

STRCMP: Integrating Graph Structural Priors with Language Models for Combinatorial Optimization

Xijun Li^{1,2}, Jiexiang Yang², Jinghao Wang², Bo Peng^{1,2}, Jianguo Yao^{1,2}, Haibing Guan^{1,2}

¹Shanghai Key Laboratory of Scalable Computing and Systems

²School of Computer Science, Shanghai Jiao Tong University

{lixijun, jianguo.yao}@sjtu.edu.cn

Abstract

Combinatorial optimization (CO) problems, central to operation research and theoretical computer science, present significant computational challenges due to their \mathcal{NP} -hard nature. While large language models (LLMs) have emerged as promising tools for CO—either by directly generating solutions or synthesizing solver-specific codes—existing approaches often *neglect critical structural priors inherent to CO problems*, leading to suboptimality and iterative inefficiency. Inspired by human experts’ success in leveraging CO structures for algorithm design, we propose STRCMP, a novel structure-aware LLM-based algorithm discovery framework that systematically integrates structure priors to enhance solution quality and solving efficiency. Our framework combines a graph neural network (GNN) for extracting structural embeddings from CO instances with an LLM conditioned on these embeddings to identify high-performing algorithms in the form of solver-specific codes. This composite architecture ensures syntactic correctness, preserves problem topology, and aligns with natural language objectives, while an evolutionary refinement process iteratively optimizes generated algorithm. Extensive evaluations across Mixed Integer Linear Programming and Boolean Satisfiability problems, using nine benchmark datasets, demonstrate that our proposed STRCMP outperforms five strong neural and LLM-based methods by a large margin, in terms of both solution optimality and computational efficiency. The code and learned model will be publicly available upon the acceptance of the paper.

1 Introduction

Making complex plans subject to multiple constraints is a time- and labor-intensive process, but is critical in many aspects of our lives such as scheduling [1], logistics [2], and robotics [3]. These problems are frequently modeled as combinatorial optimization (CO) problem, a cornerstone of operation research and theoretical computer science, where the objective is to identify optimal solutions within discrete, highly constrained search spaces. However, the inherent \mathcal{NP} -hardness of many CO problems renders obtaining exact solutions computationally intractable, posing significant challenges in solving them efficiently and accurately. Consequently, substantial research efforts have endeavored to developing algorithms that balance solution quality with computational cost, typically requiring specialized domain expertise and rigorous analytical modeling of problem structure [4–6].

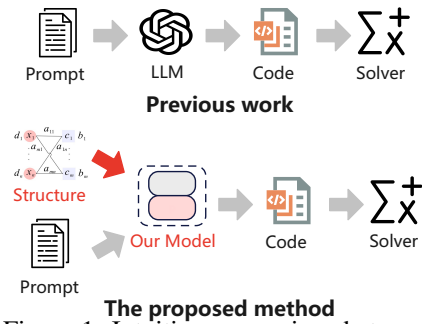


Figure 1: Intuitive comparison between prior work and the proposed framework.

Machine learning (ML) techniques, particularly deep learning and reinforcement learning, have demonstrated significant potential in addressing CO problems [7]. As many CO problems arising from similar application domains exhibit inherent structural patterns, ML methods can leverage these patterns to reduce computational complexity in traditional CO approaches through data-driven strategies. The integration of ML and CO frameworks can be broadly categorized into three paradigms[7]: (1) End-to-end neural solvers [8–10], which train ML models to directly output CO solutions; (2) ML-augmented algorithm configuration [11–13], leveraging ML models to predict optimal algorithmic configurations for specific CO algorithm to solve associated problems; and (3) Hybrid methods [14–16], embedding ML models as critical decision modules within traditional CO solvers. However, real-world adoption of above approaches remains limited due to reliance on training distributional alignment for generalization and inherently insufficient interpretability [17].

Building on the explosive advancements in large language models (LLMs) over recent years, combinatorial optimization tasks have shown potential for delegation to LLMs, particularly owing to their improved accountability and interpretability compared to conventional ML approaches. Capitalizing on their extensive world-knowledge priors and advanced code generation capabilities, numerous LLM-based approaches for CO problems have emerged. These methods bifurcate into two classes: (1) direct utilization of LLMs to solve CO problems [18, 19], and (2) employing LLMs to discover high-quality algorithm (in the form of solver-specific codes) for traditional solvers [20–22]. For example, Yang et al. [18] present Optimization by PROMpting (OPRO), which harnesses LLMs as black-box optimizers through iterative solution refinement via natural-language problem specifications and optimization trajectories. In contrast, Romera-Paredes et al. [20] proposes FunSearch that integrates a pre-trained LLM into an evolutionary algorithm to incrementally generate solver code, achieving state-of-the-art results on the cap set problem and discovering novel heuristics for online bin packing. Additionally, Huang et al. [19] demonstrates that multi-modal fusion of textual and visual prompts enhances LLM-driven optimization performance, as evidenced in capacitated vehicle routing problems.

Despite these advances, current LLM-based approaches for solving CO problems remain in their infancy. As illustrated in Figure 1, they primarily rely on textual (or occasionally visual) prompting mechanisms to interface with LLMs, *failing to effectively exploit the inherent topological structures of CO problems*. Historically, human experts have successfully leveraged structural priors of CO problems to design sophisticated and efficient algorithms [4–6]. Furthermore, existing LLM-based methods [20, 21, 18] often require multiple iterations to produce high-quality solutions or algorithm implementations, primarily due to their lack of integration with CO-specific structural priors. As highlighted in Yang’s insightful analysis [23], pre-training language model establishes strong priors for conversational tasks but weaker priors for structured domains like computer controls or video games — *challenges exacerbated in solving CO problems, as these domains differ significantly from Internet text distributions*. Given these challenges, developing a generative model that effectively integrates structural priors for CO problem solving becomes particularly compelling. As shown in Figure 1, the distinct insight lies in constructing a generative model that generates solver-specific code while respecting the intrinsic topological structure of CO problems. Theoretically, this approach aligns with the rising research directions of multi-modal generative model. Practically, such integration offers substantial benefits, dramatically reducing inference iterations while enhancing solution quality in solving CO problem.

To tackle this challenge, we present STRCMP¹, a novel structure-prior-aware LLM-based algorithm discovery framework for solving CO problems. To the best of our knowledge, STRCMP is the first framework to explicitly integrate structural priors of CO problems into LLM-driven algorithm discovery, jointly improving solution quality and computational efficiency. Our framework first constructs a composite architecture combining a graph neural network (GNN) and an LLM. The GNN extracts structural embeddings from input CO instances, which serves as inductive biases for subsequent algorithm discovery via code generation. The LLM then produces solver-specific code conditioned on these structural priors, ensuring adherence to solver syntax, preservation of CO problems’ topological characteristics, and alignment with natural language optimization objectives. This composite model is further embedded within an evolutionary algorithm-based refinement process to iteratively enhance solution quality. Besides, we provide the theoretical analysis why fusing the structure prior into LLM can benefit solving CO problem from the perspective of information theory.

¹STRCMP stands for STRucture-aware CoMPposite model that can discover and generate algorithm implementation for CO problems considering intrinsic topological structure of the problem.

Extensive experiments across two representative CO domains (Mixed Integer Linear Programming and Boolean Satisfiability), spanning nine benchmark datasets, demonstrate that STRCMP outperforms five well-recognized baselines by a large margin—including neural combinatorial optimization methods and LLM-based approaches—in both solution optimality and computational efficiency.

2 Related Work

Neural Combinatorial Optimization. Extensive research [14, 24, 25, 15, 16] has explored machine learning integration with combinatorial optimization for improved computational approaches to \mathcal{NP} -hard problems, forming Neural Combinatorial Optimization (NCO) methods that either approximate expert heuristics or learn policies via reinforcement learning. Following Bengio et al. [7]’s taxonomy, NCO encompasses: (1) End-to-end neural solvers [8–10], (2) ML-augmented algorithm configuration [11–13], and (3) Hybrid methods integrating learned components into classical frameworks [14–16]. Pointer Networks [25] represent seminal work, employing attention mechanisms [8] as dynamic pointers for CO problems, eliminating dependence on fixed output dictionaries in conventional seq2seq models [26]. The framework achieves competitive performance on convex hulls, Delaunay triangulation, and small TSP instances while generalizing to unseen sizes. In hybrid approaches, Gasse et al. [14] introduced GCNs trained via imitation learning to replace strong branching heuristics [27] in branch-and-bound algorithms for MIP solvers. While avoiding manual feature engineering through graph representations, such approaches face scalability challenges under extreme problem sizes, a key limitation of neural solver architectures. Moreover, NCO’s reliance on opaque machine learning models yields policies with insufficient interpretability—problematic for high-stakes decision-making systems demanding traceable logic [17]. Our approach addresses these gaps by furnishing optimality certificates or bounded sub-optimality guarantees via CO solver integration. By procedurally generating solver-executable code through iterative refinement, our framework ensures superior interpretability relative to black-box NCO policy learning.

Language Models for Combinatorial Optimization Problem. Recent advances in large language models (LLMs) have spurred explorations of their applications to combinatorial optimization [20, 21, 28–30]. Current approaches fall into two categories: (1) direct solution generation via LLM inference [18, 19], and (2) automated generation of solver-compatible formalizations [20–22, 30]. In the first paradigm, Yang et al. [18] propose Optimization by PROMpting (OPRO), leveraging LLMs as black-box optimizers through iterative refinement of natural-language problem descriptions. While achieving comparable performance to heuristics on small TSP instances, OPRO scales poorly beyond 50 nodes due to context limitations and solution-space complexity. For the second paradigm, Romera-Paredes et al. [20] introduce FunSearch, combining evolutionary methods with LLM-guided program synthesis to obtain breakthroughs on the cap set problem [31] and generate novel bin packing heuristics [32]. Similarly, [21] develop Evolution of Heuristics (EoH), integrating evolutionary algorithms with LLMs to co-optimize natural language "thoughts" and code implementations through iterative prompting, outperforming existing methods like FunSearch in query efficiency [20]. Existing approaches predominantly employ natural language (or occasionally visual [19]) prompts combined with evolutionary frameworks for iterative code generation to solve CO problems. However, *these methods universally neglect the topological structural characteristics intrinsic to combinatorial optimization problems*, which are systematically exploited by human experts during algorithm design [4–6]. Furthermore, evolutionary framework-based code generation with LLMs often necessitates multiple iterations for convergence while incurring significant computational overhead from repeated solver invocations during evaluation. To overcome these limitations, we propose a composite model that effectively incorporates structural priors of CO problems during algorithmic discovery. By developing composite architectures tailored to CO problem structures, our method substantially improves both solution quality and computational efficiency compared to existing LLM-based solving approaches.

3 Problem Statement

Combinatorial Optimization. Following [33], we formulate a general combinatorial optimization problem Q (e.g., Boolean Satisfiability (SAT) and Mixed Integer Linear Programming (MILP)) as a constrained discrete optimization problem. For an instance q of Q , the formulation becomes:

$$\min_{x \in S(q)} c(x; q) + f(x; q), \quad (1)$$

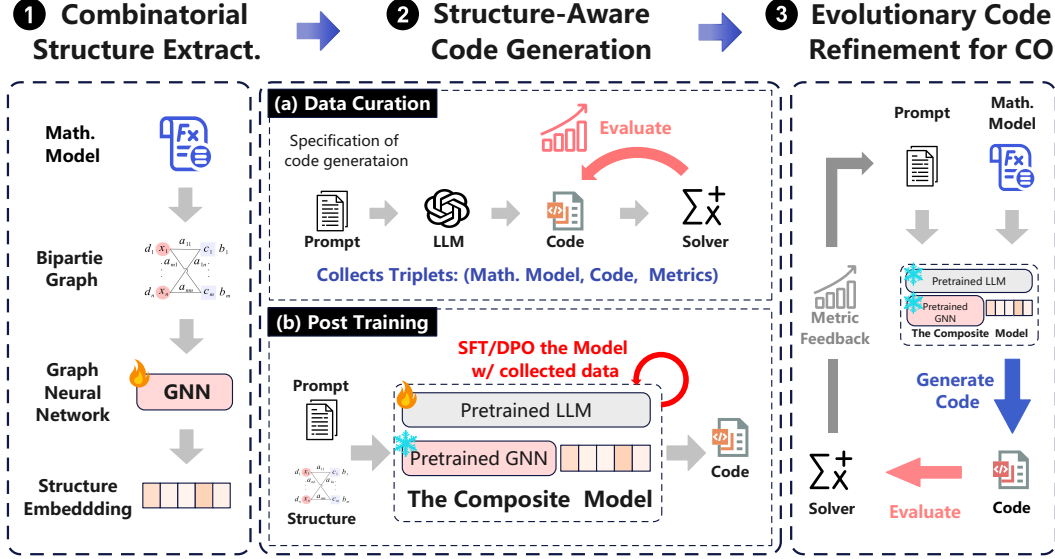


Figure 2: Overview of the proposed STRCMP. **① Combinatorial Structure Extraction.** We utilize a graph neural network (GNN) to encode the topological structure of combinatorial optimization problems into latent embeddings, capturing problem-specific structural invariants. **② Structure-Aware Code Generation:** (a) Data Curation: For a given CO problem’s mathematical model, target solver and the specific prompt, an LLM generates candidate algorithm in the form of code snippets, which are automatically validated via the solver execution to generate performance metrics. This yields a curated dataset comprising (mathematical model, code snippet, metric) triplets. (b) Post Training: A composite architecture integrating a frozen pretrained GNN with an LLM is fine-tuned on this dataset, ensuring code generation respects both the CO’s intrinsic topology and solver-specific syntax. **③ Evolutionary Code Refinement.** Drawing on [20], the composite model is embedded within an evolutionary framework to evolve the algorithm discovery process through performance-driven iterations.

where x denotes decision variables subject to solution space $S(q)$; $c(x; q)$ represents the objective function to minimize, and $f(x; q)$ corresponds to constraint penalties (zero when all constraints are satisfied). In SAT problems, the objective function $c(x; q)$ is absent since only constraint satisfaction is required. Conversely, MILP problems feature both objective and constraint functions.

