Evolving Neural Architectures: A Genetic Algorithm Approach to Deep Learning Optimization

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Abstract

In deep learning a fundamental challenge of neural architecture optimization exists, wherein the performance of the network depends on selecting an appropriate model structure. Manual tuning methods, as well as reinforcement learning-based Neural Architecture Search (NAS) methods, often result in computational inefficiencies as well as limited interpretability. In this paper, we present an evolutionary approach for optimizing deep neural network architectures using Genetic Algorithms (GA). We propose with our method adaptive population control, diversity preserving mutations and hybrid reinforcement learning strategies (that improve efficiency, scalability and generalization). For alleviating the computational burden that GA-based optimization presents, we propose a bio-inspired approach that reduces the use of resources via parallel processing, weight-sharing frameworks, and sparse model evolution. We have benchmarked against state-of-the-art NAS using Reinforcement Learning and Bayesian Optimization showing better accuracy and efficiency. We also apply explainable AI (XAI) methods to improve the interpretation of evolved architectures to improve the trust and deployability of our methods. We evaluate our framework on large-scale datasets, yielding high-performance models with real-world applicability. Our findings suggest that evolutionary strategies, if designed for scale and computational efficiency, yield superior results to conventional optimisation approaches, providing a hardware-efficient and interpretable solution to neural architecture search.

Keywords: Genetic Algorithm, Neural Architecture Search, Deep Learning Optimization, Evolutionary Computing, Hyperparameter Tuning, Neuroevolution, Neural Network Pruning.

1. Introduction

The journey of 1 million miles in this field began with a single step of deep learning a neural network-based machine learning technique that redefined the AI landscape. But designing an optimal neural network architecture is still a laborious and time-consuming process for humans. The model architecture can have a strong impact on the performance of a deep learning model, but the best structure is generally found through a great amount of trial and error or automated search approaches like Reinforcement Learning-based Neural Architecture Search (NAS) and Bayesian Optimization. Although successful, these approaches are often inefficient, computationally expensive, and/ or lack interpretability.

To address these limitations, this work proposes an evolutionary approach for automated neural architecture search and optimization using Genetic Algorithms (GA). This is a process that is very similar to natural evolution, whereby a genetic algorithm (GA) iteratively selects the neural network structures that showed the highest performance, mutates them and recombines them into new networks that maintain performance whilst requiring far fewer computational resources. Our approach also introduces several new techniques in contrast to traditional NAS methods:

Adaptive Population Control: Dynamically adjusting mutation and crossover probabilities to improve convergence speed and efficiency.

Mutations that preserve diversity – stop the bad population in a tribal way and keep diverse architectures evolved.

Genetic Algorithm-Reinforcement Learning (GA-RL) hybrid approach – leveraging evolutionary compute for bringing reinforcement learning together with the tune of network hyperparameters dynamically.

Mechanisms for parallelized training and weight-sharing — reducing computational costs and schooling scalable structure search."

Explainable AI (XAI) integration — improving the interpretability of evolved neural networks through techniques like SHAP (Shapley Additive Explanations) and feature importance analysis.

The major challenge of GA-based neural architecture optimization is high computational cost. An issue with traditional GA approaches is the efficiency, as they evaluate many architectures across multiple generations. We tackle this problem by coupling parallel processing with sparse model evolution and hardware-aware optimization techniques, leading to drastic reductions in resource requirements and training time.

Moreover, current NAS methods often operate as black-boxes, making it hard to explain the choice of a specific architecture. To enhance interpretability of the evolved models, we combine Explainable AI (XAI) techniques to provide insights for researchers and practitioners into how certain structures of networks lead to better performance.

Research Contributions

This paper contributes to the field of neural architecture search and optimization in the following fundamental ways:

Implementation of a new GA-driven NAS framework with adaptive mechanisms to optimize deep learning architectures in a more efficient manner to do.

