OPT-Engine: Benchmarking the Limits of LLMs in Optimization Modeling via Complexity Scaling

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Outline

Limitations: The "Static" Benchmark Gap

- **Small-Scale & Static:** Existing benchmarks (e.g., IndustryOR) are often restricted to textbook-size instances with fixed parameters(problem size <20) [2].
- **Evaluation Blind Spot:** Cannot distinguish between failures in *mathematical formulation* vs. *numerical execution*.
- **Data Contamination:** Static problems are likely present in LLM pre-training sets, leading to "memorized" rather than "reasoned" solutions.

Dataset	**Number After Correction**	**Affiliation**	problem size
NL4OPT	245	NeurIPS 2022 Competition	5-10
MAMO_EasyLP	642	CUHK-SZ	5-15
MAMO_ComplexLP	203	CUHK-SZ	5-15
IndustryOR	100	Cardinal Operations	5-20
OptMATH	166	PKH	5-20
Optibench	605	HKUST & Huawei	5-20

The Need

A benchmark that moves beyond "fixed snapshots" to **controllable complexity scaling**.

Research Directions: PTR vs. SIR

Research bifurcation in how LLMs approach optimization:

Pure-Text Reasoning (PTR)

Paradigm: End-to-end deduction [8, 4]

- **Mechanism:** Chain-of-Thought (CoT) text derivation [7].
- **Strength:** Mimics human intuition; no external tools needed.
- **Weakness:** Vulnerable to calculation errors.

Solver-Integrated Reasoning (SIR)

Paradigm: Formulation + Execution

- **Mechanism:** NL $\rightarrow$ Code (Pyomo/Gurobi) $\rightarrow$ Solver.
- **Strength:** Global Constraint modeling guarantees + numerical precision.
- **Weakness:** Requires strict syntax modeling.

The Hybrid Frontier: **CompPTR**

Augmenting text reasoning with **computational code tools** (e.g., calculators) to bridge the gap without full solver integration.

The Paradox: Superhuman Math vs. Brittle Optimization

- **The Phenomenon:** SOTA LLMs achieve $> 95\%$ on MATH500 [1], yet their performance **drops sharply** on optimization tasks of comparable difficulty [5].
- **Why the Gap?** Optimization modeling is a **subset** of mathematical reasoning — but with two critical differences:
  - Requires **numerical precision** across multiple interdependent variables
  - Demands **global constraint satisfaction**, not just a local or approximate answer.

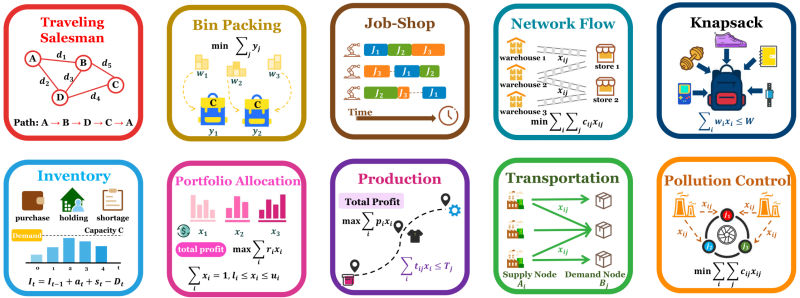
Research Question:

Why does a persistent performance gap exist between LLMs' deductive reasoning capabilities (for math) and their capacity for robust optimization modeling?

Our Proposal: The OPT-Engine Framework

OPT-Engine: An extensible framework with quantifiable and controllable complexity.

- Covers 10 canonical OR problems (from LP to MILP).
- Dynamically scales structural parameters (Constraints, Variables).



