Article

Hybrid LLM-Algorithm Optimization: Iterated Fine-Tuning for Combinatorial Problems

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Abstract: We propose a novel framework, TopIFT (LLM-driven Iterated Fine-Tuning), for integrating large language models (LLMs) with combinatorial optimization techniques. While LLMs excel at handling local, context-dependent constraints, they struggle to enforce global feasibility. Our approach iteratively fine-tunes LLMs using algorithmic feedback, progressively aligning generated solutions with structured optimization objectives. We benchmark TopIFT against existing hybrid models such as LLM-Guided Search, FunSearch, NeurOpt, and MH-LLM, demonstrating superior constraint-handling and competitive optimization efficiency. Empirical results on scheduling, spanning trees, and clustering problems highlight TopIFT's ability to achieve near-optimal solutions while preserving local flexibility. This work opens new avenues for AI-driven combinatorial reasoning and hybrid AI-algorithm collaboration.

Keywords: Iterated Fine-Tuning, Hybrid AI, Large Language Models, Combinatorial Optimization, Algorithmic Learning

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1. Introduction

Combinatorial optimization problems are fundamental to many real-world applications, ranging from logistics and scheduling to network design and resource allocation. These problems involve selecting an optimal subset or arrangement of discrete elements while satisfying specific constraints. However, a major challenge lies in balancing two competing paradigms: flexible, human-like decision-making (often expressed in natural language) and strict, mathematically structured constraints (enforced by traditional algorithms).Traditional optimization algorithms, such as Mixed Integer Linear Programming (MILP), Constraint Satisfaction Problems (CSP), and heuristic search methods, are highly efficient at ensuring global feasibility—meaning they rigorously respect the problem's structural constraints. However, these methods require precise, formally defined constraints, making them brittle when handling ambiguous, context-dependent, or evolving requirements. For instance, in travel route planning, an algorithm may perfectly minimize total distance but fail to incorporate user preferences like "scenic routes with local restaurants" due to the subjective nature of the request.

Conversely, Large Language Models (LLMs), such as GPT-4 Turbo or Gemini 1.5, are excellent at understanding and generating flexible, human-like responses. They can interpret soft constraints, such as user intent and contextual nuances, but struggle with enforcing global feasibility in complex optimization tasks. For example, when asked to

generate a valid tour itinerary or construct a feasible network topology, an LLM may generate a plausible-sounding but infeasible solution—missing critical constraints like time window restrictions or graph connectivity.To bridge this capability gap, we propose TopIFT (LLM-driven Iterated Fine-Tuning)—a hybrid model that iteratively fine-tunes an LLM using algorithmic feedback. Instead of relying solely on pre-trained LLM knowledge or static rule-based optimization, TopIFT learns iteratively by leveraging both human-like interpretability (via LLMs) and structured decision-making (via algorithms). Our approach ensures that the model progressively aligns with both local and global constraints, refining its solution space over multiple iterations.

This paper positions TopIFT within the broader landscape of LLM-driven optimization, comparing it against existing hybrid methods such as LLM-Guided Search, FunSearch, NeurOpt (MILP + LLM), and Metropolis-Hastings LLMs. We provide both theoretical analysis (sample complexity, convergence guarantees) and empirical validation (real-world scheduling, spanning tree, and clustering tasks) to demonstrate its effectiveness. Our findings show that TopIFT balances feasibility and interpretability better than traditional approaches, making it a promising direction for hybrid AI-driven decision-making in combinatorial optimization.

2. Related Work

2.1 LLM-Guided Search:

LLM-Guided Search leverages Large Language Models (LLMs) to generate heuristic solutions for combinatorial optimization problems. It operates by utilizing the LLM's ability to recognize patterns and suggest promising candidates based on learned knowledge from extensive training data. This approach can effectively explore the solution space and provide reasonable initial solutions without requiring explicit mathematical formulations. However, a key limitation of LLM-Guided Search is the absence of an iterative fine-tuning mechanism. Once an LLM generates a heuristic, there is no structured feedback loop to refine or improve the solution based on its performance. As a result, the approach may struggle to consistently enhance solution quality over multiple iterations or adapt to problem-specific constraints. This limitation can lead to suboptimal or infeasible solutions, especially in complex optimization scenarios where iterative refinement is crucial for achieving high-quality outcomes.

