PRIME: Policy-Reinforced Iterative Multi-Agent Execution for Algorithmic Reasoning in Large Language Models

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Article

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Abstract

Large language models have demonstrated remarkable capabilities across diverse reasoning tasks, yet their performance on algorithmic reasoning remains limited. To handle this limitation, we propose PRIME (Policy-Reinforced Iterative Multi-agent Execution), a framework comprising three specialized agents, an executor for step-by-step reasoning, a verifier for constraint checking, and a coordinator for backtracking control, optimized through group relative policy optimization. For comprehensive evaluation, we introduce PRIME-Bench, the largest algorithmic reasoning benchmark to date, comprising 86 tasks across 12 categories with 51,600 instances. Tasks span sorting algorithms, graph and tree structures, automata and state machines, symbolic reasoning, and constraint-based puzzles, with execution traces reaching over one million steps. Compared to baseline approach, PRIME improves average accuracy from 26.8% to 93.8%, a 250% relative gain. The largest improvements occur on tasks requiring sustained state tracking, with Turing machine simulation improving from 9% to 92% and long division from 16% to 94%. Ablation studies identify iterative verification as the primary contributor, preventing the error propagation that causes baseline approaches to fail catastrophically. Analysis across model scales (8B–120B parameters) reveals that smaller models benefit disproportionately, achieving accuracy comparable to models 8× larger.

Keywords: algorithmic reasoning; multi-agent framework; large language models; reinforcement learning; iterative verification

1. Introduction

Large language models (LLMs) have transformed artificial intelligence, demonstrating remarkable capabilities in language understanding, code generation, and complex reasoning [1] that extend beyond simple pattern matching [2]. Recent investigations into the cognitive parallels between LLMs and human reasoning have revealed striking similarities in how these systems process structured information [3]. Yet a fundamental question remains: Can LLMs reliably execute algorithmic reasoning tasks that require precise, multi-step procedural execution under formal constraints? This question bridges the divide between neural and symbolic computation paradigms and carries significant implications for deploying AI systems in domains that demand rigorous formal reasoning.

Algorithmic reasoning presents unique challenges that distinguish it from other reasoning tasks. Unlike mathematical word problems or commonsense inference, algorithmic tasks demand exact state tracking across potentially thousands of steps, where a single error can invalidate the entire execution. Consider sorting an array of 100 elements: the model must correctly execute hundreds of comparisons and swaps while maintaining precise array state throughout. Similarly, simulating

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a Turing machine requires tracking tape contents, head position, and machine state across extended execution sequences. These tasks admit no partial credit—the final answer is either correct or wrong, and errors compound catastrophically rather than averaging out. The computational complexity of such tasks is well-established, with many algorithmic problems exhibiting combinatorial explosion as solution spaces grow exponentially in problem size [4]. This combinatorial structure poses fundamental challenges for any reasoning systems.

Recent advances in prompt engineering have demonstrated that the manner in which queries are presented to LLMs significantly influences their reasoning performance [5]. Chain-of-thought prompting showed that adding intermediate reasoning steps can dramatically improve performance on both mathematical and logical tasks [6]. Building on this observation, researchers have proposed more advanced strategies including zero-shot reasoning elicitation [7], self-consistency decoding through multiple reasoning paths [8], and tree-of-thoughts prompting for exploring branching trajectories [9]. However, these approaches rely on single-pass generation without external verification, where errors can propagate through subsequent steps, corrupting the entire chain. Recent work has shown that LLM reasoning inevitably becomes derailed after a few hundred steps [10], with performance degrading catastrophically on tasks requiring multi-round execution. Furthermore, prompt engineering requires manual effort for each task type and does not generalize automatically across domains. These limitations motivate a critical question: Can we design a more systematic approach that combines structured execution with explicit verification and error recovery?

Rigorous evaluation of algorithmic reasoning requires benchmarks that span diverse task types with sufficient scale and complexity. However, existing benchmarks are limited in scope. GSM8K [11] focuses on grade-school arithmetic with approximately ten reasoning steps; MATH [12] addresses competition problems but does not require execution trace verification; BIG-Bench [13] includes diverse tasks but lacks systematic coverage of algorithmic domains. Critically, none of these benchmarks evaluate sustained multi-step execution at the scale required for true algorithmic reasoning, nor do they require complete execution trace verification. This gap raises another important question: What benchmark can comprehensively evaluate LLM performance across the full spectrum of algorithmic reasoning tasks?

The relationship between model scale and task performance has been extensively studied through neural scaling laws [14], which establish power-law relationships between model parameters, dataset size, compute budget, and test loss [15]. While larger models generally exhibit superior capabilities, the marginal utility of additional parameters varies considerably across task types. This observation raises a practical question with significant deployment implications: How does model scale interact with prompt optimization for algorithmic reasoning tasks? If smaller models can achieve comparable performance to larger ones through better prompting, this would enable more resource-efficient deployment. Conversely, if certain tasks require scale regardless of prompt quality, this informs decisions about minimum model requirements. Understanding these dynamics is essential for practitioners who must balance computational constraints against reasoning quality.

This paper presents a comprehensive empirical investigation addressing these interconnected questions. We evaluate seven open-source language models spanning a 15× range in parameter count on the N-Queens problem, systematically comparing baseline prompting against an optimized structured prompt designed to elicit constraint-aware reasoning. Our experimental framework encompasses 2,800 trials across board sizes ranging from 4×4 to 12×12, enabling fine-grained analysis of performance scaling with respect to both model capacity and problem complexity.

This work makes dual contributions that advance the state of the art in LLM algorithmic reasoning: we introduce both a novel methodology (PRIME) and a comprehensive evaluation framework (PRIME-Bench). While the main text presents the N-Queens problem as a representative case study to illustrate key principles, the complete evaluation spanning all 86 tasks with formal specifications, execution traces, and detailed results is provided in the Appendices.

The contributions of this work are fourfold:

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1. **PRIME-Bench: The Most Comprehensive Algorithmic Reasoning Benchmark.** We introduce PRIME-Bench, comprising **86 tasks** across **12 categories** with **51,600 total instances**—the largest and most comprehensive benchmark for evaluating LLM algorithmic reasoning to date. PRIME-Bench spans 28 sorting algorithms, 8 automata types (including Turing machines and PDAs), 6 theorem proving tasks, and 8 real-world system simulations, providing unprecedented coverage of computational complexity from $\mathcal{O}(n)$ to $\mathcal{O}(n^{2.7})$ with step counts ranging from 500 to over 1,000,000. This benchmark is **5–10× larger** than existing algorithmic reasoning benchmarks such as BIG-Bench, GSM8K, and MATH, and uniquely includes execution trace verification requiring sustained state tracking over extended sequences.
2. **Structured Prompting Analysis.** Through systematic evaluation on the N-Queens problem domain, we demonstrate that structured prompt engineering can yield transformative improvements, with accuracy increasing from 37.4% to 90.0% (a relative gain of 140.6%) while maintaining acceptable latency overhead of 1.56×. These insights inform the design of our PRIME framework, which achieves even larger gains (26.8% to 93.8%) across the full PRIME-Bench benchmark.
3. **Scale-Sensitivity Characterization.** We characterize the nuanced relationship between model scale and prompt sensitivity, revealing that smaller models exhibit substantially larger relative gains from prompt optimization (244.9% for 8B vs. 66.8% for 120B), with important implications for resource-efficient deployment.
4. **PRIME Framework: A Novel Multi-Agent Reasoning Architecture.** We introduce PRIME (Policy-Reinforced Iterative Multi-agent Execution), the first framework to unify multi-agent decomposition, reinforcement learning-based policy optimization via Group Relative Policy Optimization (GRPO), and iterative constraint verification within a single coherent architecture. Unlike prior approaches that address individual components in isolation, PRIME's synergistic integration enables breakthrough performance: 93.8% average accuracy across 86 diverse algorithmic tasks, representing a **250.0% improvement** over baseline approaches. PRIME achieves near-perfect performance (>95%) on 11 of 12 task categories, including tasks where vanilla LLMs fail catastrophically (Turing machine simulation: 8.9% → 92.4%).

