Compound AI Systems Optimization: A Survey of Methods, Challenges, and Future Directions

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Abstract

Recent advancements in large language models (LLMs) and AI systems have led to a paradigm shift in the design and optimization of complex AI workflows. By integrating multiple components, compound AI systems have become increasingly adept at performing sophisticated tasks. However, as these systems grow in complexity, new challenges arise in optimizing not only individual components but also their interactions. While traditional optimization methods such as supervised fine-tuning (SFT) and reinforcement learning (RL) remain foundational, the rise of natural language feedback introduces promising new approaches, especially for optimizing non-differentiable systems. This paper provides a systematic review of recent progress in optimizing compound AI systems, encompassing both numerical and language-based techniques. We formalize the notion of compound AI system optimization, classify existing methods along several key dimensions, and highlight open research challenges and future directions in this rapidly evolving field.[1]

1 Introduction

The community has witnessed a new generation of AI systems centered on large language models (LLMs), incorporating several sophisticated components such as simulators, code interpreters, web search tools, and retrieval-augmented generation (RAG) modules. These systems have shown remarkable capabilities across domains and typically outperform standalone LLMs. For instance, LLMs communicating with symbolic solvers can tackle Olympiad-level math problems (Trinh et al., 2024), integrate with search engines and code interpreters to match human programmers' performance (Li et al., 2022; Yang et al., 2024b), and when coupled with knowledge graphs, drive biological materials discovery (Ghafarollahi and Buehler, 2024).

*Equal contribution
[1] https://github.com/MiuLab/AISysOpt-Survey

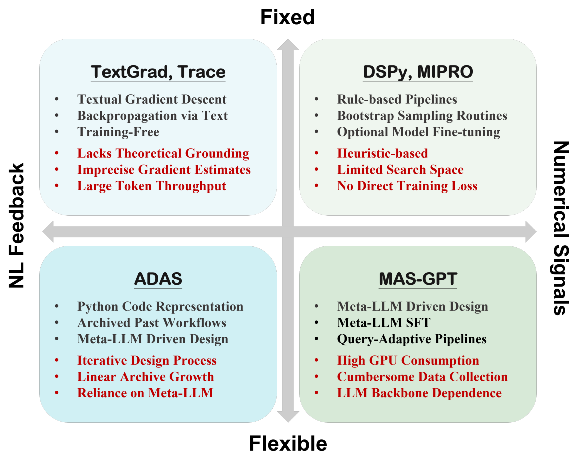

Figure 1: **The proposed 2×2 taxonomy** spans Structural Flexibility (y-axis) and Learning Signals (x-axis). Representative methods for each quadrant along with their key designs and potential drawbacks.

However, even with mature toolkits that streamline the design process of compound AI systems, such as, LangChain (Chase, 2022) and LlamaIndex (Liu, 2022), substantial human intervention remains essential to tailor these systems toward targeted downstream applications (Xia et al., 2024; Zhang et al., 2024c), often involving trial-and-error tuning prompt templates and system pipelines based on heuristics. This limitation has motivated recent efforts to develop principled, automated methods for end-to-end AI system optimization. Yet, the operational schemes of these approaches diverge significantly depending on whether they permit modifications to the system topology and how they transmit learning signals. Moreover, the field still lacks standardized terminology or a cohesive conceptual framework, making some articles difficult for newcomers to navigate (Cheng et al., 2024; Khattab et al., 2023). Despite existing surveys (Lin et al., 2024; Liu et al., 2025) have provided helpful frameworks, they focus on optimization driven by natural language, overlook critical

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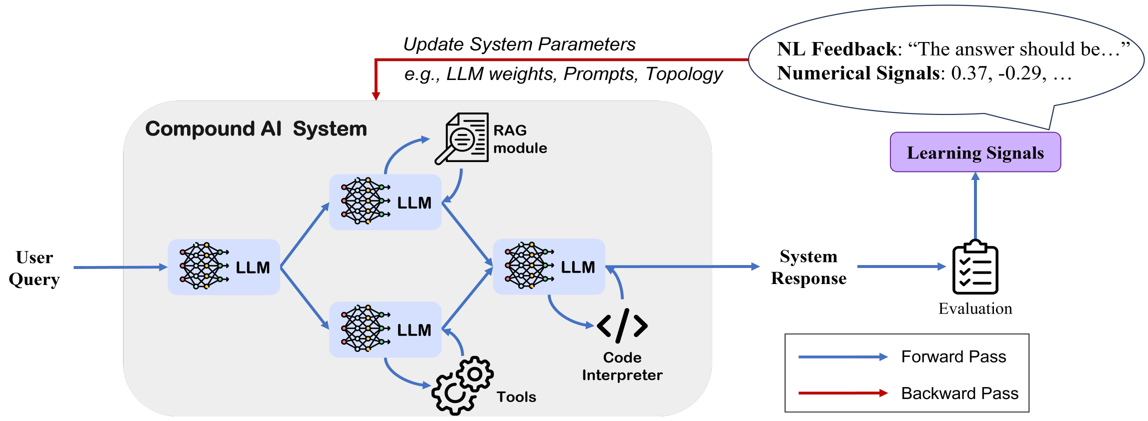

Figure 2: **Example of a compound AI system and its optimization.** Centered on LLMs and coupled with multiple interacting modules, the system handles complex user queries. Automated optimization strategies leverage two types of learning signals, i.e., natural language feedback and numerical signals (defined in Sec. 3.1), to backpropagate errors and guide system updates toward improved performance.

schemes that permit updates to system topology and do not cover the most recent advances.