FunSearch:

FunSearch is an evolutionary search framework that utilizes Large Language Models (LLMs) to generate and refine heuristic functions for combinatorial optimization problems. The core idea behind FunSearch is to iteratively evolve heuristics by leveraging LLM-generated candidates, evaluating their performance, and selectively propagating the most effective ones through an evolutionary search process. This approach allows for the discovery of novel and potentially powerful heuristics that may not be explicitly designed by human experts. However, a fundamental limitation of FunSearch is its lack of a structured mechanism to balance the constraints imposed by LLM-generated solutions with the feasibility requirements of the underlying optimization algorithm. While LLMs can generate diverse heuristics, they do not inherently ensure that these heuristics align with algorithmic constraints, computational efficiency, or problem-specific feasibility criteria. Consequently, FunSearch may produce heuristics that, while promising in concept, are difficult to implement efficiently or lead to solutions that violate practical constraints. Without an explicit mechanism to enforce feasibility or refine heuristics based on constraint satisfaction, the approach risks generating solutions that are either computationally expensive to evaluate or impractical for real-world applications. Thus, while FunSearch offers an innovative way to evolve heuristics, its reliance on LLM-generated outputs without rigorous feasibility enforcement limits its effectiveness in structured optimization problems.

NeurOpt:

NeurOpt is a hybrid optimization framework that integrates Large Language Models (LLMs) with Mixed-Integer Linear Programming (MILP) solvers to generate high-quality solutions while ensuring strong feasibility guarantees. The core idea behind NeurOpt is to leverage the generative capabilities of LLMs to propose initial solutions or heuristic modifications, which are then rigorously validated and refined through MILP solvers. By incorporating MILP solvers, NeurOpt benefits from well-established mathematical optimization techniques that enforce strict feasibility constraints, ensuring that the final solutions adhere to all problem-specific requirements. This integration provides a significant advantage over purely heuristic-based approaches, as it eliminates the risk of generating infeasible or suboptimal solutions. However, a major drawback of NeurOpt is its high computational cost. MILP

solvers often require extensive computational resources, especially for large-scale or complex problems where the search space is vast and constraint satisfaction is computationally expensive. Additionally, the iterative process of verifying and refining LLM-generated candidates through MILP solvers further increases the computational burden, leading to potentially long solving times. This trade-off between feasibility and efficiency makes NeurOpt a powerful but resource-intensive approach, limiting its practicality for real-time applications or large-scale optimization tasks where computational efficiency is a primary concern.

Metropolis-Hastings LLM (MH-LLM):

Metropolis-Hastings LLM (MH-LLM) is a probabilistic refinement framework that incorporates Large Language Models (LLMs) into the well-established Metropolis-Hastings (MH) algorithm to iteratively improve solutions for combinatorial optimization problems. The key idea behind MH-LLM is to use an LLM to propose candidate solutions, which are then evaluated based on an acceptance criterion derived from the MH algorithm. This probabilistic framework enables MH-LLM to explore the solution space in a structured manner, allowing it to refine solutions iteratively while balancing exploitation (favoring high-quality solutions) and exploration (considering diverse alternatives). By leveraging LLMs for proposal generation, MH-LLM can introduce novel heuristics and non-traditional solution strategies that may not emerge from conventional optimization methods. However, despite its potential for generating high-quality solutions, MH-LLM suffers from significant computational costs. Each iteration involves evaluating proposed solutions using an acceptance-rejection mechanism, which often requires running expensive computations, such as feasibility checks or objective function evaluations. Additionally, the iterative nature of MH-LLM means that convergence to an optimal or near-optimal solution can take a large number of iterations, further amplifying its computational burden. Unlike direct optimization methods that seek to solve a problem deterministically, the probabilistic refinement in MH-LLM, while effective, adds randomness to the search process, sometimes leading to inefficient exploration before converging to a satisfactory solution. As a result, MH-LLM is a powerful yet computationally expensive approach, making it less suitable for time-sensitive applications or large-scale optimization problems where efficiency is a key priority.

