Self-Evolving Multi-Agent Systems via Textual Backpropagation

Anonymous ACL submission

Abstract

Leveraging multiple Large Language Models (LLMs) has proven effective for addressing complex, high-dimensional tasks, but current approaches often rely on static, manually engineered multi-agent configurations. To overcome these constraints, we present the Agentic Neural Network ($\mathcal{ANN}$), a framework that conceptualizes multi-agent collaboration as a layered neural network architecture. In this design, each agent operates as a node, and each layer forms a cooperative team focused on a specific subtask. Agentic Neural Network follows a two-phase optimization strategy: (1) Forward Phase - Drawing inspiration from neural network forward passes, tasks are dynamically decomposed into subtasks, and cooperative agent teams with suitable aggregation methods are constructed layer by layer. (2) Backward Phase - Mirroring backpropagation, we refine both global and local collaboration through iterative feedback, allowing agents to self-evolve their roles, prompts, and coordination. This neuro-symbolic approach enables $\mathcal{ANN}$ to create new or specialized agent teams post-training, delivering notable gains in accuracy and adaptability. Across six benchmark datasets, $\mathcal{ANN}$ surpasses leading multi-agent baselines under the same configurations, showing consistent performance improvements.

1 Introduction

Large Language Models (LLMs) have ushered in a new era of artificial intelligence, exhibiting strong capabilities in reasoning, content generation, and multi-step problem-solving (Kojima et al., 2022; Ouyang et al., 2022). By grouping these models into *multi-agent systems* (MAS), researchers have addressed an array of complex tasks, ranging from code generation and debugging (Jimenez et al., 2023) to retrieval-augmented generation (Khattab et al., 2023a; Lewis et al., 2020; Gao et al., 2023) and data analysis (Hong et al., 2024; Hu et al., 2024). Often, MAS outperform their single-agent equivalents by bringing together diverse agent roles and expertise, including verifier agents (Shinn et al., 2023) or debating agents (Qian et al., 2024; Zhuge et al., 2024b), thus creating more adaptable and robust solutions. However, designing and deploying effective MAS remains demanding. Developers frequently invest substantial effort into prompt engineering, role assignment, and topology definition by trial and error (Chen et al., 2023; Hong et al., 2023), especially for dynamic, high-dimensional tasks.

Recent advances in automating aspects of MAS design aim to relieve these challenges. For instance, Khattab et al. (2024) introduced systematic methods for generating in-context exemplars; Hu et al. (2025) presented a meta-agent capable of creating new topologies in code; and Zhang et al. (2024) employed Monte Carlo Tree Search to find improved workflow configurations; Ke et al. (2025) proposed an automatic MAS optimization architecture under zero supervision and demonstrated significant gains. These innovations mirror earlier developments in MAS design research, where layer-wise optimization gave way to holistic, end-to-end backpropagation (Jacobs et al., 1991; Hinton et al., 2006). Similarly, *symbolic* or *agent-level* frameworks that model entire multi-agent pipelines as computational graphs have emerged (Khattab et al., 2023a; Zhuge et al., 2024a; Zhou et al., 2024).

Building on these insights, we introduce the *Agentic Neural Network ($\mathcal{ANN}$)*, a framework that adapts principles from classic neural networks to orchestrate multiple LLM agents. As shown in Figure 1, conventional neural networks rely on learnable weights and numeric optimizers for end-to-end training via gradient-based updates, whereas $\mathcal{ANN}$ considers each layer as a team of language agents, jointly optimizing roles, prompts, and tools through textual gradients (Yuksekgonul et al., 2024). While MoE and MoA architectures

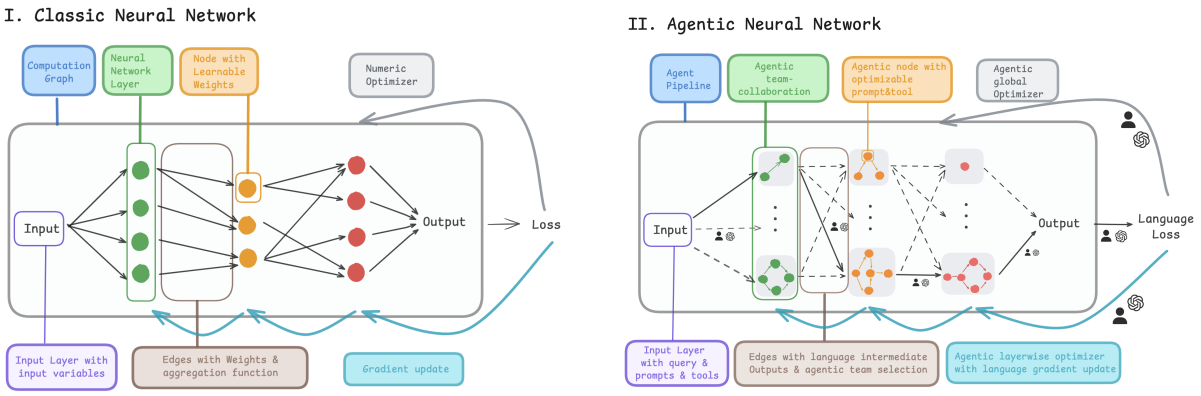

Figure 1: A conceptual comparison between classic neural networks (left) and our $\mathcal{ANN}$ (right). In the right-hand agentic diagram, the brown module labeled *"Edges with language intermediate Outputs & agentic team selection"* represents the choice among multiple candidate collaboration strategies between agent teams. **Solid lines** indicate selected collaboration modes that form the pipeline connection between layers, while **dashed lines** represent alternative strategies that were not selected at that step.

aim to scale model capacity through gated expert selection within a monolithic model (Shazeer et al., 2017; Wang et al., 2024b), $\mathcal{ANN}$ organizes layerwise teams of language agents that collaborate through multi-step reasoning and are refined via textual gradients (Yuksekgonul et al., 2024). This design enables $\mathcal{ANN}$ to support flexible, role-based agent coordination beyond the scope of numeric expert gating.

Instead of a purely engineering-driven approach, $\mathcal{ANN}$ divides a complex task into smaller subproblems, assigning each to a layer of specialized agents, and iteratively refines both local design (i.e., agent prompts and configurations) and global coordination (i.e., inter-layer flows and topologies). Our approach proceeds in two stages. First, during the forward agent team generation phase, the main task is decomposed into subtasks, with specialized agent teams dynamically assigned layer by layer, ensuring each layer is responsible for a distinct subtask. Then, if performance is suboptimal, the backward agent team optimization phase backpropagates textual feedback to isolate errors and propose targeted adjustments. These textual critiques act like gradient signals, guiding prompt updates and connection refinements (Yao et al., 2022; Verma, 2024; Khattab et al., 2023a).

To illustrate the capabilities of our framework, we evaluate $\mathcal{ANN}$ on four challenging datasets: MATH (Hendrycks et al., 2021) for mathematical reasoning, DABench (Hu et al., 2024) for data analysis, Creative Writing (Zhou et al., 2024) for open-ended writing tasks, HumanEval (Chen et al., 2021) for code generation, and MMLU (Hendrycks et al., 2020) for multiple-choice question answering. Our experiments show that our framework not only simplifies MAS design by automating prompt tuning, role assignment, and agent collaboration but also outperforms existing baselines in accuracy. Through this process, the framework acquires self-evolving capabilities, dynamically reconfiguring its agent teams and coordination strategies to meet the demands of novel tasks.

2 Related Works

In this section, we review the evolution of AI agents into LLM-based systems, discuss the emerging concept of agentic workflows, survey automated methods for optimizing agent configurations, and outline the remaining challenges in multi-agent settings.

Evolution of AI Agents Early AI agents were highly specialized and depended chiefly on symbolic reasoning, as seen in board-game-playing systems like Chess and Go. Subsequent innovations introduced reactive and reinforcement learning agents with greater adaptability. More recently, LLM-based agents have appeared, incorporating large-scale language models (Radford et al., 2018, 2019; Ouyang et al., 2022) at their foundation. By processing natural language inputs and outputs, these agents enable more flexible, human-like interactions and reasoning.

LLM-Based Agentic Workflows Modern workflows often rely on multiple LLM invocations to address complex, multi-step tasks (Wei et al., 2022; Madaan et al., 2023; Gao et al., 2022). In these

agentic workflows, each stage or node corresponds to specific subtasks like prompt creation, tool utilization, or domain-specific strategies (Hong et al., 2023; Yang et al., 2023; Cai et al., 2023). Through specialized roles—including data analyzers, verifiers, or debaters—LLM-based agents can collaborate efficiently on a range of domain challenges, from code generation (Hong et al., 2024; Lee et al., 2023) to advanced data analysis (Li et al., 2024a).

