

NADER: Neural Architecture Design via Multi-Agent Collaboration

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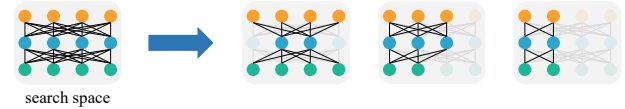
Abstract

Designing effective neural architectures poses a significant challenge in deep learning. While Neural Architecture Search (NAS) automates the search for optimal architectures, existing methods are often constrained by predetermined search spaces and may miss critical neural architectures. In this paper, we introduce NADER (Neural Architecture Design via multi-agent collaboration), a novel framework that formulates neural architecture design (NAD) as a LLM-based multi-agent collaboration problem. NADER employs a team of specialized agents to enhance a base architecture through iterative modification. Current LLM-based NAD methods typically operate independently, lacking the ability to learn from past experiences, which results in repeated mistakes and inefficient exploration. To address this issue, we propose the Reflector, which effectively learns from immediate feedback and long-term experiences. Additionally, unlike previous LLM-based methods that use code to represent neural architectures, we utilize a graph-based representation. This approach allows agents to focus on design aspects without being distracted by coding. We demonstrate the effectiveness of NADER in discovering high-performing architectures beyond predetermined search spaces through extensive experiments on benchmark tasks, showcasing its advantages over state-of-the-art methods. The code is available at <https://github.com/yang-zekang/NADER>.

1. Introduction

Recent advancements in Large Language Models (LLMs) have significantly impacted various fields thanks to their exceptional ability to integrate knowledge and follow instructions [1, 35]. Leveraging techniques such as chain-of-thought reasoning [37], Retrieval-Augmented Generation (RAG) [18], and multi-agent collaboration frameworks [26], LLMs show great potential in creative tasks,

Neural Architecture Search (NAS)



Neural Architecture Design (NAD)

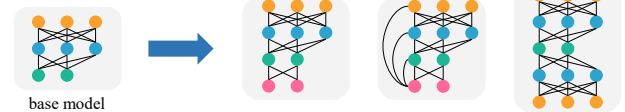


Figure 1. Traditional Neural Architecture Search (NAS) approaches aim to discover high-performing neural architectures within an expert-defined search space. In contrast, Neural Architecture Design (NAD) is not constrained by predefined search spaces, allowing for the exploration of entirely new architectures.

including software development [14], neural architecture search [48], hyperparameter optimization [43, 46], and scientific discovery [23]. Designing neural architectures that meet specific performance criteria (e.g., high accuracy or low latency) remains a significant challenge in deep learning. This process often involves extensive manual efforts and costly trial-and-error cycles. To address these challenges, existing studies have leveraged Neural Architecture Search (NAS) to automate the discovery of high-performing architectures, achieving notable results across diverse domains [21, 49]. However, as shown in Figure 1, traditional NAS methods rely on expert-defined search spaces, limiting their capacity to uncover truly novel architectures.

Motivated by advancements in large language models (LLMs), recent research has explored a new direction in Neural Architecture Design (NAD) driven by LLMs, moving beyond conventional predetermined search spaces. Unlike traditional NAS approaches, NAD fosters innovation by enabling the exploration of entirely new architectures within an open architecture space. However, this endeavor presents several challenges. First, many existing studies [3, 7] rely on evolutionary computation or reinforcement learning for architecture modifications, which often result in inefficient, undirected exploration, leading to training and evaluation of an overwhelming number of neural network

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architectures. Second, existing LLM-based methods [30, 36] perform NAD tasks independently, without benefiting from immediate feedback or past experiences, leading to repeated mistakes and unnecessary trial-and-error processes. Additionally, code-generating LLMs [3, 30] often struggle to maintain focus on neural architecture design, becoming sidetracked by non-essential aspects like text style and code syntax. Such distractions can significantly diminish the efficiency of the automatic exploration.

To tackle these challenges, we propose NADER (Neural Architecture Design via multi-Agent collaboRation), an LLM-driven NAD method. NADER begins with a well-established network, such as ResNet [13], and seeks to enhance it through iterative modifications. The framework comprises a research team and a development team, each consisting of multiple collaborating agents. This multi-agent approach facilitates more efficient and directed exploration. The research team is responsible for proposing improvement proposals based on insights drawn from recent academic literature and model optimization trees. Each proposal contains a model to be improved and a modification suggestion. Subsequently, the development team implements these proposals and evaluate the performance of the modified network. The performance is then relayed back to the research team, informing subsequent proposals and fostering a continuous cycle of improvement.

“Error is often the correct guide.” We introduce the Reflector, which effectively incorporates immediate feedback from the external environment and leverages historical experiences. Reflector tracks the behavior of Modifier and reflect on it to gain experience. Given the proposed modification suggestions, the Reflector queries the experience pool to retrieve relevant experience, providing the Modifier with contextual information for implementation. This reduces the likelihood of repeating past mistakes and increases the success rate of a good modifications.

Furthermore, to help the development team concentrate on network structure, we propose a graph-based network representation. Instead of generating executable code directly, NADER represents neural architectures as single directed acyclic graphs (DAGs), where nodes represent operations (*e.g.*, convolution, normalization) and edges denote information flow. This graph representation allows NADER to prioritize high-level structural decisions, avoiding distractions from low-level code implementation details.