Generation Task. Given a combinatorial optimization problem Q , our goal is to find an algorithm A that can consistently solve Q well:

$$\min_{A \sim \mathcal{A}} \mathbb{E}_{q \sim Q, x \sim A(q)} [c(x; q) + f(x; q)] \quad (2)$$

where \mathcal{A} denotes the algorithm search space. This work focuses on symbolic search spaces where \mathcal{A} comprises algorithms representable as code snippets executable within a combinatorial optimization solver. We resort to a generative model to synthesize the target algorithm through code generation.

4 Proposed Solution

The proposed framework is illustrated in Figure 2. We first describe the technical interplay among components within the proposed framework, highlighting design motivations and synergistic interactions. Subsequently, we provide a theoretical analysis demonstrating that integrating structural priors into LLMs enhances performance in solving combinatorial optimization problems.

4.1 Methodology

① Combinatorial Structure Extraction. Combinatorial optimization problem is equivalently converted to a bipartite graph. Thus, the intrinsic structure of the combinatorial optimization problem can be easily captured by a graph neural network, as has been done in many previous work [16, 24, 14].

As shown in the leftmost part of Figure 2, we continue to use this technique to extract structure embedding of given CO problem, benefiting the following algorithm discovery process.

Specifically, a bipartite graph $G = (C, E, V)$ is constructed for the CO problem instance q , where C corresponds to the constraints of q ; V denotes the variables of q ; and an edge $e_{ij} \in E$ between a constraint node i and a variable node j if they have a connection. A graph neural network θ_G takes as input the bipartite graph to generate the structural embedding $\mathbf{h}_q \in \mathbb{R}^d$ of the problem instance q . We simply train θ_G via a classification task, where a group of CO problems and their class label are given. The problems falling into the same class means that they originates from the same scenario/domain, such as traveling salesman problems [34], production planning [35], vehicle routing problem [36], *etc.* The data representation, training, implementation details are left to Appendix B.1. In this way, GNNs can capture structure priors of CO problem (such as symmetry, sparsity, and degeneracy), which are critical for solver decisions. The extracted embeddings transfers structural insights to downstream code generation task, facilitating generalization across problem classes.

② Structure-Aware Code Generation. In this step, we construct a composite generative model to achieve structure-aware algorithm discovery for CO problem. The composite model is essentially a concatenation of a GNN and an LLM. GNN is obtained via training method mentioned in Step ① and frozen in the composite model, which provides the structure embedding of given CO problem to LLM. The LLM takes as input the natural language description of the problem and of the code generation task. Then the LLM generates candidate algorithm in the form of code snippet conditioned on the natural language description and structure embedding for a specific solver, as shown in the middle part of Figure 2. The code generation procedure can be formulated below:

$$P(w_1, w_2, \dots, w_T) = \prod_{t=1}^T P_{\theta_L}(w_t | w_{<t}; \mathbf{h}_q, NL), \quad (3)$$

where $\{w_i | i = 1, \dots, T\}$ is the code snippet predicted by the composite model; \mathbf{h}_q is the structure embedding of given CO problem instance q ; NL is the natural language description of q and of code generation task; θ_L is the parameter of LLM.

As anticipated, the composite model exhibits suboptimal performance on code generation tasks for CO problems due to architectural incompatibilities that disrupt the native token prediction mechanism of the underlying LLM. To address this architectural mismatch, we implement a two-phase training protocol consisting of: (a) **data curation** through systematic problem sampling, and (b) parameter optimization via **post-training**. This phased approach enables effective adaptation of the composite architecture while preserving the structural integrity of the original CO problem representations.

(a) Data Curation. To facilitate the post-training phase, we aim to collect four key categories of data: 1) mathematical formulations of CO problems; 2) natural language specifications detailing problem requirements alongside corresponding code generation objectives for targeted CO solvers; 3) executable code implementations derived from these specifications; and 4) quantitative performance metrics evaluating solution quality and computational efficiency of the implemented code.

(b) Post-Training. In this phase, we only train the parameter θ_L of the composite model, which means that structural embeddings remain consistent during post-training. We conduct Supervised Fine-Tuning (SFT) on θ_L using the curated dataset, followed by Direct Preference Optimization (DPO) [37] initialized from the SFT checkpoint to derive the final composite model. All details, including prompt template, data curation and post-training, are presented in Appendix B.2.

③ Evolutionary Code Refinement for Combinatorial Optimization Problem. Prior work [30, 20, 29] leverages LLMs’ code generation and algorithm design capabilities within Evolutionary Algorithms (EAs) to address combinatorial optimization problems through iterative feedback frameworks. The iterative nature of evolutionary algorithms introduces significant computational overhead as the primary limitation of prior approaches [30, 20, 29] for identifying optimal code snippets or algorithms to solve combinatorial optimization problems. Convergence typically requires numerous iterations, exacerbated by the prolonged execution times required for solver-based evaluation of generated code or algorithm candidates.

Our evolutionary code optimization framework for combinatorial optimization adopts the core principles of prior work [30, 20, 29], with the significant distinction lying in the composite model learned in Step ② (see Figure 2 right panel). Our framework jointly processes both textual problem descriptions with algorithm discovery objectives and formal mathematical model of CO problems.

The composite model generates solver-specific, structure-aware code through standard EA operators (selection, crossover, mutation), producing higher-quality algorithm implementation within fewer iterations – a capability empirically validated in our experiments. By integrating this model into EA-based algorithm discovery frameworks, we achieve superior optimization performance while maintaining compatibility with existing evolutionary algorithm design paradigms, suggesting broader applicability across LLM-driven optimization methodologies.

4.2 Theoretical Analysis

In the following, we give the theoretical analysis why fusing the structure prior into the generative model helps algorithm discovery for solving CO problem on the basis of information theory [38] and multi-modal co-learning [39]. Specifically, we prove that a generative model with an additional prior will not lower the upper bound of its performance on the downstream task. Note that we leave all proofs into the Appendix A due to the space limitation.

Definition 1 (Upper Bound of Model Performance). *The performance upper bound of generative model, denoted by $\sup(\mathcal{P})$, is utilized to measure the maximum expected performance of a generative model for a downstream task $p(\mathbf{w}|\mathbf{c})$, where \mathbf{w} is the generated content conditional on the different kinds of prior \mathbf{c} . Formally, $\sup(\mathcal{P})$ associated with kinds of prior \mathcal{C} can be expressed as*

$$\sup(\mathcal{P}_{\mathcal{C}}) = \sum_{\mathbf{c} \in \mathcal{C}} \sum_{\mathbf{w}} p(\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}), \quad (4)$$

where Φ is the performance evaluator for given generated content \mathbf{w} ; \mathcal{C} is the complete set of different priors and \mathbf{C} is a type of prior belonging to the prior set \mathcal{C} .

Theorem 1. *Given a prior dataset \mathcal{D} whose data samples comprises M types of prior $\mathcal{C} = \{\mathbf{C}_1, \dots, \mathbf{C}_M\}$, the distinct priors follow respective true distribution $p(\mathbf{C}_i|\mathbf{w})$. Let \mathbf{c}_i be a sample drawn from the distribution, i.e., $\mathbf{c}_i \sim p(\mathbf{C}_i|\mathbf{w})$. A generative model with an additional type of prior will not lower the upper bound of model performance $\sup(\mathcal{P})$.*

Remark 1. *Theorem 1 establishes that introducing additional priors cannot reduce a generative model’s performance upper bound, while decreasing its entropy. Consequently, integrating combinatorial optimization structural priors into LLMs does not degrade their performance in generating code for solving CO problems.*

Definition 2 (Performance-Enhancing Prior). *Assume a type of prior \mathbf{C} can boost the performance of a generative model compared to the one without the prior, then \mathbf{C} is the performance-enhancing prior to the generative model. It can be formally expressed as*

$$\exists \mathbf{w}' \neq \mathbf{w}^*, p(\mathbf{w}'|\mathbf{c}) \Phi(\mathbf{w}')_{\mathbf{c} \in \mathcal{C}} > p(\mathbf{w}^*|\mathbf{c}) \Phi(\mathbf{w}^*)_{\mathbf{c} \in \mathcal{C} \setminus \{\mathbf{C}\}}, \quad (5)$$

where $\mathbf{w}^* = \arg \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w})_{\mathbf{c} \in \mathcal{C} \setminus \{\mathbf{C}\}}$.

Theorem 2. *If prior \mathbf{C}_{pe} is a performance-enhancing prior, a generative model neglecting prior \mathbf{C}_{pe} will decrease the upper bound of model performance. It can be expressed as*

$$\sup(\mathcal{P}_{\mathcal{C} \setminus \{\mathbf{C}_{pe}\}}) < \sup(\mathcal{P}_{\mathcal{C}}) \quad (6)$$

Remark 2. *Theorem 2 demonstrates that generative models equipped with performance-enhancing priors achieve superior performance relative to their prior-free counterparts. Specifically, the structural prior serves as such performance-enhancing prior for LLMs in code generation tasks targeting CO problems, which is empirically validated through our comprehensive experiments.*

5 Experimental Evaluation

To empirically evaluate the efficacy of our proposed STRCMP in solving combinatorial optimization problems, we conduct extensive experiments across two fundamental CO problem classes: mixed-integer linear programming and Boolean satisfiability, evaluated on over nine benchmark datasets. We benchmark our approach against five well-established baselines encompassing both neural optimization methods and contemporary LLM-based approaches. We aim to answer the following research questions:

Research Questions

- RQ1:** Does the proposed STRCMP identify superior algorithmic implementations compared to existing algorithm discovery approaches?
- RQ2:** Does the proposed composite model effectively reduce computational overhead in existing algorithm discovery frameworks?
- RQ3:** Does the structural prior benefit the generative model in solving combinatorial optimization problems?

5.1 Settings

Baselines. We evaluate our framework against two categories of baselines: neural combinatorial optimization methods and LLM-based evolutionary code optimization frameworks, covering mixed-integer linear programming (MILP) and Boolean satisfiability (SAT). More details of baselines and used backend solvers can be found in Appendix C.

- *Neural Combinatorial Optimization:* For MILP, we compare with the seminal work **L2B** [14], which employs graph convolutional networks for variable selection to replace the strong branching policy, and **HEM** [15, 16], a hierarchical sequence model for cut selection in branch-and-bound solvers. For SAT, we include **NeuroSAT** [40], a message-passing neural network trained with single-bit supervision for SAT solving.
- *Evolutionary Code Optimization:* While numerous LLM-based evolutionary code optimization approaches exist for combinatorial optimization, we specifically compare with two methods specialized for SAT and MILP: **AutoSAT** [29] and **LLM4Solver** [30]. **AutoSAT** leverages LLMs to automate heuristic optimization in SAT solvers, minimizing manual intervention. **LLM4Solver** integrates LLMs with multi-objective evolutionary algorithms to automatically design effective diving heuristics for MILP solvers².

Dataset. We perform the empirical evaluation over ten widely-used benchmark dataset for SAT and MILP respectively. More details and statistics of the used datasets can be found in Appendix D.

- *Mixed-integer linear programming (MILP):* The datasets for MILP solver evaluation contain three difficulty tiers [15, 16, 30]: (1) **Easy** features synthetic benchmarks (Set Covering [41], Maximum Independent Set [42], Multiple Knapsack [43]) generated using protocols from [44, 45]; (2) **Medium** includes MIK [46] and CORLAT [47]; (3) **Hard** contains the Google-inspired Load Balancing problem and the industrial-scale Anonymous problem [48].
- *Boolean satisfiability (SAT):* The dataset comprises two sources: SAT Competition problems [49] and automatically generated instances via Picat [29]. **SAT Competition data** includes Profitable-Robust-Product (PRP) and Chromatic-Number-of-the-Plane (CNP) problems, while **Picat-generated data** contains CoinsGrid and Zamkeller instances. We adhere to the generation protocol established in [29].