Automated Optimization Approaches As task workflows grow more involved, automated methods aim to minimize manual engineering. *Prompt optimization* tailors textual inputs to steer LLM outputs (Khattab et al., 2023a; Zhuge et al., 2024b). *Hyperparameter tuning* fine-tunes model parameters or scheduling (Liu et al., 2024a), and *workflow optimization* revises entire computational graphs or code structures (Hu et al., 2025; Zhang et al., 2024; Zhuge et al., 2024a). Symbolic learning frameworks (Hong et al., 2024; Zhuge et al., 2024b; Zhou et al., 2024) optimize prompts, tools, and node configurations collectively, mitigating local optima that can emerge from optimizing each component independently. Furthermore, Lee et al. (2025) propose a systematic taxonomy for AI systems optimization, enabling benchmarking of MAS designs and evaluation of collaborative frameworks.

MAS Integration and Key Challenges In multi-agent systems, LLMs facilitate inter-agent communication, strategic planning, and iterative task decomposition (Yao et al., 2022; Wang et al., 2024a). However, scaling these agents prompts concerns about computational overhead, privacy, and the opaque "black box" nature of large models (Liu et al., 2024b; Verma, 2024). These considerations highlight the need for robust design, continuous oversight, and data-centric strategies that balance performance and interpretability.

Overall, the field has moved from manually designed agent architectures to more data-driven, automated approaches that harness LLMs' language capabilities. Despite noteworthy gains in prompt tuning, structural optimization, and integrated workflows, a gap remains for frameworks that unify these methods into efficient, adaptable, and end-to-end automated systems suited for large-scale real-world deployments.

3 Methodology

This section details the Agentic Neural Network ($\mathcal{ANN}$) methodology, a multi-agent system framework designed to solve complex, multi-step computational tasks. $\mathcal{ANN}$ is inspired by classic neural networks but replaces numerical weight optimizations with dynamic agent-based team selection and iterative textual refinement. Figure 2 shows the architecture of our $\mathcal{ANN}$.By structuring multi-agent collaboration hierarchically, $\mathcal{ANN}$ enables dynamic role assignment, adaptive aggregation, and data-driven coordination improvements through a forward-pass team selection process and a backward-pass optimization strategy.

3.1 Forward Dynamic Team Selection

The $\mathcal{ANN}$ framework initiates task processing by decomposing the problem into structured subtasks. These subtasks are assigned across multiple layers, where each layer comprises a team of specialized agents working collaboratively on their designated subtask. Unlike static multi-agent workflows, $\mathcal{ANN}$ dynamically constructs these teams and their aggregation mechanisms based on task complexity. Two primary processes guide this phase: (1) defining the $\mathcal{ANN}$ structure and (2) selecting agentic teams that determine how agents collaborate.

3.1.1 Structure of the Agentic Neural Network

The architecture of $\mathcal{ANN}$ is inspired by neural networks, where each layer consists of nodes represented by agents. These agents are connected in a sequence that facilitates seamless information flow from one layer to the next, ensuring that outputs from a layer serve as structured inputs for the subsequent layer. This modular yet interconnected design enables efficient data processing, flexible task decomposition, and adaptive decision-making. Unlike static agent configurations, $\mathcal{ANN}$ dynamically refines its internal collaboration structure based on performance feedback, enhancing scalability and adaptability.

3.1.2 Selection of Layer-wise Agentic Teams

At each layer, $\mathcal{ANN}$ employs a mechanism to dynamically determine the most appropriate agentic teams, which dictates how multiple agents collaborate. This selection process considers the specific subtask requirements and complexity, ensuring that

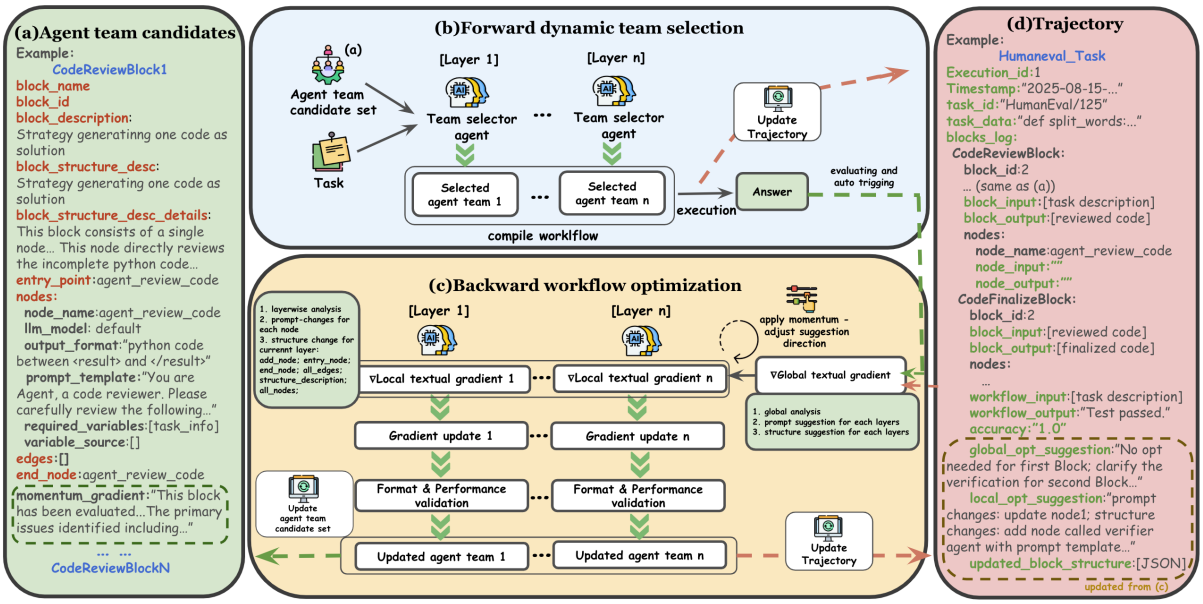

Figure 2: Overview of our $\mathcal{ANN}$ framework with textual backpropagation, which dynamically selects and refines agent teams layer by layer. (a) Agent team candidates: layer-wise candidate sets F_ℓ are represented as structured blocks composed of nodes, edges, and prompts. (b) Forward dynamic team selection: a team-selector agent selects agent team for each layer, compiles the workflow, executes the task, and records the trajectory. (c) Backward workflow optimization: task evaluation and the recorded trajectory generate a textual gradient ∇_{text}, which decomposes into a global gradient for workflow structure and local gradients for updating prompts, nodes, and edges at each layer. Momentum-based updates and format/performance validation ensure stable refinement before integrating changes into the candidate pools. (d) Trajectory: a structured record capturing the inputs and outputs of each node, layer, and workflow, along with global and local suggestions that not only guide agent team updates but are also stored as momentum gradients within the corresponding blocks, providing historical optimization references for adaptive refinement in future executions. A detailed explanation of each component is provided in Section 3

the most suitable collaborative strategy is applied to maximize performance.

Let $\mathcal{F}_\ell$ be the set of candidate agent teams available for layer ℓ, I_ℓ the input to the layer, and I the task-specific information. The dynamic team selection at each layer is determined by

$$f_\ell = \text{DynamicRoutingSelect}(\mathcal{F}_\ell, \ell, I_\ell, I),$$

where DynamicRoutingSelect denotes a process in which a team selector agent chooses the most appropriate agentic team from the candidate set based on task complexity. The selection is informed by both subtask-specific information and a structural summary of each candidate team, which are provided to the team selector agent(See Appendix B.2.Prompt 6 for details). Here, f_ℓ represents the selected agentic team. Once an agentic team is selected, the layer processes input as:

$$O_\ell = \text{ExecuteLayer}(\ell, f_\ell, I_\ell, I),$$

where the selected agentic team f_ℓ is incorporated into the overall workflow and is responsible for executing the subtask assigned to layer ℓ. The resulting output O_ℓ is then propagated as the input to the next layer, i.e., $I_{\ell+1} = O_\ell$. This dynamic selection mechanism enables $\mathcal{ANN}$ to adapt to changing task conditions, thereby optimizing efficiency and accuracy in multi-agent collaboration.

3.2 Backward Optimization

Upon completion of the forward phase, the system evaluates its performance. If the predefined performance thresholds are not met, $\mathcal{ANN}$ triggers a backward optimization phase to refine agentic collaboration team at both the global (system-wide) and local (layer-specific) levels.