We demonstrate the effectiveness of NADER in discovering high-performing neural architectures that extend beyond predetermined search spaces. Through extensive experiments, we showcase the advantages of NADER over state-of-the-art NAS and NAD methods. Our contributions are summarized as follows:

- We introduce NADER, a novel LLM-driven framework for neural architecture design that utilizes a multi-agent

collaboration strategy to automatically explore novel neural architectures beyond predetermined search spaces.

- We introduce Reflector, which effectively incorporates immediate feedback from the external environment and experiences reflected from historical trajectories, thereby reducing repeated mistakes and enhancing efficiency.
- We introduce a graph-based representation for neural network architectures, facilitating a focus on high-level structural decisions while minimizing distractions from low-level coding details.

2. Related Work

2.1. Neural Architecture Search (NAS)

NAS aims to automatically discover optimal neural network architectures from predefined search spaces. NAS methods have achieved impressive success across various tasks. Early approaches relied on reinforcement learning [27, 38], evolutionary strategies [31] and Bayesian optimisation [16] to explore the search space. More recent methods have shifted towards weight sharing techniques. These approaches [5, 8, 9, 15, 21, 41, 42, 44, 45] train a single super-network, enabling efficient exploration of various sub-networks (architectures) within the search space. However, these methods often rely on predetermined search spaces, which limits their ability to discover truly novel architectures. In contrast, our approach addresses the Neural Architecture Design (NAD) task, which is not restricted by predetermined search spaces.

2.2. LLM Agents

As large language models have demonstrated impressive emergent capabilities and have gained immense popularity, recent research has focused on LLM-based autonomous agents to solve complex problems [40]. These agents utilize the foundational capabilities of LLMs, displaying remarkable skills in memory [26], planning [22], tool use [29, 32], and reflection [34, 47]. Systems like Visual ChatGPT [39] and HuggingGPT [33] employ LLMs to orchestrate diverse AI models for complex tasks. Visual programming approaches like [12] utilize LLMs to generate programs for solving visual tasks based on natural language instructions. There are also studies on multi-agent communication [20] and collaboration [4, 14, 28]. For example, MetaGPT [14] utilizes an assembly line paradigm, assigning roles to LLM-based agents for collaborative problem-solving. Our work extends this concept by introducing a team of specialized LLM agents for neural architecture design.

2.3. LLMs for NAS

Emerging research explores the use of LLMs for NAS. GENIUS [48] is a LLM-based NAS algorithm that adopts a straightforward prompt-based search process that prompts

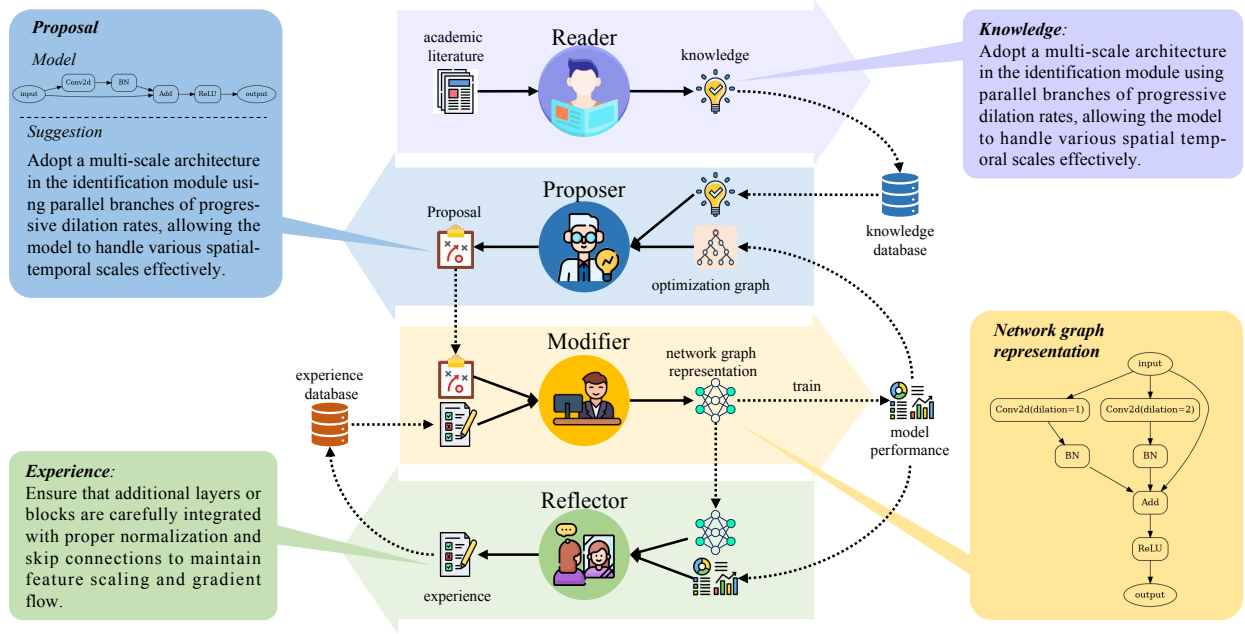


Figure 2. Overview of NADER framework. The Reader continuously learns from academic literature, while the Proposer identifies the most promising candidate networks and suggests modifications. The Modifier implements these suggestions, and the Reflector analyzes and provides feedback on the results. The performance of the modified network is relayed back to the Proposer, informing subsequent proposals and fostering a continuous cycle of improvement.