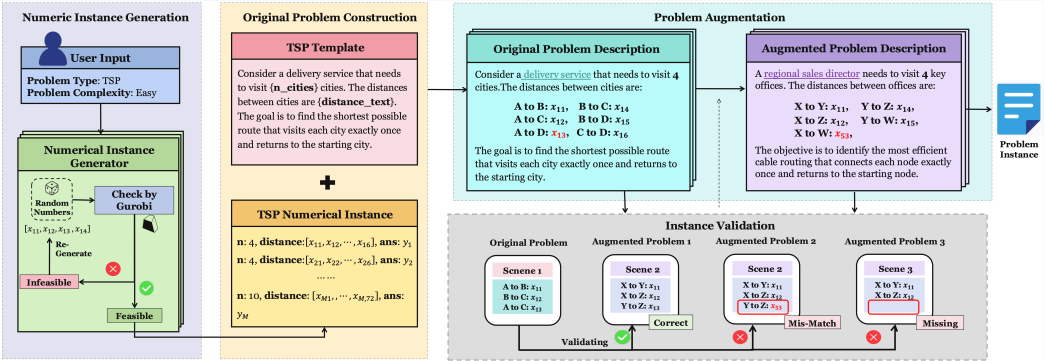
Key Research Questions

Three Pivotal Questions Addressed by OPT-Engine:

1. **Scalability:** While the current SOTA adopts Solver-Integrated Reasoning (SIR), can Pure-Text Reasoning (PTR) via classical Chain-of-Thought efficiently tackle optimization tasks as complexity scales?
2. **Tool Utility:** Can integrating external computational tools mitigate PTR's arithmetic weaknesses and achieve performance comparable to SIR?
3. **Bottleneck Identification:** What is the critical bottleneck limiting the efficacy of the current SOTA SIR approach throughout its generation process?
   - **Linguistic Ambiguity & Complexity:** Investigating whether performance degradation stems from the model's inability to parse nuanced natural language descriptions into precise mathematical variables.
   - **Objective Function Perturbations:** Assessing the model's sensitivity to changes in the objective goal.
   - **Scaling via Constraint Augmentation:** Stress-testing the "reasoning load" by incrementally increasing the number and type of constraints

OPT-Engine: Pipeline Workflow

1. **Numeric instance generation**: $G : \mathcal{D} \times \Theta \to \mathcal{I}$, with solver-based ground truth.
2. **Canonical problem construction**: $M : \mathcal{I} \times \mathcal{T} \to \mathcal{S}_C$.
3. **Problem augmentation**: $R : \mathcal{S}_C \times \mathcal{L} \to \mathcal{S}_R$ (LLM rephrasing).
4. **Instance validation**: LLM-as-judge + rule-based verifier ensures consistency.



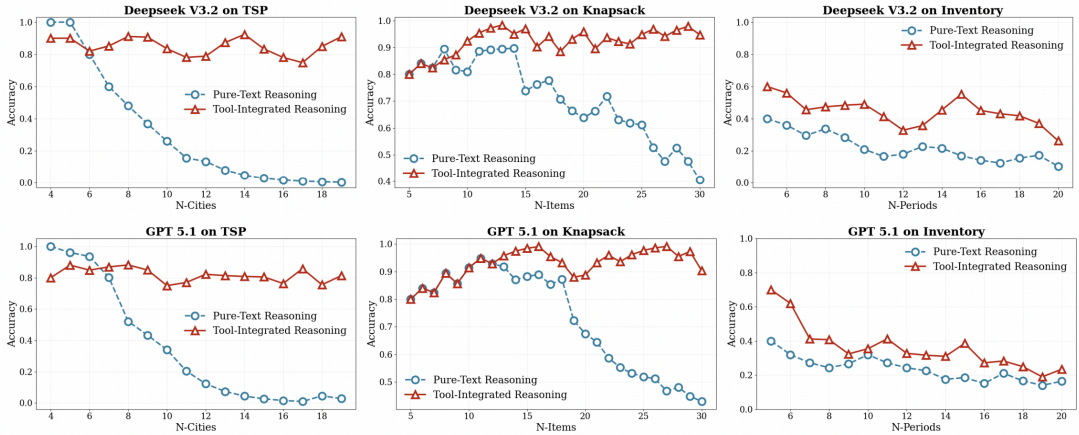
Experimental Setup & Bottleneck Analysis