3.2.1 Global Optimization

Global optimization analyzes inter-layer coordination, refining interconnections and data flow to improve overall system performance. This process provides suggestions for updating the subtask descriptions of each layer and optimizing the configuration of agent teams at the inter-layer level, primarily identifying the modules that require structural

improvement. As shown in Appendix B.2.Prompt 3 for details, it further optimizes information transfer across layers to ensure that local layer behaviors align with global objectives. Mathematically, the global gradient is computed as:

$$\mathcal{G}_{\text{global}} = \text{ComputeGlobalGradient}(S, \tau),$$

where S represents the global workflow, and τ denotes the trajectory of execution, which includes agent interactions and input-output information transformations. The system structure is then updated accordingly:

$$\mathcal{S}_{\text{global}} \leftarrow \text{GlobalGradientUpdate}(\mathcal{G}_{\text{global}}, \tau).$$

The resulting optimization suggestions are subsequently used to refine the structural composition of agent teams, enabling more coherent coordination across layers.

3.2.2 Local Optimization

While global optimization refines inter-layer interactions, local optimization focuses on improving the collaboration structure of agents within each layer, adjusting their nodes, edges, and prompts based on fine-grained performance feedback. The local gradient for each layer is computed as:

$$\mathcal{G}^t_{\text{local},\ell} = \beta \mathcal{G}_{\text{global}} + (1-\beta) \times \text{ComputeLocalGradient}(\ell, f_\ell, \tau),$$

where β is a weighting factor that balances the influence of global optimization and layer-specific gradients. At the t-th step, the agentic team is updated as:

$$f^{t+1}_\ell = f^t_\ell \times \mathcal{G}^t_{\text{local},\ell},$$

where the update is guided by the local gradient feedback, which provides suggestions to refine the structural configuration and prompt design of the current agentic team. The resulting optimized team f^{t+1}_ℓ integrates these improvements to enhance layer-level performance. Appendix B.1 provides pseudo-code and Appendix B.2.Prompt 4 provides prompts used to obtain textual local gradients. **Momentum.** To improve stability, $\mathcal{ANN}$ employs momentum-based optimization, preventing sudden changes in agent parameters. The momentum-adjusted update rule is:

$$\mathcal{G}^t_{\text{local},\ell'} = \alpha \mathcal{G}^t_{\text{local},\ell} + (1-\alpha)\mathcal{G}^{t-1}_{\text{local},\ell},$$

where α is the momentum coefficient, controlling how past updates influence the current optimization step. In essence, momentum provides the model with a memory of past optimization directions. As illustrated in Appendix B.2.Prompt 5, it records how an agent team was previously adjusted (the previous adjustment direction) and combines this historical trajectory with the current feedback. By analyzing why the previous optimization failed to solve the present task, the framework refines the update direction, ensuring that new improvements build upon, rather than contradict, earlier progress. This helps the system maintain a clearer and more stable sense of optimization direction across iterations.

Format Validation. It verifies that the updated structures conform to standard agent interaction formats, including proper edge definitions, variable references, and prompt templates, thereby maintaining consistency and reliability across the system.

Performance Validation. a validation agent evaluates the newly generated team against prior configurations, measuring structural similarity to prevent redundant designs and ensuring that each adjustment contributes positively to the system's overall functionality.

4 Experiments

4.1 Experimental Settings

Datasets We evaluate our framework on six benchmarks: HumanEval(Chen et al., 2021), Creative Writing(Zhou et al., 2024), MATH(Hendrycks et al., 2021), DABench(Hu et al., 2024), MMLU(Hendrycks et al., 2020) and Natural Plan(Zheng et al., 2024). HumanEval contains human-written coding problems and remains a standard benchmark for code generation. Creative Writing provides four-sentence prompts to craft a coherent story that ends with those sentences. MATH compiles challenging competition problems that demand multi-step symbolic reasoning across diverse fields. DABench covers data-analysis tasks such as feature engineering and statistics; MMLU–Machine Learning is a subset from the Massive Multitask Language Understanding (MMLU) benchmark and offers multiple-choice questions on core ML concepts. Natural Plan focuses on scheduling tasks that require proposing feasible times under availability constraints in natural language. Following prior work (Zhou et al., 2024; Song et al., 2024; Yuksekgonul et al., 2024; Zhang et al., 2025), we

split the datasets into training and validation sets for each benchmark, ensuring direct comparability with their reported baselines.

LLM Backbones To contain costs while maintaining strong performance, we unify the training process using the GPT-4o-mini model (Achiam et al., 2023) for optimization. During validation, we evaluate datasets HumanEval, CW, MATH, DABench using three backbone variants: GPT-3.5-turbo, GPT-4o-mini, and GPT-4. Because neither (Zhou et al., 2024) nor (Song et al., 2024) report GPT-4o-mini results, our findings add a new dimension to the performance landscape, showing how a budget-friendly large language model can still match or surpass top-tier methods on standard tasks. We evaluate datasets MMLU and Natural Plan using model GPT-4o and GPT-4o-0806 to follow the previous work . This setup enables us to demonstrate that our approach generalizes across different model capacities. We aim to demonstrate the flexibility and robustness of our framework in real-world various scenarios.

Baselines and Comparisons We compare $\mathcal{ANN}$ (ours) with various baseline approaches, each drawn from the references: GPTs (Brown et al., 2020; Chen et al., 2021) – A direct usage of GPT-based models with carefully designed prompts. Agents (Zhou et al., 2023) – A language-agent method that organizes multi-step reasoning and tool usage through a pipeline of prompts. Agents w/ AutoPE (Yang et al., 2024) – A variant wherein each prompt node is optimized by an LLM, but without full language gradient backpropagation. DSPy/ToT (Khattab et al., 2023b) – A pipeline optimization framework that performs search-based tuning of prompt components. Applicable mostly to tasks with a tractable evaluation function. Symbolic (Zhou et al., 2024) – An agent-based system employing symbolic learning methods for dynamic prompt improvements. Vanilla LLM – A single-turn GPT-based approach without agent collaboration. Meta-prompting(Suzgun and Kalai, 2024) – An adaptive prompting strategy that attempts to generate meta-level instructions for new tasks. AutoAgents (Chen et al., 2024) – An automated agent system that attempts to orchestrate multi-agent interactions but can be unstable in large-scale settings. DyLAN (Liu et al., 2024c) – A dynamic language-agent approach to break down tasks with feedback loops. AgentVerse(Chen et al., 2023) – A multi-agent platform emphasizing flexible agent composition. AutoGen (Wu et al., 2023) – A system featuring an "Assistant + Executor" design for multi-step problem-solving. Captain Agent (Song et al., 2024) – An adaptive team-building agent framework that spawns specialized sub-agents based on task progress. CoT (Chain-of-Thought)(Wei et al., 2023) – A prompting strategy that encourages intermediate reasoning steps, often used to enhance zero-shot performance on complex QA tasks. TextGrad (Yuksekgonul et al., 2024) – A framework that performs solution-level optimization by using text gradient. ADAS (Automated Design of Agentic Systems)(Hu et al., 2025) – A framework where a meta-agent autonomously generates agentic architectures for multi-agent designs.

Method	HumanEval	Creative Writing
	gpt-3.5/4o-mini/4	gpt-3.5/4o-mini/4
GPTs	59.2 / - / 71.7	4.0 / - / 6.0
Agents	59.5 / - / 85.0	4.2 / - / 6.0
Agents w/ AutoPE	63.5 / - / 82.3	4.4 / - / 6.5
DSPy / ToT	66.7 / - / 77.3	3.8 / - / 6.8
Symbolic	64.5 / - / 85.8	6.9 / - / 7.4
$\mathcal{ANN}$ **(ours)**	**72.7** / 90.9 / **87.8**	**9.0** / 8.6 / **7.9**

Table 1: Comparison results on HumanEval and Creative Writing benchmarks. The best results in each category are marked in bold.