GPT-4 to propose designs from a given search space with a handful of examples. EvoPrompting [3] utilizes code-LLMs as mutation and crossover operators for an evolutionary neural architecture search (NAS) algorithm. LL-Matic [25] extends EvoPrompting by introducing quality diversity algorithms to discover diverse and robust solutions. Our work differentiates them by introducing a multi-agent framework, allowing for a more sophisticated and collaborative exploration of the search space.

3. Neural Architecture Design via Multi-Agent Collaboration

3.1. Overview

We present the Neural Architecture Design via Multi-Agent Collaboration (NADER) system, a novel approach for neural architecture design that harnesses the capabilities of large language models (LLMs) and multi-agent collaboration. This system begins with a base network and iteratively refines its structure for optimal performance.

As illustrated in Figure 2, NADER is composed of a Research Team (Reader and Proposer) and a Development Team (Modifier and Reflector). The Reader is responsible for extracting knowledge from the latest academic literature, ensuring that the system stays current with recent advancements. The Proposer utilizes the knowledge provided by the Reader to generate modification proposals, which in-

clude a candidate network and a corresponding modification suggestion. The Modifier practically implements these proposals to get new networks and their corresponding performance metrics. Algorithm 2 shows the design process of neural architecture. The Reflector tracks and reflects on Modifier’s logs and offers guidance to Modifier.

3.2. Graph-based Neural Architecture Representation

The initial step in Neural Architecture Design (NAD) involves defining a representation for network architectures. While LLMs excel at understanding and generating program code, this can be suboptimal for NAD scenarios. Program code often contains extraneous information, such as text style and formatting, which can distract LLMs from focusing on the network structure, thereby reducing exploration efficiency. To address this issue, we introduce a graph-based representation for network structures. As shown in Figure 3, each neural network architecture can be represented as a single directed acyclic graph (DAG). In this graph, nodes correspond to input, output and fundamental operators within a neural network (e.g., convolutional layer, matrix addition), and an edge from operator N_i to operator N_j indicates that N_j receives the output of N_i as input.

This graph representation eliminates irrelevant factors, allowing LLMs to concentrate solely on network structure design without being bogged down by low-level implemen-

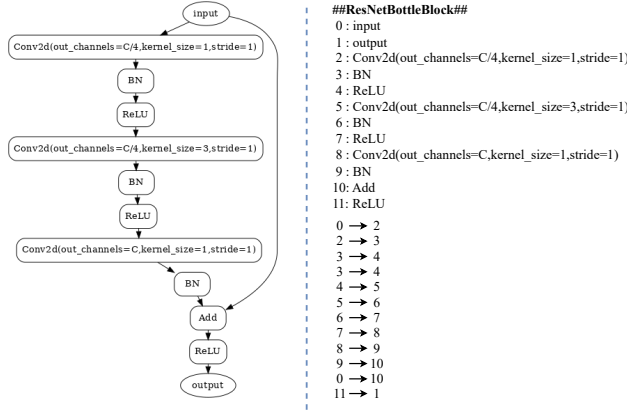


Figure 3. Illustration of graph-based neural architecture representation. **Left:** Visualization of DAG. **Right:** Text representation of DAG for LLM understanding.

tation details. Meanwhile, the graph representation can easily and accurately check whether different neural architectures are isomorphic, which can help organize neural architecture optimization paths more effectively. Furthermore, the graph representation is more compact and efficient, as it can be represented with fewer tokens. In addition, such a representation is more readable and easier to understand. In NADER, this graph representation is utilized for both the input and output of the agents.

3.3. Research Team

The Research Team is responsible for providing high-level network improvement proposals, a crucial aspect of NAD. The team is comprised of a Reader agent and a Proposer agent. The Reader agent distills knowledge from academic literature, ensuring the system is informed by the latest developments. The Proposer agent then leverages this knowledge to generate high-quality improvement proposals.

3.3.1. Reader

Staying current with the latest academic developments is crucial for neural architecture design. However, LLMs often lag behind the latest knowledge and struggle to absorb new information, hindering their ability to propose novel and valuable improvements. To overcome this challenge, we propose the Reader agent for literature-based knowledge discovery. Algorithm 1 illustrates this process. The Reader agent analyzes recent academic papers on neural architectures and related advancements. It automatically downloads recent articles from websites, evaluates their relevance to neural architecture design, and extracts key knowledge and novel ideas that could potentially improve neural network performance. These knowledge are then archived in a database for future use. **Relevant Papers Selection.** A large number of crawled papers may not be relevant to neural architecture design. Reader quickly find potentially use-

Algorithm 1 Knowledge extraction process of Reader

Require: Papers $\{P_i\}_{i=1}^N$ and their abstracts $\{A_i\}_{i=1}^N$; Knowledge vector database $\mathcal{K}$; A pre-trained LLM; Text to embedding model $\mathcal{M}$.

Ensure: Updated $\mathcal{D}_{insp}$.

```

1: Initialize the agent Reader with the LLM.
2: for  $i \leftarrow 1$  to  $N$  do
3:   if Reader judge the  $P_i$  is relevant based on  $A_i$  then
4:      $ks \leftarrow$  Reader extracts knowledge from  $P_i$ .
5:     for each element  $k$  in  $ks$  do
6:        $embed \leftarrow \mathcal{M}$  extracts the embedding of  $k$ .
7:        $\mathcal{K} \leftarrow$  Update  $\mathcal{K}$  with  $embed$  and  $k$ .
8:     end for
9:   end if
10: end for

```

ful papers by reading paper abstracts. **Knowledge Extraction.** The content of a paper is usually lengthy. By focusing on the method section of the paper, Reader can better extract the core innovation of the paper and summarize the inspiration that may be useful for neural architecture design.