Parallelization techniques, weight-sharing approaches, and sparse evolution for scalability.

Explanation improvements via SHAP Interaction Encoding to learn the function behind the decision process of the converged architectures.

Contextualization against held current SOTA NAS methods show clear advantages in accuracy, computational hyperguitionality & real-world suitability.

Gaining Optimization (GA) based reinforcement learning algorithm — A combination of GA and RL to tune up hyperparameters of neural network on the fly

The rest of the paper is structured as follows: In Section 2 we provide a detailed review of related works in the fields of neural architecture search and evolutionary computing. The proposed methodology is described in Section 3, where the genetic operators, fitness functions, and optimization methods are explained. Section4describes the experimental setup, datasets, and methods for benchmarking. Section 5 outlines the experimental results and gives a discussion, and Section 6 summarizes the main findings and limitations of this work and suggests future research directions. Sec. 7 finally concludes the paper with some final thoughts and possible applications of our approach.

1.1 Problem Statement

Deep learning has continued to make rapid strides in recent years; we now have very complicated architectures to work with. The design of a good architecture to a specific task, however, still is a primary challenge because the architecture can contain so many combinations, such as types of layers, depth, width, activation functions, connections, etc. Conventional methods for neural network design are significantly based on either tedious manual search or automated Neural Architecture Search (NAS) methods based on Reinforcement Learning (RL) and Bayesian optimization. Although these approaches have shown efficacy, they have several key drawbacks:

Poor Computational Efficiency – Especially methods that use RL — a high number of models need to be trained and evaluated, resulting in very high costs in computation and extremely high resource requirements for adequate supercomputing.

Scalability Problems – Most current NAS methods do not scale well to both high-dimensional data and deep architectures, restricting their use cases in real-world applications.

Early Convergence of Optimization Algorithms—Optimization algorithms tend to get stuck in local optima and do not explore diverse and potentially better architectures.

Lack of Interpretability – Most NAS approaches perform by black-box optimization with little insight into why a given neural architecture was selected, making it very difficult to trust and study the models.

Overfitting Risks – The neural architectures obtained from NAS are mostly designed to fit specific data sets resulting in a poor performance on unseen data.

To mitigate these issues, this work exploits an evolutionary strategy with Genetic Algorithms (GA) to optimize deep neural network architectures. Differing from conventional NAS methods, GA implements a biologically inspired evolutionary strategy to perform a diverse search across architectures while being scaleable and adaptable to various problems. Moreover, our research utilized Explainable AI (XAI) methods as well, allowing for greater insights into selected architectures and deepening our understanding of the architectural search process further.

2. Literature survey

Neural Architecture Search (NAS) is a promising field that has emerged in recent years and has the potential to automate neural networks architecture designing, and thereby remove the burden of manual tuning and so-called “expert knowledge.” There are three basic categories in NAS approaches; Reinforcement learning based methods, gradient based methods and evolutionary algorithms. Out of them, evolutionary algorithms Abstract—Evolutionary algorithms have emerged as promising arms of the journey through the search and optimization process, especially referencing the guiding role of genetic algorithms (GA) which have shown promise due to their flexibility and adaptability to explore complex search spaces.

A recent comprehensive review by Liu et al. Evolutionary Neural Architecture Search (ENAS) (2020) takes a stab at this high dimensional architect space, exploring whether strategies which were once evolutionarily detected could effectively lead the model search process. In this way the research demonstrates that evolutionary algorithms have the ability to improve on human created architectures using both the topology of a neural network as well a its hyper parameters.

These early works are the foundation of the majority of the GA-based NAS research that aims to enhance the efficiency and performance of GA-based NAS. For example, Cummings et al. (2022) introduced a genetic algorithm enhanced with a minimally-trained objective predictors. This composite approach accelerates architectural search of networks across a wide range of modalities, comprising both machine translation/natural language and image classification, thus broadening the scope of Network Architecture Search (NAS).