Metrics. To evaluate the effectiveness of the proposed framework, we analyze solving time to optimality or solution quality attainable within a fixed time budget. For solving efficiency evaluation, we measure the number of iterations or training steps required for convergence. Specifically, for MILP domain, critical metrics include **solving time** and **primal-dual (PD) integral** which are widely used in benchmarking the MILP solvers [15, 16, 14]. For SAT domain, key metrics encompass **solving time**, **PAR-2**, and **number of timeout** frequently measured in evaluating SAT solvers [29, 40]. Metrics such as solving time, PD integral, number of timeout, and PAR-2 are minimized through optimization. More details of the used metrics are presented in Appendix E.

5.2 Implementation

Model Architecture. The proposed composite model comprises two components: a GNN and a structure-prior-aware LLM. We implement the GNN using graph convolution operators from `torch_geometric`, structured with three sequential convolutional layers terminated by global mean

²For fair comparison, we slightly adjusted **LLM4Solver**'s optimization focus from diving heuristics to cut selection for MILP solver.

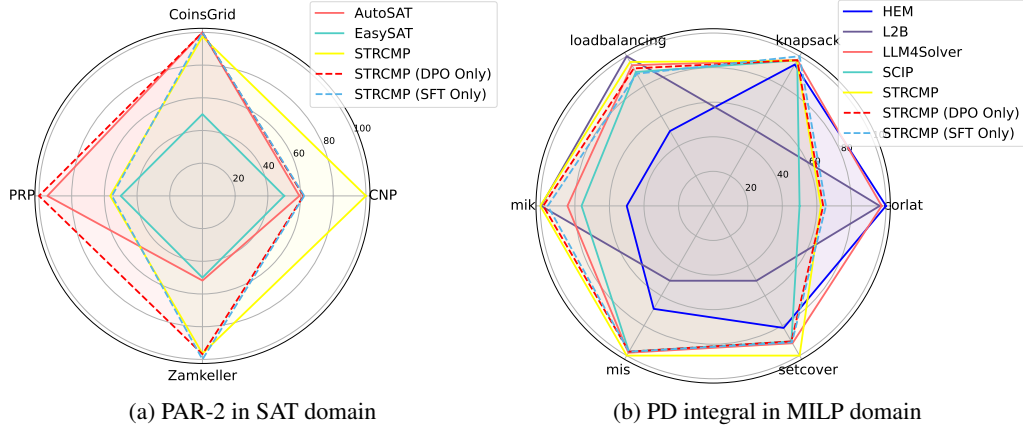


Figure 3: Optimization performance over different CO domains. Aligned with [29], we normalize each benchmark’s indicator values using $1 - \frac{value - min}{2 \times (max - min)}$, where *value* represents the method’s measured indicator, with *min* and *max* denoting respectively the minimum and maximum values observed during evaluation. A larger shaded area corresponds to superior performance.

pooling. We adapt the LLM component based on Qwen2.5-Coder-7B-Instructor model through modifying its architecture, forward propagation dynamics and inference paradigm. Comprehensive implementation details including hyperparameter configurations, adaptations, and software dependencies are provided in Appendix B.1 and B.2.

Training, Inference and Used Hardware. We first train domain-specific GNNs for SAT and MILP problems using aforementioned benchmark dataset. The GNNs are trained for three epochs on SAT instances and four epochs on MILP instances, followed by conducting post-training of the adapted LLM with a specialized corpus. All post-training data is collected via queries to Qwen2.5-Coder-7B-Instructor, aligned with the model used in the post training. The adapted LLM undergoes three epochs of post training per domain. Both GNN and LLM selecting optimal checkpoints based on validation prediction loss. We then integrate the composite model (*i.e.* the trained GNN and adapted LLM) into an EA-based framework to discover solver-specific algorithm configurations optimized for training instances. Finally, we evaluate the performance of identified algorithms on held-out test sets. All experiments are conducted on hardware platform with dual AMD EPYC 9534 64-core processors @ 2.45GHz and two NVIDIA H800 80GB GPUs connected via PCIe. More training specifics and data curation are detailed in Appendix B.1 and B.2 respectively.

5.3 Results

Optimization Performance (Answer to RQ1).

The comparative optimization results are presented in Figure 3 and Table 1 (“CGD” and “ZAM” denotes CoinsGrid and Zamkeller dataset respectively) with respect to primary objective metrics (*i.e.* PAR-2 and Number of Timeout for SAT and PD integral for MILP domains). Comprehensive results for all evaluation metrics are provided in Appendix G.1). As evidenced in Figure 3 and Table 1, our STRCMP with various post-training variants consistently matches or exceeds all baseline performance across both SAT and MILP domains. Specifically for SAT, STRCMP demonstrates universal superiority over its closest counterpart AutoSAT, particularly achieving significant reductions in terms of timeout (77.8% on Zamkeller: 18→4; 66.7% on PRP: 9→3) and solving time (on PRP: 22967 seconds → 21146 seconds; on Zamkeller: 20772 seconds → 6929 seconds). On MILP benchmarks, STRCMP maintains strong performance parity with NCO methods L2B/HEM and its direct competitor LLM4Solver. These

Table 1: Optimization performance result w.r.t. Number of Timeout between different methods over SAT domain.

Compared Methods	Number of Timeout (↓)			
	CNP	CGD	PRP	ZAM
AutoSAT [29]	32	16	9	18
EasySAT	32	25	50	18
NeuroSAT [40]	44	18	46	29
STRCMP	<u>31</u>	17	44	5
STRCMP (DPO Only)	32	<u>16</u>	<u>3</u>	5
STRCMP (SFT Only)	33	<u>16</u>	45	<u>4</u>
STRCMP w/o GNN	32	<u>16</u>	44	14

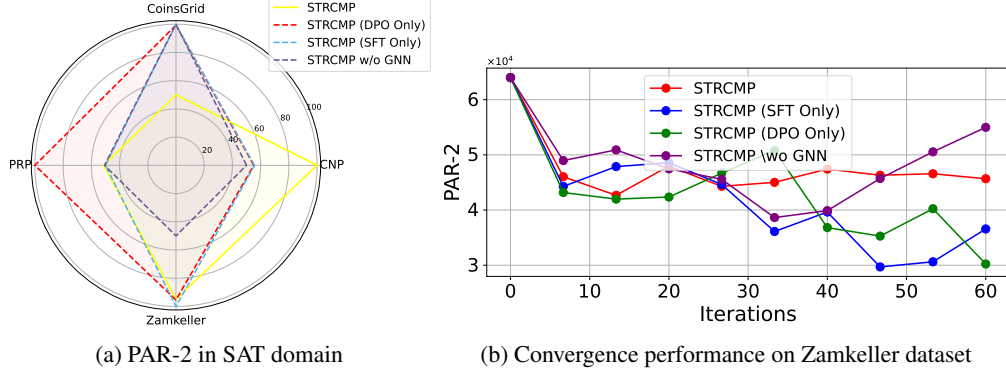


Figure 5: Ablation studies in terms of optimization performance and convergence rate.

empirical findings conclusively address RQ1: *STRCMP successfully identifies superior algorithmic configurations compared to existing strong baselines.*

Efficiency Improvement (Answer to RQ2).

Next, we assess the efficiency of our proposed STRCMP framework in discovering high-performance algorithms via iterative search for combinatorial optimization problems. The representative convergence comparison for SAT domain are presented in Figures 4. More evaluations over other SAT datasets and MILP domain across additional metrics are provided in Appendix G.2. Our experiments reveal that STRCMP achieves convergence significantly faster than existing evolutionary-based algorithm discovery frameworks. Furthermore, the framework attains markedly higher-quality convergence points compared to baseline methods AutoSAT and LLM4Solver. Notably, STRCMP achieves stable convergence while AutoSAT exhibits persistent oscillations even after convergence. These findings validate that *our proposed STRCMP substantially reduces computational overhead in evolutionary-based algorithm discovery frameworks.*

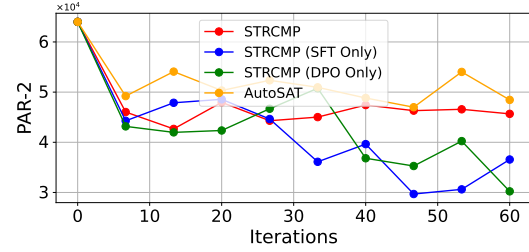


Figure 4: Convergence comparison (w.r.t. PAR-2) between evolutionary-based algorithm discovery frameworks on Zamkeller dataset of SAT domain.

Ablation Studies (Answer to RQ3). To address RQ3, we conduct comprehensive ablation studies on our composite model by systematically deactivating individual components and evaluating their impact on optimization performance and computational efficiency. Representative results are shown in Figure 5, with full ablation studies detailed in Appendix G.3. Analysis of Figure 5 reveals that *the structural prior provides measurable benefits for code generation in combinatorial optimization tasks: the STRCMP w/o GNN variant (lacking structural guidance) exhibits consistently inferior optimization performance compared to counterparts incorporating the prior.* Furthermore, this variant demonstrates increased solution variability during algorithmic search iterations, potentially resulting in higher computational costs. Counterintuitively, the full STRCMP model (with complete post-training) does not uniformly outperform its ablations STRCMP (SFT Only) and STRCMP (DPO Only) across all benchmarks, suggesting underlying conflicts within the post-training data distribution. We plan to investigate this phenomenon in subsequent research.

6 Conclusion

We propose STRCMP, a novel structure-aware LLM-based algorithm discovery framework for combinatorial optimization problems. To our knowledge, this represents the first methodology that explicitly incorporates structural priors of combinatorial optimization problems into LLM-driven algorithm discovery, simultaneously enhancing solution quality and computational efficiency. We validate the effectiveness of STRCMP through theoretical analysis and extensive empirical evaluations across SAT and MILP problems, demonstrating consistent improvements in both solving efficiency and solution optimality. Our framework offers a principled foundation for future research integrating additional modal priors into LLMs for solving combinatorial optimization problems.

References

- [1] David M Ryan and Brian A Foster. An integer programming approach to scheduling. *Computer scheduling of public transport urban passenger vehicle and crew scheduling*, pages 269–280, 1981.
- [2] Xijun Li, Mingxuan Yuan, Di Chen, Jianguo Yao, and Jia Zeng. A data-driven three-layer algorithm for split delivery vehicle routing problem with 3d container loading constraint. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 528–536, 2018.
- [3] Bo Liu, Yuqian Jiang, Xiaohan Zhang, Qiang Liu, Shiqi Zhang, Joydeep Biswas, and Peter Stone. Llm+ p: Empowering large language models with optimal planning proficiency. *arXiv preprint arXiv:2304.11477*, 2023.
- [4] Etienne De Klerk. Exploiting special structure in semidefinite programming: A survey of theory and applications. *European Journal of Operational Research*, 201(1):1–10, 2010.
- [5] Maria Kandyba-Chimani. *Exact algorithms for network design problems using graph orientations*. PhD thesis, Citeseer, 2011.
- [6] Bruce Hendrickson. The molecule problem: Exploiting structure in global optimization. *SIAM Journal on Optimization*, 5(4):835–857, 1995.
- [7] Yoshua Bengio, Andrea Lodi, and Antoine Prouvost. Machine learning for combinatorial optimization: a methodological tour d’horizon. *European Journal of Operational Research*, 290(2):405–421, 2021.
- [8] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural information processing systems*, 30, 2017.
- [9] Irwan Bello, Hieu Pham, Quoc V Le, Mohammad Norouzi, and Samy Bengio. Neural combinatorial optimization with reinforcement learning. *arXiv preprint arXiv:1611.09940*, 2016.
- [10] Elias B Khalil, Christopher Morris, and Andrea Lodi. Mip-gnn: A data-driven framework for guiding combinatorial solvers. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pages 10219–10227, 2022.
- [11] Carlos Ansótegui, Britta Heymann, Josep Pon, Meinolf Sellmann, and Kevin Tierney. Hyper-reactive tabu search for maxsat. In *Learning and Intelligent Optimization: 12th International Conference, LION 12, Kalamata, Greece, June 10–15, 2018, Revised Selected Papers 12*, pages 309–325. Springer, 2019.
- [12] Markus Kruber, Marco E Lübbecke, and Axel Parmentier. Learning when to use a decomposition. In *International conference on AI and OR techniques in constraint programming for combinatorial optimization problems*, pages 202–210. Springer, 2017.
- [13] Pierre Bonami, Andrea Lodi, and Giulia Zarpellon. Learning a classification of mixed-integer quadratic programming problems. In *International conference on the integration of constraint programming, artificial intelligence, and operations research*, pages 595–604. Springer, 2018.
- [14] Maxime Gasse, Didier Chételat, Nicola Ferroni, Laurent Charlin, and Andrea Lodi. Exact combinatorial optimization with graph convolutional neural networks. *arXiv preprint arXiv:1906.01629*, 2019.
- [15] Zhihai Wang, Xijun Li, Jie Wang, Yufei Kuang, Mingxuan Yuan, Jia Zeng, Yongdong Zhang, and Feng Wu. Learning cut selection for mixed-integer linear programming via hierarchical sequence model. *arXiv preprint arXiv:2302.00244*, 2023.
- [16] Jie Wang, Zhihai Wang, Xijun Li, Yufei Kuang, Zhihao Shi, Fangzhou Zhu, Mingxuan Yuan, Jia Zeng, Yongdong Zhang, and Feng Wu. Learning to cut via hierarchical sequence/set model for efficient mixed-integer programming. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2024.