Our results contribute to the growing body of knowledge on prompt-performance dynamics and offer practical guidance for practitioners seeking to leverage LLMs for combinatorial reasoning applications. The extended evaluation across ten algorithmic tasks—including Tower of Hanoi, Bubble Sort simulation, Turing machine execution, and extended Zebra puzzles—demonstrates that the principles underlying structured prompting generalize beyond the N-Queens domain to a broad class of algorithmic reasoning challenges.

2. Related Work

The intersection of large language models and structured reasoning has attracted considerable research attention, spanning theoretical investigations of emergent capabilities, empirical evaluations across diverse benchmarks, and methodological innovations in prompt engineering. This section situates our work within this broader context, highlighting the gaps our study addresses.

2.1. Transformer Architecture and Language Modeling

The transformer architecture, introduced by Vaswani et al., revolutionized sequence modeling by replacing recurrent connections with self-attention mechanisms [16]. The core operation computes attention weights through scaled dot-product attention:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V \tag{1}$$

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where Q, K, V represent query, key, and value matrices, and d_k is the key dimension. This formulation enables parallel computation across sequence positions while capturing long-range dependencies. Multi-head attention extends this by projecting inputs into multiple subspaces:

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W^O \tag{2}$$

where each $\text{head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$ operates on a projected subspace. Modern language models stack these attention layers with feed-forward networks and layer normalization, achieving remarkable generalization across diverse tasks [1].

The GPT family established autoregressive language modeling as a dominant paradigm [17]. These models maximize the likelihood $P(x) = \prod_{t=1}^{T} P(x_t|x_{<t})$ over training corpora, learning rich representations that transfer to downstream tasks. Open-source alternatives have proliferated, including the LLaMA family [18] and its successors [19], the OPT models [20], and Mistral [21], enabling reproducible research. The Qwen series introduced architectural refinements including grouped-query attention and rotary position embeddings [22]. Gemma models incorporated multi-query attention with GeGLU activations, building on findings that gated linear units improve transformer performance [23,24]. The PaLM architecture demonstrated scaling to 540B parameters with strong reasoning capabilities [25]. Proprietary models including Claude 3 have achieved competitive performance [26]. Comprehensive evaluation frameworks assess these models systematically [27].

2.2. LLM Reasoning and Benchmarking

The reasoning capabilities of large language models have been extensively probed through standardized benchmarks, as documented in comprehensive surveys of the field [28]. The BIG-Bench project assembled over 200 tasks designed to assess model capabilities across diverse cognitive dimensions [13]. Mathematical reasoning has received particular scrutiny, with the GSM8K benchmark evaluating grade-school arithmetic [11]. The MATH dataset posed substantially harder competition-level problems, revealing fundamental limitations of scaling alone [12]. Specialized mathematical models such as Minerva demonstrated that domain-specific training yields substantial gains [29]. Code generation benchmarks, including HumanEval, demonstrated that LLMs can produce functionally correct programs [30]. Evaluation frameworks such as MT-Bench have enabled systematic comparison across model families [31].

The phenomenon of emergent abilities, wherein capabilities appear discontinuously above certain scale thresholds, has attracted significant theoretical interest [32]. Chain-of-thought reasoning exemplifies such emergence: models below approximately 100 billion parameters produce incoherent reasoning chains, while larger models exhibit qualitatively different behavior [6]. This discontinuity suggests that certain reasoning capabilities may require sufficient model capacity to manifest, though recent work has questioned whether emergence reflects genuine phase transitions or artifacts of evaluation metrics.

However, the evaluation of LLMs on classical constraint satisfaction problems remains notably sparse in the literature. While puzzle-solving tasks have appeared in various benchmarks, systematic investigations of performance scaling and prompt sensitivity on well-characterized combinatorial problems are lacking. The N-Queens problem, despite its historical significance as a benchmark for traditional constraint satisfaction solvers, has not been rigorously evaluated as an LLM reasoning task. Our work addresses this gap by establishing comprehensive baseline metrics and analyzing the factors influencing performance.

2.3. Prompt Engineering and Optimization

The discovery that prompting strategies profoundly influence LLM performance has catalyzed a substantial body of research. Chain-of-thought prompting, which encourages models to generate intermediate reasoning steps before producing final answers, emerged as a watershed development [6]. The technique can be formalized as augmenting the input x with a reasoning trace r such that the

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model generates (r, y) jointly, where r provides an interpretable path to the answer y. Subsequent work demonstrated that even simpler interventions, such as appending "Let's think step by step" to prompts, can elicit improved reasoning in zero-shot settings without any exemplars [7].

Self-consistency decoding extended these ideas by sampling K independent reasoning chains $\{(r_1, y_1), \ldots, (r_K, y_K)\}$ and selecting the most frequent conclusion through majority voting [8]:

$$\hat{y} = \arg\max_{y} \sum_{k=1}^{K} \mathbf{1}[y_k = y] \tag{3}$$

This approach exploits the observation that correct reasoning paths tend to converge, while erroneous chains scatter across multiple conclusions. Tree-of-thoughts prompting generalized the linear chain structure to branching search, enabling backtracking and lookahead [9]. Program-aided language models demonstrated that offloading computation to external interpreters improves numerical accuracy [33]. The program-of-thoughts approach explicitly separates reasoning from computation [34].

Beyond manual prompt design, researchers have explored automated approaches to prompt optimization. Zhou et al. demonstrated that LLMs can themselves generate effective prompts when provided with task descriptions and examples [35]. Evolutionary approaches, such as Promptbreeder, iteratively refine prompts through mutation and selection [36]. Recent work on cross-model chain-of-thought transfer has shown that reasoning patterns can be effectively adapted across different model architectures [37]. Comprehensive taxonomies of prompting methods have been established by survey work [38]. A foundational survey formalized the pre-train, prompt, and predict paradigm [5].

An important finding from Min et al. revealed that in-context learning does not require accurate input-output mappings in demonstrations [39]. Rather, demonstrations primarily convey the label space, input distribution, and sequence format. This suggests that prompt effectiveness derives from structural cues rather than exemplar fidelity, with implications for understanding how LLMs process contextual information.

2.4. Scaling Laws and Model Capacity

The relationship between model scale and performance has been formalized through neural scaling laws. Kaplan et al. established power-law relationships between model size, dataset size, compute budget, and test loss [14]. The cross-entropy loss L can be expressed as a function of parameters N and data D:

$$L(N, D) = \left[\left(\frac{N_c}{N} \right)^{\alpha_N / \alpha_D} + \frac{D_c}{D} \right]^{\alpha_D} \tag{4}$$

where the exponents and constants are determined empirically. The Chinchilla study refined these insights, demonstrating that many models are undertrained relative to their parameter counts [15]. The compute-optimal frontier follows $N^* \propto C^{0.5}$ and $D^* \propto C^{0.5}$, implying roughly equal allocation of compute to model size and training data.

Recent investigations have extended scaling analysis to reasoning quality, establishing efficiency frontiers that characterize trade-offs between computational resources and output quality [40]. Unified scaling laws for mixture-of-experts models have revealed distinct parameter efficiency characteristics compared to dense architectures [41]. Studies comparing mixture-of-experts with dense models across specific domains have shown that parameter efficiency varies substantially with task type [42]. The PaLM 2 technical report documented scaling properties across model variants [43]. These findings have practical implications for model selection and deployment decisions.