To address these gaps, this study introduces four key dimensions for examining existing methods and, drawing on two of these dimensions, constructs a 2×2 taxonomy (Fig. 1) that holistically covers 26 representative works. Setting a reasonable scope for our survey, we excluded related but not directly relevant work. These include prompt optimization techniques for a single LLM (Zhou et al., 2022b; Pryzant et al., 2023; Yang et al., 2023; Das et al., 2024; Guo et al., 2025), systems built for task-specific applications without optimization (Zhuge et al., 2023; Hong et al., 2023), and papers that do not explicitly frame their problem as system optimization (Zhou et al., 2022a; Sordoni et al., 2023). The proposed taxonomy is inherently adaptable to future research, and we hope it will enable developers of compound AI systems to gain a high-level overview before delving into technical details, while allowing researchers proposing novel algorithms to better situate and compare their contributions.

The remainder of this paper is organized as follows: Sec. 2 provides the necessary background and formalization for compound AI systems and their optimization. Sec. 3.1 discusses the four key dimensions, followed by Sec. 3.2, which presents a detailed review of surveyed papers based on the proposed 2×2 taxonomy. Sec. 4 identifies the main challenges facing current methods and their corresponding future directions, and Sec. 5 concludes with a summary of our contributions.

2 Background and Preliminaries

2.1 Compound AI Systems

In contrast to single AI models that function as statistical models (e.g., the Transformer (Vaswani et al., 2017) for next-token prediction), compound AI systems are defined as systems that tackle AI tasks using multiple interacting components (Zaharia et al., 2024) (see Fig. 2). The term compound AI system somehow overlaps with related concepts and is often used interchangeably in the field. These include multi-agent systems (MAS) (Zhou et al., 2025; Wang et al., 2025b), language model pipelines (Khattab et al., 2023; Soylu et al., 2024), and language model programs (Opsahl-Ong et al., 2024). Hence, in this survey, we include any method that aims to optimize AI systems composed of multiple components, and adopt "compound AI system" as a unifying label.

Although end-to-end optimization of single models such as neural networks implemented in PyTorch (Paszke, 2019) is straightforward thanks to gradient-based backpropagation (Rumelhart et al., 1986) on their fully differentiable layer connections, compound AI systems are built from non-differentiable components and thus require novel optimization methods. Representative examples include heuristic bootstrap-based methods (Khattab et al., 2023) applied to find optimal in-context examples in LLM prompts, as well as approaches leveraging an auxiliary LLM to provide textual feedback on prompt updates (Yuksekgonul et al., 2025) or propose improved system topologies (Hu et al., 2024).

2.2 Formal Definitions

Due to inconsistent mathematical descriptions across the surveyed papers, we develop a unified graph-based formalization as well as notations for compound AI systems and their optimization[2].

Specifically, we use $\Phi = (G, \mathcal{F})$ to denote a compound AI system that inputs a user query $q \in \mathcal{Q}$ and outputs a response (answer) $a \in \mathcal{A}$. In particular, $G = (V, E)$ is a directed graph and $\mathcal{F} = \{f_i\}_{i=1}^{|V|}$ is a set of operations (e.g., LLM forward pass, RAG step, external tool calling). Each f_i is attached to node v_i, producing

$$Y_i = f_i(X_i;\, \Theta_i), \tag{1}$$

where X_i is the input to v_i, Y_i its output, and Θ_i its parameters. The edge matrix $E = [c_{ij}]$ comprises Boolean functions $c_{ij} : \Omega \to \{0, 1\}$ that determine whether the potential edge from v_i to v_j is active. This means given the contextual state $\tau \in \Omega$, the edge $(v_i \to v_j)$ is active if and only if $c_{ij}(\tau) = 1$. Consequently, even though G and $\mathcal{F}$ are fixed after optimization, the Φ's effective topology varies with τ, reflecting dependencies on both the input query q and intermediate outputs of the system, as visualized in Appendix Fig. 5.

In more detail, the node input is set by

$$X_i \;\leftarrow \bigoplus_{j:\, c_{ji}(\tau)=1} Y_j, \tag{2}$$

where $\oplus$ denotes concatenation of the outputs Y_j from all nodes v_j whose edge $v_j \to v_i$ is active. The node parameter Θ_i decomposes as $\Theta_i = (\theta_{i,N}, \theta_{i,T})$, where $\theta_{i,N}$ are numerical parameters (e.g., LLM weights, temperature) and $\theta_{i,T}$ are textual parameters (e.g., LLM prompts). Due to space constraints, descriptions of the input node v_{in}, the output node v_{out}, and our formalism's ability to either support or prohibit cyclic structures are deferred to Appendix Sec. A.

Given a training set $\mathcal{D} = \{(q_i, m_i)\}_{i=1}^N$, where each query q_i is associated with optional metadata $m_i \in \mathcal{M}$, such as output labels or hints useful for evaluating system correctness, and a performance metric $\mu : \mathcal{A} \times \mathcal{M} \to \mathbb{R}$, the goal of compound AI system optimization is defined by solving:

$$\max_{\Phi} \frac{1}{N} \sum_{i=1}^{N} \mu\big(\Phi(q_i), m_i\big). \tag{3}$$

[2]If our notations conflict with that of any original work, our definitions take precedence.

3 Compound AI System Optimization

With background established, we now turn to the core of our survey. Sec. 3.1 first present four principled dimensions underlying the optimization of compound AI systems, i.e., *Structural Flexibility*, *Learning Signals*, *Component Options*, and *System Representations*. Sec. 3.2 then review existing methods in the proposed 2×2 taxonomy.

3.1 Four Principled Dimensions

Structural Flexibility As described in Sec. 2.2, the pipeline of Φ can be modeled as a computation graph $G = (V, E)$. The concept of *Structural Flexibility* thus refers to the degree to which an optimization method can modify this graph. One class of methods, termed *Fixed Structure*, assumes a predefined topology (V, E) and focuses exclusively on optimizing the node parameters $\{\Theta_i\}$ (e.g., LLM prompts). In contrast, more recent methods acknowledge the importance of identifying optimal system topologies (Zhuge et al., 2024; Hu et al., 2024) and propose to jointly optimize both the node parameters and the graph structure itself, such as edge connections E, node counts $|V|$, and even the types of operations in $\mathcal{F}$. These methods, termed *Flexible Structure*, broaden the search space of Φ, enabling more effective orchestration of the system toward targeted tasks.