3.3.2. Proposer

The Proposer agent is responsible for guiding the architecture modification process. By strategically navigating the model modification graph and selecting the most promising candidate network and proposing modification suggestions, the Proposer agent optimizes the overall architecture design process, maximizing the potential for performance improvements while minimizing the risk of exploring unproductive paths. **Network Modification Tree.** Network modification tree records the history of modification during NAD. The tree's root represents the basic network, with each node representing a modified network architecture and each edge representing an applied modification suggestion. The performance of each node is recorded within the graph. **Candidate Network Selection.** Given the network modification graph, the Proposer selects the most promising node as the candidate network for the next modification. The Proposer leverages the performance data recorded within the graph to guide its selection. It prioritizes nodes with higher performance scores, indicating successful past modifications. Specifically, it explores the network modification graph using a combination of depth-first search (DFS) and breadth-first search (BFS). DFS allows for a deeper exploration of promising paths within the graph, while BFS ensures a wider coverage of the search space. **Modification Suggestion Selection.** The knowledge pool constructed by the Reader are abundant and vary in quality. The Proposer selects a set of promising knowledge from the database as the suggestions to be applied to the chosen candidate network. It uses reflections from previous experiences to retrieve modification suggestions at different similarity levels, balancing exploration of novel ideas with the exploitation of

Algorithm 2 Neural architecture design process of NADER

Require: The initial architecture $arch_0$; A pre-trained LLM; Knowledge database $\mathcal{K}$; Design experience database $\mathcal{E}$; Number of architectures to generate N ; Max number of retry after failed max_retry .

Ensure: Best architecture $arch_{best}$; Historical records $\mathcal{H}$; Network modification tree $\mathcal{T}$.

```
1: Initialize the Proposer and Modifier with LLM.
2: Initialize model optimization tree  $\mathcal{T}$  with  $arch_0$ .
3:  $n \leftarrow 0$  Initialize the number of architectures generated.
4: while  $n < N$  do
5:    $insps \leftarrow$  Retrieve inspirations from  $\mathcal{K}$ .
6:    $prop \leftarrow$  Proposer generate a proposal based on  $insps$  and  $\mathcal{T}$ .
7:    $e \leftarrow$  Retrieve experiences from  $\mathcal{E}$  by query  $prop$ .
8:    $conv \leftarrow$  Initialize conversation with  $prop$  and  $e$ .
9:   for  $i \leftarrow 1$  to  $max\_retry$  do
10:     $arch_n \leftarrow$  Modifier generate a new architecture according to  $conv$ .
11:     $error \leftarrow$  Check the correctness of  $arch_n$ .
12:     $conv \leftarrow$  Update  $conv$  with  $arch_n$  and  $error$ .
13:    if  $error$  is empty then break
14:  end for
15:  if  $error$  is empty then
16:     $arch\_acc_n \leftarrow$  Train architecture  $arch_n$  on train dataset and get its test accuracy on test dataset.
17:     $\mathcal{T} \leftarrow$  Update  $\mathcal{T}$  with  $prop$ ,  $arch_n$  and  $arch\_acc_n$ .
18:     $n \leftarrow n + 1$ 
19:  end if
20:   $\mathcal{H} \leftarrow$  Update  $\mathcal{H}$  with  $prop$ ,  $conv$  and  $arch\_acc_n$ .
21: end while
22:  $arch_{best} \leftarrow$  Get the best architecture from  $\{arch_i\}_{i=1}^N$ .
```

past successes. It prioritizes suggestions that have proven effective in similar contexts or that address common error patterns identified during past modifications.

3.4. Development Team

The Development Team is responsible for implementing the architectural modifications suggested by the Research Team. Its goal is to make reasonable and accurate changes to the neural architecture. The team consists of the Modifier and the Reflector, which collaborate through a multi-round dialogue to refine and correct the design.

3.4.1. Modifier

The Modifier agent modifies the given architecture based on the modification suggestions. It performs modifications hierarchically, starting from a single block and progressing to the entire network. Initially, it implements a new cell block using the candidate block and modification suggestions. This process considers both macro-level guidance (e.g., introducing multi-scale information) and micro-level design experience (e.g., residual connections before out-

Algorithm 3 Design experience extraction process

Require: Historical records $\mathcal{H}$; Design experience vector database $\mathcal{E}$; Network modification tree $\mathcal{T}$; A pre-trained LLM; Text to embedding model $\mathcal{M}$.