- **Models:** DeepSeek-V3.2, GPT-5.1, Qwen3-4B-Instruct, Qwen3-4B-RL.
- **Accuracy Criterion:** Relative error $< 10^{-3}$. For each problem class and complexity level, we generate ten distinct instances. A solution $\hat{y}_i^{(p)}$ is correct if:

$$\frac{|\hat{y}_i^{(p)} - y_i^*|}{|y_i^*| + 10^{-6}} < 10^{-3}.$$

  We report avg@10 (mean success rate over the ten instances) as the standard accuracy measure.
- **Optimization task reasoning approaches:**
  - **SIR:** Gurobi execution (100s time limit).
  - **PTR:** Pure Chain-of-Thought, no tools.
  - **CompPTR:** PTR augmented with Python (numpy, itertools) but **no external solvers**.
- **Bottleneck Identification – What limits current SOTA SIR?**
  1. **Linguistic ambiguity & complexity:** base on base problem template generate problem with different PPL perperxity.
  2. **Objective function perturbations:** do both linear and nolinear pertuabation when generate new questions.
  3.
  4. **Constraint augmentation:** incrementally increase the number and type of constraints

SIR vs PTR: Frontier Models



- **SIR (red)**: accuracy remains high or degrades only slightly as problem scale increases.
- **PTR (blue)**: severe performance ceiling – accuracy collapses as as problem scale increases..

SIR vs PTR: Qwen3-4B Series

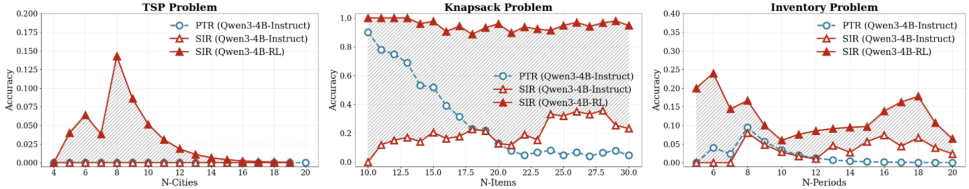


Figure 4. **Performance scaling of PTR (blue) vs. SIR (red) on the Qwen3-4B series**. The panel displays results from Qwen3-4B-RL, indicating RLVR training significantly enhances SIR mode accuracy.

Baseline Performance

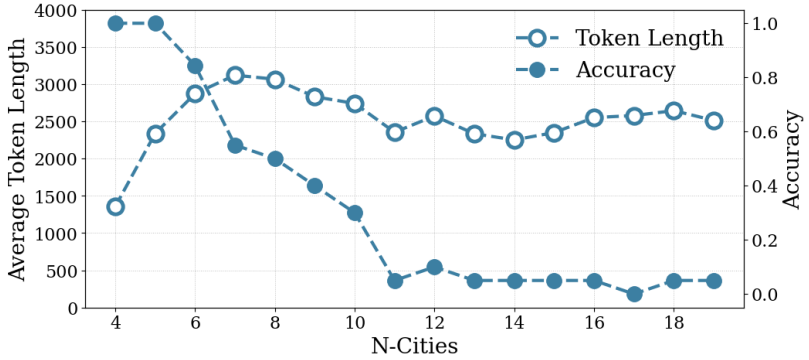
- **PTR vs. SIR:** At low complexity, **PTR** initially leads due to the Instruct model's limited code generation capacity.
- **Execution Ceiling:** Pure text reasoning acts as a temporary fallback for weaker coding models.

Impact of RLVR Fine-tuning

- **Scaling Shift:** Post-RLVR, **SIR** consistently surpasses PTR across all complexity levels.
- **Diagnostic:** RLVR significantly elevates code execution success rates, transforming SIR from a bottleneck into a strength.

Case Study: PTR Behavior on the TSP Problem

- **Small problem sizes:** Explicit enumeration of Hamiltonian cycles → high accuracy, token usage grows with complexity.
- **Beyond a critical threshold:** Lightweight heuristics (nearest neighbor, cheapest insertion) → token usage plateaus, solution quality drops.
- the model dynamically shifts to near-optimal, practical heuristics when exact solutions become intractable.



Implication: This adaptive strategy explains the efficacy of PTR in prior work [4, 6].

Constraint Infeasibility vs. Computational Inaccuracy

Hypothesis: PTR functions as a *stochastic approximation* — directionally accurate but numerically imprecise.

- **Feasibility:** Measures violations of hard logical or physical constraints.
- **Accuracy:** Measures numerical precision and residual computational errors.