Less understood is how model scale interacts with prompt sensitivity. Anecdotal evidence suggests that larger models may be more robust to suboptimal prompts, while smaller models require more careful prompt engineering to achieve acceptable performance. However, this hypothesis has not been systematically tested across a controlled task. Our experimental design, which evaluates

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models spanning a 15× range in parameter count under identical prompting conditions, enables direct examination of scale-prompt interactions.

2.5. Multi-Agent LLM Systems and Reinforcement Learning

The deployment of LLMs within multi-agent frameworks represents an emerging paradigm for complex reasoning tasks. Recent surveys have documented the landscape of LLM-based multi-agent reinforcement learning, highlighting challenges in coordination and communication among agents [44]. The AGILE framework introduced novel agent architectures that combine LLM reasoning with RL-based action selection [45]. Multi-Agent Group Relative Policy Optimization (MAGRPO) extends single-agent methods to cooperative multi-agent settings, demonstrating improved collaboration on writing and coding tasks [46].

Reinforcement learning from human feedback (RLHF) has become the dominant approach for aligning LLM behavior with human preferences [47,48]. The standard pipeline involves training a reward model on preference data and optimizing the policy using Proximal Policy Optimization (PPO) [49]. Constitutional AI extends this paradigm through AI-generated feedback [50], while Direct Preference Optimization (DPO) offers an alternative that bypasses explicit reward modeling [51].

Group Relative Policy Optimization (GRPO) [52], introduced in DeepSeekMath, represents a significant advance in efficient policy optimization. By eliminating the value network and using group-based advantage estimation, GRPO reduces memory requirements while maintaining training stability. The method samples multiple responses per query and computes advantages relative to the group mean, enabling effective optimization without a separate critic model. This approach has been adopted in subsequent work on reasoning models, including DeepSeek-R1.

Process supervision has emerged as a powerful alternative to outcome-based training [53]. By providing feedback on intermediate reasoning steps rather than only final answers, process supervision enables more effective credit assignment in multi-step reasoning chains. Recent work on test-time compute scaling has demonstrated that increased inference computation can be more effective than scaling model parameters for certain reasoning tasks [54]. Our PRIME framework builds on these developments, integrating GRPO with iterative verification and multi-agent coordination.

Brain-inspired architectures have also shown promise for LLM planning tasks [55]. The Modular Agentic Planner (MAP) decomposes planning into specialized modules, achieving significant improvements on graph traversal, Tower of Hanoi, and PlanBench benchmarks. The MAKER system demonstrated that extreme task decomposition into focused micro-agents can enable reliable execution across million-step tasks [10], addressing the fundamental limitation that LLM reasoning degrades after a few hundred sequential steps.

Parameter-efficient fine-tuning methods, including LoRA [56] and QLoRA [57], have democratized model adaptation by reducing memory requirements. These techniques are particularly relevant for multi-agent systems where multiple specialized models must be maintained. Our PRIME framework leverages these methods for efficient agent specialization within the multi-agent architecture.

3. Methods

This section details the PRIME framework and the experimental protocol used to evaluate algorithmic reasoning. We first formalize our multi-agent architecture and optimization strategy, then describe the specific constraint satisfaction task (N-Queens) and prompting baselines used to diagnose latent reasoning capabilities. We present a controlled study designed to isolate the effects of prompt engineering on LLM performance across varying model scales and problem complexities.

3.1. The PRIME Framework

To address the fundamental limitation that LLM reasoning inevitably becomes derailed after a few hundred steps [10], we introduce **PRIME** (Policy-Reinforced Iterative Multi-agent Execution). Unlike standard Chain-of-Thought (CoT) prompting which relies on a single linear generation pass,

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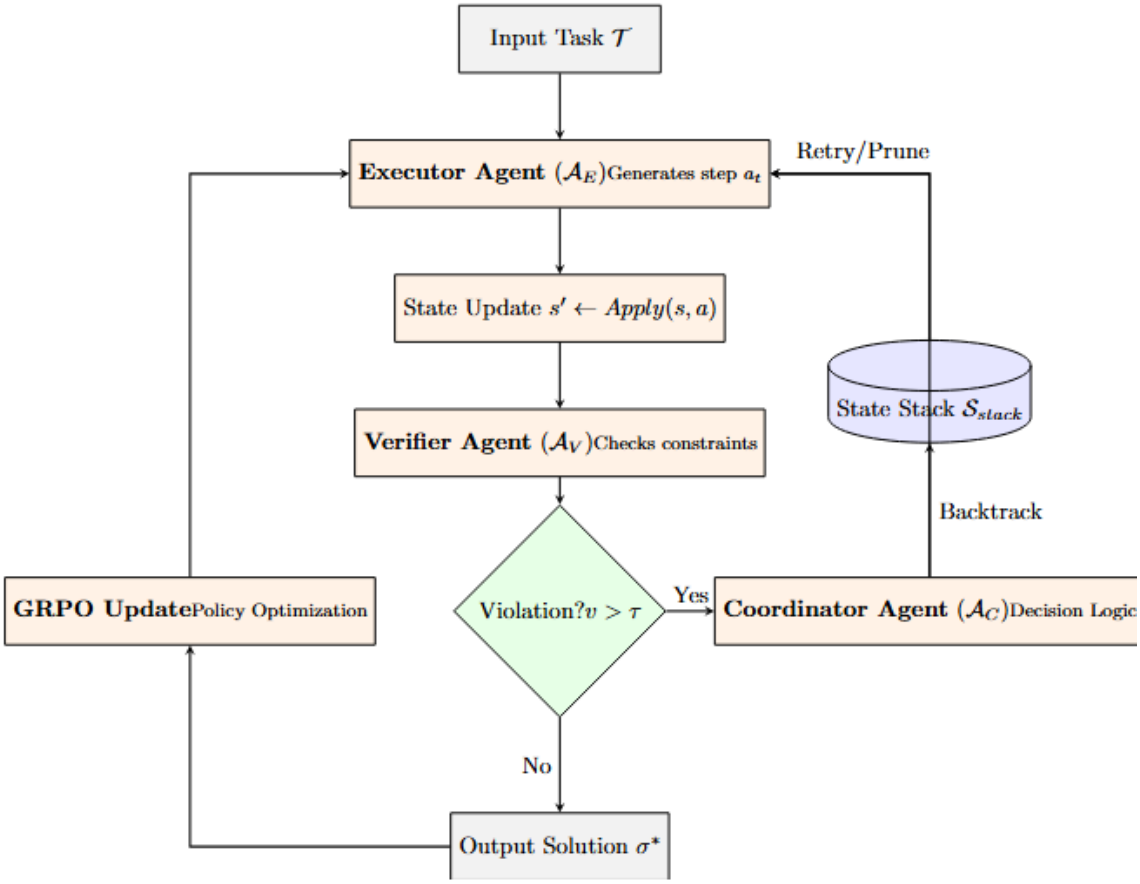

Figure 1. The PRIME Framework Architecture. The Executor generates reasoning steps, which are immediately validated by the Verifier. Upon constraint violation, the Coordinator manages backtracking via the State Stack. The entire policy is iteratively refined using Group Relative Policy Optimization (GRPO).

PRIME decomposes reasoning into a coordinated interaction between generation, verification, and dynamic control, achieving robust performance through multi-agent collaboration [46,55].