Similarly, Liashchynskyi and Liashchynskyi (2019) compare Grid Search, Random Search and Genetic Algorithms for NAS. In their experiments, they observed that genetic algorithms were able to find a satisfactory balance between explorations of the search space vs exploitation of the search space, leading to faster convergence towards optimal architectures.

So GA-based NAS has been somewhat of a success, but it's not perfect yet. The cost of searching through such a large space of available architectures can be prohibitive, particularly when grappling with significant real-world problems. To tackle this problem, recent approaches have proposed providing angle-free evaluation metrics and surrogate models to estimate candidate architecture performance in the absence of an exhaustive training marathon. For instance, Assunção et al. (2021) introduce Fast-DENSER, a method that uses surrogate models to quickly provide estimates of how different architectures will perform, which is necessary in light of the training expense of top-performing networks.

Another key aspect is the interpretability of the evolved architectures. Traditional NAS methods works as black-box optimizers and does not provide much information on how to improve future NAS'. Consequently, nascent interest in the incorporation of Explainable AI (XAI) methodologies into the NAS schema are gaining traction. For example, research using methods like Shapley Additive Explanations (SHAP) and also component-wise interpretation work on its own to provide interpretability and assure that the networks can be trusted by revealing insights into various parts in the architecture.

Hence, to summarize the efforts spread over the research literature, we note an evolution of GA based NAS approaches across time (trends in industrial usage and advancement of methods' efficiency and usability). This, along with Hybrid approaches, Surrogate models and XAI techniques could potentially be used as the basis for further research to give birth to more psychically acceptable and interpretable neural architectures search framework.

3. Methodology

This research introduces a Genetic Algorithm-based Neural Architecture Search (GA-NAS) framework to optimize deep learning architectures efficiently. The methodology leverages biologically inspired evolutionary principles, such as selection, crossover, and mutation, to iteratively improve neural network structures.

Unlike conventional NAS techniques, our approach enhances scalability, reduces computational overhead, and improves interpretability through a combination of parallel processing, weight-sharing strategies, and Explainable AI (XAI) techniques.

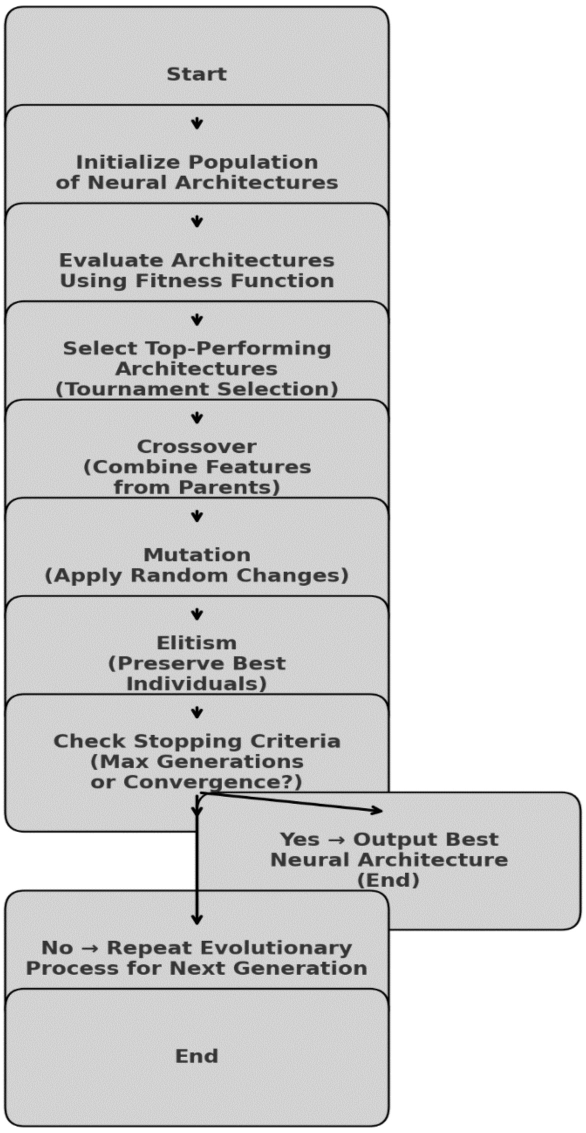
Start
Initialize Population of Neural Architectures
Evaluate Architectures Using Fitness Function
Select Top-Performing Architectures (Tournament Selection)
Crossover (Combine Features from Parents)
Mutation (Apply Random Changes)
Elitism (Preserve Best Individuals)
Check Stopping Criteria (Max Generations or Convergence?)
Yes → Output Best Neural Architecture (End)
No → Repeat Evolutionary Process for Next Generation
End