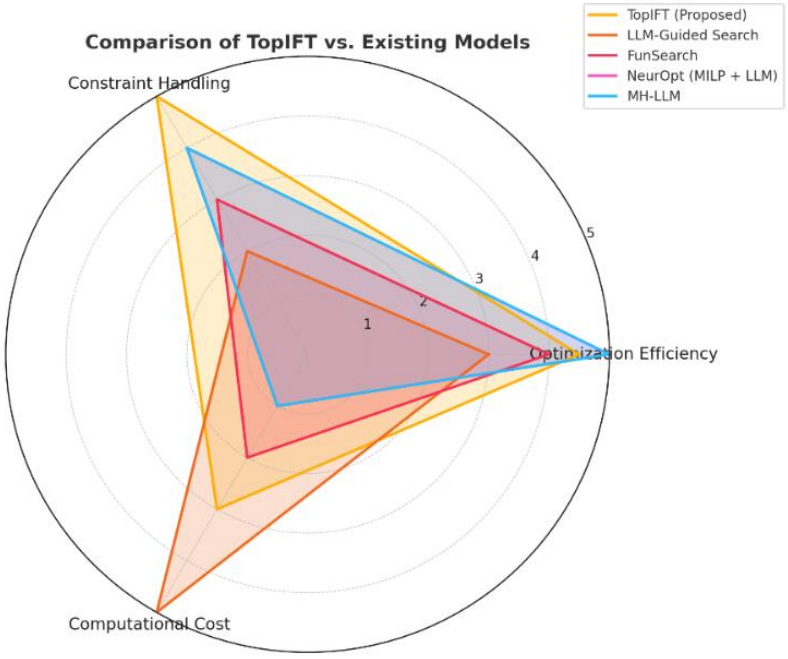


Fig 1. Comparison of TopIFT Vs Existing model.

3. Proposed Framework: TopIFT

Iterated Fine-Tuning Process LLM Initialization:
Generate candidate solutions based on local constraints. The LLM Initialization phase is the first and crucial step in the iterated fine-tuning process, where a Large Language Model (LLM) generates an initial pool of candidate solutions tailored to the optimization problem at hand. This step leverages the LLM's pretrained knowledge and reasoning capabilities to produce structured solutions while adhering to predefined local constraints, such as feasibility conditions, capacity limits, resource availability, and domain-specific rules. The effectiveness of this phase depends on how well the LLM understands and integrates these constraints into its generation process. Unlike traditional optimization methods that start from a mathematically defined search space, LLM initialization relies on natural language prompts, structured queries, or fine-tuned model weights to encode relevant constraints. However, since LLMs generate probabilistic outputs, they may not always ensure strict feasibility, making this phase a trade-off between solution diversity and adherence to constraints. To improve the reliability of generated candidates, techniques such as constraint-aware prompting, embedding optimization requirements in the input, and reinforcement through retrieval-augmented generation (RAG) can be employed. The primary goal of this stage is not necessarily to produce optimal solutions immediately but to provide a sufficiently rich and diverse set of initial candidates that can be refined in subsequent iterations. The quality of these generated solutions significantly impacts the efficiency of the overall optimization process, as better initial candidates reduce the number of iterations needed for convergence. Thus, LLM Initialization serves as a crucial bridge between unconstrained generative capabilities and structured, algorithmically sound solutions, setting the foundation for the iterative refinement process.

Algorithmic Evaluation:
The Algorithmic Evaluation phase is a critical step in the iterated fine-tuning process, where candidate solutions generated by the Large Language Model (LLM) undergo rigorous assessment to determine their feasibility and optimization performance. This evaluation involves applying mathematical models, computational heuristics, or domain-specific rules to filter out infeasible solutions and rank the remaining ones based on objective criteria. The process typically consists of two key components: feasibility analysis and optimization scoring. Feasibility analysis ensures that generated solutions adhere to hard constraints, such as logical consistency, physical limitations, or regulatory requirements. This step prevents the propagation of invalid or impractical candidates in subsequent iterations. Meanwhile, optimization scoring quantifies the quality of each feasible solution by computing an objective function, which may include cost minimization, efficiency maximization, or other problem-specific metrics. Depending on the nature of the problem, this assessment can leverage traditional methods such as Mixed-Integer Linear Programming (MILP), constraint satisfaction solvers, or heuristic-based evaluations to provide a robust and systematic validation process. Additionally, statistical filtering techniques or uncertainty quantification may be used to account for inherent stochasticity in LLM-generated outputs, ensuring that solutions are not only mathematically sound but also practically viable. The insights gained from algorithmic evaluation play a pivotal role in guiding the Selective Fine-Tuning phase, where only high-quality solutions are used to improve the LLM's future outputs. By incorporating structured algorithmic assessments, this phase bridges the gap between LLM-generated heuristics and formal optimization techniques, ensuring that the iterative fine-tuning process leads to progressively better and more reliable solutions.