4.2 Experimental Results

4.2.1 Main Results

Table 1 compares our method with prior approaches on HumanEval and CW. Because (Zhou et al., 2024) provide baseline results only for GPT-3.5-turbo, hereafter referred to as GPT-3.5 and GPT-4, we supplement these with our own evaluations under GPT-4o-mini for a thorough comparison. We note the following key findings: On HumanEval, our $\mathcal{ANN}$ approach consistently surpasses all baselines. We achieve **72.7**% and **87.8**% for GPT-3.5 and GPT-4, respectively, outperforming the best baseline by a clear margin. Notably, even our GPT-4o-mini results(**90.9**/%) show competitive or superior performance despite GPT-4o-mini being a lower-cost model. For open-ended text generation tasks in CW, our method scores **9.0/7.9** on GPT-3.5/GPT-4. We attribute this to $\mathcal{ANN}$'s structured layer-wise approach, which fosters creative synergy among specialized agents while maintaining

Method	MATH	DABench
Vanilla LLM	51.53	6.61
Meta-prompting	68.88	39.69
AutoAgents	56.12	57.98
DyLAN	62.24	-
AgentVerse	69.38	-
AutoGen	74.49	82.88
Captain Agent	77.55	88.32
$\mathcal{ANN}$ (gpt-4)	<u>80.0</u>	**92.0**
$\mathcal{ANN}$ (gpt-3.5-turbo)	55.0	76.0
$\mathcal{ANN}$ (gpt-4o-mini)	**82.5**	**92.0**

Table 2: Comparison results on the MATH and DABench datasets. The best results in each column are marked in bold, and the second-best results are underlined. All results without special annotation are based on GPT-4.

Method	MMLU	Natural Plan		
	ML	Trip Planning	Meeting Planning	Calendar Scheduling
CoT	85.7	1.0	50.0	60.0
ADAS	–	3.1	43.0	66.0
TextGrad	88.4	–	–	–
$\mathcal{ANN}$	**89.1**	**7.9**	**55.0**	**73.0**

Table 3: Accuracy on MMLU-ML[1] and the Natural Plan benchmark, which consists of three task domains: TP (Trip Planning), MP (Meeting Planning), and CS (Calendar Scheduling). Our method outperforms CoT(Wei et al., 2023), ADAS(Hu et al., 2025), and TextGrad(Yuksekgonul et al., 2024) baselines, highlighting the effectiveness of layerwise feedback and structure refinement.

logical consistency in narrative structure.

In Table 2, we contrast our method with baseline results from (Song et al., 2024) on MATH and DABench. Notably, (Song et al., 2024) report results using GPT-4 but omit GPT-3.5 and GPT-4o-mini. On MATH, We record 55.0, **82.5**, and 80.0 across GPT-3.5, 4o-mini, and GPT-4. Despite using GPT-4o-mini in training, our method exhibits strong generalization to both GPT-3.5 and GPT-4. On GPT-4, our **80.0**% accuracy significantly outperforms Captain Agent (77.55%) and AutoGen (74.49%). On DABench, which focuses on data-analysis tasks, our method ($\mathcal{ANN}$) attains 76.0%, **92.0%**, and 92.0% on GPT-3.5, GPT-4o-mini, and GPT-4, respectively, consistently outperforming prior baselines. We observe that GPT-4o-mini again surprisingly yields top-tier results, indicating that data-centric tasks can benefit from well-structured agent orchestration without always requiring the largest language models.

Following (Zhang et al., 2025), it employs distinct models for optimization and execution. Specifically, we use GPT-4o-mini for training-phase with optimization, and select GPT-4o for validation-phase only with execution. We contrast our method with baseline results from (Yuksekgonul et al., 2024; Zhang et al., 2025) on the MMLU-ML and Natural Plan (see Table 3. For MMLU, our method achieves **89.1**% accuracy, outperforming CoT (85.7%) and TextGrad (88.4%). For the Natural Plan benchmark, our method achieves accuracies of **7.9/55.0/73.0**, outperforming CoT (1.0/50.0/60.0) and ADAS (3.1/43.0/66.0). This result demonstrates the advantage of our layerwise optimization approach in highly structured reasoning settings.

4.2.2 Robustness to Backbone Variation

To address concerns regarding our use of a single backbone during training, we conducted an additional experiment using GPT-3.5-turbo as the training model while retaining GPT-3.5-turbo, GPT-4o-mini, and GPT-4 as evaluation backbones. Results across HumanEval, CW, Math, and DABench benchmarks (see Table 4) show that $\mathcal{ANN}$ achieves strong generalization even when trained on GPT-3.5-turbo, a smaller-capacity model. This suggests that the agentic orchestration and textual backpropagation mechanisms in $\mathcal{ANN}$ are robust to changes in underlying language model capacity. Experiments demonstrate that the multi-agent architecture discovered by our $\mathcal{ANN}$ framework, even when using the weaker GPT-4o-mini, can generalize effectively to more powerful LLMs, achieving superior performance. Additionally, our results highlight GPT-4o-mini as a cost-effective yet high-performing alternative, reinforcing $\mathcal{ANN}$'s robustness across different model scales.

4.2.3 Ablation Studies

We conduct a unified ablation study using only GPT-4o-mini to further investigate the design choices in our $\mathcal{ANN}$ framework. Specifically, we compare four variants: (1) **Full $\mathcal{ANN}$:** Our complete approach with momentum-based optimiza-

[1]We report results on the MMLU-ML subset for fair comparison, as TextGrad provides separate results on this subset.

Train / Eval	HumanEval	Creative Writing	MATH	DABench	*Total Train Cost*
Backbones	GPT-3.5/4o-mini/4	GPT-3.5/4o-mini/4	GPT-3.5/4o-mini/4	GPT-3.5/4o-mini/4	(in USD)
GPT-3.5	73.7 / 85.5 / 86.3	8.9 / 8.5 / 8.1	53.5 / 80.0 / 77.5	71.2 / 88.0 / 91.5	≈$122.30
GPT-4o-mini	72.7 / 90.9 / 87.8	9.0 / 8.6 / 7.9	55.0 / 82.5 / 80.0	76.0 / 92.0 / 92.0	≈$73.40

Table 4: **Evaluation results across four benchmarks (HumanEval, CW, Math, and DABench)** with two different training backbones (GPT-3.5 vs GPT-4o mini), evaluated across GPT-3.5, GPT-4o, and GPT-4. Training costs are estimated based on approximately 244.6M input tokens.

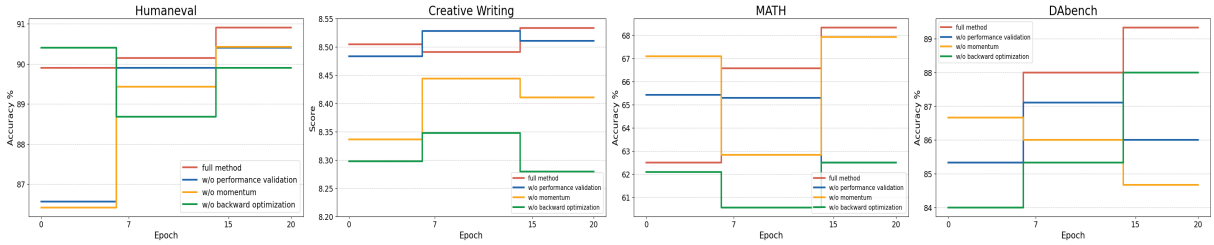

Figure 3: Ablation results on HumanEval, CW, MATH, and DABench using the GPT-4o-mini model for both training and validation. We compare the full $\mathcal{ANN}$ framework (red curve) against three ablated variants: w/o Validation Performance (blue curve), w/o Momentum (purple curve), and w/o Backward Optimization (green curve). Each curve shows average validation accuracy (or equivalent score) over three runs. The full $\mathcal{ANN}$ consistently outperforms all ablations, confirming the necessity of each component.

tion, validation-based performance checks, and backward optimization. (2) **w/o Momentum:** Disables the momentum technique in textual gradient refinement. (3)**w/o Validation Performance:** Skips the validation-based filtering stage when selecting improved prompts and agent roles. (4)**w/o Backward Optimization:** Does not use the backward pass to refine prompts; i.e., omits textual gradients for *error signals*.

Training Procedure. All four variants are trained for 20 epochs on each dataset (HumanEval, CW, MATH, DABench) using the training splits described above. To mitigate the randomness inherent in LLM sampling, we repeat each condition *three times* and report the *average* results on the validation set at regular epoch intervals.

Results and Analysis. Figure 3 illustrates the validation accuracy (or relevant score) as a function of training epoch. We observe a consistent upward trend across all four datasets, with the full $\mathcal{ANN}$ approach converging to the highest performance. Detailed findings indicate that the **impact of momentum** is substantial: removing momentum (w/o Momentum) leads to the largest performance drop on HumanEval, suggesting that gradual accumulation of textual gradient signals is crucial for code-generation tasks that require precise correctness. **Validation-based checks** also play an important role—omitting validation performance filtering can cause more erratic updates, particularly evident in MATH, where narrative consistency can degrade if suboptimal agent prompts are accepted too frequently. Finally, **backward optimization** proves essential: without the backward pass, we lose a key mechanism for refining agentic team. Overall, our ablation highlights that each component contributes significantly to performance, and combining them yields the most reliable and robust improvements.