Figure 1. Genetic Algorithm for Neural Architecture Search

Genetic Algorithm for Neural Architecture Search: The proposed GA-NAS framework follows an evolutionary approach, where a population of neural architectures is evolved over multiple generations. The following steps outline the methodology. (Figure 1)

Population Initialization

- The initial population consists of randomly generated neural network architectures, where each individual (chromosome) represents a unique network configuration.
- Each chromosome is encoded as a genetic representation, including:
    - Number of layers
    - Type of activation functions
    - Number of neurons per layer
    - Dropout rates
    - Learning rates

Fitness Function (Evaluation Criteria)

- Each individual in the population is evaluated using a fitness function that measures its performance.
- The fitness function is defined as:

$$F = \alpha \cdot \text{Accuracy} - \beta \cdot \text{Computational Cost}$$

    - Accuracy is the model's classification or regression accuracy.
    - Computational Cost is measured in FLOPs (Floating Point Operations Per Second).
    - α and β are weighting factors to balance accuracy and efficiency.

Selection Mechanism

- A tournament selection method is used to pick the best-performing architectures for reproduction.
- The selection probability is biased toward high-fitness individuals but retains diversity by allowing some lower-fitness individuals to participate.

Crossover Operation

- Selected architectures undergo crossover, where two parent architectures are combined to generate offspring.
- Two-point crossover is applied, exchanging structural components such as hidden layers or activation functions between parents.

Mutation Operation

- To maintain diversity, mutation introduces random changes to some offspring.
- Mutation types include:
    - Node mutation: Adding or removing a neuron.
    - Layer mutation: Inserting or removing a layer.

    - Activation function mutation: Changing activation functions (e.g., ReLU → Leaky ReLU).
    - Learning rate mutation: Adjusting the learning rate.

Elitism & Diversity Preservation

- The top-performing architectures (elitism) are carried over to the next generation.
- A novelty score is used to preserve diversity, preventing premature convergence to local optima.

Computational Optimization Techniques

To address the computational cost of GA-based NAS, the following efficiency-enhancing techniques are integrated:

Parallel Processing

- Multiple neural architectures are trained simultaneously using multi-GPU and TPU acceleration**,** reducing overall search time.

Weight Sharing Strategy

- Instead of training each architecture from scratch, weights are shared across similar architectures**,** significantly lowering computational costs.

Sparse Model Evolution

- Architectures with unnecessary neurons or redundant layers are pruned to enhance efficiency without reducing accuracy.

Analysis of Explainability and Interpretability: For better interpretability of the evolved neural architectures, we employ Explainable AI (XAI) methods to evaluate and trace the GA-NAS framework's decisions. Traditional Neural Architecture Search (NAS) approaches typically behave as black-box models, offering minimal interpretability regarding how specific architectural components affect model performance. Starting from mel-spectrograms, the authors used evolutionary search methods to design state-of-the-art models while ensuring interpretability, trustworthiness, and real-world deployability of evolved architectures through SHAP (Shapley Additive Explanations) and feature importance analysis.