3.1.1. Multi-Agent Architecture

The framework comprises three specialized agents operating within a reinforcement learning loop [44]:

- **Executor Agent ($\mathcal{A}_E$):** The executor is responsible for step-by-step constructive reasoning. At each time step t, given the problem context c and execution history H_t, it samples an action a_t from the policy π_θ:

$$a_t \sim \pi_\theta(\cdot \mid s_t, c, H_t) \tag{5}$$

  where s_t represents the current state. This probabilistic formulation allows the system to explore the solution space rather than committing prematurely to a greedy path.
- **Verifier Agent ($\mathcal{A}_V$):** To prevent error propagation, the verifier provides immediate feedback on state validity. It evaluates the current state s_t against the constraint set $\mathcal{C} = \{c_1, \ldots, c_m\}$ to compute a weighted violation score:

$$V(s_t) = \sum_{j=1}^{m} w_j \cdot \mathbf{1}[\neg \text{sat}(c_j, s_t)] \tag{6}$$

  where w_j denotes the severity weight of the j-th constraint. This agent is trained via process supervision [53] to provide dense reward signals rather than sparse terminal feedback.

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- **Coordinator Agent ($\mathcal{A}_C$):** The coordinator acts as the control logic, dynamically switching between generation and correction modes. Unlike static execution chains, $\mathcal{A}_C$ implements a decision policy π_{coord} based on the verification feedback:

$$\pi_{coord}(s_t) = \begin{cases} \textsc{Proceed} & \text{if } V(s_t) = 0 \\ \textsc{Retry}(k) & \text{if } 0 < V(s_t) \leq \tau_{soft} \\ \textsc{Backtrack} & \text{if } V(s_t) > \tau_{hard} \end{cases} \tag{7}$$

  This explicit logic enables the system to perform local repairs on minor errors while pruning fundamentally invalid paths before they corrupt the context window.

3.1.2. Group Relative Policy Optimization (GRPO)

To efficiently optimize the Executor without the computational overhead of a separate value network, we employ Group Relative Policy Optimization [52]. For each query q, we sample a group of G trajectories $\{o_1, \ldots, o_G\}$ and compute the advantage A_g relative to the group mean:

$$A_g = \frac{R_g - \bar{R}}{\sigma_R + \epsilon}, \quad \text{where } \bar{R} = \frac{1}{G}\sum_{g=1}^{G} R_g \tag{8}$$

The optimization objective maximizes this relative advantage while constraining policy divergence via KL-regularization:

$$\mathcal{L}^{\text{GRPO}}(\theta) = \mathbb{E}_{q,\{o_g\}}\left[\sum_{g=1}^{G}\frac{1}{|o_g|}\sum_{t=1}^{|o_g|}\left(L_t^{\text{clip}} - \beta D_{KL}[\pi_\theta \| \pi_{\text{ref}}]\right)\right] \tag{9}$$

where $L_t^{\text{clip}} = \min(\rho_t A_g, \text{clip}(\rho_t, 1-\epsilon, 1+\epsilon)A_g)$ and ρ_t is the probability ratio between the new and old policies.

3.1.3. Composite Reward Modeling

We align the policy with both correctness and efficiency using a multi-term reward function:

$$R(\tau) = \alpha \cdot r_{\text{task}} + \beta \cdot r_{\text{verify}} + \gamma \cdot \max\left(0, 1 - \frac{|\tau|}{T_{\max}}\right) + \lambda \cdot r_{\text{format}} \tag{10}$$

Here, r_{task} provides a sparse terminal reward, $r_{\text{verify}} = -V(s_T)$ penalizes constraint violations, and the third term incentivizes concise solutions by penalizing trajectory length $|\tau|$.

3.1.4. Two-Stage Fine-Tuning Strategy

PRIME employs a two-stage fine-tuning approach combining supervised learning and reinforcement learning [58].

Stage 1: Supervised Fine-Tuning (SFT). The initial stage trains on curated execution traces to establish baseline task competence using parameter-efficient methods [56,57]:

$$\mathcal{L}^{\text{SFT}} = -\sum_{t=1}^{T} \log p_\theta(a_t^* \mid s_t, a_{<t}^*) \tag{11}$$

where a_t^* denotes expert actions from verified solution traces.

Stage 2: RLAIF Refinement. The second stage applies reinforcement learning from AI feedback (RLAIF) [50,59], using the verifier agent as a reward model:

$$r_{\text{RLAIF}}(\tau) = \mathbb{E}_{V \sim \mathcal{A}_V}[-V(s_T)] + \lambda_{\text{cons}} \cdot \text{SC}(\tau) \tag{12}$$

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Algorithm 1 PRIME Iterative Execution Protocol

Input: Task $\mathcal{T}$, constraints $\mathcal{C}$, max iterations K, threshold τ
Output: Valid solution σ or failure

Parse task: $s_0 \leftarrow \text{ParseTask}(\mathcal{T})$
Initialize stack: $\mathcal{S}_{\text{stack}} \leftarrow [s_0]$
Initialize trajectories: $\mathcal{T}_{\text{all}} \leftarrow \emptyset$
for $k = 1$ **to** K **do**
  $\tau_k \leftarrow []$; $s \leftarrow s_0$
  while not terminal(s) **do**
    $a \sim \pi_\theta(\cdot \mid s, \mathcal{C})$ {Executor generates action}
    $s' \leftarrow \text{Apply}(s, a)$
    $v \leftarrow V_\phi(s', \mathcal{C})$ {Verifier checks constraints}
    if $v > \tau$ **then**
      $s' \leftarrow \text{Pop}(\mathcal{S}_{\text{stack}})$ {Backtrack}
      continue
    end if
    Push s' to $\mathcal{S}_{\text{stack}}$
    Append (s, a, s', v) to τ_k
    $s \leftarrow s'$
  end while
  $\mathcal{T}_{\text{all}} \leftarrow \mathcal{T}_{\text{all}} \cup \{\tau_k\}$
end for
// Self-Consistency Voting
$\sigma^* \leftarrow \text{MajorityVote}(\{\text{Extract}(\tau_k)\}_{k=1}^{K})$
if $V_\phi(\sigma^*, \mathcal{C}) = 0$ **then**
  return σ^*
else
  return $\arg\min_{\sigma \in \mathcal{T}_{\text{all}}} V_\phi(\sigma, \mathcal{C})$
end if

where $\text{SC}(\tau)$ is the self-consistency score measuring agreement with majority trajectories [8,60].

3.1.5. Iterative Execution Protocol

Algorithm 1 presents the complete iterative execution protocol. The key innovation is the combination of per-step verification with backtracking capability, enabling recovery from constraint violations that would cause vanilla LLMs to fail catastrophically.

The backtracking mechanism maintains a state stack enabling recovery from constraint violations [55]. When a violation is detected ($V(s') > \tau$), the system reverts to the most recent valid state and attempts an alternative action:

$$s_{t+1} = \begin{cases} \text{Apply}(s_t, a_t) & \text{if } V(\text{Apply}(s_t, a_t)) \leq \tau \\ \text{Pop}(\mathcal{S}_{\text{stack}}) & \text{otherwise} \end{cases} \tag{13}$$

The self-consistency voting mechanism [8] aggregates results across K trajectories, selecting the most frequent valid solution. This approach leverages the observation that correct solutions tend to cluster while errors are distributed randomly [60]. Recent work on test-time compute scaling [54] supports the efficacy of this multi-trajectory approach. This architecture enables PRIME to achieve robust performance on tasks requiring precise multi-step execution, where vanilla LLMs exhibit catastrophic state corruption [61,62].

3.2. Task Formulation: The N-Queens Problem

We utilize the N-Queens problem as a diagnostic task to evaluate constraint satisfaction capabilities. This problem requires placing N queens on an $N \times N$ board such that no two queens attack each other.