5 Conclusion

Our experimental results establish that $\mathcal{ANN}$ achieves high accuracy and adaptability across tasks ranging from code generation to creative writing, surpassing traditional static configurations. Through a dynamic formation of agent teams and a two-phase optimization pipeline, the framework delivers robust performance rooted in neural network design principles. These findings underscore the potential of $\mathcal{ANN}$ as an efficient solution for orchestrating complex multi-agent workflows. Detailed ablation studies highlight the significance of each component. Ultimately, this integrated agentic paradigm paves the way for fully automated and self-evolving multi-agent systems, effectively combining symbolic coordination with connectionist optimization.

Limitations

Despite its advantages, the Agentic Neural Network framework has limitations. Its reliance on manually defined structures and prompts reduces adaptability across tasks, which could be improved through meta-prompt learning to automate structure generation. Moreover, candidate selection becomes computationally expensive as the pool grows, requiring periodic pruning, though this risks homogenization, which could be mitigated by stochastic retention of lower-ranked candidates. Future work will address these limitations by integrating meta-prompt learning, adaptive pruning, and dynamic role adjustments to enhance $\mathcal{AN}\mathcal{N}$'s scalability and adaptability.

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Framework	Layerwise	Backward Optimization	Momentum Adjustment	Global Optimization	Local Optimization	Dynamic Teaming	Training Requirement
Symbolic (Zhou et al., 2024))	✗	✓	✗	✓	✓	✗	✓
AutoGen (Wu et al., 2023)	✗	✗	✗	✓	✓	✓	✗
InfiAgent-DAbench (Hu et al., 2024)	✗	✗	✗	✓	✗	✓	✗
MetaGPT (Hong et al., 2023)	✗	✗	✗	✗	✓	✓	✗
DyLan (Liu et al., 2024c)	✗	✓	✗	✓	✓	✓	✓
Adaptive Team (Song et al., 2024)	✗	✗	✓	✗	✓	✓	✗
Chain-of-Thought (Wei et al., 2023)	✗	✗	✗	✗	✓	✗	✗
GPTSwarm (Zhuge et al., 2024b)	✗	✗	✓	✓	✓	✓	✓
Aflow (Li et al., 2024b)	✗	✗	✗	✓	✗	✓	✗
$\mathcal{ANN}$ **(Ours)**	✓	✓	✓	✓	✓	✓	✓

Table 5: Framework-level comparison across layerwise design, optimization strategies (backward, momentum, global/local), dynamic team composition, and training requirements. ✓/✗ indicate support.

A Comparison

With the rapid advancement and widespread adoption of deep learning techniques (Liu et al., 2022, 2023; Lu and Chen, 2019, 2022, 2023; Tian et al., 2023a, 2024, 2023b; Wan et al., 2024; Liu et al., 2025; Xiao et al., 2024, 2023), large language models (Bi et al., 2024, 2025b,a; Du et al., 2025b,a; Wang et al., 2025a) have emerged as a transformative force across diverse domains (Chen et al., 2025a; Rong et al., 2025; Zhang et al., 2023; Chen et al., 2025b; Zhao and Zhang, 2024; Yu et al., 2025; Huang et al., 2024; Zeng et al., 2024; Xu et al., 2024; Lu et al., 2024, 2023; Xuankun et al., 2025; Liu et al., 2022; Wang et al., 2025c, 2024c, 2025b). Their ability to understand, generate, and reason over natural language has enabled a new generation of intelligent systems, particularly in the orchestration and coordination of multi-agent frameworks. As these models continue to evolve, numerous architectures have been proposed to harness their capabilities in increasingly sophisticated and dynamic environments.

To situate $\mathcal{ANN}$ in the rapidly evolving ecosystem of multi-agent orchestration, we benchmark it against nine representative frameworks drawn from recent literature—*Symbolic* (Zhou et al., 2024), *AutoGen* (Wu et al., 2023), *InfiAgent-DAbench* (Hu et al., 2024), *MetaGPT* (Hong et al., 2023), *DyLan* (Liu et al., 2024c), *Adaptive Team* (Song et al., 2024), *Chain-of-Thought* (Wei et al., 2023), *GPTSwarm* (Zhuge et al., 2024b), and *Aflow* (Li et al., 2024b). Collectively, these baselines cover symbolic planning, agentic workflow coordination, dynamic team formation, and optimisation-driven routines, thus furnishing a balanced backdrop for assessing architectural and functional advances.

Table 5 distils the comparison along seven orthogonal dimensions: (i) *layerwise decomposition*, (ii) *back-propagated optimisation*, (iii) *momentum-based adjustment*, (iv) *global optimisation scope*, (v) *local-only optimisation*, (vi) *dynamic team selection*, and (vii) *task-specific training requirements*. A check mark (✓) indicates native support; a cross (✗) denotes absence. As the table shows, $\mathcal{ANN}$ is the only framework that provides *full* coverage across all criteria—combining layerwise granularity with momentum-augmented backward optimisation, unifying global and local objectives, and eliminating the need for costly task-specific fine-tuning through on-the-fly team selection.

B Implementation

B.1 Pseudo Code

This section provides pseudocode for the system's overall architecture and the local gradient optimization process. Algorithm 1 outlines how the network leverages a dynamic routing mechanism alongside an agentic neural network structure, integrating both global optimization and layerwise optimization. Dynamic routing selects the most suitable path for a given task, thereby enhancing overall system

Algorithm 1: Agentic Neural Network with Dynamic Routing and Adaptive Optimization

Require: I: dataset input; L: layers in the workflow; F_ℓ: set of possible aggregation functions for each layer ℓ; S: workflow updation for optimization

Ensure: Updated structure and prompts for the agentic neural network

Traj $\leftarrow$ [] ▷ Initialize Trajectory
$I_\ell \leftarrow I$ ▷ Initialize input of first layer
Forward Pass with Dynamic Routing and Aggregation
for each layer ℓ in L **do**
  $f_\ell \leftarrow \text{DynamicRoutingSelect}(F_\ell, \ell, I_\ell, I)$
  $O_\ell \leftarrow \text{ExecuteLayer}(\ell, f_\ell, I_\ell, I)$
  Append $(\ell, f_\ell, I_\ell, O_\ell)$ to Traj
  $I_{\ell+1} \leftarrow O_\ell$
end for
Backpropagation:
Global Optimization
$\mathcal{G}_{\text{global}} \leftarrow \text{ComputeGlobalGradient}(S, \text{Traj})$
$\mathcal{S}_{\text{global}} \leftarrow \text{GlobalGradientUpdate}(\mathcal{G}_{\text{global}}, \text{Traj})$
Layerwise Optimization
for each layer ℓ in reverse(L) **do**
  $\mathcal{G}^t_{local,\ell} \leftarrow \text{ComputeLocalGradient}(\ell, f_\ell, \text{Traj}, \mathcal{L}_{\text{global}})$
  if momentum_needed **then**
    $\mathcal{S}_{\text{local}} \leftarrow \text{LocalGradientUpdate}(\ell, f_\ell, \mathcal{G}^t_{local,\ell}, \mathcal{S}_{\text{global}})$
  else
    $\mathcal{G}^t_{local,\ell'} \leftarrow \text{ApplyMomentum}(\ell, \text{Traj}, \mathcal{G}^t_{local,\ell}, \mathcal{G}^{t-1}_{local,\ell})$
    $\mathcal{S}_{\text{local}} \leftarrow \text{LocalGradientUpdate}(\ell, f_\ell, \mathcal{G}^t_{local,\ell'}, \mathcal{S}_{\text{global}})$
  end if
end for
return (F_ℓ, Traj)

performance and stability. Global optimization steers the entire network toward optimal solutions, while layerwise optimization fine-tunes each layer for improved learning efficiency and reliability. Algorithm 2 focuses on local optimization within each specialized layer. By applying localized gradient updates, each module can concentrate on its respective sub-task. Such targeted adjustments accelerate convergence, improve learning efficiency, and, in conjunction with the global optimization strategy, enhance the system's overall performance.