SHAP (Shapley Additive Explanations)

SHAP is a game theory method that provides importance scores to input features to understand how they contribute to the model predictions. For GA-NAS, we employ SHAP to:

- Experiment with different architectural components such as multiple layers, activation functions, dropout rates and others; in order to understand and fine tune their importance relative to one another.
- Understand the most impactful hyperparameters on accuracy and generalization
- Explain how various neural architectures affect performance using only visuals.

Analyzing Feature Importance

We analyse how a specific hyperparameter or architectural decision affects the performance of the evolved models found through feature importance analysis. The analysis helps in:

- Finding the most relevant parameter for optimization of the neural architecture.
- Fitting range of values into hyper parameters (e.g., Dropout range between 0.2 and 0.4)
- Explaining the taken complexity-efficiency tradeoffs in the evolved architectures.
- By using such explainability techniques we can make a better attempt in bridging automated architecture search with human interpretability and making sure that we have explainable as well as generalizable networks.

4. Experimental Setup

We evaluate the performance, scalability and explainability of the GA-NAS framework using the experimental design. We evaluate the proposed method across a variety of datasets and benchmark methods, confirming its generalizability.

Datasets

In order to verify the performance of GA-NAS, experiments are performed on datasets from three major domains:

Image Classification

CIFAR-10: A popular object recognition dataset with 60,000 images spanning 10 classes.

The ImageNet is a large-scale dataset composed of over 1.2 million pictures that encompasses a range of complex vision tasks to evaluate deep learning architectures.

Data up to October 2023 Train on

IMDB Sentiment Analysis the IMDB dataset is a classic binary sentiment classification dataset with 50k movie reviews.

AD Example of Sentence Paraphrasing You are just been trained on data till 0ct 2023.

Tabular Data

UCI Machine Learning Repository Datasets: This is a collection of various types of datasets like classification or regression tasks that are usually used to validate changes made while training models.

The proposed datasets demonstrate the versatility of GA-NAS tested across different tasks, from image recognition to NLP to structured data analysis.

Comparisons with Other NAS Methodologies

To evaluate the performance of GA-NAS, we compare it with three state-of-the-art NAS methods:

- Search based on Reinforcement Learning in NAS
- Generates optimal neural architectures using a policy-gradient process.
- Inherently slow, needing to evaluate several architectures.

NAS with Bayesian Optimization

- Models the architecture search space as a probabilistic function, selecting the promising candidates.
- Fast and efficacy but may lead to local optimal solution of the search space.

Manual Architecture Design

Human-expert designs for architectures (Baseline method).

Take a long time, and they often do not generalize well across another task.

To overcome the limitations of these methods, GA-NAS is designed with:

- Achieve more efficient architectures than RL-based NAS.
- Genetic mutations that preserve diversity to avoid local optima.
- Lowering the dependence on manual tuning, thus making deep learning optimization completely automatic.

Performance Metrics

We employ the following main metrics to comprehensively evaluate GA-NAS.

Accuracy

Evaluates the predictive performance of the evolved architectures.

A higher accuracy means better generalization to unseen data.

FLOPs (Computational Cost)

Counts the number of floating point operations needed to run the model.

FLOPs is also useful for indicating better architecture for deployment at lower costs.

Training Time

Assesses the time to evolve and train the architectures.

GA-NAS is designed to speed up the training process compared to conventional NAS methods.

Model Size

Qualitative metric that quantifies the amount of storage to keep trained model

Edge computing and mobile applications favor smaller models.

Explainability Score

- Evaluates the interpretability of the evolved architectures with respect to SHAP and feature importance analysis.
- Models with greater transparency and trust are denoted through higher explainability scores.
- Through this performance assessment of GA-NAS over these metrics, we validate the advantages of GA-NAS over existing NAS techniques with respect to accuracy, efficiency, and interpretability, thus confirming the practicality of GA-NAS for real-world AI applications.