Learning Signals Regardless of structural flexibility, effective optimization of Φ requires *Learning Signals* that steer system updates toward improved task performance (Fig. 2). These signals naturally originate from system performance metric $\mu\big(\Phi(q_i), m_i\big)$, and can be conveyed in two distinct forms. The first type is natural language feedback (denoted as *NL Feedback*), where signals are generated by an auxiliary LLM that is separate from those used within the system itself (Yuksekgonul et al., 2025; Cheng et al., 2024; Hu et al., 2024). This approach leverages the reasoning capabilities of LLMs to provide textual guidance for system optimization. The second type, termed *Numerical Signals*, encompasses methods in which learning signals are represented numerically. We further categorize numerical signals into four different forms, as illustrated in Fig. 3.

Component Options This dimension distinguishes optimization methods by their considered types of operations in $\mathcal{F}$. Though most Φ center around LLMs, many frameworks integrate addi-

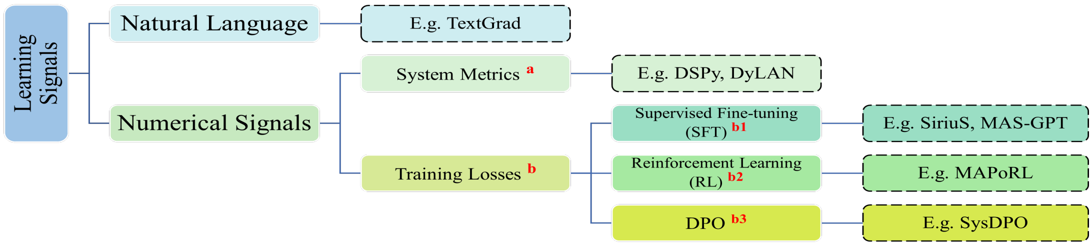

Figure 3: **Learning Signals** are classified into two categories, with Numerical Signals further divided by their utilization schemes: (a) one class of methods devises rule-based algorithms that directly learn from raw system performance metrics, and (b) another class transforms system evaluation results into formalized training objectives. These objectives are further split as (b1) supervised fine-tuning (SFT) losses, (b2) reinforcement learning (RL) reward functions, and (b3) direct preference optimization (DPO) (Rafailov et al., 2023) losses.

tional components to enrich domain knowledge or perform specialized tasks. These include RAG modules (Yin and Wang, 2025), code interpreters (CI) (Hu et al., 2024; Wang et al., 2025b), or Tools calling such as web search (Zhuge et al., 2024). In multi-modal contexts, additional components such as image generation models (IGM) are employed (Wang et al., 2025a). Note that some works assume an unrestricted components pool (Yuksekgonul et al., 2025) or do not explicitly specify their supported component options (Hu et al., 2024; Wang et al., 2025b). In those cases, we infer their component options by examining the components used in their experimental setups or by inspecting their system representations.[3]

System Representations Different representations are used to characterize Φ's operational topology across methods. The most common choice is to model Φ as a graph. A directed acyclic graph (DAG) ensures that each node is invoked at most once per forward pass (Khattab et al., 2023; Zhuge et al., 2024), while a cyclic graph supports schemes such as multi-turn debates (Subramaniam et al., 2025; Park et al., 2025) or multi-hop RAG (Yin and Wang, 2025). Although Liu et al. (2024) employs feed-forward networks as system representations, we also label them as graphs, given their equivalence. Acknowledging the potential limitations to optimize system topologies in graph space (Hu et al., 2024), another line of research represents Φ's workflow as natural language program (Li et al., 2024) or Python code (Hu et al., 2024; Zhang et al., 2024a; Ye et al., 2025), which supports conditional logic and loops without any acyclicity constraints.

[3]Methods that use Python code as *System Representations* inherently support code interpreters (CI).

3.2 Representative Methods

Equipped with the discussed four principled dimensions, here we review existing methods along two major axes: *Structural Flexibility* (Fixed vs. Flexible Structure) and *Learning Signals* (NL Feedback vs. Numerical Signals)[4]. All considered papers are listed in Table 1.

Fixed Structure, NL Feedback Most existing methods leverage LLMs' ability to generate rich, general natural language suggestions for prompt optimization in standalone LLMs (Zhou et al., 2022b; Pryzant et al., 2023; Yang et al., 2023). TextGrad (Yuksekgonul et al., 2025) is among the first to extend this idea to compound AI systems by updating their node parameters, e.g., LLM prompts ($\{\theta_{i,T}\}$). Drawing inspiration from numerical gradient descent in PyTorch (Paszke, 2019), TextGrad defines each node in the system graph as an independent computational unit, where optimization unfolds in three stages: (1) an *evaluator* LLM assesses the system's output $\Phi(q_i)$ against an expected reference m_i and generates textual loss signals; (2) for each participating node, a *gradient estimator* LLM generates node-specific textual suggestions conditioned on system dialogue and backpropagated loss; and (3) an *optimizer* LLM at each node refines node parameters using these suggestions. This process mirrors backpropagation via natural language, simulating differentiability across discrete modules.

Several works have since built upon TextGrad's framework. AIME (Patel et al., 2024) shows that for complex code generation tasks, using a single

[4]For a few methods that use both types of learning signals, we still categorize them into a single category. See Appendix Sec. C for more details.

