 64 statistical indicators [10]. Bayesian Optimization (BO) with Genetic Algorithm (GA), Differential Evolution (DE), and Covariance Matrix Adaptation–Evolutionary Strategy (CMA-ES) was applied to optimize AutoML hyperparameters for image classification tasks. Results show that CMA-ES and DE achieved highly accurate performance, outperforming standard BO, while GA produced lower results. However, BO remained less effective when GA was used for acquisition function optimization [11]. Constraint-Aware Automated Machine Learning (CAML) with Meta-Learning (ML) was applied to automatically adapt AutoML parameters, including search strategy, validation strategy, and search space, for constraint-aware pipeline optimization. Findings indicated CAML achieved up to 95% predictive performance while satisfying runtime and resource constraints, outperforming static AutoML configurations. Nonetheless, existing AutoML systems lacked automatic adaptation to specific use-case requirements [12]. ML, Deep Learning (DL), and AutoML were applied to forecast cryptocurrency prices using historical data to improve prediction accuracy and explore automated model selection. Results showed that Long Short-Term Memory (LSTM) achieved RMSE = 0.027, MAE = 0.021, R^2 = 0.91, outperforming AutoML (Root Mean Square Error (RMSE) = 0.045, Mean Absolute Error (MAE) = 0.037, R^2 = 0.78). Nevertheless, AutoML remains underdeveloped and requires further research [13]. ML and AutoML tools like PyCaret, AutoGluon, and AutoKeras were applied to heart disease datasets to automate model selection and improve prediction accuracy. Findings proved that AutoGluon achieved 78-86% accuracy, outperforming traditional ML (55–60%). Nonetheless, AutoML performance varied across datasets, indicating limitations in consistency and reliability [14]. The imputation algorithms: Denoise AutoEncoder, MissForest, and Mean/Mode (MM) were tested in an AutoML environment for missing data, and to boost predictive modeling. The results indicated that Denoise AutoEncoder achieved the highest average accuracy = 0.813 on real datasets, followed by MissForest with accuracy = 0.796 on simulated datasets, and MM with accuracy = 0.789 that performed similarly. But there was a high computational cost and all feature values are needed for the new samples in Neural Network–based imputation [15]. Parameter space exploration and benchmarking of data acquisition strategies were performed by automated ML techniques, based on active learning (AL) and design of experiments (DOE). The results showed that models had $R^2 > 0.90$ with 200,000 test data points and the precision in the evaluation was within ±0.002, whereas the replication-oriented strategies worked better in noisy conditions. However, some of the AL strategies performed better than the traditional DOE strategies under different data sets complexity and size [16].

A multimodal ML pipeline autoML framework based on pre-trained transformers and Bayesian Optimization was designed to synthesize efficient ML pipelines. It was tested on 23 multimodal datasets and performed on average with an accuracy = 0.872 and an F1-score = 0.861 while also accelerating computation time by ~35%. However, the performance was found to be different for different datasets and limited resources [17]. Five AutoML models, namely, auto-sklearn, TPOT, H2O AutoML, AutoKeras, and MLBox, were employed to predict streamflow on a daily basis based on time-lagged streamflow and rainfall data along with remote-sensing data. The model performance for the 3-day forecasts were found to be between 12.4 m^3/s and 15.7 m^3/s for Root Mean Square Error (RMSE) and 0.82–0.89 for Nash–Sutcliffe Efficiency (NSE). But, the small number of training samples was limiting the models' generalizability [18]. Well production forecasting was done on 19 selected geological, engineering and production features using the AutoGluon framework with 5-fold cross-validation, bagging and stacking. The value of R^2 was 0.79, which is a good fit. In spite of this, the performance of the models was reliant on the selection of the features and data quality [19]. In the field of intelligent manufacturing, the use of AI to provide transparent explanations has been proposed as a way to enhance the transparency of AI models, and the use of Shapley Additive Explanations (SHAP) to explain the decisions made by AI models has also been suggested to improve the interpretability of AI models. Results showed that 60-90% of processing time was spent on AI data preprocessing and that the proposed techniques increased the sensitivity, accuracy and robustness. However, the method has mainly been applied to tool wear monitoring [20].