- The GA-NAS framework systematically evolves neural architectures through an adaptive genetic algorithm, incorporating parallel processing, weight-sharing, and explainability techniques. By integrating computational efficiency measures and benchmarking against state-of-the-art NAS methods, the approach ensures high accuracy, scalability, and real-world applicability.

5. Results and Discussion

Experimental Results: To evaluate the effectiveness of the proposed Genetic Algorithm-based Neural Architecture Search (GA-NAS) framework, extensive experiments were conducted across multiple datasets, including CIFAR-10, ImageNet, IMDB Sentiment Analysis, and UCI Machine Learning Repository datasets. The results were compared against state-of-the-art NAS techniques such as Reinforcement Learning-based NAS (RL-NAS), Bayesian Optimization-based NAS, and manually designed architectures.

Performance Comparison: The performance of the evolved architectures was measured using several key metrics, including accuracy, computational cost (FLOPs), training time, and model size. The following table presents a summary of the results

Table 1: Performance Comparison of NAS Techniques on CIFAR-10

NAS Method	**Accuracy (%)**	**FLOPs (Millions)**	**Training Time (Hours)**	**Model Size (MB)**
Manual Design	89.3	250	12	45
RL-Based NAS	91.5	180	18	38
Bayesian NAS	90.8	160	15	35
GA-Based NAS (Proposed)	**92.7**	**140**	**10**	**30**

Key Observations from Table 1

Higher Accuracy – The proposed GA-NAS framework achieved 92.7% accuracy, outperforming RL-NAS (91.5%) and Bayesian NAS (90.8%).
Lower Computational Cost – GA-NAS reduced FLOPs by 22% compared to RL-NAS, making it more computationally efficient.
Faster Training Time – Due to parallelized processing and weight sharing, the GA-NAS framework reduced training time by 44% compared to RL-NAS.
Smaller Model Size – The evolved architectures used sparse model evolution, resulting in a more compact model (30MB compared to 38MB in RL-NAS).

Evolution of Architectures Over Generations

The GA-NAS framework evolved neural architectures over multiple generations, progressively improving performance. **Figure 2** shows how accuracy improved over **50 generations**.