Methods	Structural Flexibility	Learning Signals	Component Options	System Representations
TextGrad (2025)	Fixed	NL Feedback	LLM	Graph†
Trace (2024)	Fixed	NL Feedback	LLM	Graph†
AIME (2024)	Fixed	NL Feedback	LLM	Graph†
Revolve (2024b)	Fixed	NL Feedback	LLM	Graph†
GASO (2024a)	Fixed	NL Feedback	LLM	Graph†
LLM-AutoDiff (2025)	Fixed	NL Feedback	LLM; RAG	Graph
DSPy (2023)	Fixed	Numerical Signals^{a}	LLM	Graph†
MIPRO (2024)	Fixed	Numerical Signals^{a}	LLM; RAG	Graph
BetterTogether$*$ (2024)	Fixed	Numerical Signals^{a,b_1}	LLM; RAG	Graph†
SiriuS$*$ (2025)	Fixed	Numerical Signals^{b_1}	LLM	Graph
MAPoRL$*$ (2025)	Fixed	Numerical Signals^{b_2}	LLM	Graph
SysDPO$*$ (2025a)	Fixed	Numerical Signals^{b_3}	LLM; IGM	Graph†
Multiagent Finetuning$*$ (2025)	Fixed	Numerical Signals^{b_1}	LLM	Graph
Agent Symbolic Learning (2024)	Flexible	NL Feedback	LLM; RAG	Graph†
ADAS (2024)	Flexible	NL Feedback	LLM; CI	Python Code
AFlow (2024a)	Flexible	NL Feedback	LLM; CI	Python Code
MASS (2025)	Flexible	NL Feedback	LLM	Graph
DebFlow (2025)	Flexible	NL Feedback	LLM	Graph
DyLAN (2024)	Flexible	Numerical Signals^{a}	LLM	Graph
GPTSwarm (2024)	Flexible	Numerical Signals^{b_2}	LLM; Tools	Graph†
AutoFlow$*$ (2024)	Flexible	Numerical Signals^{b_2}	LLM	NL Programs
MaAS (2025)	Flexible	Numerical Signals^{b_2}	LLM; Tools; CI	Graph†
ScoreFlow$*$ (2025b)	Flexible	Numerical Signals^{b_3}	LLM; CI	Python Code
MAS-GPT$*$ (2025)	Flexible	Numerical Signals^{b_1}	LLM; CI	Python Code
W4S$*$ (2025)	Flexible	Numerical Signals^{b_2}	LLM; CI	Python Code
FlowReasoner$*$ (2025)	Flexible	Numerical Signals^{b_1,b_2}	LLM; CI	Python Code

Table 1: **Compound AI System Optimization methods**, sorted by their first publication date on arXiv. All methods and their properties along the four principled dimensions are listed. Superscripts ^{a}, ^{b_1}, ^{b_2}, and ^{b_3} denote the type of numerical signal each method employs (Fig. 3). An asterisk ($*$) indicates methods that require model fine-tuning. For graph-based system representations, a dagger (†) marks methods restricted to acyclic structures (i.e., DAGs).

evaluator LLM often allows errors in the generated code to go undetected, whereas concatenating outputs from multiple *evaluator* LLMs can mitigate this issue. REVOLVE (Zhang et al., 2024b) observes that *NL Feedback* is often applied in a first-order manner, causing stagnation and oscillations during system optimization. It therefore enriches the *gradient estimator* LLMs' input with a concise execution history of past prompts and responses, enabling the generation of curvature-aware feedback, similar to the Hessian in numerical optimization. GASO (Wang et al., 2024b) identifies the negligence of sibling-input interactions in TextGrad's backpropagation scheme, thus proposes semantic gradient descent to compute context-aware gradients and aggregate them for credit assignment. LLM-AutoDiff (Yin and Wang, 2025) addresses the intricacy of multi-component (e.g., large $|V|$, diverse $\mathcal{F}$) and cyclic system structures that prior work has not fully explored. In particular, it introduces *time-sequential gradients* to accumulate multiple textual gradients for nodes invoked repeatedly during a forward pass, and proposes an optional *skip-connections* mechanism, serving as powerful building block for optimizing large-scale systems via natural language.

Trace (Cheng et al., 2024), developed concurrently with TextGrad, introduces a joint optimization that updates all LLM prompts at once. It first obtains global *NL Feedback* from an *evaluator* LLM and then, in a single LLM invocation, updates every involved node by presenting the model with an minimal subgraph (analogous to execution trace in Python). This process address two caveats (Lin et al., 2024) in the backpropagation scheme of TextGrad: (i) error accumulation due to imprecise *NL Feedback*, and (ii) the linear growth in LLM calls with the number of nodes.

Serving as pioneers in the field, these methods demonstrate that learning from text is possible not only for single AI models but also for systems composed of discrete modules. Nevertheless, their successes are supported mainly by empirical results without theoretical grounding. In addition, the common reliance on proprietary LLMs to generate NL feedback incurs high API costs.

Fixed Structure, Numerical Signals Rather than relying on textual signals, methods in this category use numerical signals to update node parameters. DSPy (Khattab et al., 2023) provides a Python library[5] featuring declarative programming modules for designing and optimizing Φ. As a method that learns directly from raw system metrics, it introduces a suite of rejection-sampling–based routines (`Bootstrap-*`) for generating high-quality in-context demonstrations informed by corresponding system performance. Users may optionally fine-tune LLM weights ($\theta_{i,N}$) on the collected demonstrations via `BootstrapFinetune` procedure. MIPRO (Opsahl-Ong et al., 2024) advances by jointly optimizing demonstrations and instructions. Specifically, it employs a Bayesian surrogate model to maintain and update posterior distributions over instruction–demonstration configurations, favoring those that yield high performance. BetterTogether (Soylu et al., 2024) extends by alternating between LLM prompt and weight optimization, enabling LLMs to iteratively teach themselves and outperform single-strategy baselines.