3. Methodology

The methodology is based on structured, high dimensional benchmark datasets and intelligent AutoML techniques with CNN and GNN models. The learning of hyper parameters is done using Whale and Aquila Optimization algorithms and combined with a Hybrid Whale-Aquila Optimization (HWAO) model. This can be used to achieve adaptive, efficient model selection, optimized parameter tuning, and better prediction performance in the AutoML environment. The CNN and GNN with Hybrid Whale-Aquila Optimization method is seen to be used for adaptive hyperparameter tuning in AutoML as shown in figure 1.

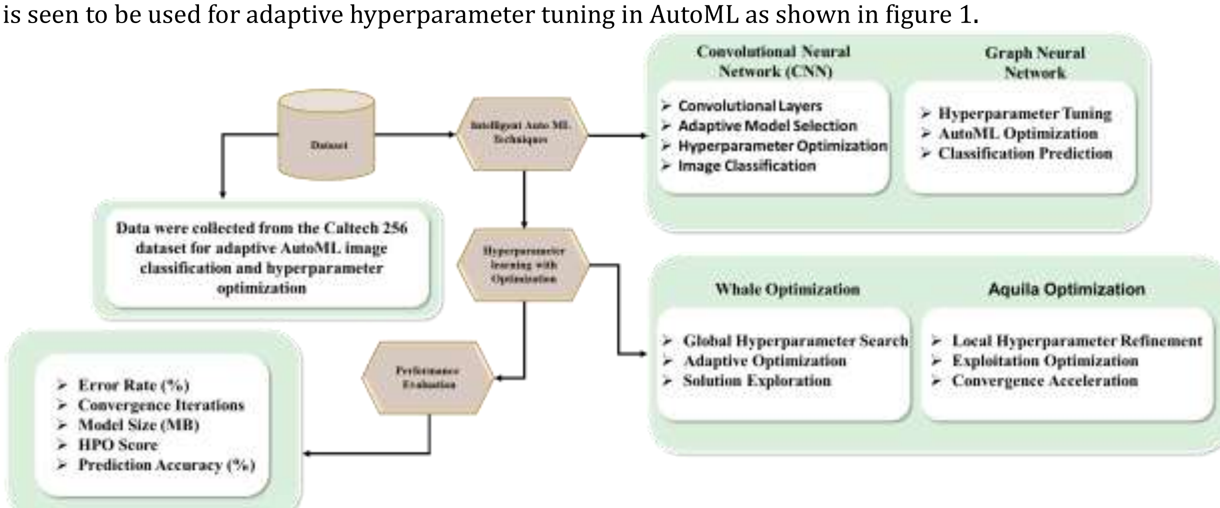

Figure 1: Proposed Flow of the Research Framework

3.1 Data collection

The Caltech 256 dataset comprises 30.6k images spanning 256 object categories and a background class, collected to support image classification and object recognition tasks, which is publicly available on Kaggle (https://www.kaggle.com/datasets/jessicali9530/caltech256). Each category contains at least 80 images of varying sizes, resolutions, and viewpoints. The dataset includes diverse objects with intra-class variations, where category labels are targets. Images undergo preprocessing, including resizing and normalization, and are split into 80% training and 20% testing sets for unbiased evaluation of automated classification models.

3.2 Intelligent AutoML techniques for Object Detection

The suggested AutoML architecture utilizes CNN to extract the hierarchical features from the high-dimensional image data for object detection purposes and GNN to model the relationship between the objects identified. Another feature of this system is automatic tuning and selection of optimum model for efficient object detection.