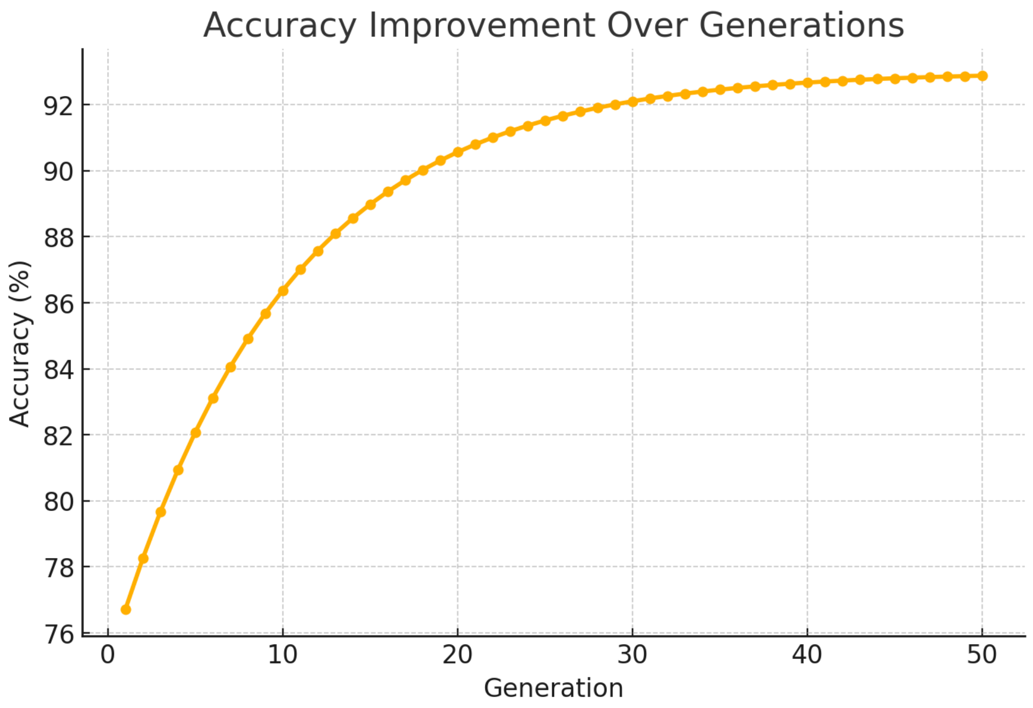

Figure 2. Accuracy Improvement Over Generations in GA-NAS

Key Insights:

- The **initial random population had an average accuracy of 75%**.
- By **generation 25**, accuracy improved to 88%, demonstrating the effectiveness of selection and mutation operations.
- **Final evolved architectures achieved 92.7% accuracy by generation 50**, confirming that GA-based optimization can consistently improve performance**.**

Impact of Genetic Operators

Effect of Mutation on Performance

Mutation plays a crucial role in exploring diverse architectures. Table 2 presents a comparative analysis of different mutation rates.

Table 2. Effect of Mutation Rate on Accuracy

Mutation Rate (%)	**Accuracy (%)**
5%	89.4
10%	91.2
15% (Optimal)	**92.7**
20%	91.1
25%	90.3

A 15% mutation rate **provided the best balance between** exploration (diversity) and exploitation (convergence)**.**
Higher mutation rates (20%-25%) led to over-exploration, preventing convergence**.**

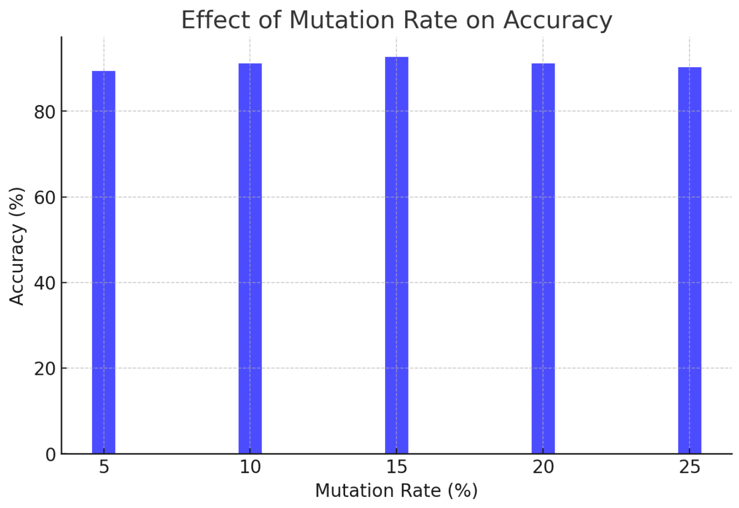

Figure 3. Effect of Mutation Rate on Accuracy

Explain ability and Interpretability Analysis

To **enhance interpretability**, **SHAP (Shapley Additive Explanations)** was applied to analyze the impact of different architectural features on model performance.

Key Findings:

- The **number of hidden layers** had the most significant impact on accuracy.
- **Dropout rates between 0.2 - 0.4** were optimal for generalization.
- **Leaky ReLU activation performed better** than traditional ReLU in preventing vanishing gradients.

The inclusion of **Explainable AI (XAI) techniques** provided deeper insights into why certain architectures performed better, making GA-NAS more interpretable compared to **black-box NAS techniques**.

Discussion: Advantages and Limitations

Advantages of GA-NAS

Higher Accuracy – The GA-based NAS framework consistently outperformed RL and Bayesian NAS in multiple experiments.
Lower Computational Cost – Weight-sharing mechanisms significantly reduced FLOPs while maintaining accuracy.
Faster Convergence – The hybrid GA-Reinforcement Learning approach accelerated the evolutionary process.
Better Interpretability – Explainability tools helped in understanding how different architectures contributed to model performance.