Ensure: Updated $\mathcal{E}$.

```
1: Initialize the agent Reflector with LLM.
2: for each  $h_i$  in  $\mathcal{H}$  do
3:    $p_i, arch_i, arch\_acc_i, error_i \leftarrow$  Get proposal, architecture, test accuracy and error information from  $h_i$ .
4:    $arch_j, arch\_acc_j \leftarrow$  Get the father architecture and its test accuracy of  $arch_i$  from  $\mathcal{T}$ .
5:    $e_i \leftarrow$  Reflector reflects on  $(arch_i, arch\_acc_i, arch_j, arch\_acc_j, error_i)$ .
6:    $pe_i \leftarrow \mathcal{M}$  extracts the embedding of  $p_i$ .
7:    $\mathcal{E} \leftarrow$  Update  $\mathcal{E}$  with key  $pe_i$  and value  $e_i$ .
8: end for
```

put). Given the new cell block, it then implements corresponding and compatible stem and downsample blocks. The prompt for this step includes: (1) the cell block structure, (2) examples cell blocks and their corresponding stem blocks, and (3) design principles (e.g., downsampling by at least $2\times$ in the stem to prevent memory overflow). **Isomorphic Graph Checking.** When the newly generated neural architecture is detected to be isomorphic to the existing neural architecture, no repeated training is performed. **Graph-to-Code Conversion.** NADER adopts the graph representation for neural network architectures. Once a valid computational graph is designed, this component translates the graph representation into executable code.

3.4.2. Reflector

The Reflector agent tracks, analyzes and reflects on the results of the Modifier to support the modification process. **Learn from Immediate Feedback (LIF).** We have developed a computational graph flow verification tool to ensure the generated neural architecture is valid and executable. It checks the connectivity and information flow within the computational graph, verifying that all operations are properly connected and that the overall structure is coherent. Given the neural architecture implemented by the Modifier, the Reflector utilizes this verification tool to analyze its executability. If an invalid structure is generated, the agent communicates with the Modifier to retry and correct the errors. **Learn from Design Experience (LDE).** The Reflector also plays a crucial role in learning from historical records and summarizing design experience to guide future design process, Algorithm 3 demonstrates the process by which Reflector extracts design experience from historical records. It tracks the Modifier’s historical records, including both successes and failures. (1) Failure Records: This category stores records of modifications that led to a decrease in performance or resulted in an invalid architecture. (2) Failure-to-Success Records: This cate-

gory stores records of modifications that initially failed but were later corrected. (3) Success Records: This category stores records of successful modifications that led to an improvement in performance. The Reflector analyzes the error causes associated with each failure record, generating design experience and categorizing them based on the type of error (*e.g.*, invalid connection, memory overflow, performance degradation). This analysis helps identify common error patterns and develop strategies for avoiding them in future design. To facilitate efficient retrieval of relevant experience, the Reflector utilizes a database where queries are modification suggestions, and keys are lists of error/success experience for base, stem, and downsample blocks. For each modification trial, the Reflector queries the database using the proposed modification suggestion as input. It then retrieves 5 related design experience from the database, based on the similarity between the current suggestion and past records. The Reflector then provides these 5 relevant experience as context to the Modifier. The Modifier leverages the context to make more informed decisions during the design process, reducing the likelihood of repeating past errors and increasing the success rate of the design.

4. Experiment and Analysis

4.1. NAD Benchmark

To facilitate developing and evaluating LLM-based Neural Architecture Design (NAD), we create a comprehensive benchmark dataset. We established five types of basic blocks as our starting points: (1) ResNet base block, (2) ResNet bottleneck block, (3) GoogLeNet block, (4) ConvNeXt block and (5) SE-ResNet block. For each basic block, we used GPT-4o to generate some initial macro-level and micro-level modification suggestions. We manually inspected and modified the generated modification suggestions, resulting in 10 high-quality macro-level and 10 micro-level modification suggestions for each basic block. There are $(10 + 10) \times 5 = 100$ test samples in total. This allows us to evaluate the system’s performance on a diverse set of architectural modifications, ranging from basic blocks to more complex structures inspired by state-of-the-art models. Macro-level modification suggestions don’t have definitive answers and are more open-ended, while the micro-level modification suggestions have more specific, ground-truth answers. For each pair of basic block and its corresponding modification suggestions, we manually checked and generated ground-truth resulting blocks for reference. It is ensured that the resulting blocks reflect the modification suggestions and were executable.

Evaluation Metrics. To assess the performance of our approach, we use the 100 test samples from the NAD benchmark to evaluate the ability to generate valid and executable architectures that adhere to both macro-level and micro-

level modification suggestions. **Executability (E):** This metric quantifies the agents’ ability to generate executable code as the percentage of successfully executable modified architectures. **Quality (Q):** This metric assesses the ability of agents to generate a neural architecture that meets the modification suggestions, quantified as the percentage of modified architectures that successfully implement the specified modification suggestions among the executable ones. **Success Rate (SR):** The success rate is a holistic metric that considers both executability and quality, providing a comprehensive measure of the approach’s effectiveness. **Number of Tokens (# Tokens):** This metric represents the cost per execution, with a higher number of generated tokens indicating increased computational expense.

4.2. Comparison with State-of-the-art Models

Experimental Setup. We conduct experiments to compare both NAS and NAD methods using the well-known NAS-Bench-201 [10] benchmark, covering evaluations on CIFAR10, CIFAR100 [17], and ImageNet16-120 [6]. The results are demonstrated in Table 1. Our NADER accepts any network as the initial network. In our experiments, we report the results of utilizing ResNet [13] as the initial network and the results of using randomly selected networks from the NAS-Bench-201 search space. We report results for designing 5 and 10 new architectures. Each result reflects the mean and standard deviation from three repeated runs with different random seed.