Convolutional Neural Network (CNN): This research uses a CNN to accurately process and identify/classify image data by automatically learning the hierarchical spatial feature. CNNs use convolutional layers to extract local patterns like edges, textures, and shapes, while using pooling layers to downsample and retain key features. It is able to identify strong features in high-dimensional and diverse images, including the Caltech 256 dataset images. For classification tasks, CNN is used as the main model component in the proposed AutoML model, where it is used to adaptively perform HPO and auto model selection. CNN captures complex visual patterns and increases the accuracy of the model, generalization, and overall performance of automated image recognition workflows, as shown in Equation (1).

$$Z_t = \sum_{j=1}^{m} v_i \, p_{i-m+1} + A \tag{1}$$

The output $Z_t$aggregates input features $v_i$weighted by kernel parameters $p_{i-m+1}$and includes a bias term A. The summation operator $\sum_{j=1}^{m}$ indicates aggregation over the past mvalues or features. It captures the influence of multiple prior data points or parameters, enabling CNN to learn hierarchical spatial patterns, supporting adaptive hyperparameter learning and automated model selection in AutoML.

Graph Neural Network (GNN): Graph Neural Networks (GNN) were used to learn and understand graph-structured data, which means that information is defined in terms of nodes and their connections. Contrary to regular neural networks, the GNN allows the information to spread over the nodes of the graphs to learn about dependencies, interactions, and structures within the data. The GNN contributes to the AutoML process by offering automatic selection of the model and the best hyperparameters, leading to accurate classifications and predictions with respect to structured input data. With the help of Graph Neural Networks, accurate predictions can be made using relational data defined in Equation (2).

$$b_{pq} = \begin{cases} 1, & \text{if } \Delta H_{pq} \in F \\ 0, & \text{if } \Delta H_{pq} \notin F \end{cases} \tag{2}$$

A binary indicator, b_{pq}represents whether nodes pand qare connected within the graph used for GNN-based learning in the AutoML framework. The difference or edge weight, ΔH_{pq}, quantifies relationships between nodes, and Fdenotes the set of relevant edges. If $\Delta H_{pq} \in F$, $b_{pq} = 1$; otherwise, it equals 0, ensuring that only meaningful connections influence adaptive model selection and HPO according to Equation (3).

$$M_0(u) = \{u\} \tag{3}$$

The 0-th order neighborhood, denoted by $M_0(u)$, is defined as the set containing only the node uitself. Here, $M_0(u)$represents the neighborhood of uat order zero, and urefers to an individual node in the graph. Including u's intrinsic features ensures that the GNN can perform adaptive model selection and HPO effectively within the AutoML model, represented by Equation (4).

$$M_1(u) = \{v \mid (u, v) \in F \text{ or } (v, u) \in F\} \tag{4}$$

The first-order neighborhood $M_1(u)$contains all nodes vdirectly connected to node u, where uis the reference node whose features are being updated and v represents neighboring nodes providing relational information. The connections are defined by the set of valid edges F. This structure enables the GNN to aggregate meaningful neighbor features, supporting adaptive model selection and HPO in the AutoML framework.

3.3 Hyperparameter learning with HWAO

The proposed HWAO AutoML scheme uses WOA for the global search and AO for local optimization of the hyperparameters. The strength of AO is the enhancement of possible solutions while the power of WOA is in the diversity of search in large dimensions. This helps CNN and GNN networks to learn more efficiently, converge, and generalize.

Whale Optimization Algorithm (WOA): The WO algorithm is included to enable global searching of hyperparameters in the proposed automatic ML technique. Based on the bubble-net hunting process used by humpback whales, the WOA algorithm conducts a systematic search in the high-dimensional and complex hyperparameter space to locate potential areas where optimal sets of hyperparameters can exist. The global search mechanism of WOA ensures diversity among potential solutions, thereby preventing any premature convergence toward sub-optimal solutions. This technique improves adaptability, stability, generalization, and performance of the model represented by Equation (5).

$$H(t+1) = H^{*}(t) - B \cdot \Delta H \tag{5}$$

The updated solution $H(t+1)$is computed from the best current solution $H^{*}(t)$, where B controls step size and ΔH represents parameter differences, enabling adaptive hyperparameter learning in AutoML, defined in Equation (6).