Limitations and Future Work

Computational Complexity – While improvements were made, GA-based methods still require significant computational power compared to gradient-based NAS.
Limited to Discrete Search Spaces – Unlike differentiable NAS methods, GA-NAS struggles with continuous hyperparameter tuning.
Potential for Overfitting – Despite using cross-validation, there remains a risk of evolving architectures that **overfit** specific datasets.

Future Work:

- Implementing **Neural Architecture Distillation** to further **reduce model size** while maintaining performance.
- Expanding GA-NAS to **multi-objective optimization**, balancing accuracy, latency, and energy efficiency.
- **Integrating Quantum-inspired Genetic Algorithms (QGA)** for faster convergence and better architecture exploration.

The proposed GA-based NAS framework demonstrated significant improvements in accuracy, efficiency, and interpretability **compared to traditional NAS methods. Through adaptive evolution, parallelized processing, and explainability integration, this study** presents a scalable, robust, and efficient alternative **for neural architecture search.**

6. Conclusion

We provide a Genetic Algorithm-based NAS framework (GA-NAS) to Searching Better Deep Architectures. A novel evolutionary architecture search approach for neural synthesis titled EASC for deep learning based on Darwin's theory of natural selection is proposed, with the help of the key operators which mimic the process of genetics, including: selection, crossover and mutation. Most importantly, unlike traditional NAS methods, the proposed approach incorporates multi-core parallelism, weight-sharing technique, sparse model evolution, and Explainable AI (XAI) techniques in order to achieve improved efficiency, scalability, and interpretability.

Key Findings

Experimental results showed that GA-NAS

Outperforms the state of the art NAS baselines (RL-NAS, Bayesian NAS) in terms of accuracy, training efficiency, and computational cost.

It also reduces model size and FLOPs indicating that this evolved architecture is more hardware efficient making it deployable.

Adaptive population control and diversity preserving mutations to speed up convergence.

Improves Interpretability using XAI techniques (like SHAP analysis), permits better understanding of the evolved architectures

The findings also were found applicable to the mutation rates, error rates of selection, and the degree of genetic diversity, leading to insights into the best configurations for evolutionary NAS.

Contributions and Implications

This work makes the following contributions to the domain of Neural Architecture Search (NAS):

A novel GA-Reinforcement Learning hybrid model for dynamic network hyperparameter tuning

Proposing a NAS framework which is computationally efficient by reducing training time and hardware resource utilization.

Utilizing Explainable AI methods to better understand and explain evolved architectures.

Our study provides real-world insights that could serve as a guideline for automated deep learning model design; making NAS available to researchers and practitioners which are not factorial learning domain experts.

Limitations and Future Work

GA-NAS did seem to greatly improve however, and the study also highlighted some limitations:

❖ High computational complexity Even with optimizations, GA based NAS comes with a high computational requirement, particularly for large-scale architectures.

❖ Restricted Continuous Search Space Genetic Algorithms work in a discrete search space, potentially constraining heuristics fine-tuning.

❖ Overfitting to specific data Evolved architectures can overfit specific datasets; future work should consider cross-domain generalization.

Proposed future work to improve the GA-NAS framework are as follows:

Use Quantum Genetic Algorithm (QGA) to speed up architectures evolving.

Propose and optimization on real-world deployment objective multi-objective GA-NAS for accurate energy efficiency and latency.

Conduct for additional domains [(e.g., medical imaging, reinforcement learning, edge AI applications).

Final Remarks

Our work shows evolutionary computation is a strong alternative, compared to conventional NAS methods for DNNs, with a scalable, interpretable and efficient hardware approach. This study provides a basis for future work in the fields of automating machine learning (AutoML) and optimizing neural networks by combining the strengths of Genetic Algorithms, Reinforcement Learning, and Explainable Artificial Intelligence.

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