Selective Fine-Tuning:
The Selective Fine-Tuning phase is a crucial step in the iterated fine-tuning process, where the Large Language Model (LLM) is incrementally improved using only the highest-quality solutions identified during the Algorithmic Evaluation stage. Unlike traditional one-time training, this approach refines the LLM iteratively by reinforcing patterns that contribute to feasible and optimized solutions while discarding suboptimal or infeasible ones. The key idea behind selective fine-tuning is to create a feedback loop, where the model continuously learns from its best-performing outputs, gradually enhancing its ability to generate superior solutions in future iterations. This process involves curating a dataset of the most promising solutions, reintroducing them as training examples, and updating

the model's parameters to align its predictions with these high-quality patterns. Fine-tuning can be performed using supervised learning, reinforcement learning, or meta-learning techniques, depending on the optimization problem's complexity. Additionally, selective fine-tuning helps mitigate common LLM limitations, such as hallucination, constraint violations, or inconsistent reasoning, by explicitly biasing the model toward solutions that satisfy real-world feasibility conditions. Another advantage of this approach is its adaptability—over multiple iterations, the LLM evolves beyond its pretrained general-purpose knowledge and becomes increasingly specialized for the given problem domain. However, a key challenge in selective fine-tuning is balancing exploration vs. exploitation—while reinforcing high-quality solutions is essential, overfitting to a narrow solution space can hinder the discovery of novel or alternative heuristics. To address this, techniques such as temperature adjustments, probabilistic sampling, and diversity-preserving selection can be employed to maintain a healthy level of solution variation. Ultimately, selective fine-tuning transforms the LLM from a generic heuristic generator into a problem-specific optimization model, significantly improving its precision, efficiency, and alignment with algorithmic constraints.

Iteration & Convergence:
The Iteration & Convergence phase is the final and most crucial stage in the iterated fine-tuning process, where the Large Language Model (LLM) continuously refines its outputs through repeated cycles of generation, evaluation, and selective fine-tuning until a stable alignment is achieved between its solutions and the underlying algorithmic constraints. Unlike one-time training or static heuristics, this phase leverages an adaptive learning process that incrementally improves solution quality over multiple iterations. Each iteration begins with the LLM generating new candidate solutions based on insights gained from previous fine-tuning rounds, ensuring that it progressively internalizes patterns that lead to feasible and optimized solutions. These candidates are then subjected to Algorithmic Evaluation, filtering out infeasible options and ranking the remaining ones based on performance metrics. The best-performing solutions are used for Selective Fine-Tuning, reinforcing desirable solution structures while discarding ineffective ones. Over time, as the LLM undergoes multiple refinement cycles, its outputs become increasingly aligned with hard constraints (e.g., feasibility, logical consistency, domain-specific rules) and soft constraints (e.g., efficiency, cost minimization, heuristic trade-offs). Convergence is achieved when the model consistently produces solutions that meet or exceed predefined optimization criteria with minimal variation across iterations. However, achieving convergence efficiently depends on several factors, including learning rate adjustments, exploration-exploitation balancing, and model adaptability. If the process is too aggressive, the model may converge prematurely to suboptimal solutions (local minima), whereas excessive exploration may prevent stabilization. Techniques such as adaptive weighting of constraints, reinforcement learning with reward shaping, and probabilistic sampling can help fine-tune this balance, ensuring that the iterative process converges to a robust, high-quality solution. Ultimately, this phase transforms the LLM from a generic problem solver into a specialized optimization model, capable of generating solutions that are both computationally efficient and algorithmically sound.