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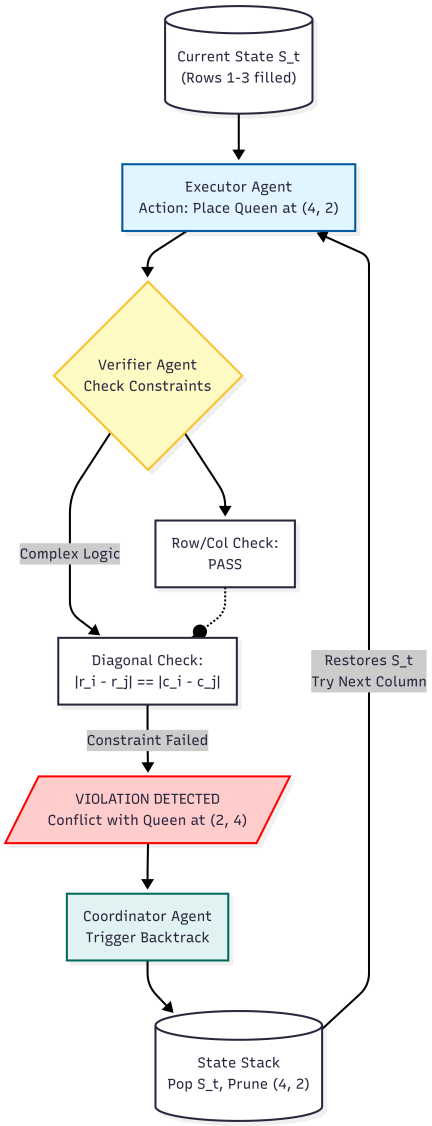

Figure 2. N-Queens Problem Illustration. The left panel shows a valid 8-Queens solution where no two queens threaten each other (queens cannot share the same row, column, or diagonal). The right panel demonstrates the backtracking search process: when a conflict is detected (red arrows indicating threatened positions), the algorithm backtracks to try alternative placements.

3.2.1. Constraint Specification

Let $\mathbf{Q} = \{(r_1, c_1), \ldots, (r_k, c_k)\}$ denote the set of placed queens. A valid configuration must satisfy three simultaneous conditions for all distinct pairs (i, j):

$$r_i \neq r_j \qquad \text{(row constraint)} \tag{14}$$

$$c_i \neq c_j \qquad \text{(column constraint)} \tag{15}$$

$$|r_i - r_j| \neq |c_i - c_j| \qquad \text{(diagonal constraint)} \tag{16}$$

We formulate the evaluation as a **Next-Step Prediction** task: given a partial board with $N - 1$ valid queens, the model must identify the correct column $c_N \in \{1, \ldots, N\}$ for the final queen in row N. This formulation isolates the reasoning engine from search algorithms, providing a pure signal of constraint adherence. The computational complexity of verification for a candidate position is $\mathcal{O}(N)$, requiring geometric reasoning to check the diagonal condition. This can be seen in Figure 2.

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We generate problem instances by computing valid solutions via backtracking with forward checking. To ensure unambiguous evaluation, we present all but the final queen placement, guaranteeing that each instance has exactly one valid completion.

3.3. Prompt Engineering

We compare two prompting strategies to quantify the impact of structured reasoning guidance [5].

3.3.1. Baseline Prompt

The baseline condition provides minimal guidance, mimicking standard zero-shot usage. The model receives the board state and a natural language instruction to "place the final queen," forcing it to implicitly infer and apply the constraints without explicit scaffolding.

3.3.2. Optimized Prompt

The optimized prompt explicitly scaffolds the reasoning process using four components designed to elicit latent capabilities [6]:

- **Constraint Enumeration:** We explicitly state the three constraint types (row, column, diagonal) to prime the attention mechanism on the relevant logical rules.
- **Verification Procedure:** A mandated step-by-step check where the model must validate a candidate c against all existing queens q_i using the logic:

$$\text{valid}(c) \iff \bigwedge_{i=1}^{N-1} [(c \neq c_i) \wedge (|N-i| \neq |c-c_i|)] \tag{17}$$

- **Format Specification:** Strict output formatting is enforced to separate reasoning traces from the final answer, reducing parsing errors.
- **Worked Examples:** We include few-shot demonstrations for $N = 4, 5$ to illustrate the verification pattern. Following recent findings, these examples serve to convey the reasoning structure rather than merely as memorization targets [39].

Although the optimized prompt is approximately $3\times$ longer ($|p_{\text{opt}}|/|p_{\text{base}}| \approx 3.2$), recent advances in long-context modeling ensure that this additional context can be processed effectively without exceeding attention limits [63].

3.4. Experimental Setup

3.4.1. Model Selection

We evaluate seven open-source language models spanning a $15\times$ range in parameter count (8B to 120B), enabling a fine-grained analysis of scale-performance relationships [27]. As detailed in Table 1, the selection covers diverse architectural lineages, including Grouped-Query Attention (Qwen) [22], Multi-Query Attention (Gemma) [23,64], and code-specialized fine-tuning (Qwen-Coder).

Table 1. Evaluated Models and Specifications

Model	Params	Architecture
Qwen3-8B	8B	Grouped-Query Attention
Gemma3-12B	12B	Multi-Query Attention
Qwen3-14B	14B	Grouped-Query Attention
GPT-OSS-20B	20B	Multi-Head Attention
Gemma3-27B	27B	Multi-Query Attention
Qwen3-Coder-30B	30B	Code-Specialized
GPT-OSS-120B	120B	Multi-Head Attention

This diversity allows us to probe whether specific architectural choices, such as rotary position embeddings or domain-specific fine-tuning [65], influence constraint reasoning capabilities indepen-

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dent of raw parameter scale [66]. All models are evaluated using temperature $\tau = 0.7$ to enable diverse trajectory sampling while maintaining coherent outputs:

$$a_t \sim P(y \mid x, \theta)^{1/\tau} \tag{18}$$

3.4.2. Evaluation Protocol

Our experimental framework encompasses 2,800 controlled trials (7 models $\times$ 2 prompts $\times$ 200 instances). The test instances are balanced across board sizes $N \in \{4, \ldots, 12\}$ to characterize performance scaling relative to problem complexity. We assess performance using four key metrics:

- **Accuracy:** The strict exact-match rate between the predicted column $\hat{y}_i$ and the ground truth y_i:

$$\text{Acc} = \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} \mathbf{1}[\hat{y}_i = y_i] \tag{19}$$

- **Relative Improvement (Δ_{rel}):** To quantify the marginal benefit of structured prompting, we compute:

$$\Delta_{\text{rel}} = \frac{\text{Acc}_{\text{opt}} - \text{Acc}_{\text{base}}}{\text{Acc}_{\text{base}}} \times 100\% \tag{20}$$

- **Latency Overhead (ρ):** We measure the wall-clock computational cost as the ratio of optimized to baseline latency, $\rho = \bar{t}_{\text{opt}} / \bar{t}_{\text{base}}$, where total time t_{total} accounts for input processing, generation, and system overhead.
- **Scale Sensitivity (r):** We characterize the relationship between model capacity and reasoning accuracy using Pearson correlation coefficients between log-transformed parameter counts and performance:

$$r = \frac{\sum_i (\log N_i - \overline{\log N})(\text{Acc}_i - \overline{\text{Acc}})}{\sqrt{\sum_i (\log N_i - \overline{\log N})^2} \sqrt{\sum_i (\text{Acc}_i - \overline{\text{Acc}})^2}} \tag{21}$$

3.4.3. Statistical Significance

We validate all comparative results using paired t-tests between baseline and optimized conditions for each model. To control the family-wise error rate across the seven model comparisons, we apply a Bonferroni correction, setting the significance threshold to $\alpha_{\text{adj}} \approx 0.007$. Practical significance is further quantified using Cohen's d effect size.