Remaining methods in this category involve model fine-tuning, where numerical signals from system evaluation are instantiated as different types of training losses, as discussed in Fig. 3. In the SFT category, SiriuS (Zhao et al., 2025) constructs several system schemes by assigning predefined roles to its LLM nodes (e.g., "Physicist" and "Mathematician"). It then gathers reasoning trajectories, i.e., intermediate dialogue outputs, for queries q_i with high $\mu\big(\Phi(q_i), m_i\big)$ and independently supervised fine-tunes each LLM node using its corresponding input–output pairs. For q_i that results in failed attempts, SiriuS performs *trajectory augmentation* by resampling original attempts with feedback from an additional agent. Concurrent with SiriuS but building on the multiagent debate (Du et al., 2023) scheme, *multiagent finetuning* (Subramaniam et al., 2025) introduces novel rules for collecting training data for each *generation* and *critic* model for subsequent SFT.

Belonging to the RL category, MAPoRL (Park et al., 2025) targets the multiagent debate (Du et al., 2023) scenario as well. It differs from Subramaniam et al. (2025) by training a *verifier* LLM to assign immediate correctness rewards to each LLM node, and introduces influence-aware reward shaping to incentivize collaboration. Finally, in the DPO category, SysDPO (Wang et al., 2025a) features a system characterized by an LLM and a diffusion model (Rombach et al., 2022). Aiming at image generation tasks, SysDPO curates a preference dataset by computing preference scores based on images' *order consistency* and *distribution evenness*. Unlike original DPO loss, SysDPO incorporates probability decomposition to enable fine-tuning multiple components in Φ.

These methods introduce novel ways to leverage system performance signals, effectively mitigating the imprecision of natural language. However, excessive human-designed rules may limit generalizability. Additionally, fine-tuning each LLM in Φ incurs substantial GPU resource demands.

Flexible Structure, NL Feedback Methods discussed previously tune only node parameters within a predefined system topology. To overcome this constraints, methods in this category leverage NL Feedback to jointly optimize both node parameters and overall system structure. Concurrent with TextGrad (Yuksekgonul et al., 2025), Agent Symbolic Learning (Zhou et al., 2024) designs optimizers with three components: *PromptOptimizer*, *ToolOptimizer*, and *PipelineOptimizer*, making it goes beyond node tuning because the latter two components support tool creation as well as node addition, deletion, and movement. Through a series of analytical experiments, MASS (Zhou et al., 2025) demonstrates that optimizing LLM prompts $\{\theta_{i,T}\}$ can deliver performance gains in compound AI systems more easily than exploring the topology (V, E). Building on this insight, MASS devises a three-stage framework in which prompt optimization precedes topology search.

Recognizing that previous approaches using graphs as system representations may not fully cover the space of possible system designs and that this space is inherently difficult to search, ADAS (Hu et al., 2024) is the first to adopt Python code as system representation. Specifically, conditioned on an archive maintaining prior code and its corresponding performance metric, a meta LLM is asked to iteratively design novel workflows. Owing to the vast search space of code representations, ADAS faces challenges in its linear heuristic search processes and coarse workflow storage, which lead to the accumulation of irrelevant information for the meta LLM (Zhang et al., 2024a). Identifying this, AFlow (Zhang et al., 2024a) leverages the tree structure of Monte Carlo Tree Search (MCTS)

[5] `http://dspy.ai`

to preserve past experience and employs a set of predefined operators to efficiently identify optimal system designs. DebFlow (Su et al., 2025) argues the limitation posed by using a single meta LLM in this scheme, and introduces an innovative debate framework where multiple *debaters* propose their opinions on system designs, with a *judge* helping to conclude the refined workflow.

Methods in this category demonstrate how novel algorithms can leverage the power of proprietary LLMs for direct workflow design. Nonetheless, effective engagement with these meta LLMs demands high token consumption (Hu et al., 2024) or multiple LLM inferences (Su et al., 2025). Also, evaluations on less powerful open-source models remain scarce.

Flexible Structure, Numerical Signals Completing our review, this passage describes methods that employ *Numerical Signals* to refine Φ without posing fixed topology constraints. DyLAN (Liu et al., 2024) and GPTSwarm (Zhuge et al., 2024) are methods in this category that do not involve model fine-tuning. DyLAN models multiturn debate as a temporal feed-forward network in which agents prompted with distinct roles are unrolled across layers. The system is optimized through pruning unhelpful agents and adaptively connect the surviving agents between consecutive layers. Rule-based algorithms are employed to score each agent's importance, positioning DyLAN within the category that leverages raw system metrics as learning signals. GPTSwarm models Φ as a hierarchical framework composed of *nodes* ($v_i \in V$), *agents* (graphs that link nodes), and *swarms* (composite graphs that interconnect multiple agents), then employs an optimization procedure to refine the edge connections among *agents*. A parameterized probabilistic distribution D_θ is introduced to govern the connectivity within the swarm graph, which is then optimized using a gradient-ascent variant of the REINFORCE (Williams, 1992) algorithm, placing GPTSwarm within the class of RL methods.

Before discussing the remaining methods, we note that they operate in a query-adaptive manner, i.e., instantiating a new Φ for each q_i. This operating scheme contrasts with methods discussed so far in which a single task-specific Φ, once optimized, is used for all q_i. Similar to ADAS (Hu et al., 2024) and AFlow (Zhang et al., 2024a), these methods leverage a meta LLM to generate optimal system designs. However, rather than relying solely on inference, they fine-tune the meta LLM using constructed training datasets or reward functions to enable effective pipeline generation, given the limited prior knowledge about compound AI system design within LLMs

Starting from the SFT category, MAS-GPT (Ye et al., 2025) first constructs a *query pool* from open-source queries across various domains, and a *MAS pool* by manually implementing over 40 common system designs in Python code. Through *evaluation*, *selection*, and *refinement* of query–MAS pairs, MAS-GPT curates a training dataset that ensures consistency, minimizing ambiguity when fine-tuning the meta LLM.