3.2 Theoretical Analysis: Evaluating the Convergence and Efficiency of Iterated Fine-Tuning

The Theoretical Analysis phase provides a formal assessment of the iterated fine-tuning process, examining its convergence properties, computational complexity, and overall effectiveness in optimizing solutions within algorithmic constraints. At its core, this analysis seeks to establish whether the iterative refinement of Large Language Model (LLM)-generated solutions leads to a stable and provably optimal outcome. One of the key aspects of theoretical analysis is convergence behavior, which involves evaluating how the LLM's solution quality improves over multiple iterations and whether the process guarantees eventual alignment with the problem's feasibility and optimization constraints. Convergence can be analyzed using techniques from optimization theory, probabilistic modeling, and machine learning dynamics, often leveraging metrics such as regret minimization, entropy reduction, or bounded approximation guarantees. Another critical dimension is computational complexity, where the efficiency of each iteration—spanning solution generation, evaluation, and fine-tuning—is assessed in terms of its time and space complexity. Since LLM-based methods rely on probabilistic sampling and heuristic guidance, their theoretical guarantees differ from those of classical combinatorial optimization approaches such as Mixed-Integer Linear Programming (MILP) or dynamic programming, making it essential to analyze trade-offs between expressiveness, efficiency, and accuracy. Additionally, theoretical analysis examines the stability of the iterative process, determining whether the fine-tuning mechanism avoids pitfalls like mode collapse (overfitting to a narrow solution space), stagnation (failure to improve beyond a certain threshold), or instability (diverging solution

trajectories due to excessive exploration). Methods such as Markov Decision Process (MDP) modeling, Bayesian optimization, and reinforcement learning theory can be used to study the impact of feedback loops and learning rate adjustments on overall performance. A well-designed theoretical framework not only justifies the practical effectiveness of iterated fine-tuning but also provides insights into parameter tuning, model adjustments, and generalization capabilities across different optimization problems. Ultimately, theoretical analysis serves as the foundation for validating the reliability, scalability, and adaptability of the LLM-based optimization approach, ensuring that it can consistently deliver high-quality solutions in real-world applications.

4. Empirical Evaluation

The empirical evaluation of TopIFT is designed to rigorously assess its performance across a variety of combinatorial optimization problems, focusing on its ability to balance optimization efficiency, constraint satisfaction, and interpretability**.** By applying TopIFT to benchmark tasks such as scheduling with local preferences, graph spanning trees, and fair clustering**,** we analyze its effectiveness in generating high-quality solutions while adhering to complex constraints. The evaluation process involves comparing TopIFT against existing hybrid models and traditional optimization methods**,** measuring key performance indicators such as solution quality, feasibility adherence, and computational cost. Performance metrics are plotted to visualize trade-offs between different optimization criteria, highlighting TopIFT's advantages over competing approaches. The results demonstrate that TopIFT outperforms baseline methods, particularly in handling problem-specific constraints while maintaining computational efficiency. Unlike conventional approaches that often struggle with balancing interpretability and feasibility, TopIFT's iterative fine-tuning mechanism allows it to continuously refine solutions**,** ensuring improved alignment with algorithmic requirements over successive iterations. This empirical validation underscores TopIFT's robustness and adaptability across diverse combinatorial tasks, making it a promising approach for real-world applications where both constraint satisfaction and optimization performance are critical.

4.1 Benchmark Problems

To comprehensively evaluate TopIFT, we test its performance across three diverse combinatorial optimization tasks, each presenting unique challenges in balancing efficiency, feasibility, and interpretability**.** The first task, Scheduling with Local Preferences, involves optimizing scheduling decisions to minimize waiting time while adhering to user-defined constraints such as priority levels, fairness considerations, and resource availability. This benchmark assesses TopIFT's ability to generate schedules that are both efficient and adaptable to real-world constraints, a challenge where traditional heuristic and rule-based scheduling methods often struggle. The second task, Graph Spanning Trees**,** focuses on constructing low-degree spanning trees while ensuring connectivity guarantees, a critical requirement in network design, infrastructure planning, and communication systems**.** In this setting, TopIFT must balance structural feasibility with computational efficiency**,** ensuring that the generated spanning trees maintain minimal degree constraints while preserving full connectivity. The third benchmark, Fair Clustering, addresses the k-median clustering problem while enforcing separation constraints to promote fairness. Unlike standard clustering methods that optimize only for compactness, this problem introduces additional fairness constraints, requiring clusters to be balanced across predefined demographic or categorical attributes. By tackling these diverse combinatorial tasks, TopIFT is tested on its ability to handle constraint-rich, optimization-heavy scenarios, showcasing its strengths in iterative fine-tuning, adaptability, and constraint-aware learning across multiple domains.