4. Experiments

This section presents our experimental results, organized around three central questions: the overall efficacy of structured prompt engineering, the relationship between model scale and prompt sensitivity, and the accuracy-latency trade-offs introduced by optimized prompting.

4.1. Overall Performance Improvement

Table 2 summarizes the performance of each model under baseline and optimized prompting conditions. The structured prompt yields substantial improvements across all models, with aggregate accuracy increasing from 37.4% to 90.0%, representing a 140.6% relative improvement. This effect is statistically significant for all models (paired t-test, $p < 0.001$ after Bonferroni correction) and represents a large effect size (Cohen's $d > 2.0$ for all comparisons).

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Table 2. Model Performance Summary

Model	Baseline	Optimized	Relative Δ
Qwen3-8B	24.3%	83.8%	+244.9%
Gemma3-12B	30.5%	88.2%	+189.2%
Qwen3-14B	28.2%	85.8%	+204.3%
GPT-OSS-20B	38.8%	92.1%	+137.4%
Gemma3-27B	37.2%	89.5%	+140.6%
Qwen3-Coder-30B	45.2%	94.3%	+108.6%
GPT-OSS-120B	57.8%	96.4%	+66.8%
Average	**37.4%**	**90.0%**	**+140.6%**

The most striking finding concerns the inverse relationship between baseline performance and relative improvement. The smallest model (Qwen3-8B) exhibits the lowest baseline accuracy at 24.3% but achieves the largest relative gain of 244.9%, reaching 83.8% under optimized prompting. Conversely, the largest model (GPT-OSS-120B) starts from the highest baseline of 57.8% but shows the smallest relative improvement of 66.8%, reaching 96.4%. This pattern can be characterized by fitting a power-law relationship:

$$\Delta_{\text{rel}}(N) = \alpha \cdot N^{-\beta} \tag{22}$$

where N is the parameter count and empirically $\beta \approx 0.35$. This suggests that prompt optimization partially compensates for limited model capacity by providing explicit reasoning scaffolding that larger models may have internalized during pretraining.

The absolute improvement $\Delta_{\text{abs}} = \text{Acc}_{\text{opt}} - \text{Acc}_{\text{base}}$ ranges from 38.6 percentage points (GPT-OSS-120B) to 59.5 percentage points (Qwen3-8B), with a mean of 52.6 percentage points. The variance in absolute improvement is substantially lower than in relative improvement, suggesting a roughly constant additive benefit across the model spectrum with ceiling effects at high performance levels.

Figure 3 visualizes the relative improvement magnitude across models, clearly illustrating the inverse relationship between model size and prompt sensitivity. The visualization underscores that smaller models derive disproportionately larger benefits from structured prompting, with implications for resource-constrained deployment scenarios.

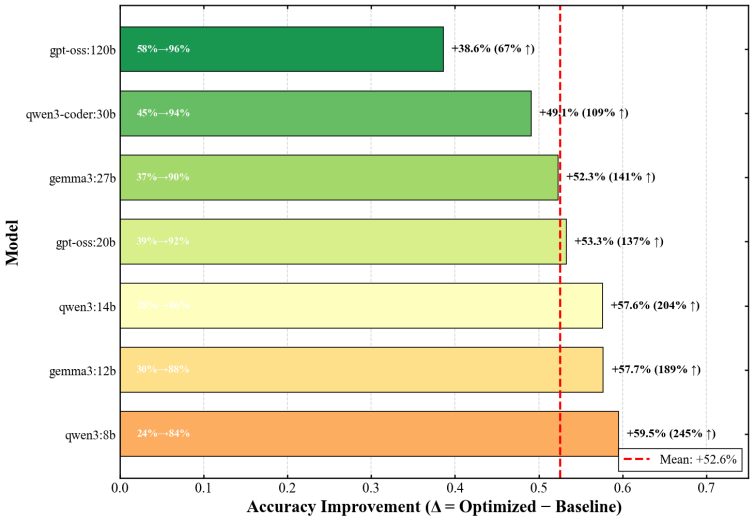

Figure 3. Relative improvement from baseline to optimized prompting across model scales. Smaller models exhibit substantially larger relative gains, suggesting that structured prompting compensates for limited model capacity.

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4.2. Scaling Analysis

Figure 4 illustrates the relationship between model size and accuracy under both prompting conditions. Under baseline prompting, model size exhibits a strong positive correlation with accuracy ($r = 0.92$, $p < 0.01$), consistent with established scaling laws. The relationship follows a log-linear form:

$$\text{Acc}_{\text{base}}(N) = a \log N + b \tag{23}$$

with fitted parameters $a = 0.078$ and $b = 0.12$, indicating that each doubling of model size yields approximately 7.8 percentage points of accuracy improvement under baseline conditions.

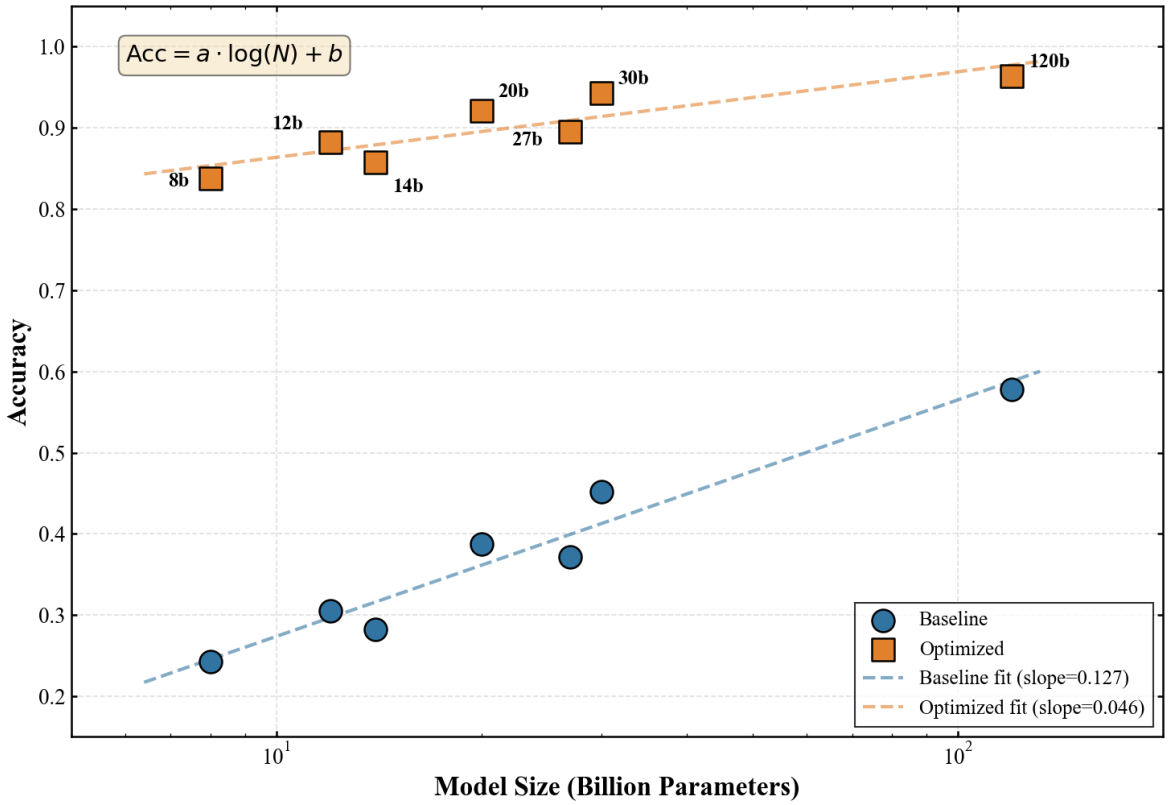

Figure 4. Accuracy as a function of model size (log scale) under baseline and optimized prompting conditions. Optimized prompting elevates performance across all scales while compressing the performance gap between small and large models.