- [17] Weiwei Sun, Shengyu Feng, Shanda Li, and Yiming Yang. Co-bench: Benchmarking language model agents in algorithm search for combinatorial optimization. *arXiv preprint arXiv:2504.04310*, 2025.
- [18] Chengrun Yang, Xuezhi Wang, Yifeng Lu, Hanxiao Liu, Quoc V Le, Denny Zhou, and Xinyun Chen. Large language models as optimizers. *arXiv preprint arXiv:2309.03409*, 2023.
- [19] Yuxiao Huang, Wenjie Zhang, Liang Feng, Xingyu Wu, and Kay Chen Tan. How multimodal integration boost the performance of llm for optimization: Case study on capacitated vehicle routing problems. *arXiv preprint arXiv:2403.01757*, 2024.
- [20] Bernardino Romera-Paredes, Mohammadamin Barekatin, Alexander Novikov, Matej Balog, M Pawan Kumar, Emilien Dupont, Francisco JR Ruiz, Jordan S Ellenberg, Pengming Wang, Omar Fawzi, et al. Mathematical discoveries from program search with large language models. *Nature*, 625(7995):468–475, 2024.
- [21] Fei Liu, Xialiang Tong, Mingxuan Yuan, Xi Lin, Fu Luo, Zhenkun Wang, Zhichao Lu, and Qingfu Zhang. Evolution of heuristics: Towards efficient automatic algorithm design using large language model. *arXiv preprint arXiv:2401.02051*, 2024.
- [22] Haoran Ye, Jiarui Wang, Zhiguang Cao, Federico Berto, Chuanbo Hua, Haeyeon Kim, Jinkyoo Park, and Guojie Song. Reevo: Large language models as hyper-heuristics with reflective evolution. *arXiv preprint arXiv:2402.01145*, 2024.
- [23] Shunyu Yao. The Second Half. <https://ysmyth.github.io/The-Second-Half/>, 2025.
- [24] Xijun Li, Qingyu Qu, Fangzhou Zhu, Mingxuan Yuan, Jia Zeng, and Jie Wang. Accelerating linear programming solving by exploiting the performance variability via reinforcement learning. 2023.
- [25] Oriol Vinyals, Meire Fortunato, and Navdeep Jaitly. Pointer networks. *Advances in neural information processing systems*, 28, 2015.
- [26] Ilya Sutskever, Oriol Vinyals, and Quoc V Le. Sequence to sequence learning with neural networks. *Advances in neural information processing systems*, 27, 2014.
- [27] Santanu S Dey, Yatharth Dubey, Marco Molinaro, and Prachi Shah. A theoretical and computational analysis of full strong-branching. *Mathematical Programming*, 205(1):303–336, 2024.
- [28] Fei Liu, Yiming Yao, Ping Guo, Zhiyuan Yang, Zhe Zhao, Xi Lin, Xialiang Tong, Mingxuan Yuan, Zhichao Lu, Zhenkun Wang, et al. A systematic survey on large language models for algorithm design. *arXiv preprint arXiv:2410.14716*, 2024.
- [29] Yiwen Sun, Furong Ye, Xianyin Zhang, Shiyu Huang, Bingzhen Zhang, Ke Wei, and Shaowei Cai. Autosat: Automatically optimize sat solvers via large language models. *arXiv preprint arXiv:2402.10705*, 2024.
- [30] Yuyan Zhou, Jie Wang, Yufei Kuang, Xijun Li, Weilin Luo, Jianye HAO, and Feng Wu. Llm4solver: Large language model for efficient algorithm design of combinatorial optimization solver.
- [31] Ernie Croot, Vsevolod F Lev, and Péter Pál Pach. Past and future of the cap set problem. *arXiv preprint arXiv:2408.02328*, 2024.
- [32] Baoying Wang, Zhaohui Lin, Weijie Kong, and Huixu Dong. Bin packing optimization via deep reinforcement learning. *IEEE Robotics and Automation Letters*, 2025.
- [33] Christos H Papadimitriou and Kenneth Steiglitz. *Combinatorial optimization: algorithms and complexity*. Courier Corporation, 1998.
- [34] Karla L Hoffman, Manfred Padberg, Giovanni Rinaldi, et al. Traveling salesman problem. *Encyclopedia of operations research and management science*, 1:1573–1578, 2013.

- [35] Ludo F Gelders and Luk N Van Wassenhove. Production planning: a review. *European Journal of Operational Research*, 7(2):101–110, 1981.
- [36] Paolo Toth and Daniele Vigo. *The vehicle routing problem*. SIAM, 2002.
- [37] Rafael Rafailov, Archit Sharma, Eric Mitchell, Christopher D Manning, Stefano Ermon, and Chelsea Finn. Direct preference optimization: Your language model is secretly a reward model. *Advances in Neural Information Processing Systems*, 36:53728–53741, 2023.
- [38] Robert B Ash. *Information theory*. Courier Corporation, 2012.
- [39] Amir Zadeh, Paul Pu Liang, and Louis-Philippe Morency. Foundations of multimodal co-learning. *Information Fusion*, 64:188–193, 2020.
- [40] Daniel Selsam, Matthew Lamm, Benedikt Bünz, Percy Liang, Leonardo de Moura, and David L Dill. Learning a sat solver from single-bit supervision. *arXiv preprint arXiv:1802.03685*, 2018.
- [41] Egon Balas and Andrew Ho. Set covering algorithms using cutting planes, heuristics, and subgradient optimization: a computational study. In *Combinatorial Optimization*, pages 37–60. Springer, 1980.
- [42] David Bergman, Andre A Cire, Willem-Jan Van Hoes, and John Hooker. *Decision diagrams for optimization*, volume 1. Springer, 2016.
- [43] Lara Scavuzzo, Feng Yang Chen, Didier Chételat, Maxime Gasse, Andrea Lodi, Neil Yorke-Smith, and Karen Aardal. Learning to branch with tree mdps. *arXiv preprint arXiv:2205.11107*, 2022.
- [44] Maxime Gasse, Didier Chételat, Nicola Ferroni, Laurent Charlin, and Andrea Lodi. Exact combinatorial optimization with graph convolutional neural networks. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.
- [45] Haoran Sun, Wenbo Chen, Hui Li, and Le Song. Improving learning to branch via reinforcement learning. In *Learning Meets Combinatorial Algorithms at NeurIPS2020*, 2020.
- [46] Alper Atamtürk. On the facets of the mixed-integer knapsack polyhedron. *Mathematical Programming*, 98(1):145–175, 2003.
- [47] Carla P Gomes, Willem-Jan van Hoes, and Ashish Sabharwal. Connections in networks: A hybrid approach. In *International Conference on Integration of Artificial Intelligence (AI) and Operations Research (OR) Techniques in Constraint Programming*, pages 303–307. Springer, 2008.
- [48] Simon Bowly, Quentin Cappart, Jonas Charfreitag, Laurent Charlin, Didier Chételat, Antonia Chmiela, Justin Dumouchelle, Maxime Gasse, Ambros Gleixner, Aleksandr M, Kazachkov, Elias B, Khalil, Pawel Lichocki, Andrea Lodi, Miles Lubin, Chris J, Maddison, Christopher Morris, Dimitri J, Papageorgiou, Augustin Parjadis, Sebastian Pokutta, Antoine Prouvost, Lara Scavuzzo, and Giulia Zarpellon. Machine learning for combinatorial optimization, 2021. URL <https://www.ecole.ai/2021/ml4co-competition/>.
- [49] Tomas Balyo, Marijn Heule, Markus Iser, Matti Jarvisalo, and Martin Suda. Proceedings of sat competition 2023: Solver, benchmark and proof checker descriptions. 2023.
- [50] Antoine Prouvost, Justin Dumouchelle, Lara Scavuzzo, Maxime Gasse, Didier Chételat, and Andrea Lodi. Ecole: A gym-like library for machine learning in combinatorial optimization solvers. *arXiv preprint arXiv:2011.06069*, 2020.
- [51] Yang Li, Xinyan Chen, Wenxuan Guo, Xijun Li, Wanqian Luo, Junhua Huang, Hui-Ling Zhen, Mingxuan Yuan, and Junchi Yan. Hardsatgen: Understanding the difficulty of hard sat formula generation and a strong structure-hardness-aware baseline. In *Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, pages 4414–4425, 2023.

- [52] Ksenia Bestuzheva, Mathieu Besançon, Wei-Kun Chen, Antonia Chmiela, Tim Donkiewicz, Jasper van Doornmalen, Leon Eifler, Oliver Gaul, Gerald Gamrath, Ambros Gleixner, et al. The scip optimization suite 8.0. *arXiv preprint arXiv:2112.08872*, 2021.
- [53] Vinod Nair, Sergey Bartunov, Felix Gimeno, Ingrid von Glehn, Pawel Lichocki, Ivan Lobov, Brendan O’Donoghue, Nicolas Sonnerat, Christian Tjandraatmadja, Pengming Wang, et al. Solving mixed integer programs using neural networks. *arXiv preprint arXiv:2012.13349*, 2020.
- [54] He He, Hal Daume III, and Jason M Eisner. Learning to search in branch and bound algorithms. In Z. Ghahramani, M. Welling, C. Cortes, N. Lawrence, and K.Q. Weinberger, editors, *Advances in Neural Information Processing Systems*, volume 27. Curran Associates, Inc., 2014.
- [55] Frank Hutter, Holger H Hoos, and Kevin Leyton-Brown. Automated configuration of mixed integer programming solvers. In *International Conference on Integration of Artificial Intelligence (AI) and Operations Research (OR) Techniques in Constraint Programming*, pages 186–202. Springer, 2010.

Contents

1	Introduction	1
2	Related Work	3
3	Problem Statement	3
4	Proposed Solution	4
4.1	Methodology	4
4.2	Theoretical Analysis	6
5	Experimental Evaluation	6
5.1	Settings	7
5.2	Implementation	7
5.3	Results	8
6	Conclusion	9
A	Proofs	15
B	Implementation Details	16
B.1	Combinatorial Structure Extraction	16
B.2	Structure-Aware Code Generation	18
C	Baseline Details	19
C.1	Solver Adoption	19
C.2	Baselines Setting	19
C.2.1	Neural Combinatorial Optimization	19
C.2.2	Evolutionary Code Optimization	20
D	Dataset Details	21
D.1	SAT Domain	21
D.2	MILP Domain	21
E	Metric Details	22
E.1	Metrics related to MILP	22
E.2	Metrics related to SAT	22
F	Discussion	23
G	Additional Experimental Results	24
G.1	Optimization Performance Result	24
G.2	Convergence Comparison Result	25
G.3	Ablation Studies Result	27
H	Experiment Statistical Significance	28

A Proofs

Theorem 1. Given a prior dataset \mathcal{D} whose data samples comprises M types of prior $\mathcal{C} = \{\mathbf{C}_1, \dots, \mathbf{C}_M\}$, the distinct priors follow respective true distribution $p(\mathbf{C}_i|\mathbf{w})$. Let \mathbf{c}_i be a sample drawn from the distribution, i.e., $\mathbf{c}_i \sim p(\mathbf{C}_i|\mathbf{w})$. A generative model with an additional type of prior will not lower the upper bound of model performance $\sup(\mathcal{P})$.