Next, within the RL category, AutoFlow (Li et al., 2024) prompts the meta LLM to generate Φ using CoRE (Xu et al., 2024b) syntax, then iteratively fine-tunes it with the average score on task data $\mathcal{D}$ as the reward. It also offers a workaround for closed-source meta LLMs by in-context learning. MaAS (Zhang et al., 2025) constructs and optimizes an *agentic supernet*, a probabilistic distribution over agentic architectures. The token cost incurred during system execution is also considered as a loss term to achieve a trade-off between system performance and complexity. W4S (Nie et al., 2025) maximizes the meta LLM's flexibility by constraining only the workflow interfaces, without predefining any system modules. By using a small (weak) model to reduce training cost, W4S casts the problem as a multi-turn Markov Decision Process (MDP), in which the meta LLM progressively learns to design and refine Φ based on environmental feedback. FlowReasoner (Gao et al., 2025) combines SFT and RL by first fine-tuning the meta LLM for basic reasoning regarding system generation, and then applying RL with a multi-purpose reward to further optimize the model.

Finally, ScoreFlow (Wang et al., 2025b) introduces Score-DPO, an extension of the original DPO. During each iteration, for every query q_i, multiple candidate Φ are sampled from the meta LLM and evaluated by an LLM executor; preference data are then collected based on the observed differences in system performance.

Recent trends in this category frame compound system optimization as a meta LLM fine-tuning problem, thereby sidestepping the non-differentiability of modules within Φ. However, substantial effort is still required to curate high-quality training data, and the lack of comprehensive evaluation across different model families limits the practical applicability of these methods.

4 Challenges and Future Directions

After reviewing representative methods, this section presents several key challenges and their future directions. Due to space constraints, additional discussion is deferred to Appendix Sec. B.

Manual Hyperparameter Configuration Despite aiming to automate the optimization process, we identify residual human interventions in existing methods, particularly in the configuration of algorithm-related hyperparameters, that challenge automation claims and limit practical value.

In particular, methods in the Fixed Structure category require users to configure system topologies based on domain expertise. Although some studies evaluate their algorithms across multiple system designs (Yin and Wang, 2025; Zhao et al., 2025), there is no guarantee that these configurations will meet the requirements of all target applications. Textual hyperparameters also frequently appear in various methods. For example, the prompt templates used for the *evaluator*, *gradient estimator*, and *optimizer* in TextGrad (Yuksekgonul et al., 2025), as well as those for the meta LLM in ADAS (Hu et al., 2024), are handcrafted by the original authors and often lack a clear design rationale or sensitivity analysis of their wording.

Numerical hyperparameter decisions persist as well; for instance, the number of bootstrap samples in DSPy (Khattab et al., 2023) remains user-tunable and cannot be automated. Even seemingly automated numerical flexible-structure methods, such as MAS-GPT (Ye et al., 2025), require manual configuration, as evidenced by the prompt templates for *pair refinement*.

Despite the efforts of metaTextGrad (Xu et al., 2024a), which applies meta-learning to automatically optimize templates for *evaluator*, human intervention remains to craft the meta-learner's prompts. To move toward truly automated system optimization, akin to near hyperparameter-free neural network training, we urge future research to reduce reliance on both textual and numerical hyperparameters. For any hyperparameters that remain, we advocate thorough sensitivity analyses to help users understand each method's behavior and robustness.

Excessive Computation Burden Optimization of compound AI systems is inherently more challenging than tuning individual models. Existing approaches thus resort to various workarounds, leading to substantially higher computational overhead.

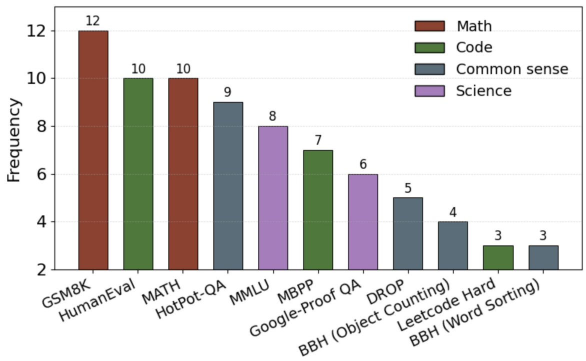

Figure 4: The frequency statistics of benchmarks tested in the surveyed 26 papers.

In NL feedback learning, methods such as TextGrad require multiple LLM calls to approximate a single gradient step. Although methods like Trace (Cheng et al., 2024) and ADAS (Hu et al., 2024) use global LLM call(s) per optimization step, they must embed extensive context in their prompts (e.g., *minimal subgraphs* or *agent archives*), which increases token throughput. Since these methods typically rely on proprietary models (Achiam et al., 2023), they incur substantial API costs. Conversely, numerical signal-based methods often leverage open-source LLMs to avoid API expenses. These models typically require fine-tuning to perform well, thereby shifting the burden to GPU resources. Developers are thus faced with a trade-off between API costs and GPU consumption.

Moreover, computational burden also arises during inference. By focusing primarily on system performance, current Flexible Structure methods often overlook the need to regularize system complexity (e.g., multi-round loops or lengthy executions), resulting in unbounded resource consumption at run time. Although a few methods (Zhang et al., 2025; Gao et al., 2025) have begun to encourage less complex system designs (e.g., lower token consumption), their applicability and scalability in large-scale deployments remain to be tested (Liu et al., 2025). We therefore suggest that future research develop resource-efficient optimization algorithms and at the same time devise principled ways to constrain system complexity without compromising performance.