For NAD, the newly designed architecture can be out of the scope of the search space. To ensure fairness, (1) we constrain the architectures generated by NADER to have the same macro skeleton with NAS-Bench-201. (2) We constrain the FLOPs and parameter count of NAD methods not to exceed the largest network within the NAS search space: parameters no more than 1.5M for all datasets, FLOPs no more than 0.2 GFLOPs for CIFAR10 and CIFAR100, and FLOPs no more than 0.05 GFLOPs for ImageNet16-120. (3) Model training adhered strictly to the NAS-Bench-201 settings, maintaining the original train/validation/test splits without altering any hyperparameters.

Comparisons with NAS methods. NAS methods operate within a predetermined search space, focusing primarily on designing cell blocks for neural architectures. Given five operation choices and four nodes for each cell, the total search space expands to $5^6 = 15625$ candidate cells. We evaluated several prominent NAS algorithms, categorized as follows: (1) Random search algorithms: random search (RS) [2] and random search with parameter sharing (RSPS) [19]; (2) ES methods: REA [31]; (3) RL algorithms: REINFORCE [38] and ENAS [27]; (4) HPO methods: BOHB [11]; (5) Differentiable algorithms: DARTS [21], SETN [8], DSNAS [15], PC-DARTS [42], SNAS [41], iDARTS [45], GDAS [9], DRNAS [5], β -DARTS [44], A-

Table 1. Comparisons with state-of-the-art NAS and NAD methods. NAS is limited by the expert-defined search space, *i.e.* NAS-Bench-201, while NAD enables the exploration of entirely new architectures beyond the search space. We compare with $\diamond$ methods with parameter sharing, $\heartsuit$ methods without parameter sharing, $\star$ LLM-based methods. We report the mean validation and test accuracies for 5 three runs.

	Method	Search (archs)	CIFAR-10		CIFAR-100		ImageNet16-120	
			validation	test	validation	test	validation	test
NAS	$\diamond$ ENAS [27]	-	37.51 $\pm$ 3.19	53.89 $\pm$ 0.58	13.37 $\pm$ 2.35	13.96 $\pm$ 2.33	15.06 $\pm$ 1.95	14.84 $\pm$ 2.10
	$\diamond$ DARTS [21]	-	39.77 $\pm$ 0.00	54.30 $\pm$ 0.00	38.57 $\pm$ 0.00	15.61 $\pm$ 0.00	18.87 $\pm$ 0.00	16.32 $\pm$ 0.00
	$\diamond$ SETN [8]	-	84.04 $\pm$ 0.28	87.64 $\pm$ 0.00	58.86 $\pm$ 0.06	59.05 $\pm$ 0.24	33.06 $\pm$ 0.02	32.52 $\pm$ 0.21
	$\diamond$ DSNAS [15]	-	89.66 $\pm$ 0.29	93.08 $\pm$ 0.13	30.87 $\pm$ 16.40	31.01 $\pm$ 16.38	40.61 $\pm$ 0.09	41.07 $\pm$ 0.09
	$\diamond$ PC-DARTS [42]	-	89.96 $\pm$ 0.15	93.41 $\pm$ 0.30	67.12 $\pm$ 0.39	67.48 $\pm$ 0.89	40.83 $\pm$ 0.08	41.31 $\pm$ 0.22
	$\diamond$ SNAS [41]	-	90.10 $\pm$ 1.04	92.77 $\pm$ 0.83	69.69 $\pm$ 2.39	69.34 $\pm$ 1.98	42.84 $\pm$ 1.79	43.16 $\pm$ 2.64
	$\diamond$ iDARTS [45]	-	89.86 $\pm$ 0.60	93.58 $\pm$ 0.32	70.57 $\pm$ 0.24	70.83 $\pm$ 0.48	40.38 $\pm$ 0.59	40.89 $\pm$ 0.68
	$\diamond$ GDAS [9]	-	89.89 $\pm$ 0.08	93.61 $\pm$ 0.09	71.34 $\pm$ 0.04	70.70 $\pm$ 0.30	41.59 $\pm$ 1.33	41.71 $\pm$ 0.98
	$\diamond$ DRNAS [5]	-	91.55 $\pm$ 0.00	94.36 $\pm$ 0.00	73.49 $\pm$ 0.00	73.51 $\pm$ 0.00	46.37 $\pm$ 0.00	46.34 $\pm$ 0.00
	$\diamond$ β -DARTS [44]	-	91.55 $\pm$ 0.00	94.36 $\pm$ 0.00	73.49 $\pm$ 0.00	73.51 $\pm$ 0.00	46.37 $\pm$ 0.00	46.34 $\pm$ 0.00
	$\diamond$ Λ -DARTS [24]	-	91.55 $\pm$ 0.00	94.36 $\pm$ 0.00	73.49 $\pm$ 0.00	73.51 $\pm$ 0.00	46.37 $\pm$ 0.00	46.34 $\pm$ 0.00
	$\heartsuit$ REA [31]	500	91.19 $\pm$ 0.31	93.92 $\pm$ 0.30	71.81 $\pm$ 1.12	71.84 $\pm$ 0.99	45.15 $\pm$ 0.89	45.54 $\pm$ 1.03
	$\heartsuit$ RS [2]	500	90.93 $\pm$ 0.36	93.70 $\pm$ 0.36	70.93 $\pm$ 1.09	71.04 $\pm$ 1.07	44.45 $\pm$ 1.10	44.57 $\pm$ 1.25
	$\heartsuit$ REINFORCE [38]	500	91.09 $\pm$ 0.37	93.85 $\pm$ 0.37	71.61 $\pm$ 1.12	71.71 $\pm$ 1.09	45.05 $\pm$ 1.02	45.24 $\pm$ 1.18
	$\heartsuit$ BOHB [11]	500	90.82 $\pm$ 0.53	93.61 $\pm$ 0.52	70.74 $\pm$ 1.29	70.85 $\pm$ 1.28	44.26 $\pm$ 1.36	44.42 $\pm$ 1.49
	$\star$ GENIUS [48]	10	91.07 $\pm$ 0.20	93.79 $\pm$ 0.09	70.96 $\pm$ 0.33	70.91 $\pm$ 0.72	45.29 $\pm$ 0.81	44.96 $\pm$ 1.02
	$\star$ LLMatic [25]	2000	-	94.26 $\pm$ 0.13	-	71.62 $\pm$ 1.73	-	45.87 $\pm$ 0.96
	<i>Optimal</i>	-	91.61	94.37	73.49	73.51	46.77	47.31
NAD	$\star$ LeMo-NADe-Gemini [30]	30	82.94	81.76	52.12	52.96	30.34	31.02
	$\star$ LeMo-NADe-GPT4 [30]	30	90.90	89.41	63.38	67.90	27.05	27.70
	$\star$ NADER (Random)	0	87.67 $\pm$ 2.88	90.36 $\pm$ 2.94	64.89 $\pm$ 4.94	64.81 $\pm$ 5.13	36.56 $\pm$ 6.60	36.51 $\pm$ 7.11
		5	90.91 $\pm$ 0.46	94.20 $\pm$ 0.38	74.11 $\pm$ 0.25	74.02 $\pm$ 0.33	48.73 $\pm$ 0.19	48.72 $\pm$ 0.14
		10	91.16 $\pm$ 0.36	94.40 $\pm$ 0.23	74.41 $\pm$ 0.34	74.51 $\pm$ 0.16	<u>50.07$\pm$0.75</u>	<u>49.63$\pm$0.80</u>
	$\star$ NADER (ResNet)	0	90.83	93.97	70.42	70.86	44.53	43.63
		5	91.17 $\pm$ 0.24	94.52 $\pm$ 0.22	73.29 $\pm$ 1.86	73.12 $\pm$ 1.09	47.98 $\pm$ 0.73	47.99 $\pm$ 0.38
		10	91.18 $\pm$ 0.23	<u>94.52$\pm$0.22</u>	<u>74.71$\pm$0.45</u>	<u>74.65$\pm$0.33</u>	48.56 $\pm$ 0.83	48.61 $\pm$ 0.76
		500	91.55	94.62	75.72	76.00	50.20	50.52