Problem	Approaches	Easy		Medium		Hard	
		Feas/Acc	OptGap	Feas/Acc	OptGap	Feas/Acc	OptGap
TSP	PTR	73.3% / 58.3%	1.07%	70.0% / 10.0%	10.14%	64.0% / 2.0%	11.72%
	SIR	98.3% / 91.7%	0.01%	96.0% / 86.0%	0.25%	88.0% / 80.0%	0.24%
Knapsack	PTR	93.9% / 89.2%	5.62%	93.2% / 78.0%	0.29%	61.8% / 45.6%	0.42%
	SIR	100.0% / 92.3%	0.00%	100.0% / 91.7%	0.00%	100.0% / 95.7%	0.00%
Netflow	PTR	40.0% / 10.0%	3.57%	15.0% / 0.0%	2.64%	0.0% / 0.0%	0.00%
	SIR	100.0% / 100.0%	0.00%	100.0% / 100.0%	0.00%	100.0% / 100.0%	0.00%

Divergent Failure Signatures:

1. **SIR (Structural Logic):** Success is strictly contingent on **feasibility**. The solver guarantees optimality provided the logical grounding (constraints + objectives) is well-defined.
2. **PTR (Probabilistic Inference):** Exhibits a **dual-failure trajectory**:
   - **Reasoning Collapse:** Loss of global constraint consistency (feasibility) as task complexity scales.
   - **Precision Deficit:** Inherent lack of deterministic **accuracy**, even when operating on a correct logical manifold.

Can Computational Tools Rescue PTR?

Mechanism: CompPTR augments PTR with a Python interpreter for local arithmetic and deterministic sub-tasks (excluding solver calls).

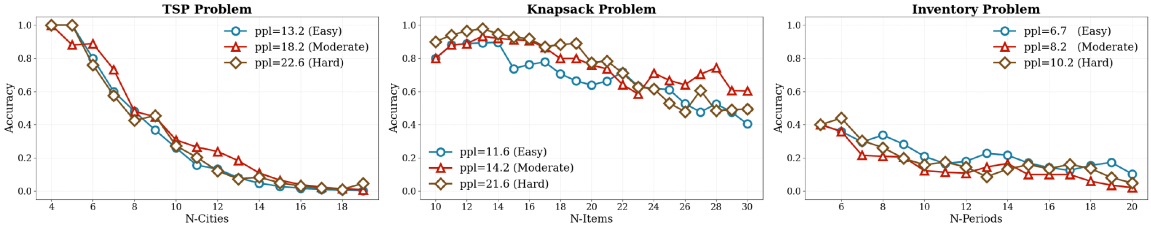
Problem	Approaches	Easy		Medium		Hard	
		Feas/Acc	OptGap	Feas/Acc	OptGap	Feas/Acc	OptGap
TSP	PTR	73.3% / 58.3%	1.07%	70.0% / 10.0%	10.14%	64.0% / 2.0%	11.72%
	CompPTR	86.7% / 85.0%	0.15%	72.0% / 70.0%	0.05%	52.0% / 44.0%	0.43%
Knapsack	PTR	93.9% / 89.2%	5.62%	93.2% / 78.0%	0.29%	61.8% / 45.6%	0.42%
	CompPTR	98.5% / 87.7%	0.00%	98.3% / 83.3%	0.01%	87.1% / 78.6%	0.00%
Netflow	PTR	40.0% / 10.0%	3.57%	15.0% / 0.0%	2.64%	0.0% / 0.0%	0.00%
	CompPTR	90.0% / 90.0%	0.00%	85.0% / 85.0%	0.00%	75.0% / 75.0%	0.00%

Conclusion: The "Global" Ceiling

External tools mitigate **local execution errors** but fail to enforce the **global optimization strategy** required for combinatorial consistency.

Bottleneck Analysis:Linguistic Complexity

- Start from a canonical problem template.
- Create two derivative versions with progressive syntactic and lexical complexity.
- All three templates share the **same numeric instance and constraint set** $\rightarrow$ linguistic variation is the sole independent factor.



When the underlying mathematical structure is held fixed, solution accuracy remains stable as Perplexity (PPL) [3] increases.