Limited Experimental Scope Since compound AI systems are expected to address complex problems, it is important to investigate their effectiveness on more challenging tasks. Yet, papers in the field primarily evaluate their proposed methods on datasets widely used for single LLMs (Fig. 4), such as those for math reasoning (e.g., GSM8K (Cobbe et al., 2021)), commonsense reasoning (e.g., MMLU (Hendrycks et al., 2021)), and code generation (e.g., HumanEval (Chen et al., 2021) and MBPP (Austin et al., 2021)). While these evaluations reflect general effectiveness, we argue that it is also important to include benchmarks involving more complex tasks. For instance, AgentBench (Liu et al., 2023) and AgentGym (Xi et al., 2024) comprise multiple tasks requiring different LLMs within the system to cooperate and discuss, and GAIA (Mialon et al., 2023) examines system effectiveness in real-world scenarios requiring various tool usage. Furthermore, given the broad utility of compound AI systems (e.g., healthcare systems with doctors embedded as nodes in Φ (Chen et al., 2024)), it is necessary to evaluate algorithmic performance when humans function as nodes within the system and to devise principled methods for modeling their behavior.

Empirical NL Feedback While NL Feedback methods have shown promising empirical results, they lack theoretical guarantees. For example, the convergence of textual gradient descent remains unproven, whereas classical gradient descent are supported by formal convergence proofs (Cheridito et al., 2022; Hutzenthaler et al., 2021). Such proofs provide a solid foundation for the continuous advancement of single-model optimization. We therefore advocate future work to deliver rigorous convergence and optimality analyses for learning via NL Feedback, which will offer deeper insights and strengthen the field's theoretical underpinnings.

Potential Safety Risks While safety issues and corresponding defenses for single models have been extensively studied, such as jailbreak attacks on LLMs and their mitigation (Yi et al., 2024) and human-engineered AI pipelines to reduce harmful prompts and outputs (Han et al., 2024), the attack surface expands considerably in compound AI systems (Banerjee et al., 2024). For instance, Debenedetti et al. (2024) demonstrate that privacy-preserving models can still leak sensitive data when integrated as a component of a larger system. Furthermore, because compound AI systems are often embodied and executed as code within enterprise environments, latent failure modes may remain undetected and undermine system reliability even in the absence of explicit adversarial attacks. Despite these risks, research on compound AI system optimization that extends beyond downstream performance has so far addressed mainly execution efficiency (Zhang et al., 2025), with little attention to system-level alignment or safety (Zheng et al., 2025). Given the mature alignment and safeguarding optimization techniques available for single models (Achiam et al., 2017; Dai et al., 2023), we urge future work to adapt and extend these strategies to compound systems in order to balance capability enhancements with safety guarantees (Yang et al., 2024a).

Inconsistent Library Support During our survey, we observed a lack of a standardized and widely adopted library in the field. Although some well-maintained libraries such as TextGrad (Yuksekgonul et al., 2025) and DSPy (Khattab et al., 2023) have gained popularity among practitioners, still a great portion of existing works implement compound AI systems optimization using custom, self-crafted codebases. While frameworks such as TensorFlow (Abadi et al., 2015) and PyTorch (Paszke, 2019) dominate single-model training, best practices for implementing and optimizing compound AI systems are still under development. We suggest that future efforts focus on systematically benchmarking and comparing existing libraries for compound AI system optimization. Such efforts could support their improvement and help establish clearer guidelines for developers and researchers—for example, regarding when to use which library—as is done in the context of single-model training (Novac et al., 2022).

5 Conclusions

We survey recent advances in optimizing compound AI systems composed of interacting components like agents and tools. To unify diverse research efforts, we propose a graph-based formalism with conditional edges, enabling structured analysis of system interactions. With this framework, we examine existing methods across four principled dimensions and organize them into a 2×2 taxonomy. Our survey highlights key trends and trade-offs, including computational overhead, the NL interface, and challenges in scaling and generalization. We also identify open problems and outline future directions to guide continued progress in the field.

Limitations

We acknowledge several limitations of this survey. First, due to the lack of a universally accepted definition of "compound AI systems," we also include works that self-identify as optimizing multi-agent systems (MAS) or LM programs, without systematically analyzing their conceptual overlaps and distinctions.

Second, we focus exclusively on methods that explicitly optimize systems of multiple nodes, thereby excluding traditional prompt optimization techniques for standalone LLMs and contributions not framed as system optimization. Despite our efforts to draw a clear boundary, some relevant papers may have been inadvertently omitted; moreover, as this field is actively evolving during the preparation of this manuscript, studies published in the last two months may be only partially covered. To address this, we maintain an open-source repository where readers can submit works we may have missed.

Third, due to page limits, we highlight only the core motivation and algorithmic design of each method and omit details such as experimental setups and results. Readers are encouraged to consult the original papers and code repositories for full technical details once they have gained an overview from our survey.

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A More Details on Formal Definitions

Special Nodes In our formalism of compound AI systems, two special nodes play key roles:
(1) the input node $v_{\text{in}} \in V$, which receives the user query $q \in \mathcal{Q}$ as the system's entry point; and
(2) the output node $v_{\text{out}} \in V$, which terminates system execution. In our definition, the operation attached to v_{out} is the identity function I, so that it simply parses its input as the final system answer:

$$Y_{\text{out}} = I\big(X_{\text{out}}\big)\,,$$
$$a = Y_{\text{out}}\,.$$

Additionally, all outgoing conditional edges from v_{out} are set to zero ($c_{\text{out},j} = 0, \forall j$), ensuring that the system does not route its output back to other nodes. This terminal structure effectively signals computation completion, similar to how end-of-sequence tokens function in language models.