Proof. Assume that there is a generative model, which is associated with a set of prior $\mathcal{C}_K = \{\mathbf{C}_1, \dots, \mathbf{C}_K\}$. Its upper bound of model performance is denoted by $\sup(\mathcal{P}_{\mathcal{C}_K})$. According to Definition 1, $\sup(\mathcal{P}_{\mathcal{C}_K})$ can be expanded as

$$\begin{aligned}
\sup(\mathcal{P}_{\mathcal{C}_K}) &= \sum_{\mathbf{C} \in \mathcal{C}_K} \sum_{\mathbf{c} \in \mathbf{C}} p(\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}) \\
&= \sum_{\mathbf{C} \in \mathcal{C}_K} \sum_{\mathbf{c} \in \mathbf{C}} p(\mathbf{c}) \max_{\mathbf{w}} \sum_{\mathbf{c}_i \in \mathbf{C}_i} p(\mathbf{c}_i|\mathbf{c}) p(\mathbf{w}|\mathbf{c}, \mathbf{c}_i) \Phi(\mathbf{w}) \\
&\leq \sum_{\mathbf{C} \in \mathcal{C}_K} \sum_{\mathbf{c} \in \mathbf{C}} \sum_{\mathbf{c}_i \in \mathbf{C}_i} p(\mathbf{c}) p(\mathbf{c}_i|\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}, \mathbf{c}_i) \Phi(\mathbf{w}) \\
&= \sum_{\mathbf{C} \in \mathcal{C}_K} \sum_{\mathbf{c} \in \mathbf{C}} \sum_{\mathbf{c}_i \in \mathbf{C}_i} p(\mathbf{c}_i, \mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}, \mathbf{c}_i) \Phi(\mathbf{w}) \\
&= \sum_{\mathbf{C} \in \mathcal{C}_K \cup \{\mathbf{C}_i\}} \sum_{\mathbf{c} \in \mathbf{C}} p(\mathbf{c}_i, \mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}, \mathbf{c}_i) \Phi(\mathbf{w}) \\
&= \sup(\mathcal{P}_{\mathcal{C}_K \cup \{\mathbf{C}_i\}})
\end{aligned} \tag{7}$$

Above proof indicates that for a given generative model with any additional modal prior \mathbf{C}_i , its performance upper bound $\sup(\mathcal{P}_{\mathcal{C}_K \cup \{\mathbf{C}_i\}})$ is greater or equal to its original performance upper bound $\sup(\mathcal{P}_{\mathcal{C}_K})$. \square

Theorem 2. If prior \mathbf{C}_{pe} is a performance-enhancing prior, a generative model neglecting prior \mathbf{C}_{pe} will decrease the upper bound of model performance. It can be expressed as

$$\sup(\mathcal{P}_{\mathcal{C} \setminus \{\mathbf{C}_{pe}\}}) < \sup(\mathcal{P}_{\mathcal{C}}) \tag{6}$$

Proof. If prior \mathbf{C}_{pe} is a performance-enhancing prior, according to Definition 2, we have

$$\begin{aligned}
\max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w})_{\mathbf{c} \in \mathcal{C} \setminus \{\mathbf{C}_{pe}\}} &< \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w})_{\mathbf{c} \in \mathcal{C}} \\
&= \sum_{\mathbf{c}_{pe} \in \mathbf{C}_{pe}} p(\mathbf{c}_{pe}|\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w})_{\mathbf{c} \in \mathcal{C}}
\end{aligned} \tag{8}$$

Then, according to Definition 1, $\sup(\mathcal{P}_{\mathcal{C} \setminus \{\mathbf{C}_{pe}\}})$ can be expanded as

$$\sup(\mathcal{P}_{\mathcal{C} \setminus \{\mathbf{C}_{pe}\}}) = \sum_{\mathbf{C} \in \mathcal{C} \setminus \{\mathbf{C}_{pe}\}} \sum_{\mathbf{c} \in \mathbf{C}} p(\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}) \tag{9}$$

Substitute Eq.(8) into Eq.(9) to derive

$$\begin{aligned}
\sup(\mathcal{P}_{\mathcal{C} \setminus \{\mathbf{C}_{pe}\}}) &= \sum_{\mathbf{C} \in \mathcal{C} \setminus \{\mathbf{C}_{pe}\}} \sum_{\mathbf{c} \in \mathbf{C}} p(\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}) \\
&< \sum_{\mathbf{C} \in \mathcal{C} \setminus \{\mathbf{C}_{pe}\}} \sum_{\mathbf{c} \in \mathbf{C}} p(\mathbf{c}) \sum_{\mathbf{c}_{pe} \in \mathbf{C}_{pe}} p(\mathbf{c}_{pe}|\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}) \\
&= \sum_{\mathbf{C} \in \mathcal{C} \setminus \{\mathbf{C}_{pe}\}} \sum_{\mathbf{c} \in \mathbf{C}} \sum_{\mathbf{c}_{pe} \in \mathbf{C}_{pe}} p(\mathbf{c}) p(\mathbf{c}_{pe}|\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}) \\
&= \sum_{\mathbf{C} \in \mathcal{C} \setminus \{\mathbf{C}_{pe}\}} \sum_{\mathbf{c} \in \mathbf{C}} \sum_{\mathbf{c}_{pe} \in \mathbf{C}_{pe}} p(\mathbf{c}_{pe}, \mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}) \\
&= \sum_{\mathbf{C} \in \mathcal{C}} \sum_{\mathbf{c} \in \mathbf{C}} p(\mathbf{c}) \max_{\mathbf{w}} p(\mathbf{w}|\mathbf{c}) \Phi(\mathbf{w}) \\
&= \sup(\mathcal{P}_{\mathcal{C}})
\end{aligned} \tag{10}$$

\square

B Implementation Details

B.1 Combinatorial Structure Extraction

Data Representation of MILP problem. A mixed-integer linear programming (MILP) problem is formally defined as:

$$\min_{\mathbf{x} \in \mathbb{R}^n} \mathbf{w}^\top \mathbf{x}, \quad \text{s.t. } \mathbf{A}\mathbf{x} \leq \mathbf{b}, \mathbf{l} \leq \mathbf{x} \leq \mathbf{u}, x_j \in \mathbb{Z}, \forall j \in \mathbb{I}, \quad (11)$$

where $\mathbf{w} \in \mathbb{R}^n$, $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$, $\mathbf{l} \in (\mathbb{R} \cup \{-\infty\})^n$, $\mathbf{u} \in (\mathbb{R} \cup \{+\infty\})^n$, and the index set $\mathbb{I} \subset \{1, 2, \dots, n\}$ specifies integer-constrained variables.

To encode MILP instances, we design a bipartite graph $\mathcal{G} = (\mathcal{C} \cup \mathcal{V}, \mathcal{E})$ with constraint-variable interactions. The constraint node set $\mathcal{C} = \{c_1, \dots, c_m\}$ corresponds to rows of $\mathbf{A}\mathbf{x} \leq \mathbf{b}$, where each node c_i is associated with a 1D feature vector $\mathbf{c}_i = (b_i)$ representing its right-hand side value. The variable node set $\mathcal{V} = \{v_1, \dots, v_n\}$ represents decision variables, each equipped with a 9D feature vector \mathbf{v}_j containing the objective coefficient w_j , variable type indicator (integer/continuous), and bound parameters l_j, u_j . Edges $\mathcal{E} = \{e_{ij}\}$ connect constraint c_i to variable v_j iff $a_{ij} \neq 0$, with edge features $\mathbf{e}_{ij} = (a_{ij})$ encoding the constraint coefficients.

Furthermore, a mixed-integer linear programming (MILP) instance is encoded as a weighted bipartite graph with feature matrices $\mathbf{G} = (\mathbf{C}, \mathbf{V}, \mathbf{E})$, where \mathbf{C} , \mathbf{V} , and \mathbf{E} aggregate constraint node features \mathbf{c}_i , variable node features \mathbf{v}_j , and edge features \mathbf{e}_{ij} , respectively. The full specification of these features is summarized in Table 2, which preserves all structural and numerical information of the original MILP problem. Following standard practice, we utilize the observation function from Ecole [50] to generate these bipartite graph representations from MILP instances.

Table 2: Description of the constraint, variable, and edge features in our bipartite graph representation for MILP instance.

Tensor	Feature	Description
\mathbf{C}	Constraint coefficient	Average of all coefficients in the constraint.
	Constraint degree	Degree of constraint nodes.
	Bias	Normalized right-hand-side of the constraint.
	Objective	Normalized objective coefficient.
\mathbf{V}	Variable coefficient	Average variable coefficient in all constraints.
	Variable degree	Degree of the variable node in the bipartite graph representation.
	Maximum variable coefficient	Maximum variable coefficient in all constraints.
	Minimum variable coefficient	Minimum variable coefficient in all constraints.
\mathbf{E}	Coefficient	Constraint coefficient.

Data Representation of SAT problem. A Boolean satisfiability (SAT) problem consists of variables x_i and logical operators \wedge , \vee , and \neg . A formula is satisfiable if there exists a variable assignment that makes all clauses evaluate to true. Following [51], we focus on formulas in conjunctive normal form (CNF) – conjunctions (\wedge) of clauses, where each clause is a disjunction (\vee) of literals (variables x_i or their negations $\neg x_i$). Any SAT formula can be converted to an equisatisfiable CNF formula in linear time. For example, $(x_1 \vee \neg x_2) \wedge (x_2 \vee \neg x_3)$ represents a CNF formula with two clauses.

We utilize the Variable-Clause Graph (VCG) to represent SAT formulas. For a SAT formula, the VCG is constructed with nodes representing literals and clauses, and edges indicating the inclusion of a literal in a clause. The bipartite structure of VCGs ensures a one-to-one correspondence between CNF formulas and their graph representations. Formally, a bipartite graph $\mathcal{G} = (\mathcal{V}_1 \cup \mathcal{V}_2, \mathcal{E})$ is defined by its vertex set $\mathcal{V}_1 \cup \mathcal{V}_2 = \{v_1, \dots, v_n\}$ and edge set $\mathcal{E} \subseteq \{(v_i, v_j) | v_i, v_j \in \mathcal{V}\}$. The vertex set is partitioned into two disjoint subsets \mathcal{V}_1 and \mathcal{V}_2 , with edges restricted to connections between nodes in distinct partitions: $\mathcal{E} \subseteq \{(v_i, v_j) | v_i \in \mathcal{V}_1, v_j \in \mathcal{V}_2\}$. In the context of VCGs, a CNF formula with n

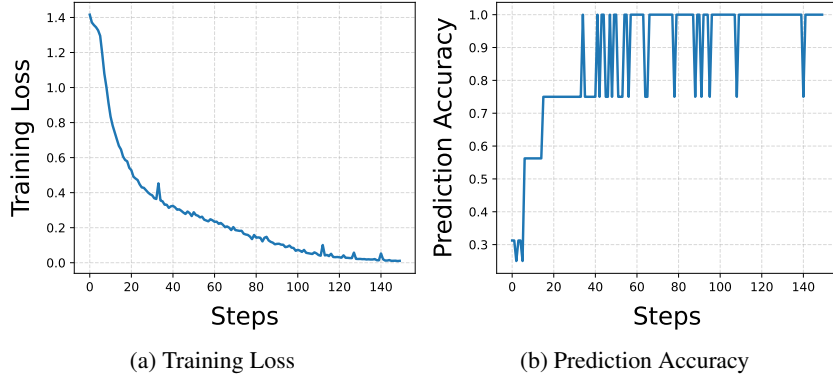


Figure 6: The convergence curve of training GNN for SAT domain.

literals and m clauses induces a bipartitioned graph where $\mathcal{V}_1 = \{l_1, \dots, l_n\}$ denotes the literal nodes and $\mathcal{V}_2 = \{c_1, \dots, c_m\}$ represents the clause nodes.

GNN Structure. The process of using GNN to extract combinatorial optimization problem can be formulated as:

$$\mathbf{v}_i^{(k+1)} \leftarrow \mathbf{f}_V(\mathbf{v}_i^{(k)}, \sum_{\substack{(i,j) \in \mathcal{E} \\ j, i \neq j}} \mathbf{g}_V(\mathbf{v}_i^{(k)}, \mathbf{v}_j^{(k)}, \mathbf{e}_{ij})), \quad (k = 0, 1, \dots, K-1) \quad (12)$$

$$\mathbf{h}_q = \text{Pool}(\{\mathbf{v}_i^{(K)}\}), \quad (13)$$

where \mathbf{f}_V and \mathbf{g}_V are perceptrons for node representation; K represents the total number of times that we perform the convolution; Pool denotes pooling function that aggregates the embedding of each node in the graph, obtaining the structure embedding $\mathbf{h}_q \in \mathbb{R}^d$ of the instance q . We denote the parameters of GNN as θ_G .

GNN Training. The loss function w.r.t. θ_G is given below:

$$\mathcal{L}(\theta_G) = -\frac{1}{N} \sum_{i=1}^N \sum_{c=1}^C y_{i,c} \log p_{\theta_G}(c|q_i), \quad (14)$$

$$p_{\theta_G}(c|q_i) = \frac{\exp(\mathbf{W}_c^T \mathbf{h}_{q_i} + \mathbf{b}_c)}{\sum_{j=1}^C \exp(\mathbf{W}_j^T \mathbf{h}_{q_i} + \mathbf{b}_j)}, \quad (15)$$

where N is the total number of CO problems in the training procedure; C denotes the number of classes; $y_{i,c} \in \{0, 1\}$ is the ground-truth label of problem instance q_i ; and $\mathbf{W}_j \in \mathbb{R}^d, \mathbf{b}_j \in \mathbb{R}, (j = 1, \dots, C)$ is the parameters of final classifying layer, which are also part of θ_G .

Implementation & Training Details. Following the training protocol outlined above, we implement separate GNN models for the SAT and MILP domains using the dataset described in Appendix D. Our GNN architecture consists of three convolutional layers ($K = 3$) followed by a global mean pooling operation. We leverage the graph convolution operator from the `torch_geometric` library, with node embedding dimensions of 16, 32, and 64 for successive layers³. To capture global graph structure, we apply mean pooling to the final convolutional layer’s node embeddings. For classification, a softmax layer processes the pooled representation to produce final predictions. The models are trained using the loss function defined in Eq.(14) with AdamW optimizer and cosine decay learning rate. Figure 6 illustrates the training convergence for SAT instance classification (5-way classification task). Upon model convergence, we compute structural prior representations for combinatorial optimization problem instances by processing their bipartite graph representations through the above GNN. The final convolutional layer’s output embeddings are extracted as the structural prior for each instance in the target domain.

³For the MILP domain, we increase the final layer’s dimensionality to 128 to account for higher problem complexity compared to SAT domain.