$$B = 2\,b \cdot s - b \tag{6}$$

The coefficient B determines the step size for global hyperparameter exploration, where b and s guide the search direction and intensity. This mechanism supports adaptive HPO and intelligent model selection within the AutoML framework, defined in Equation (7).

$$\Delta H = | F \cdot H^{*}(i) - H(i) | \tag{7}$$

The difference vector ΔH measures the deviation between the best solution $H^{*}(i)$ and current solution $H(i)$, scaled by F, enabling adaptive HPO and intelligent model selection within AutoML

Aquila Optimization (AO): The AO algorithm is introduced for local exploitation of the AutoML model parameters. Leveraging the hunt mechanisms of the Aquila eagle species, AO significantly optimizes candidate solutions by focusing on more likely spaces that were discovered in the process of global exploration. Such a setup facilitates the convergence of the algorithm toward more optimal sets of parameters and improves the accuracy of HPO. AO helps balance the search space between exploration and exploitation by employing the capabilities of the Whale Optimization algorithm, to ensure global exploration. This implementation helps improve adaptive learning of hyperparameters, generalization capabilities, and computational efficiency of the entire algorithm, thus optimizing both CNN and GNN models as represented by Equation (8).

$$Bz_{ij} = y_1 \times V_{qk} - L_{qk} + L_{qk};\ i = 1{:}\,M_p, j = 1{:}\ Dim \tag{8}$$

The updated solution Bz_{ij}adjusts local hyperparameters, where $y_1$scales the update, $V_{qk}$is solution velocity, L_{qk}defines promising regions, $i = 1{:}\,M_p$ indexes hyperparameters, $j = 1{:}$ Dimindexes dimensions, supporting adaptive hyperparameter learning in AutoML, defined in Equation (9).

$$s = (\Delta H_1 \times V) + s_1 \tag{9}$$

The step size scontrols local hyperparameter adjustments, where $\Delta H_1$is the parameter difference, V scales the change, and $s_1$is the previous step, enabling adaptive HPO and intelligent model selection in AutoML, defined in Equation (10).

$$\theta = 3 \times \frac{\pi}{2} - (Y \times \Delta H_1) \tag{10}$$

The angle θdetermines the direction for local hyperparameter updates, where Yscales the adjustment, $\Delta H_1$is the parameter difference, supporting adaptive hyperparameter learning and intelligent model selection in AutoML.

Intelligent Hybrid Whale Aquila Optimization (HWAO) algorithm: HWAO integrates WOA for global exploration and AO for local exploitation within the proposed AutoML framework. WOA broadly searches high-dimensional hyperparameter spaces, maintaining diversity to avoid premature convergence, while AO refines promising regions, accelerating convergence toward optimal parameter combinations. This is a hybrid exploration vs exploitation strategy that improves adaptive hyperparameter learning, intelligent model selection and predictive performance. By enhancing convergence stability, the model generalization and computational efficiency, HWAO facilitates the automatic selection of the optimal configuration for CNN and GNN models on complex image and graph-structured data, mitigating the manual effort required for these tasks.

4. Results

The system is trained with Keras 2.2.4 and tested with TensorFlow with Python 3.9. The results show that the HWAO can enhance the performance of the AutoML model across both CNN and GNN methods. The error rates and convergence time of HWAO are lower than Whale and Aquila optimization alone, and HWAO produces smaller models than Whale and Aquila optimization, and better HPO scores and prediction accuracy. The results show that hybrid optimization can successfully strike a balance between exploration and exploitation, leading to better adaptive hyperparameter tuning and model selection.

Performance Analysis of CNN Models with HWAO: The trained CNN models are compared to each other in terms of five performance metrics as shown in Table 1, using the Whale Optimization Algorithm, Aquila Optimization, and the HWAO approach. The goal is to investigate if hybrid optimization can enhance adaptive hyperparameter tuning and model selection in AutoML setups. The CNN-HWAO performed the best overall with an error rate of 11.0%, converged in the least number of iterations (30), required the smallest model size (115 MB), a highest HPO score of 92.1%, and high prediction accuracy of 89.0% among all models. This result shows that a combination of global and local exploration and exploitation improves the predictive accuracy, convergence efficiency and the generality of the model. Figure 2(a) shows the degree of relationship between error and prediction accuracy, where the lower the error, the higher the accuracy, and the better the point is. The benefits of CNN-HWAO for convergence speed, model compactness and the effectiveness of hyperparameter optimization are also shown in Figures 2(b), 2(c) and 2(d), respectively.