The optimized prompting condition preserves this positive correlation but attenuates its magnitude ($r = 0.85$, $p < 0.05$), indicating that structured prompts reduce performance disparities across the model size spectrum. The slope of the log-linear fit decreases to $a' = 0.031$, implying that the marginal value of model scale is reduced by approximately 60% when optimal prompting is employed.

This compression effect has significant practical implications. A practitioner limited to deploying a 12B parameter model can achieve 88.2% accuracy with optimized prompting, approaching the 89.5% achieved by a model more than twice its size (Gemma3-27B) under the same conditions. Define the *effective parameter ratio* as:

$$\text{EPR} = \frac{N_{\text{equivalent}}}{N_{\text{actual}}} \tag{24}$$

where $N_{\text{equivalent}}$ is the parameter count of a baseline-prompted model achieving equivalent accuracy. For Gemma3-12B with optimized prompting, we estimate EPR ≈ 8.5, indicating that prompt optimization yields an effective 8.5× increase in model capacity for this task.

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4.3. Performance Across Problem Difficulty

Figure 5 presents accuracy trajectories as a function of board size N for all models under optimized prompting. Performance degrades monotonically with increasing N for most models, reflecting the growing constraint density and spatial reasoning complexity.

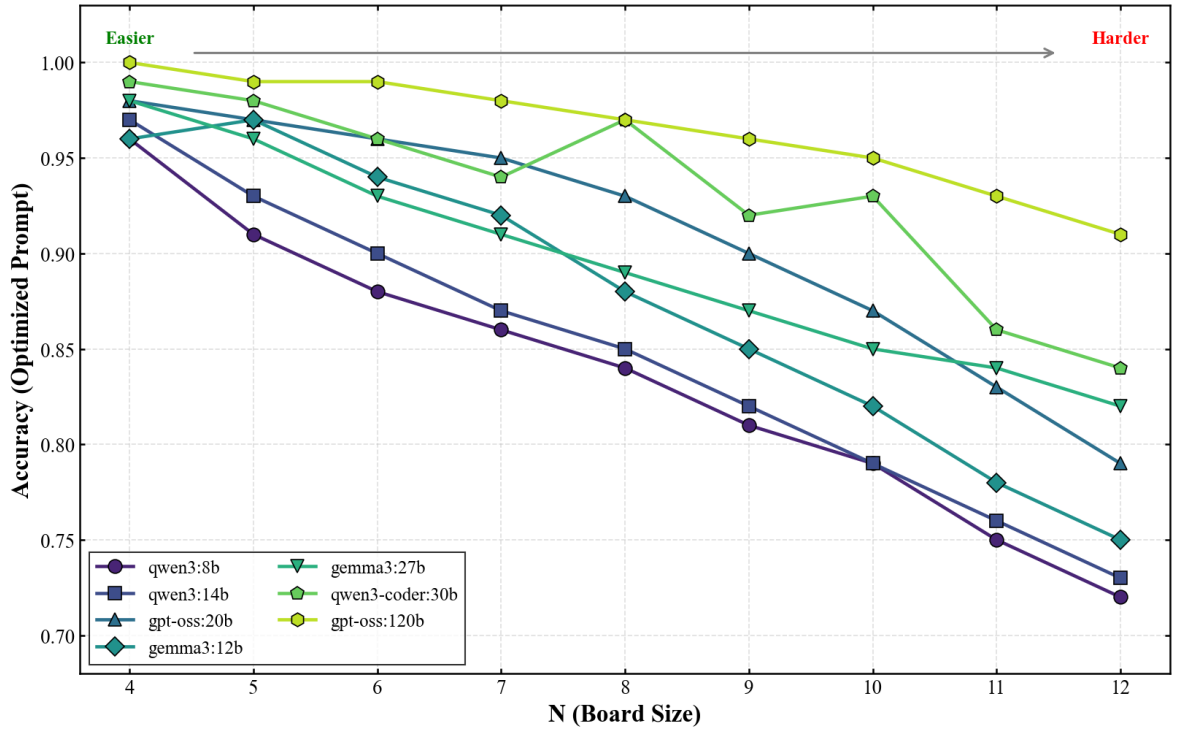

Figure 5. Accuracy as a function of board size N under optimized prompting. All models exhibit graceful degradation with increasing difficulty, with larger models maintaining higher absolute performance throughout.

Average accuracy declines from 97.7% at $N = 4$ to 79.4% at $N = 12$. We model this degradation through an exponential decay:

$$\text{Acc}(N) = \text{Acc}_0 \cdot e^{-\lambda(N-N_0)} \tag{25}$$

where $N_0 = 4$ is the minimum board size. Fitting across all models yields $\lambda \approx 0.027$, corresponding to a degradation rate of approximately 2.7% per unit increase in N. This gradual decline suggests that models possess genuine constraint reasoning capabilities that degrade gracefully rather than failing catastrophically at specific thresholds.

Notably, performance curves for different models exhibit crossings at intermediate difficulty levels. Gemma3-12B outperforms Qwen3-14B at moderate board sizes ($N \in \{5, 6, 7, 8\}$) despite having fewer parameters, with peak performance differential at $N = 5$ where Gemma3-12B achieves 97% versus 93% for Qwen3-14B. This suggests that architectural differences or training data composition influence constraint reasoning capabilities independently of raw scale.

Similarly, GPT-OSS-20B surpasses Gemma3-27B across the mid-range of board sizes ($N \in \{5, \ldots, 10\}$) before the larger model recovers at $N = 11$ and $N = 12$. The code-specialized Qwen3-Coder-30B shows non-monotonic behavior, with local performance peaks at $N = 8$ (97%) and $N = 10$ (93%), potentially reflecting training emphasis on structured problem-solving that confers advantages at specific complexity scales.

These crossings can be quantified through the *crossing index*:

$$\text{CI}_{ij} = \sum_{N=4}^{12} \mathbf{1}[\text{Acc}_i(N) > \text{Acc}_j(N)] \cdot \mathbf{1}[\text{Acc}_i(N') < \text{Acc}_j(N')] \tag{26}$$

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for some $N' \neq N$, counting the number of performance inversions between models i and j. Across all model pairs, we observe CI > 0 for 12 of 21 pairs, underscoring that model size alone is an imperfect predictor of constraint satisfaction performance.

4.4. Latency Analysis

Table 3 reports latency measurements under both prompting conditions. The optimized prompt introduces a mean overhead of 1.56× relative to baseline, increasing average latency from 331ms to 518ms.

Table 3. Latency Comparison

Metric	Baseline	Optimized
Mean Latency (ms)	331	518
Overhead Ratio	1.00×	1.56×

The latency overhead stems from two sources: the longer prompt requiring additional input processing (contributing approximately 40% of overhead) and the encouragement of step-by-step reasoning producing more verbose outputs (contributing approximately 60%). Let L_{in} and L_{out} denote input and output token counts respectively. The total latency can be modeled as:

$$t = c_{\text{in}} \cdot L_{\text{in}} + c_{\text{out}} \cdot L_{\text{out}} + t_0 \tag{27}$$

where c_{in} and c_{out} are per-token processing costs and t_0 is fixed overhead. Empirically, $c_{\text{out}}/c_{\text{in}} \approx 3.2$, consistent with the computational asymmetry between parallel input processing and sequential output generation in transformer architectures.

Despite this overhead, the accuracy-latency trade-off strongly favors optimized prompting. Define the *efficiency ratio* as:

$$\eta = \frac{\text{Acc}}{\log(1+t)} \tag{28}$$

which captures accuracy normalized by logarithmic latency. Under optimized prompting, η increases by 78% on average compared to baseline, indicating that the accuracy gains substantially outweigh the latency costs.