B.2 Structure-Aware Code Generation

Data Curation. We begin by assembling a curated collection of mathematical models for CO problems, which are directly compatible with corresponding CO solvers, alongside their natural language descriptions. Subsequently, for each CO problem, we compile a prompt that integrates the natural language description with specific code generation requirements. For instance, the code generation requirements may include details such as the function name, input/output parameters, expected function behavior, relevant background knowledge, *etc.* This prompt is then fed into an LLM to generate a code snippet. Note that to maximize the diversity of collected code snippets, we employ multiple LLM queries per prompt under high temperature settings to sample distinct candidate implementations. Each generated code snippet is evaluated by embedding it into the target solver and solving the corresponding CO problem, thereby obtaining performance metrics for the code snippet. Note that based on the principles of data curation, we collect the needed data via querying Qwen2.5-Coder-7B-Instructor same as the model adopted in the following post training procedure.

Post Training. Specifically, we first curate the collected data by processing each CO problem Q_i with its associated prompt x_i and corresponding multiple generated code snippets $y_{i,j} (j = 1, \dots, M)$. These code snippets are systematically ranked based on previously obtained performance metrics to establish quality ordering. The highest-performing code-prompt pairs are selected to form the SFT dataset $\mathcal{D}_{SFT} = \{(x_i, y_i^*)\}_{i=1}^N$. Additionally, by leveraging pairwise comparisons extracted from the established ranking hierarchy, we derive the preference dataset $\mathcal{D}_{DPO} = \{(x_i, y_w, y_l)\}_{i=1}^N$ where y_w, y_l are preferred/dispreferred code snippets. The training process can be formulated as follows:

$$\mathcal{L}_{DPO} = -\mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}_{DPO}} \left[\log \sigma \left(\beta \ln \frac{\pi_{\theta_L}(y_w|x)}{\pi_{\text{ref}}(y_w|x)} - \beta \ln \frac{\pi_{\theta_L}(y_l|x)}{\pi_{\text{ref}}(y_l|x)} \right) \right], \quad (16)$$

where σ is the Sigmoid function; β is the hyperparameter that governs the trade-off between reward maximization and KL divergence minimization; π_{ref} is the reference model trained on \mathcal{D}_{SFT} . Note that both π_{ref} and π_{θ_L} updates only the parameter θ_L of the composite model. Through above post-training, we obtain a generative model capable of structure-aware code generation that simultaneously respects combinatorial optimization problems' inherent topological constraints and solver-specific syntactic requirements. Note that based on above principle of data curation and post-training, we collect 8k and 4k post-training instances for MILP and SAT instances respectively.

Implementation & Training Details. To implement the proposed composite model, we first design a structure-prior-aware forward propagation mechanism and corresponding adapted inference framework based on the Qwen2.5-Coder-7B-Instructor⁴ model via the Transformers library.

① Structure-Prior-Aware Forward Propagation Mechanism. Specifically, we process the input prompt through the tokenizer and the model's embedding layer to obtain *input_embeds*, which are then merged with structural feature vectors of combinatorial optimization problems extracted by the previous graph neural network.

First, we align the dimensionality of the combinatorial optimization problem feature vector $\mathbf{h}_q \in \mathbb{R}^d$ with the hidden layer dimensions of the large language model via zero-padding. Given the text embedding shape $\text{embeds} \in \mathbb{R}^{B \times S \times H}$, where B is the batch size, S is the sequence length (number of tokens), and H is the hidden dimension, the dimension-adapted feature vector is obtained as:

$$\mathbf{H}_q = \text{ZeroPadding}(\mathbf{h}_q \oplus \mathbf{0}^{(H-d)}) \in \mathbb{R}^{B \times H} \quad (17)$$

where *ZeroPadding* denotes zero-padding, and \mathbf{H}_q represents the padded graph structural feature vector. Subsequently, we fuse text and structural features between the embedding layer and decoder layer by prepending the graph feature vector to the text embedding sequence, forming a hybrid input:

$$\mathcal{E}(\text{embeds}, \mathbf{H}_q) = [\text{CLS}] \oplus \mathbf{H}_q \oplus \text{embeds}[1:] \in \mathbb{R}^{B \times (1+S) \times H} \quad (18)$$

Here, *embeds* is the *input_embeds* obtained from processing the textual prompt via the tokenizer and embedding layer, enabling the self-attention mechanism to jointly model textual semantics and graph structural features. A mask of all True values is constructed and merged with the *attention_mask* to match the shape of the combined *input_embeds*, ensuring \mathbf{H}_q participates in attention computation. Let the original *attention_mask* shape be $M = \{0, 1\}^{B \times S}$; the merged *attention_mask* becomes:

$$M_{in} = [M_{0:1}; \mathbf{1}^B; M_{1:S}] \in \{0, 1\}^{B \times (1+S)} \quad (19)$$

⁴This model is available at <https://huggingface.co/Qwen/Qwen2.5-Coder-7B-Instruct>.

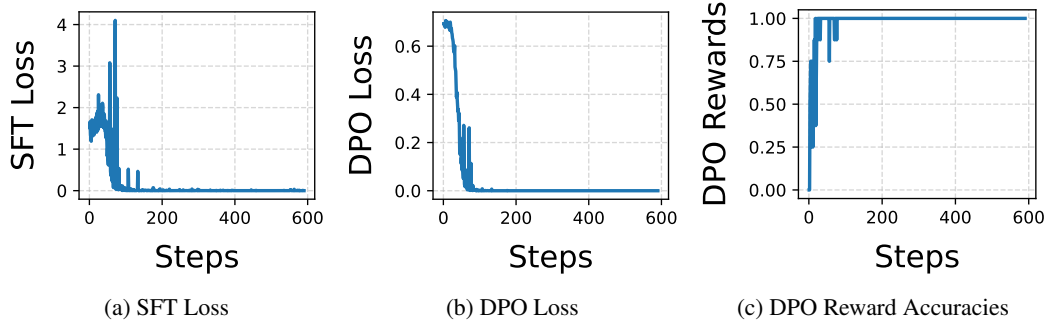


Figure 7: The convergence curve of post-training composite model for SAT domain.

The resulting *input_embeds* and *attention_mask* are then passed to the decoder layers and subsequent model structures for standard forward propagation.

② Parameter-Efficient Finetuning. We adopt LoRA for parameter-efficient fine-tuning on an autoregressive language model task. Key hyperparameters are configured as: rank dimension $r = 16$ controlling the latent dimension of low-rank adaptation matrices; scaling factor $lora_alpha = 32$ for output normalization; dropout probability 0.05 for regularization; trainable low-rank adaptation layers injected exclusively into query (q_proj) and value (v_proj) projection submodules of the Transformer architecture while keeping other parameters frozen; bias parameters set to "none" to preserve original model biases. The adapted LLM is trained with AdamW optimizer and cosine decay learning rate. An illustrative training curve of the model for SAT domain is given in Figure 7.

③ Adapted Inference Framework. Based on this modified architecture, we further adapt the LLM inference framework with structure-prior feature vector integration. During each autoregressive forward pass, logits are obtained via the feature-enhanced forward propagation, ensuring persistent influence of the structure-prior feature vector throughout the generation process rather than only affecting the initial output. We employ a hybrid sampling strategy with Top-k set to 20, Top-p to 0.8, and repetition penalty to 1.0.

C Baseline Details

C.1 Solver Adoption

MILP Solver. In all experiments related to MILP domain, we employ SCIP 8.0.0 [52] as the MILP solver backend—a leading open-source solver widely adopted in machine learning research for combinatorial optimization [44, 53]. To ensure reproducibility and fair comparisons, all SCIP parameters remain at default values. We retain the solver’s advanced features (*e.g.*, presolve, heuristics), aligning our experimental setup with real-world applications.

SAT Solver. In all experiments related to SAT domain, we use EasySAT⁵ to ensure direct comparability with AutoSAT[29]. The solver incorporates modern Conflict-Driven Clause Learning (CDCL) techniques including Literal Block Distance (LBD) heuristics, and VSIDS variable selection, and conflict-driven clause learning. All configurations (compiler versions, interfaces, time budgets) maintain parity with [29] for reproducibility.

C.2 Baselines Setting

C.2.1 Neural Combinatorial Optimization

L2B [14]. The paper addresses the challenge of variable selection in the branch-and-bound (B&B) algorithm for solving mixed-integer linear programs (MILPs), where traditional expert-designed heuristics like strong branching incur prohibitive computational costs. To overcome this, the authors propose a graph convolutional neural network (GCNN) framework that leverages the natural bipartite

⁵EasySAT: A Simple CDCL SAT Solver, <https://github.com/shaowei-cai-group/EasySAT>.

graph representation of MILPs – with variable and constraint nodes connected via edges representing their coefficients – to learn branching policies through imitation learning. Key innovations include encoding MILP states as bipartite graphs with constraint/variable features, designing permutation-invariant sum-based graph convolutions with prenormalization layers to handle variable-sized inputs, and training via behavioral cloning of strong branching decisions using cross-entropy loss. All configurations take the default value used in [14] for fair comparison.

HEM [15, 16]. The paper addresses the challenge of improving cut selection in mixed-integer linear programming (MILP) solvers by simultaneously optimizing three critical aspects: which cuts to select (P1), how many to choose (P2), and their ordering (P3). Existing learning-based methods focus primarily on scoring individual cuts while neglecting dynamic cut count determination and sequence dependencies. To overcome these limitations, the authors propose a novel hierarchical sequence model (HEM) that leverages a two-level architecture: a higher-level policy predicts the ratio of cuts to select using a tanh-Gaussian distribution, while a lower-level pointer network formulates cut selection as a sequence-to-sequence learning problem to output ordered subsets. The model is trained via hierarchical policy gradient optimization within a reinforcement learning framework, where states encode MILP relaxation features and candidate cut characteristics, actions represent ordered cut subsets, and rewards correspond to solver performance metrics like primal-dual gap integral. All hyperparameters take the default value used in [15, 16] for fair comparison.

NeuroSAT [40]. The paper proposes a message-passing neural network (MPNN) to solve the Boolean satisfiability problem by training solely on binary labels indicating satisfiability. The key innovation lies in representing SAT instances as bipartite graphs where literals and clauses are nodes connected via edges, and leveraging permutation-invariant neural architectures to process these graphs. NeuroSAT iteratively refines node embeddings through bidirectional message passing: clauses aggregate information from their constituent literals, while literals update their states based on connected clauses and complementary literals. Trained on a distribution of random SAT problems generated by incrementally adding clauses until unsat, the model learns to predict satisfiability via a cross-entropy loss on the final aggregated literal embeddings. Crucially, the architecture enforces structural symmetries (variable/clause permutation invariance, negation equivalence) and generalizes to larger instances and entirely unseen domains (*e.g.*, graph coloring, vertex cover) at test time by simply extending the message-passing iterations, despite being trained only on small random $n \leq 40$ problems. All configurations of this algorithm take the default used in [40] for fair comparison. Note that since NeuroSAT is a prediction framework for Boolean satisfiability problem, it is meaningless to measure the solving time for this framework over the SAT instances. Besides, the ground-truth dataset used to train the NeuroSAT model is those SAT instances can be proved/solved within timelimit τ . Thus, we only count the number predicted to be correct of NeuroSAT (this number must be less than the number of ground-truth labels). Then, the number of timeout for NeuroSAT is equal to the total number of test instances minus the number predicted to be correct.

C.2.2 Evolutionary Code Optimization

AutoSAT [29]. The paper introduces a framework that leverages Large Language Models (LLMs) to automatically optimize heuristics in Conflict-Driven Clause Learning (CDCL) SAT solvers. The authors address the challenge of manually designing and tuning heuristic functions in modern CDCL solvers, which is time-consuming and expert-dependent. Instead of generating solvers from scratch, AutoSAT operates within a modular search space comprising nine key heuristic functions (*e.g.*, branching, restart, and clause management) derived from an existing CDCL solver. The framework employs LLMs to iteratively refine these heuristics through two search strategies: a greedy hill climber (GHC) and a (1+1) Evolutionary Algorithm (EA), where LLMs generate candidate code modifications guided by performance feedback. All configurations of this algorithm take the default used in [29] for fair comparison.

LLM4Solver [30]. The paper proposes a novel framework that integrates large language models (LLMs) with evolutionary search to automate the design of high-performance diving heuristics for exact combinatorial optimization (CO) solvers. The key challenge addressed is the inefficiency of traditional manual and learning-based approaches in navigating the vast, discrete algorithm space for CO solver components like diving heuristics, which require domain expertise and suffer from poor generalization. The core methodology leverages LLMs as prior-knowledge-guided generators to produce candidate algorithms encoded as interpretable score functions, while a derivative-free evolutionary framework (single- or multi-objective) optimizes these candidates through iterative

population-based search. The algorithm space is defined via 13 interpretable variable features, with LLMs enabling code-level manipulations during initialization, crossover, and mutation. We slightly adjusted **LLM4Solver**'s optimization focus from diving heuristics to cut selection for MILP solver for fair comparison with previous work [15, 16]. All configurations of this algorithm take the default used in [15, 16] for fair comparison.

D Dataset Details

D.1 SAT Domain

Chromatic-Number-of-the-Plane (CNP). This problem requires coloring graph vertices such that adjacent nodes have distinct colors.

Profitable-Robust-Production (PRP). This problem seeks robust production plans maintaining profitability under uncertain/fluctuating conditions. The generation setting of PRP adhere to [29].