Bottleneck Analysis: Objective Perturbations

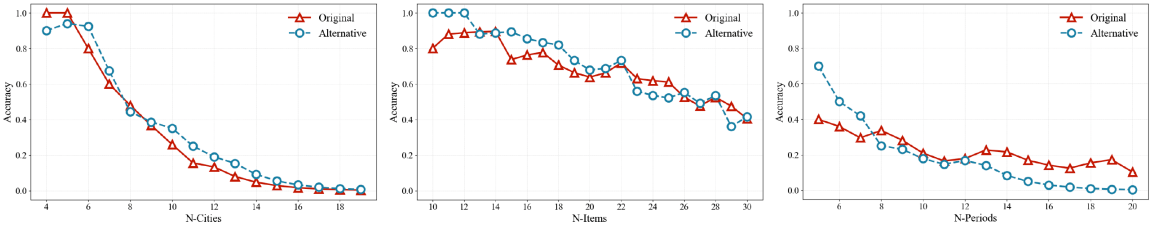
Intuition: Models might rely on "memorized signatures", a shift in the objective could potentially break heuristic-based reasoning.

Formal Perturbation Model

For an original objective $f(x)$, we apply a linear shift using a randomly sampled constant K (independent of decision variables):

$$\min_x f(x) \quad \Longrightarrow \quad \min_x f(x) + K$$

Property: The optimal solution x^* remains **invariant** under this shift.



- **Key Finding:** Empirical results show a **negligible impact** on accuracy across all problem classes.

Bottleneck Analysis: Constraint Augmentation

- **Setup:** For each problem class, we add mathematically straightforward constraints:
  - No new variables, only $\mathcal{O}(1)$ constraints $\rightarrow$ intrinsic mathematical difficulty and asymptotic complexity remain unchanged.
  - The modeling burden shifts from computation to **semantics**: the model must correctly parse and integrate auxiliary conditions.

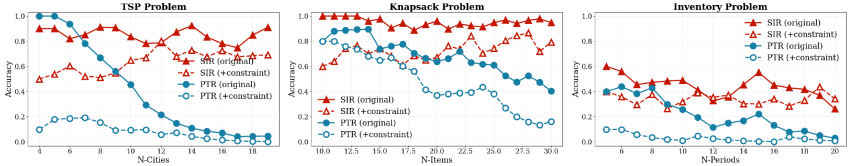


Figure 7. **Performance scaling under baseline vs. augmented constraints on the Deepseek-V3.2 Model.** PTR is shown in blue and SIR in red. Augmented constraints used in evaluation are as follows: **TSP**: Exactly one of the following two roads must be included in the tour: the road between city 1 and city 2, the road between city 2 and city 3. ($x_{01} = 0$, $x_{12} + x_{23} = 1$); **Knapsack**: Exactly one of item 1 and item 2 must be selected. If item 3 is selected, the effective backpack capacity is reduced by 2 kg. ($x_1 + x_2 = 1$, $\sum_{i=1}^{n} w_i x_i \leq C - 2x_3$); **Inventory**: On day t, the on-hand inventory must be at least $I_{\min}$ units. ($I_t \geq I_{\min}$). The introduction of augmented constraints leads to a consistent accuracy drop across problem classes.

- **Key result:** Both PTR and SIR show significant accuracy degradation compared to canonical problems.

Summary of Key Findings

1. **OPT-Engine Benchmark:** Introduced the first extensible framework capable of quantifying LLM performance across granular **complexity scaling** dimensions.
2. **The PTR Ceiling:** Pure-Text Reasoning suffers from a dual failure: **logical collapse** under high dimensionality and inherent **numerical imprecision**.
3. **CompPTR Limitations:** While tool-augmentation (Python) mitigates arithmetic errors, it remains insufficient for enforcing **global logical constraints** as problem size increases.
4. **The Formulation Bottleneck:** Structural constraint formulation is the primary barrier; even frontier models exhibit fragility when faced with incremental constraint additions.

Resource Release: Code and Data available at
`https://github.com/CardinalOperations/OPTEngine`

Conclusion and Future Directions

- **The SIR Necessity:** We establish that **Solver-Integrated Reasoning** is the essential paradigm for maintaining robustness in high-complexity industrial optimization.
- **Future Research Streams:**
  - **Advanced Metrics:** Developing tracks for reporting **optimality gaps**, computational runtime, and feasibility robustness.
  - **Heuristic Synthesis:** Evaluating LLMs' capacity to design meta-heuristics for NP-hard problems.
  - **Domain Expansion:** Extending OPT-Engine to support **nonlinear, stochastic**, and **dynamic** programming.

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