Support for Cyclic Structures Our formulation naturally accommodates both DAGs and cyclic topologies via conditional edges. Formally, a cycle at node v_i exists if and only if there is a path of length $L \geq 1$

$$\big(v_{i_0}, v_{i_1}, \ldots, v_{i_L}\big) \subseteq V$$

such that

$$v_{i_0} = v_{i_L} = v_i, \quad v_{i_t} \neq v_{\text{out}} \;\; \forall\, 0 \leq t < L,$$

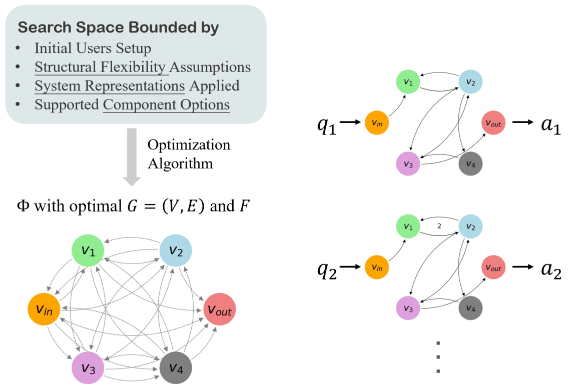
and

$$c_{i_t, i_{t+1}}(q, \tau_t) = 1 \quad \forall\, 0 \leq t < L.$$

Here, $\{v_{i_0}, \ldots, v_{i_L}\}$ denotes the sequence of nodes visited along the loop, and each $c_{i_t, i_{t+1}}(q, \tau_t) = 1$ indicates that the conditional edge from v_{i_t} to $v_{i_{t+1}}$ is active under input q and state τ_t. In other words, v_i can route its output back to itself before reaching the output node v_{out}, forming a cyclic loop.

If one would like to enforce acyclicity, it suffices to record the history of visited nodes in the state τ and disallow any transition $v_j \to v_k$ whenever v_k already appears in the history. This simple rule easily prevents the re-entry required to form a cycle.

Visualization Fig. 5 provides a visualization of system optimization under our formalism of graphs with conditional edges.



(a) Optimization Stage (b) Execution Stage

Figure 5: (a) During optimization, the algorithm explores the design space defined by user constraints and algorithmic parameters (Sec. 3.1). Although the conditional arguments in the edge matrix $E = [c_{ij}]$ are fixed once optimization completes, the actual on/off status of each c_{ij} remains undetermined. (b) At runtime, the optimized Φ instantiates different execution topologies based on $c_{ij}(\tau)$, reflecting dependence on the query input q_i and the induced contextual state τ.

B Advanced Topics and Applications

We briefly highlight several advanced topics and emerging applications in compound AI systems that may interest readers. Serving as advanced optimization methods, LLMSelector (Chen et al., 2025a) shows that selecting different LLMs at system nodes has a major effect on system performance, proposing an efficient algorithm for model selection in compound systems. Efforts have also focused on improving system execution efficiency, including network orchestration techniques (Santhanam et al., 2024) and hardware-level optimizations (Chaudhry et al., 2025). These strategies are particularly well suited for refining complex system pipelines, such as question answering with RAG or data processing with tool calling, by accounting for the run-time efficiency.

The advances in compound AI systems have also led to novel applications: SciAgents (Ghafarollahi and Buehler, 2024) leverage ontological knowledge graphs and data retrieval tools to drive automatic materials discovery that surpasses traditional human-driven research methods; AutoML-Agent (Trirat et al., 2024) devises a system to handle end-to-end AutoML pipeline, accepting user task descriptions and optional constraints and handling everything from data retrieval to model deployment; and VFlow (Wei et al., 2025) targets hardware design tasks (i.e., Verilog code generation) by augmenting AFlow (Zhang et al., 2024a) with domain-specific components, thereby optimizing system performance to achieve a higher pass@1 rate than previous methods.

Furthermore, the effectiveness of natural language feedback demonstrated by TextGrad (Yuksekgonul et al., 2025) has spurred applications in diverse domains. For example, FedTextGrad (Chen et al., 2025b) investigates the potential and challenges of integrating TextGrad into federated learning settings, where the server receives and aggregates locally optimized prompts from clients. Similarly, TPO (Li et al., 2025) proposes a method for aligning LLM preferences during inference by leveraging textual gradient signals.

C More Details of Learning Signals

Most surveyed papers leverage a single type of learning signal (i.e., either NL feedback or numerical signals) to guide the optimization of Φ. However, several works use both types of signals. For instance, GPTSwarm (Zhuge et al., 2024) employs an RL loss to numerically learn optimal connections within the swarm and then updates LLM prompts using OPRO (Yang et al., 2023), an algorithm based on NL feedback. Additionally, MaAS (Zhang et al., 2025) leverages a Bayesian Monte Carlo procedure to numerically update the probability distribution of the *agentic supernet* and uses textual gradients to refine its *operators*, including LLM prompts, temperature settings, and local node structures.

Despite the existence of these methods, we do not introduce a separate "hybrid" category for now. Instead, we classify them as either NL feedback or numerical signals based on two criteria: (1) the authors' primary design novelty—for example, GPTSwarm is categorized as numerical since OPRO is a previously designed algorithm; and (2) the signal used to update the system topology—for example, MaAS is categorized as numerical since the topology is updated via numerical signals.

To accommodate future developments, we will dynamically adjust our criteria to keep the taxonomy clear and intuitive. Introducing a "hybrid" category also remains an open option as the field evolves. We encourage future efforts that leverage both types of learning signals to leverage our proposed taxonomy and position their methods at the intersection of NL feedback and numerical signals.

D Clarification of Methods Name

Most surveyed papers introduce a single name for their method (i.e., main algorithm), while others employ multiple terms to refer to the target problem (Wang et al., 2024a; Hu et al., 2024), individual algorithms or components, or released libraries (Khattab et al., 2023). To improve readability, we assign these works a single, consistent name, chosen based on (1) its prevalence in subsequent literature and (2) its appearance in the original paper's title.