CoinsGrid. This problem, based on Tony Hurlimann's coin puzzle, involves arranging coins on a grid with row-wise, column-wise, and distance-based constraints. The generation setting of CoinsGrid adhere to [29].

Zamkeller. This problem requires finding a permutation of integers from 1 to n that maximizes differential alternations in subsequences divisible by integers 1 to k ($1 < k < n$). Instance generation follows [29].

Table 3: The statistical description of used SAT datasets. Const. and Var. stand for constraints and variables respectively.

Dataset	Size	# Const. (mean)	# Const. (std)	# Var. (mean)	# Var. (std)
CNP	150	261,260	352,379	8,798	8,893
CoinsGrid	78	1,116,972	1,068,009	154,828	148,571
PRP	80	2,120,983	1,346,344	317,635	201,185
Zamkeller	80	310,804	335,102	24,592	22,190

D.2 MILP Domain

Easy. The SCIP 8.0.0 solver solves MILP instances in the Easy dataset within one minute. This dataset comprises three synthetic problems: Set Covering [41], Maximum Independent Set [42], and Multiple Knapsack [43]. We select these classes because: (1) they serve as standard benchmarks for MILP solver evaluation [44], and (2) they encompass diverse MILP problem structures encountered in practice. Following [44, 43], we generate set covering instances (500 rows \times 1000 columns), Maximum Independent Set instances (500-node graphs with affinity 4), and multiple knapsack instances (60 items, 12 knapsacks). For each dataset within this category, we generate 1,000 training instances and hold 100 instances as test set. Besides, we set the timelimit as 60 seconds for solving problem instances within this dataset.

Medium. The SCIP 8.0.0 solver requires at least five minutes to solve this set of instances optimally. Following [54, 55, 53], this dataset combines MIK⁶ [46] (MILPs with knapsack constraints) and CORLAT⁷ [47] (real-world grizzly bear corridor planning in Northern Rockies). Each problem set is partitioned into 80% training and 20% test instances. Furthermore, we set the timelimit as 120 seconds for solving problem instances within this dataset.

Hard. The SCIP 8.0.0 solver requires more than one hour to solve Hard dataset instances to optimality. These datasets⁸ include Load Balancing from the NeurIPS 2021 ML4CO competition [48]. Load Balancing instances model server task allocation under resource constraints. Same as Medium dataset, each problem set in Hard dataset is also partitioned into 80% training and 20% test instances. Additionally, we set the timelimit as 360 seconds for solving problem instances within this dataset.

⁶MIK data can be found at <https://atamturk.ieor.berkeley.edu/data/mixed.integer.knapsack/>.

⁷CORLAT data is available at <https://bitbucket.org/mlindauer/aclib2/src/master/>.

⁸All these data can be found at <https://www.ecole.ai/2021/ml4co-competition/>.

Table 4: The statistical description of used MILP datasets.

Dataset	# Constraints (mean)	# Variables (mean)
Set Covering (SC)	500	1,000
Maximum Independent Set (MIS)	1,953	500
Knapsack	72	720
MIK	346	413
CORLAT	486	466
Load Balancing	64,304	61,000

E Metric Details

E.1 Metrics related to MILP

For fair comparison, our evaluation employs metrics aligned with HEM [15, 16, 14], which are well-established in the MILP community.

Solving Time. For MILP instances solved to optimality within time limit T , we measure the solver runtime t required to obtain certifiably optimal solutions. For those MILP instances that cannot be solved to optimality within time limit T , we utilize the following metrics.

Primal-Dual Gap. During the execution of MILP solvers, two critical bounds are maintained: the global primal bound and the global dual bound. The global primal bound represents the objective value of the incumbent feasible solution, serving as the tightest upper bound for the MILP. The global dual bound corresponds to the minimal lower bound among all active nodes in the search tree, constituting the strongest lower bound for the problem. The primal-dual gap is defined as the absolute difference between these two bounds. In SCIP 8.0.0 [52], the initial primal-dual gap is initialized to a constant value of 100.

Primal-Dual (PD) Integral. The primal-dual gap integral is defined as the area enclosed between the primal and dual bound trajectories during solver execution. Formally, given a time limit T , this integral is expressed as:

$$\int_{t=0}^T (\mathbf{w}^T \mathbf{x}_t^* - \mathbf{z}_t^*) dt, \quad (20)$$

where \mathbf{w} denotes the objective coefficient vector of the MILP instance; \mathbf{x}_t^* represents the incumbent feasible solution at time t , \mathbf{z}_t^* corresponds to the tightest dual bound at time t . This metric quantifies the cumulative optimality gap over the solving horizon and serves as an established performance benchmark for MILP solvers. Notably, the primal-dual gap integral was adopted as the primary evaluation criterion in the NeurIPS 2021 ML4CO competition [48].

E.2 Metrics related to SAT

To ensure fair comparison, our evaluation adopts metrics consistent with AutoSAT [29], which are widely recognized in the SAT community.

Solving Time. For SAT instances that can be solved/proved within a timeout limitation τ , we record the running time t of a SAT solver solving/proving these instances. For those SAT instances that cannot be solved/proved within timeout limitation τ , we measure the two following metrics.

Number of Timeout. Given a timeout limitation τ and a set of SAT instances, we record the number of SAT instances that cannot be solved/proved within τ for different compared methods. The τ is set as 5000 seconds, same as [29].

Penalized Average Runtime with a factor of 2 score (PAR-2). PAR-2 is a standard evaluation metric in SAT solver competitions and benchmarks, employed to assess and compare solver performance under incomplete executions or timeout scenarios. Specifically, the PAR-2 score aggregates runtime across test instances as follows: 1) For solved instances, record the solver’s runtime; 2) For instances where the solver exceeds the timeout limitation τ , assign twice the timeout threshold τ as the penalty—this is why we call this metric as PAR-2; 3) Compute the average across all instances by summing these values and dividing by the instance count. Lower PAR-2 scores indicate better overall solver efficiency.

Intuitively, consider a benchmark set comprising n SAT instances. Let t_i denote the solver’s runtime on the i -th instance. The PAR-2 score is formally defined as

$$\text{PAR-2} = \frac{1}{n} \sum_{i=1}^n t_i, \quad (21)$$

where

$$t_i = \begin{cases} t_i, & \text{if } t_i \leq \tau; \\ 2\tau, & \text{if } t_i > \tau \text{ or the solver fails to return a solution.} \end{cases} \quad (22)$$

F Discussion

End-to-End Training. In this work, we adopt a two-stage training procedure for our composite model: first training a graph neural network (GNN), then training a large language model (LLM) conditioned on the frozen GNN embeddings. This approach stems from our empirical observation that end-to-end joint training of the composite model presents significant optimization challenges. We hypothesize that this limitation could be mitigated by exploring more sophisticated GNN architectures or developing enhanced alignment strategies between the GNN’s structural representations and the LLM’s semantic space.

Explore Domain-specific Distributional Discrepancies. In our ablation studies, empirical results reveal that the full STRCMP model (with complete post-training) underperforms relative to its variants STRCMP (SFT Only) and STRCMP (DPO Only) across benchmark datasets, suggesting potential conflicts between optimization objectives during multi-stage post-training. This observation motivates future investigation into domain-specific distributional discrepancies that may arise from the heterogeneous nature of combinatorial optimization problems, which could inform improved alignment strategies for cross-domain post-training protocols.

Incorporating Additional Modal Priors. In this study, we focus specifically on integrating graph structural priors into LLM-based algorithm discovery for combinatorial optimization problems. While current methodologies rely on human expertise to predefine target components, we posit that LLMs’ context-aware capabilities could assimilate additional modal priors (e.g., dynamic constraint patterns or solution quality metrics) to enhance combinatorial optimization problem-solving performance. Future extensions may enable LLMs to autonomously identify computational bottlenecks through techniques such as runtime complexity profiling or constraint violation pattern analysis, thereby prioritizing component optimization.

G Additional Experimental Results

G.1 Optimization Performance Result

Table 5: The optimization performance result w.r.t. PAR-2 score between different methods over SAT domain.

Compared Methods	PAR-2 Score (\downarrow)			
	CNP	CoinsGrid	PRP	Zamkeller
AutoSAT	644.72	1098.69	639.34	807.75
EasySAT	649.42	1595.75	2000	829.38
STRCMP	624.15	1124.09	1804.46	270.62
STRCMP (DPO Only)	643.45	1098.69	482.92	265.94
STRCMP (SFT Only)	643.23	1098.47	1837.86	227.69
STRCMP w/o GNN	645.67	1098.34	1820.38	646.12

Table 6: The optimization performance result w.r.t. Solving Time between different methods over SAT domain.

Compared Methods	Solving Time (\downarrow)			
	CNP	CoinsGrid	PRP	Zamkeller
AutoSAT	32472	19158	22967	20772
EasySAT	32942	26064	50000	21810
STRCMP	31415	18971	46223	7990
STRCMP (DPO Only)	32345	19158	21146	7765
STRCMP (SFT Only)	32323	19151	46893	6929
STRCMP w/o GNN	32567	19147	47019	17014

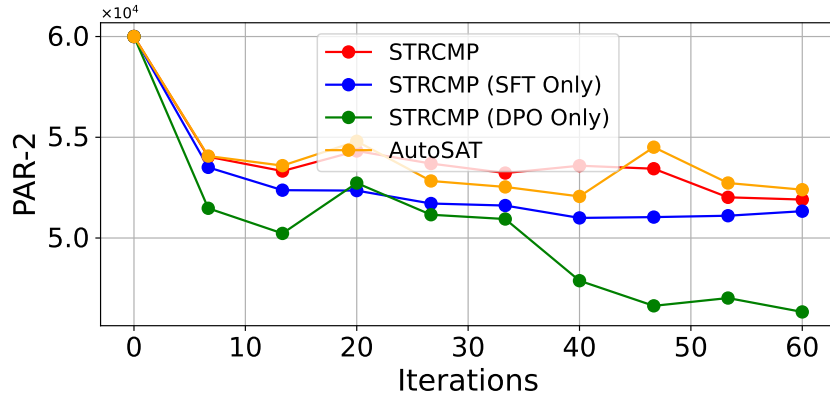


Figure 8: Convergence comparison (w.r.t. PAR-2) between evolutionary-based algorithm discovery frameworks on PRP dataset of SAT domain.

G.2 Convergence Comparison Result

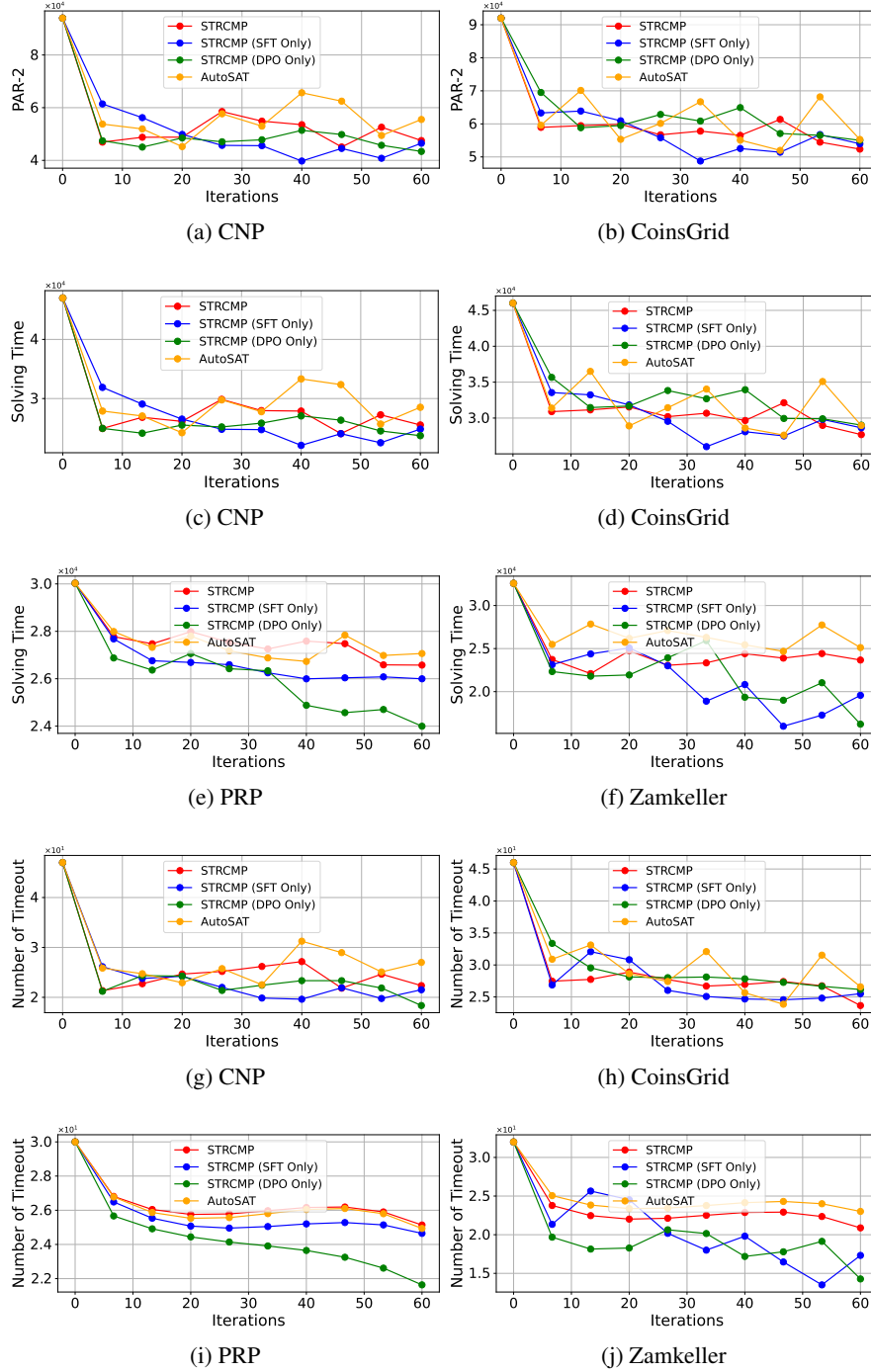


Figure 9: Convergence comparison (w.r.t. PAR-2, Solving Time, and Number of Timeout) between evolutionary-based algorithm discovery frameworks on SAT domain.