B.2 Prompt Repository

To guarantee rigorous experimentation, our framework distills complex evaluation and optimisation routines into a curated suite of six reusable examples of *prompts* for reference. Each prompt encapsulates a distinct facet of model assessment—ranging from factual exactness to strategic, multi-layer workflow repair—thereby furnishing a unified interface for loss-function design and optimiser selection. Collectively, these templates enable (i) **fine-grained answer verification**, (ii) **holistic workflow diagnosis**, and (iii) **progressive, momentum-aware refinement**, furnishing the gradient signals that steer the training loop towards globally coherent behaviour.

Answer Verification. Prompt 1 formalises a strict comparison between a model's predicted answer and an externally supplied ground truth, while Prompt 2 generalises the rubric to creative-writing settings where no canonical answer exists.

Algorithm 2: LocalGradientUpdate

Require: ℓ: current layer; f_ℓ: selected aggregation function; Traj: trajectory of execution; $\mathcal{G}_{\text{global}}$: global gradient; $\mathcal{S}_{\text{global}}$: current global structure; F_ℓ: set of possible aggregation functions for each layer ℓ

Ensure: Updated global structure $\mathcal{S}_{\text{global}}$ and valid aggregation function f_ℓ

$\mathcal{G}_{local,\ell} \leftarrow$ ComputeLocalGradient(ℓ, f_ℓ, Traj, $\mathcal{G}_{\text{global}}$) ▷ Compute local gradient in layer ℓ
$\mathcal{S}_{\text{local}} \leftarrow$ LocalGradientUpdate($\ell, f_\ell, \mathcal{G}_{local,\ell}, \mathcal{S}_{\text{global}}$): ▷ $\mathcal{S}_{\text{local}}$: Update layer-wise workflow
for $k \leftarrow 1$ to 3 **do** ▷ Attempt up to 3 updates
    $f'_\ell \leftarrow$ LocalGradientUpdate($\ell, f_\ell, \mathcal{G}_{local,\ell}, \mathcal{S}_{\text{global}}$)
    ValidateUpdate (f'_ℓ): ▷ If update passes validation
    Node Validation:
    if VariableSourcesValid(f'_ℓ) & FormatValid(f'_ℓ) **then**
        Edge Validation:
        if AllNodesHaveEdges(f'_ℓ) **then**
            Structure Validation:
            if StructureNotUnique(f'_ℓ) **then**
                if ValidatePerformance(f'_ℓ, f_ℓ) **then**
                Append f'_ℓ to F_ℓ ▷ add new agg func f'_ℓ into F_ℓ
                break ▷ Exit update loop on success
                end if
            end if
        end if
    end if
end for
return $\mathcal{S}_{\text{global}}$

Global Optimisation. Prompt 3 performs gradient-based analysis over an entire workflow trajectory, isolating error-prone sub-tasks and prescribing block-level remedies.

Layer-wise Repair. Prompt 4 zooms in on a single block, recommending structural or prompt-template adjustments that preserve inter-block consistency.

Momentum-based Adjustment. Prompt 5 fuses historical "velocity" information with fresh gradient signals to resolve recurrent faults while safeguarding previously effective changes.

Block Selection. Prompt 6 scores competing blocks against task complexity, ensuring that the most capable module is invoked for code-finalisation tasks and analogous challenges.

By systematically orchestrating these prompts, we induce *task-aligned* gradients that couple local correctness with global workflow efficiency, thereby enhancing both convergence speed and final performance.

Prompt 1: Prompt for Answer Verification with Ground Truth

```
You are a helpful AI assistant.
You will use your math skills to verify the answer.

You are given:
- A problem: {problem}
- A reply from a model: {final_answer}
- A ground truth answer: {solution}

Please do the following::
1. Extract the answer from the reply in the format:
```

```
   "The answer is <answer extracted>"

2. Compare the extracted answer with the ground truth.

3. Based on your analysis, choose only one of the following outputs:
   (a) "The answer is correct."
   (b) "The answer is approximated but should be correct."
   (c) "The answer is incorrect.
       Correct Answer: <ground truth answer> </ground truth answer> |
       Answer extracted: <answer extracted> </answer extracted>."
   (d) "The reply doesn't contain an answer."
```

Prompt 2: Prompt for Creative Writing Evaluation

```
Evaluate the following creative writing piece based on the provided task.

Inputs:
- Task Description: {task_prompt}
- Creative Writing Output: {output_from_last_layer}

Evaluation Criteria:
- Logical coherence: Is the text logically organized?
- Emotional engagement: Does the text evoke the desired emotions?
- Adherence to task requirements: Does it match the original prompt?
- Creativity: Is the text original and imaginative?

Output Format:
- Coherence: [Score out of 10, with a brief explanation]
- Engagement: [Score out of 10, with a brief explanation]
- Adherence: [Score out of 10, with a brief explanation]
- Creativity: [Score out of 10, with a brief explanation]
- Suggestions for Improvement: [Text]
- Overall Score: [Score out of 10]
```

Prompt 3: Prompt for Gradient-Based Global Optimization

```
Task:
You are an advanced global workflow analysis assistant tasked with diagnosing
inefficiencies and proposing optimizations for a multi-step process.
Your goal is to analyze the workflow trajectory and determine which aspects
need improvement to address task failures and enhance overall performance.

You will evaluate the provided consolidated information from a workflow task.
Identify which sub-task outputs or prompts likely caused the failure and
provide specific suggestions for each sub-task. Your output must strictly
follow this format:
<output\_format>\{example\_global\_loss\_format\}</output\_format>

Important Notice:
- All analyses and suggestions should be based on a general level.
- Avoid overly targeted feedback for this specific task instance.
- All required information is provided via: {initial_solution}

Global Optimization Steps:

1. Final Result Evaluation:
   Analyze the final result <final result> to determine if the task failed.

2. Solution Comparison:
   Compare <canonical solution> and <generated solution>:
   - Is the logic in <generated solution> aligned with <canonical solution>?
   - Where is the gap between the analysis and the standard answer?
   - Identify specific issues in <generated solution> that contributed to the
```

```
      failure.
    - Document these findings in the 'global_analysis' section of the
      <output_format>.

3. Block Input and Output Analysis:
   Based on the <task description> and <workflow trajectory>:
   - Do not compare the block outputs with the <canonical solution>.
   - Examine each block_input and block_output.
   - Identify which block(s) caused the task to fail.
   - Highlight any inefficiencies or redundancies.
   - Write optimization suggestions into the 'structure_suggestion' section
     of each relevant block.
   - Review each block's block_description and provide edits if necessary,
     recorded in the 'prompt_suggestions' section.
   - If no edits are needed, do not add any suggestions.

4. Node-Level Analysis Within Blocks:
   For each problematic block:
   - Analyze the internal node_input and node_output.
   - Evaluate the team collaboration structure.
   - Propose improvements to intra-block agent collaboration, if necessary.
   - Document your suggestions in the 'structure_suggestion' section of the
     corresponding block.
```

Prompt 4: Prompt for Layer-Wise Block Optimization

```
You are given a block within a workflow. Your task is to suggest
optimizations for this block, focusing on both prompt improvements and
structural changes, while ensuring consistency and efficiency.

Block Information:
- Block Name: {block_name}
- Global Loss Feedback: {global_loss_feedback}
  (This is global feedback for the entire workflow. Use as reference, but
  base suggestions on block-level reasoning.)
- Blocks Log: {blocks_log}
  (Includes architecture, node inputs/outputs, block/node descriptions.)
- Canonical Solution: {canonical_solution}
- Task Description: {task_prompt}

Evaluation Criteria:
1. Evaluate Each Node
- Check input_variables for validity and consistency.
- Valid sources include:
  * State variables: "task_data", "task_prompt", "task_id"
  * Prior node outputs: e.g., calculation_expert1_output
- For prompt modifications:
  * Include an updated prompt_template with clear instructions
  * Explicitly list all input_variables and their sources

2. Propose Structural Changes
- Add/remove nodes (max 3 additions)
- For added nodes, specify:
  * node_name, agent, output format, prompt_template
  * variable_sources, constraints
- Define from/to edges for new nodes
- Update connected nodes' input_variables if needed
- Set the new entry_node and end_node
- Ensure all nodes (except end_node) have valid outgoing edges
- Include all_edges_now and all_nodes_now

3. Impact on Other Nodes
- Maintain logical consistency with the entire workflow

4. Use Available Agents
- Refer to {available_agents} for potential agents
```

```
- Check each agent's constraints for fit
- Modify agents as needed (update prompt_template, input_variables, or define
new agents)

5. Dynamic Block ID and Naming
- Use {new_block_id} to assign a unique block_id
- Format name as {block_name}X, where X = new_block_id

6. Block Structure Description
- Include:
  * block_structure_description: high-level purpose
  * block_structure_description_details: including:
    1. Nodes and connections
    2. Node roles and logic
    3. Input/output flow
- Ensure clarity, accuracy, and alignment with structure

7. Provided Canonical Solution and Test Cases
- Don't over-optimize: block may not be the cause of failure
- Avoid overfitting: feedback should remain generalized
- Use <canonical solution> and <test cases> as reference only

8. Output Format
- All feedback must be returned in this JSON format: {layerwise_loss_format}
- Do not use arrows to represent edges!
```