Table 1: CNN Performance Using Hybrid Optimization Strategies

Model - Optimization	Error Rate (%)	Convergence Iterations	Model Size (MB)	HPO Score	Prediction Accuracy (%)
CNN-WO	12.5	45	120	78.5	87.5
CNN-AO	13.1	38	118	80.2	86.9
CNN-HWAO [Proposed]	11.0	30	115	92.1	89.0

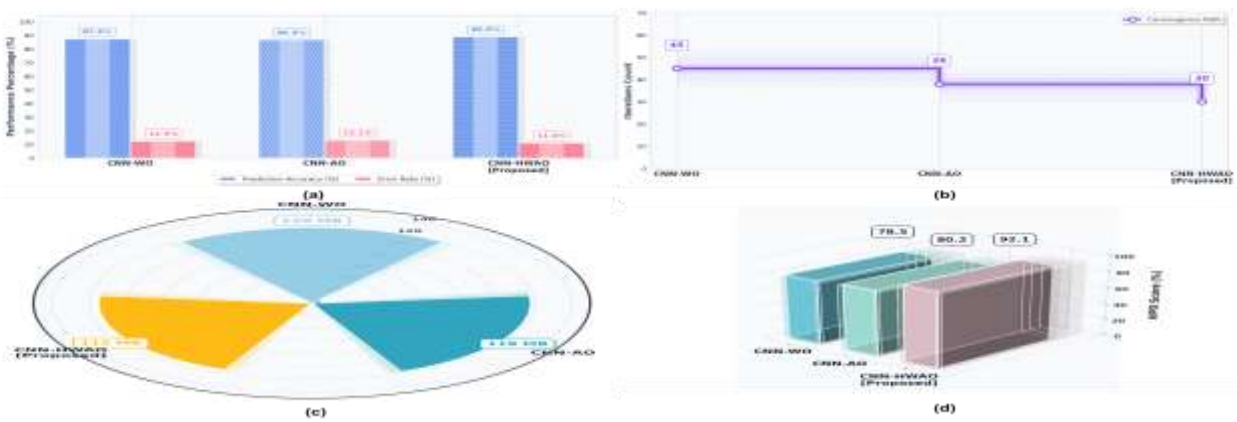

Figure 2: CNN-HWAO comparison of CNN models showing (a) error rate and prediction accuracy, (b) convergence iterations, (c) model size (MB), and (d) HPO score

Performance Analysis of GNN Models with HWAO

In the following, Table 2, a comparative evaluation of the GNN models optimized by Whale Optimization Algorithm, Aquila Optimization and Hybrid Whale Aquila Optimization (HWAO) for intelligent hyperparameter learning in AutoML is provided. GNN-HWAO model with the lowest error rate (10.2%) and the highest prediction accuracy (90.1%) among the evaluated models. Additionally, the model converged well with 32 iterations, and optimized its model size to 125 MB with the highest HPO score of 93.4%. The results indicate that the hybrid optimization strategy is effective in a balance between global exploration and local exploitation, which is reflected by the enhanced predictive ability and robust model selection ability in graph-based networks. Figures 3(a-d) show the error rate, prediction accuracy, convergence speed, and model compactness and hyperparameter optimization effectiveness, respectively.