DARTS; (6) LLM-based methods: GENIUS [48] and LLMatic [25]. We provide the optimal accuracy for reference (*Optimal*), which is the maximum accuracy that can be achieved in the NAS-bench-201 search space. Our findings indicate that the NADER framework is robust; even when initialized with a random network, it can be effectively optimized after just a few iterations. Notably, in nearly all scenarios, NADER consistently designs architectures that surpass the optimal accuracy achievable within the predetermined search space, demonstrating the advantages of NAD over traditional NAS methods.

Comparisons with NAD methods. We also compare NADER against the recent NAD method, LeMo-NADe [30], which employs advanced LLMs like Gemini and GPT4-Turbo to refine neural networks based on expert-generated instructions. While LeMo-NADe shows promise, it still falls short compared to more recent NAS methods in certain respects. Our NADER approach significantly surpasses LeMo-NADe in both effectiveness and efficiency. For instance, with a random base network, NADER achieved 49.63% accuracy on the ImageNet16-120 test set, compared to LeMo-NADe’s 31.02%. Further-

Table 2. Ablation studies of Research Team. Experiments are conducted on CIFAR10, CIFAR100, and ImageNet16-120 datasets. We report the results of neural architecture modifications for 5 iterations and show the mean and standard deviation from three repeated runs with different random seed. “R” and “P” represent Reader and Proposer respectively.

R	P	CIFAR-10		CIFAR-100		ImageNet16-120	
		validation	test	validation	test	validation	test
$\times$	$\times$	90.37 $\pm$ 0.65	94.01 $\pm$ 0.42	72.55 $\pm$ 0.27	72.49 $\pm$ 0.40	47.12 $\pm$ 1.26	47.14 $\pm$ 1.30
$\times$	$\checkmark$	90.73 $\pm$ 0.32	93.73 $\pm$ 0.38	73.55 $\pm$ 1.26	73.45 $\pm$ 1.32	47.88 $\pm$ 0.29	47.92 $\pm$ 0.34
$\checkmark$	$\times$	90.86 $\pm$ 0.19	91.72 $\pm$ 2.52	73.67 $\pm$ 0.85	73.37 $\pm$ 0.73	47.89 $\pm$ 1.16	47.91 $\pm$ 1.00
$\checkmark$	$\checkmark$	90.91$\pm$0.46	94.20$\pm$0.38	74.11$\pm$0.25	74.02$\pm$0.33	48.73$\pm$0.19	48.72$\pm$0.14

more, NADER requires only 10 trials—three times fewer than LeMo-NADe. These results highlight the potential of leveraging multi-agent collaboration for both effective and efficient NAD in an open architectural space.