Prompt 5: Prompt for Momentum-Based Adjustment

```
Task Description:
You are an advanced strategic advisor focused on enhancing team performance.
Your role is to analyze recent feedback in combination with historical
adjustments to guide team improvement for a specific workflow block.

Provided Information:
- Team Name: <team name> {block_name} </team name>
- Current Team Structure: <current team> {current_block} </current team>
- Final Result of Task Execution:
  <final result> {current_task_results} </final result>
- Current Gradient Feedback:
  <current feedback> {current_gradient} </current feedback>
- Previous Adjustment Direction:
  <previous adjustment direction> {velocity}</previous adjustment direction>
- Input and Output for Block and Nodes:
  * <team input> {block_input} </team input>
  * <team output> {block_output} </team output>
  * <input and output of all nodes> {nodes_info}
    </input and output of all nodes>

Instructions - Two-Step Strategy:

1. Overlap Handling:
- If <current feedback> overlaps with </previous adjustment direction>, focus
on these overlapping issues.
- Since the current version <current team> was formed via previous
adjustments, but <final result> still failed, analyze why earlier suggestions
did not work.
- Carefully review block_input, block_output, and nodes_info to pinpoint
reasons for failure.
- Revise the <current feedback> so it addresses overlapping issues in a more
effective way.

2. New Issues Maintenance:
- If <current feedback> introduces new problems not found in
  <previous adjustment direction>, retain those.
- Slightly refine and consolidate all suggestions to form an updated version
  of feedback.
```

```
Important Notes:
- This block may not be the root cause of task failure.
  Avoid over-optimization.
- Our optimization is dataset-level, not task-specific. Do not overfit
  feedback to this task instance.

Output Format:
Return your suggestions using the same structure as <current feedback>,
wrapped as:
<adjusted feedback> [Your updated suggestions here] </adjusted feedback>
```

Prompt 6: Prompt Example for Layer Selection Based on Task Difficulty

```
Task Description:
You are a performance evaluator tasked with selecting the most suitable block
for solving a Python code finalization task.
The complete workflow consists of three blocks: code_review_block,
code_finalize_block, and code_execute_block.

Current Block:
The block under evaluation is code_finalize_block, which represents the second
layer in the workflow.
It's purpose is to refine another agent's code output based on prior messages,
considering:
- Syntax accuracy
- Logical completeness
- Adherence to the initial coding intent

If the code meets the above standards, keep it unchanged. Otherwise, provide a
corrected version.

Task Details:
- Task Objective: Improve the agent's output code using the contextual
messages.
- Task Description: <task description> {task_prompt} </task description>

Available Blocks:
Below is a list of available blocks, including their structural roles and
descriptions:
<list of all block's structure description> {blocks_structure_descriptions}
</list of all block's structure description>

Instructions:
1. Evaluate the <task description> carefully, identifying key difficulty
points and requirements.
2. Compare block roles and structures from <list of all block's structure
description> to determine which best fits the task.
3. Select the most appropriate block based on the task complexity.

Output Format:
- Output your selection using the exact format below:
  <selected_agg_func> X </selected_agg_func>
- For example, selecting CodeFinalizeBlock3 should result in:
  <selected_agg_func> 3 </selected_agg_func>
```

C Experiment Details

D Experiment Details

D.1 Training and Validation Split

We adopt an 80/20 protocol per dataset when comparable to prior work, and otherwise follow the dataset-specific setups cited below. This keeps splits aligned with baselines while ensuring evaluation on unseen

tasks. The table fuses all details (counts, protocol, and per-task runtime).

Benchmark	Total	Train	Val	Split	Train / task	Test / task
HumanEval[a]	164	131	33	80/20	7 s ↑ 30 s	7 s
Creative Writing[a]	100	80	20	80/20	17 s ↑ 30 s	17 s
MATH (subset)[b]	196	157	39	80/20	13 s ↑ 33 s	13 s
DAbench[c]	257	206	51	80/20	15 s ↑ 34 s	15 s
MMLU–ML[d]	128	16	112	custom	8 s ↑ 28 s	8 s

Table 6: Dataset splits and approximate per-task runtimes. ↑ indicates additional time from backward optimization during training; inference is forward-only. Notes: (a) 8:2 as in Zhou et al. (2024); (b) 196-problem subset and sampling as in Song et al. (2024); (c) full dataset with 8:2; (d) ML subset as in TEXTGRAD (Yuksekgonul et al., 2024), base dataset Hendrycks et al. (2020).

E Case Study

E.1 Prompt Evolutions Examples

Figure 4 and Figure 5 illustrate representative trajectories of prompt evolution across two benchmark tasks: subtask about code review in the HumanEval dataset and subtask about task analysis in the DABench suite, respectively. These diagrams reflect both the structural transformations of block-level workflows and the fine-grained progression of node-level prompt design. Together, these visualizations exemplify how the prompt design co-evolved with structural modularity.

HumanEval: Code Review Prompt Evolution. Figure 4 demonstrates how the system's prompt architecture evolved in the context of solving the `review_code` subtask on the HumanEval dataset. Initially, the workflow consisted of a single-agent node responsible for completing partially written code. As the system matured, this simplistic design was incrementally augmented with a multi-agent framework involving two parallel reviewers and a subsequent decision node. Each reviewer agent received increasingly structured prompts, incorporating pseudo-code context, explicit reasoning criteria (e.g., correctness, efficiency, readability), and modular output constraints.

In subsequent iterations, the system integrated static analysis agents, forming a pluggable review-correction pipeline. The final prompt configuration emphasized modular roles, strict output formatting, and conditional rewriting policies, resulting in a robust, interpretable code review pipeline.

DABench: Task Analysis Prompt Evolution. Figure 5 illustrates the evolution of task analysis prompts when solving data-centric reasoning problems in the DABench benchmark. The initial system was anchored around a single agent generating a natural-language strategy and accompanying pseudo-code. Prompt instructions were general-purpose, with minimal context sensitivity or structural annotation.

With successive iterations, the system adopted a multi-agent architecture, introducing review, feedback, and revision loops. Each agent's prompt was incrementally specialized: reviewers were instructed to analyze structural logic, adherence to constraints, and planning completeness. Prompts began incorporating input-specific metadata, including task constraints, file paths, and structured output tags (e.g., `<analysis>`, `<feedback>`, `<result>`).

E.2 Team Structure Examples with Optimization

To better understand how agent team structures evolve throughout the optimization process, we present visualizations of team configurations across multiple datasets. These examples demonstrate how architectures transition from simple, linear pipelines to more dynamic, graph-based systems as the model learns to coordinate more effectively.

Figure 6 illustrates selected examples from three representative datasets: Creative Writing (Zhou et al., 2024), Math (Hendrycks et al., 2021), and MMLU–Machine Learning (Hendrycks et al., 2020). For each dataset, we choose a single layer and show how the team structure at that layer evolves over time. As optimization progresses, the agent configurations become increasingly complex and tailored to the demands of each dataset, reflecting greater specialization and improved collaboration.

Figure 7 focuses on two additional datasets: HumanEval (Chen et al., 2021) and DABench (Hu et al., 2024). In the case of DABench, we adopt the random train/validation split from (Song et al., 2024). Here, we emphasize the functional diversity among agents by using different node colors to indicate distinct roles (e.g., generation, evaluation, decision-making). These visualizations highlight how functional heterogeneity and task-specific routing emerge through optimization.

Together, these figures demonstrate how adaptive reconfiguration of agent teams enables more effective problem solving and reflects the system's ability to internalize dataset-specific strategies.