Table 2: GNN Performance Using Hybrid Optimization Strategies

Model - Optimization	Error Rate (%)	Convergence Iterations	Model Size (MB)	HPO Score	Prediction Accuracy (%)
GNN-WO	11.8	48	130	79.0	88.2
GNN-AO	12.2	40	128	81.5	87.5
GNN-HWAO [Proposed]	10.2	32	125	93.4	90.1

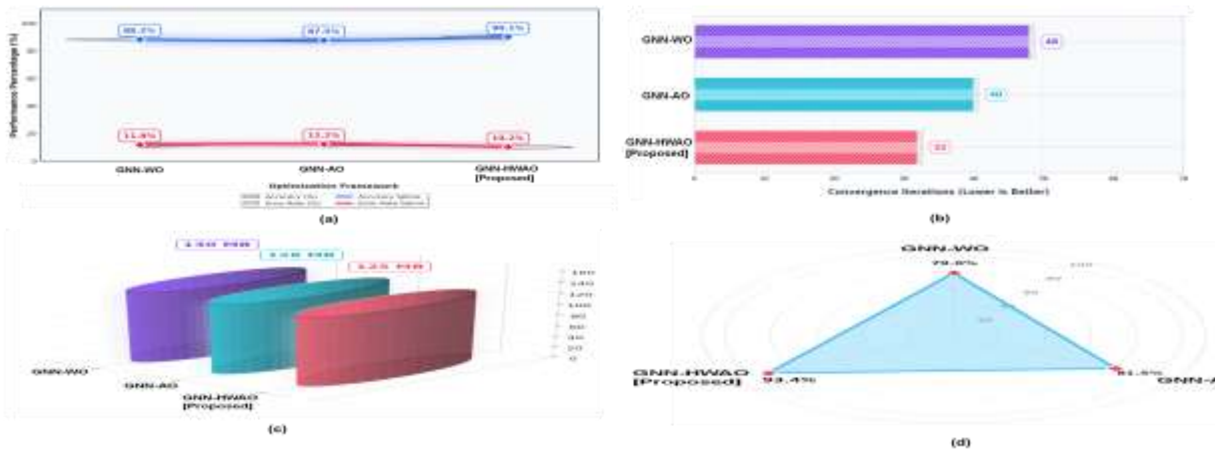

Figure 3: GNN-HWAO performance evaluation (a) error rate and prediction accuracy, (b) convergence speed, (c) model size efficiency, and (d) hyperparameter optimization (HPO) scores

4.1 Discussion

AutoML technology needs more development and research [13]; performance was inconsistent among different datasets [14]; and imputation using neural network incurs high costs and requires all features to be known [15]. Performance was dependent on diversity of data and availability of resources [17]; less training data restricts generalization of models [18]; and model performance was affected by feature selection and quality of data [19]. This research solves all the problems by incorporating feature selection and preprocessing techniques that adopt strong AutoML algorithms based on the CNN and GNN frameworks coupled with cross-validation and the different datasets to guarantee consistent outcomes. Algorithm effectiveness is obtained through pipeline optimization for computational purposes, while the usage of different imputation and predictive models avoids the need for massive datasets.

Implication of the research: This research shows that the implementation of efficient AutoML systems along with effective feature selection, imputation techniques, and varied datasets can greatly increase the accuracy, effectiveness, and reliability of predictions for various applications including finance, medicine, and climate prediction. This is a valuable approach to the creation of effective decision support systems from large volumes of data and to reducing the need for manual modelling.

5. Conclusion

To address these issues, an Intelligent AutoML-Based Adaptive HPO and Model Selection framework was designed that utilizes a hybrid Whale-Aquila Optimization (HWAO) algorithm. The proposed hybrid approach is found to be effective to combine global exploration and local exploitation to improve adaptive learning, convergence stability and model generalization. Experimental results showed that CNN-HWAO gave an error rate of 11.0% and prediction accuracy of 89.0% and GNN-HWAO gave an error rate of 10.2% with prediction accuracy of 90.1%, which were better than the standalone Whale and Aquila optimization methods. Some of its limitations are the restriction to structured, high dimensional classification data sets and the lack of examination of performance for unstructured data or regression problems. Future research might further expand the framework to a wider range of data types, real-world dynamic environments, and incorporate other evolutionary algorithms for greater adaptability, scalability, and computation efficiency in wider-ranging AutoML applications.

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