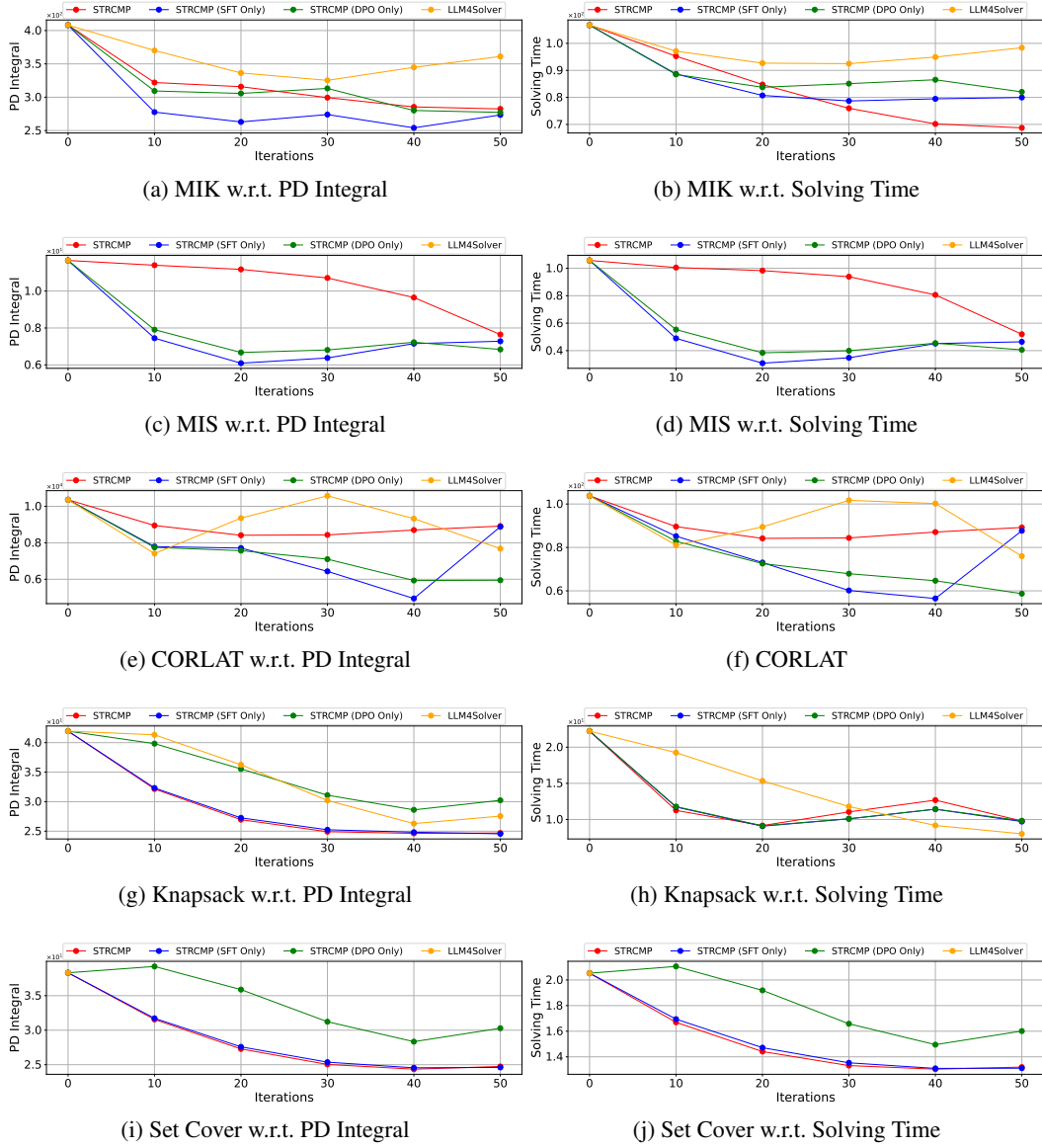


Figure 10: Convergence comparison (w.r.t. PD Integral and Solving Time) between evolutionary-based algorithm discovery frameworks on MILP domain.

G.3 Ablation Studies Result

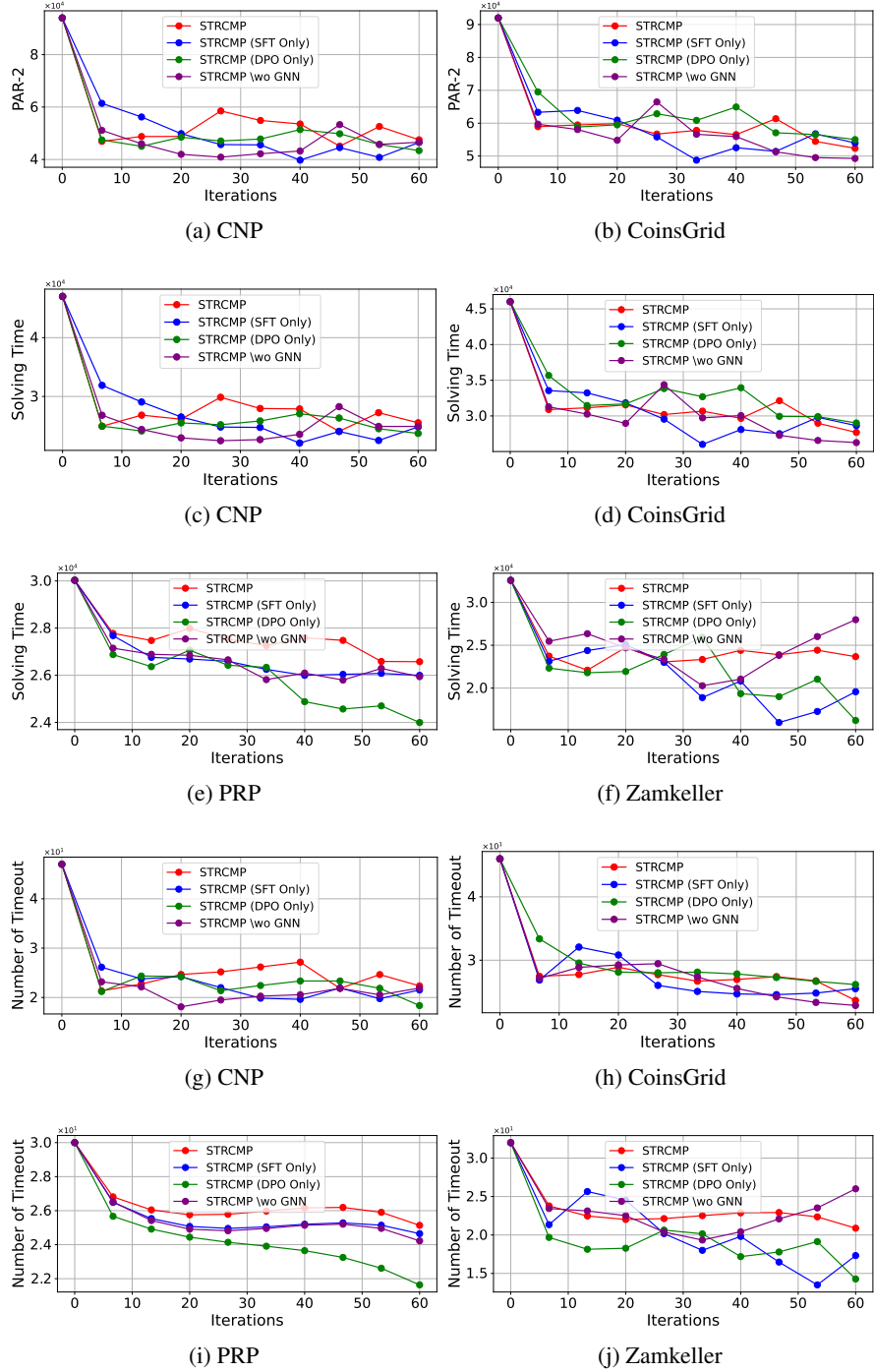


Figure 11: Ablation studies (w.r.t. PAR-2, Solving Time, and Number of Timeout) during algorithm search on SAT domain.

H Experiment Statistical Significance

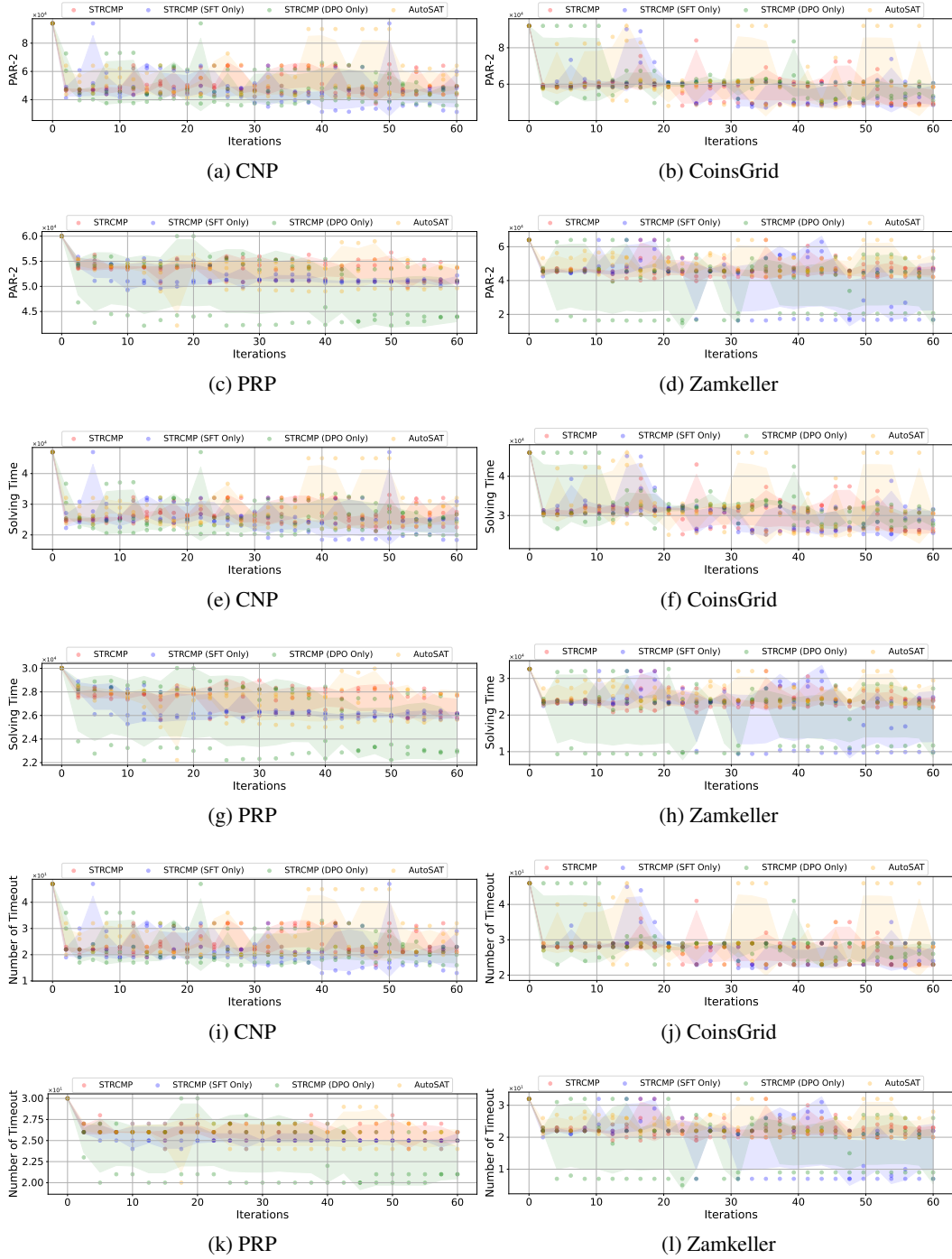


Figure 12: Convergence comparison with variance statistic (w.r.t. PAR-2, Solving Time, Number of Timeout) between evolutionary-based algorithm discovery frameworks on SAT domain.