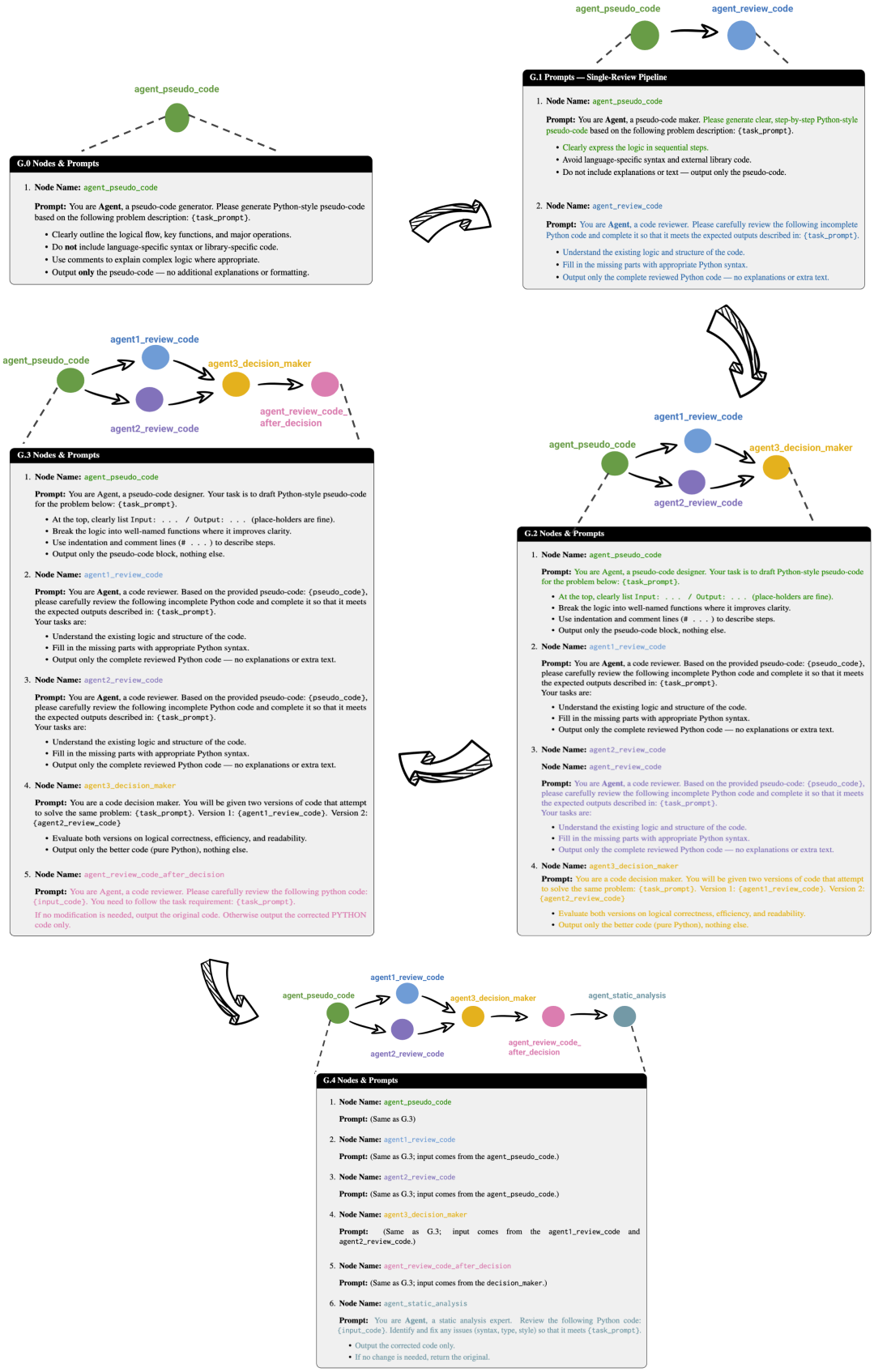

Figure 4: Prompt-evolution trajectory for the HumanEval(Chen et al., 2021) *review_code* subtask. Boxes denote agent nodes, arrows indicate information flow, and shaded regions highlight components newly introduced at each iteration.

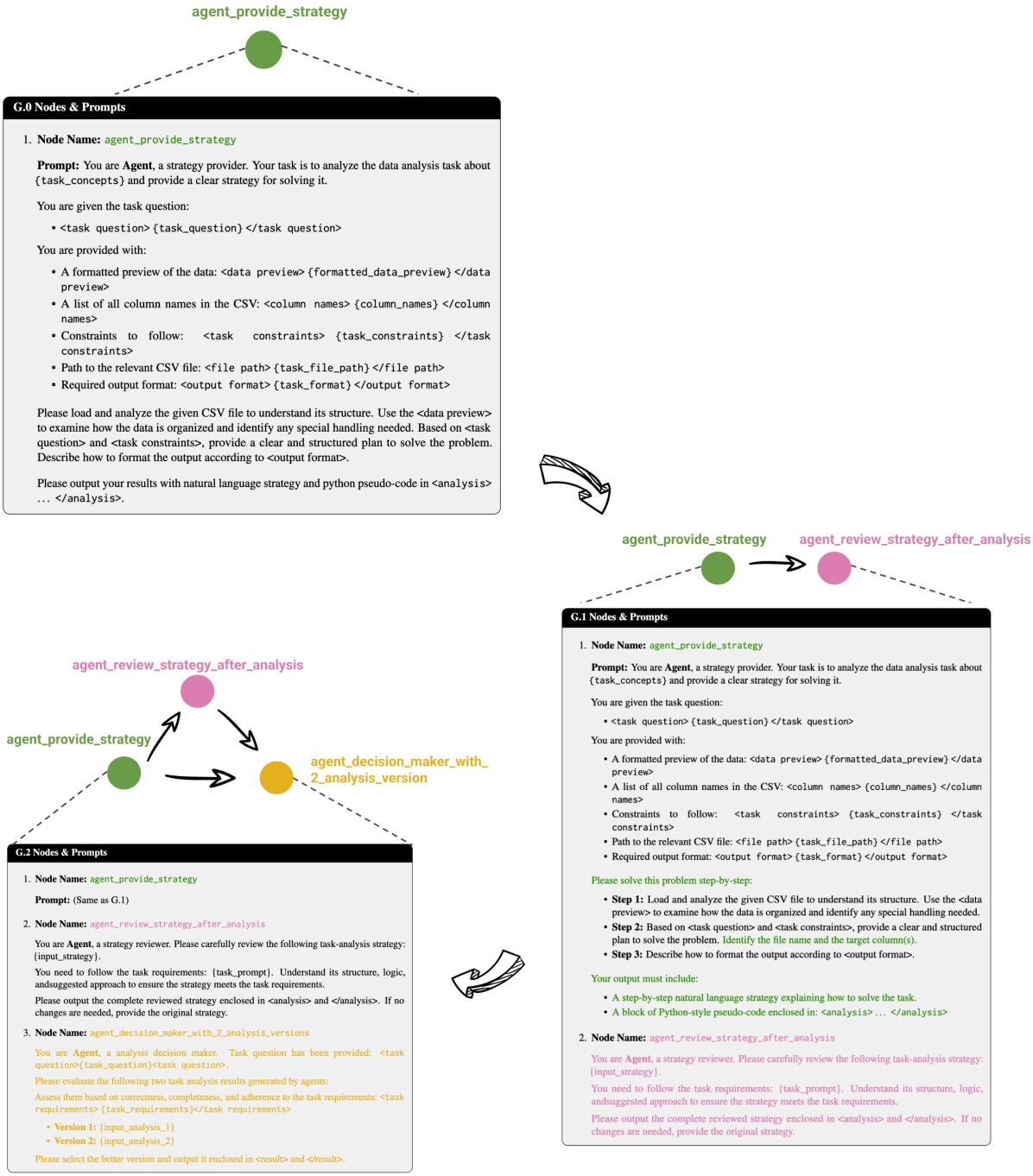

Figure 5: Prompt-evolution trajectory for the DABench(Hu et al., 2024) task-analysis benchmark. Boxes denote agent nodes, arrows indicate information flow, and shaded regions highlight components newly introduced at each iteration.

Figure 6: Evolution of agent team structures on the **Creative Writing** (Zhou et al., 2024), **Math** (Hendrycks et al., 2021), and **MMLU–Machine Learning** (Hendrycks et al., 2020) datasets. For each dataset, we visualize a representative example from one layer, showing how team configurations become progressively more structured and cooperative through optimization.

Figure 7: Team structure visualizations for the **HumanEval** (Chen et al., 2021) and **DABench** (Hu et al., 2024) datasets. Each node's color reflects its functional role within the system. The diagrams highlight how different types of agents coordinate and how task-specific configurations emerge over time.