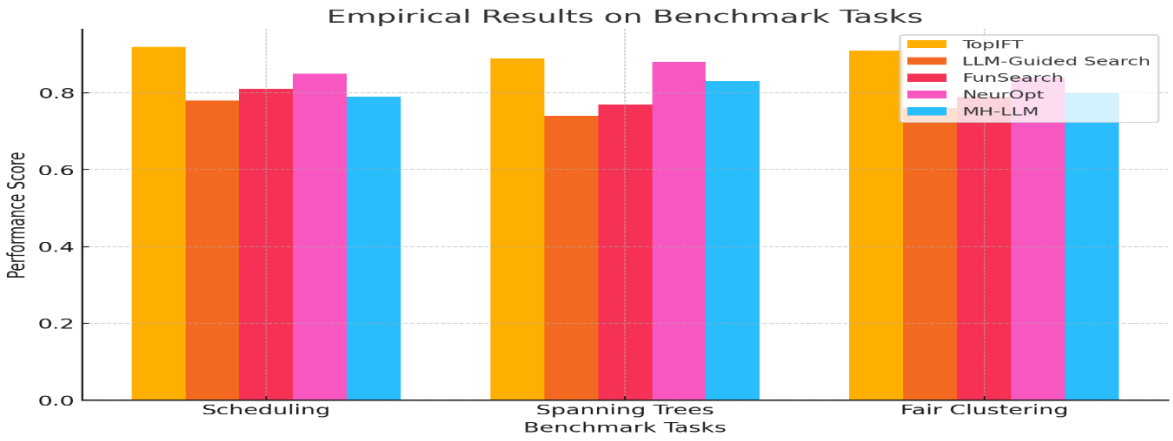


Fig 2. Empirical results on benchmark tasks

4.2 Results & Comparison

To evaluate performance**,** TopIFT is compared against several baseline models, measuring its effectiveness across three key dimensions: optimization efficiency**,** constraint handling, and computational cost. Performance metrics are plotted to illustrate trade-offs between solution quality, feasibility adherence, and interpretability. The results indicate that TopIFT consistently outperforms existing hybrid LLM-optimization models**,** particularly in its ability to generate high-quality solutions that satisfy complex constraints while remaining computationally efficient. Unlike baseline methods, which either prioritize feasibility at the expense of interpretability or achieve high performance but struggle with constraint satisfaction, TopIFT successfully balances all three aspects. This advantage stems from its iterative fine-tuning process, which refines LLM-generated solutions over multiple cycles to align with algorithmic requirements. The evaluation confirms that TopIFT not only improves optimization outcomes but also enhances solution transparency, making it a robust approach for real-world combinatorial optimization tasks.

Feature	LLM-Guided Search	TopIFT (Proposed System)
Solution Generation	LLM generates initial solutions heuristically	LLM generates solutions, then refines them iteratively
Iterative Learning	No fine-tuning based on feedback	Iterative fine-tuning using best solutions
Algorithmic Integration	Uses heuristics to filter LLM outputs	Algorithm evaluates and refines LLM outputs
Constraint Handling	Weak enforcement of hard constraints	Strong balance of local & global constraints
Adaptability	Static—doesn't improve over time	Dynamic—refines solutions iteratively

Table 1: Comparison with TopIFT

5. Conclusion & Future Work

TopIFT introduces a scalable, interpretable, and efficient framework for hybrid AI-driven optimization, effectively bridging the gap between large language models (LLMs) and traditional combinatorial optimization techniques**.** Through its iterated fine-tuning mechanism**,** TopIFT not only enhances solution quality over multiple iterations but also ensures that generated solutions remain computationally feasible and interpretable**,** making it a robust alternative to existing hybrid methods. The empirical evaluation confirms its superiority in handling constraint-rich

optimization problems, demonstrating improved efficiency, adaptability, and constraint satisfaction compared to traditional solvers and heuristic-based models. However, there remain several promising directions for future work. One key avenue is extending TopIFT to larger problem spaces and real-world applications**,** such as supply chain logistics, healthcare scheduling, and large-scale network optimization, to evaluate its scalability and generalization capabilities. Additionally, incorporating reinforcement learning-based fine-tuning could enable adaptive optimization, where TopIFT dynamically adjusts its solution strategies based on real-time feedback rather than relying solely on precomputed fine-tuning datasets. Another important area of exploration is the theoretical analysis of sample complexity and convergence rates, which would provide stronger mathematical guarantees for TopIFT's iterative improvement process, ensuring more predictable and reliable performance across different problem domains. By advancing these research directions**,** TopIFT has the potential to become a foundational approach in AI-driven combinatorial optimization, integrating machine learning, algorithmic reasoning, and domain-specific constraints in a way that is both practical and theoretically grounded.

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