4.3. Ablation Studies

Effect of Reader and Proposer. The Reader agent analyzes recent academic papers on neural architectures and related advances, and proposes key innovations and knowledge that could potentially improve neural network performance. Then the Reflector agent retrieves appropri-

Table 3. Ablation studies of the Developer Team. Experiments are conducted on our NAD benchmark. “LIF” and “LDE” mean learning from immediate feedback and learning from design experience respectively.

Task	Graph	LIF	LDE	# Tokens (K)	E	Q	SR
Macro	✗	✗	✗	2.23±0.27	0.64	0.63	0.40
	✓	✗	✗	0.58±0.66	0.54	0.78	0.42
	✓	✓	✗	0.73±0.82	0.64	0.84	0.54
	✓	✓	✓	0.53±0.68	0.78	0.87	0.68
Micro	✗	✗	✗	2.10±0.22	0.76	0.65	0.49
	✓	✗	✗	0.49±0.63	0.62	0.97	0.60
	✓	✓	✗	0.48±0.65	0.70	0.89	0.62
	✓	✓	✓	0.31±0.45	0.92	0.96	0.88

ate knowledge for the network to enhance it. To validate the effectiveness of LLM-empowered Reader and LLM-empowered Proposer, we conducted ablation experiments, and the results are shown in Table 2. we built two strong baselines. When both Reader and Proposer are absent, we adopt a set of expert designed modification suggestions used in LeMo-NADe [30] to generate design suggestions. When only the Proposer is present, we prompts LLM to propose design suggestions based on its own knowledge without accessing to the recent achievements. When only the Reader is present, we randomly select knowledge from the knowledge pool as design suggestions. We observe that both Reader and Proposer are important for improving the performance of NAD, especially on the challenging dataset, *i.e.* ImageNet16-120.

Effect of Graph-based Neural Architecture Representation. We compare the graph-based neural architecture representation with the code-generation baseline. Specifically, we carefully design the prompts to prompt the LLM to directly generate codes for modifying the neural network architecture. From the Table 3, it can be seen that while existing LLMs demonstrate impressive capabilities in generating executable program codes (64% executability), the quality is relatively low (63% quality score). By adopting the graph representation, the LLMs can focus more on designing network architecture without distracted by the code style and formatting. In addition, the graph-based representation is more compact, resulting in fewer required tokens.

Effect of Learning from Immediate Feedback (LIF). The Reflector agent plays a crucial role in improving the executability and the quality of the modified network architecture. Adding LIF improves the executability from 0.54 to 0.64, while improving the quality score from 0.78 to 0.84.

Effect of Learning from Design Experience (LDE). The integration of learning from design experience significantly enhances the performance of NAD, in terms of both the executability and the quality, resulting in improved success rate. For micro-level modifications, the code execution rate of the generated neural network reached 92% and the

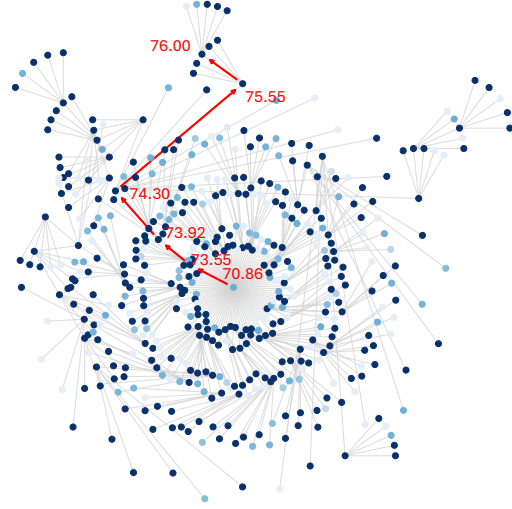


Figure 4. Large-scale NAD experiments. Each node represents a model, and the edge indicates which model is modified based on. The darker the node color, the higher the accuracy on the test set. The root node in the center is ResNet. The path highlighted by the red arrows is the improvement path of the optimal model found.

success rate is significantly improved from 0.62 to 0.88.

4.4. Large-scale NAD Experiment

To further explore the potential of NADER, we use NADER to conduct a larger-scale neural architecture design on CIFAR100. We initialize with ResNet [13] and generate 500 novel architectures using NADER. The modification process of these 500 architectures is shown in Figure 4. To obtain these 500 architectures, we used 5,371K input tokens and 987K output tokens, totaling \$23 (\$2.50 per 1M input tokens and \$10.00 per 1M output tokens), resulting in an average cost of \$0.046 per architecture. Finally, we get a novel architecture with an accuracy of 76.0% on the test dataset, which is 5.14% higher than the initial architecture. Furthermore, we evaluate this architecture on the CIFAR-10 and ImageNet16-120. The experimental results, shown in Table 1, demonstrate that the designed architecture achieves strong performance across different datasets.

5. Conclusion

In this paper, we propose NADER (Neural Architecture Design via multi-Agent collaboRation), a novel framework for neural architecture design (NAD). The framework adopts a multi-agent collaboration strategy to automatically explore novel neural architectures beyond predetermined search spaces. We propose Reader to continuously learn from recent academic literature, Proposer to raise design proposals, Modifier to implement these proposals, and Reflector to learn from feedback and historical records. Experiments demonstrate the effectiveness of the proposed method across a range of benchmark datasets.

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