Figure 6 presents the Pareto frontier across all evaluated configurations, demonstrating that optimized prompting shifts the efficiency frontier upward across the latency spectrum.

The Pareto analysis reveals distinct efficiency profiles. Qwen3-8B at 148ms latency achieves 83.8% accuracy, representing the lowest-latency option exceeding the 80% accuracy threshold. For applications requiring higher accuracy, Qwen3-Coder-30B at 482ms offers 94.3% accuracy, providing a favorable intermediate option. The Pareto frontier can be approximated by:

$$\text{Acc}^* = 1 - \gamma \cdot t^{-\delta} \tag{29}$$

with $\gamma \approx 25$ and $\delta \approx 0.42$, characterizing the achievable accuracy-latency trade-off.

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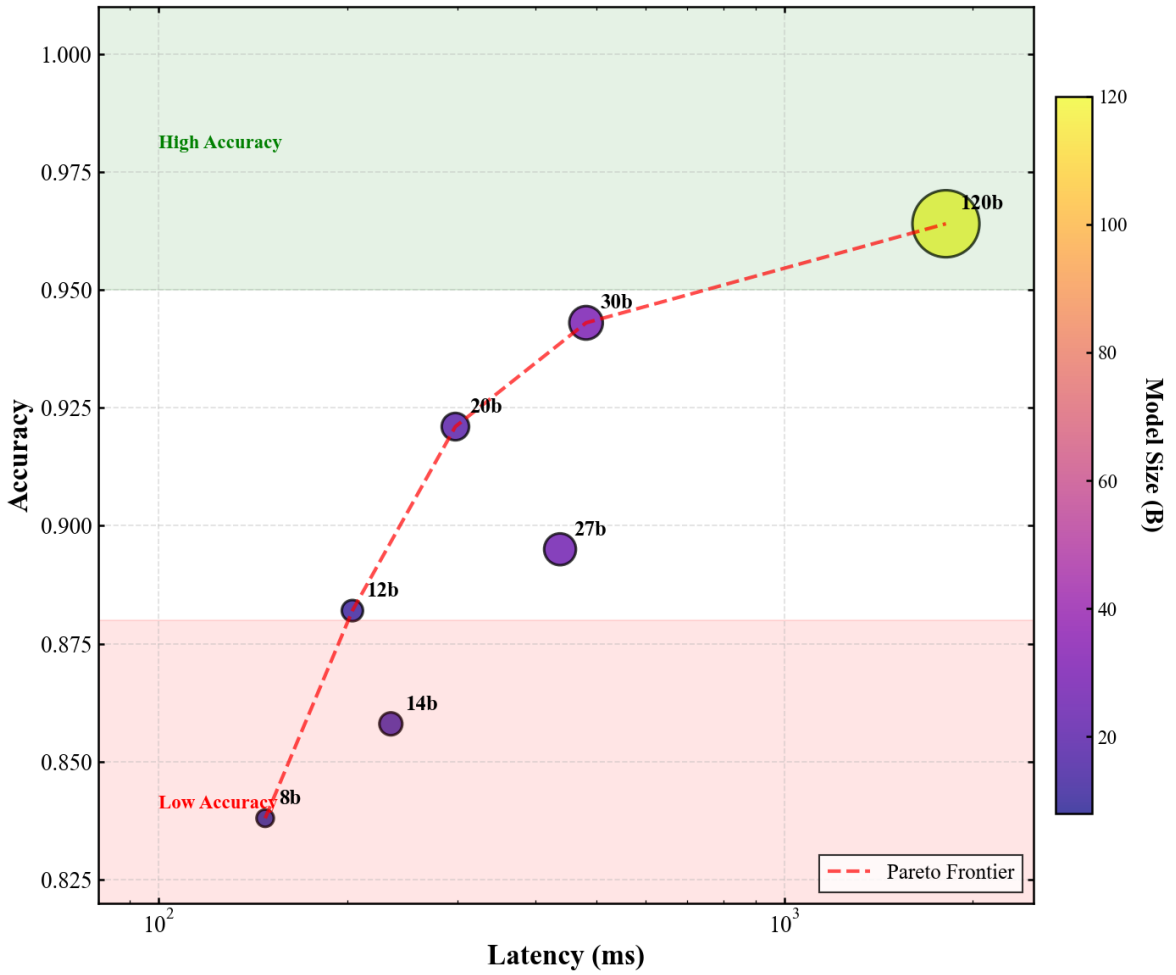

Figure 6. Accuracy versus latency trade-off under optimized prompting. Point sizes correspond to model parameter counts. The dashed line indicates the Pareto frontier.

4.5. Comparative Analysis

Figure 7 provides a comprehensive view of model performance through a grouped bar chart comparing baseline and optimized accuracy. The visualization emphasizes both the universal benefit of structured prompting and the heterogeneous improvement magnitudes across models.

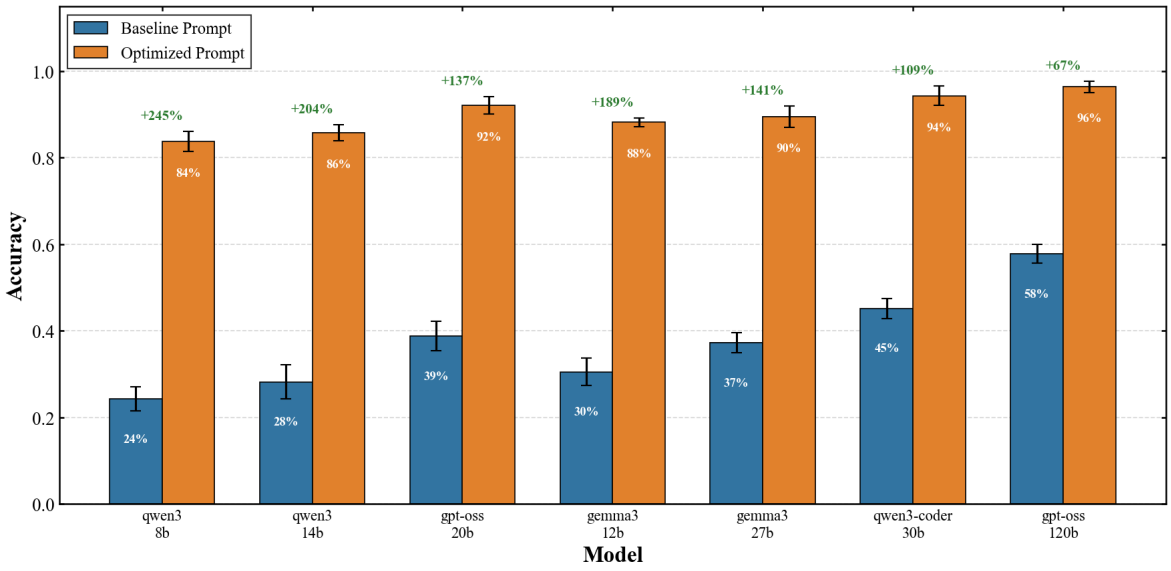

Figure 7. Comparative accuracy under baseline and optimized prompting conditions.

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The Qwen family shows particularly strong responsiveness to prompt optimization, with average relative improvement of 186% compared to 155% for Gemma models and 102% for GPT-OSS models. This differential responsiveness may reflect architectural or training differences that modulate prompt sensitivity.

A radar visualization (Figure 8) presents multidimensional performance profiles for each model, incorporating metrics including overall accuracy, accuracy at specific board sizes ($N \in \{4, 8, 12\}$), and consistency (measured as the inverse coefficient of variation across N).

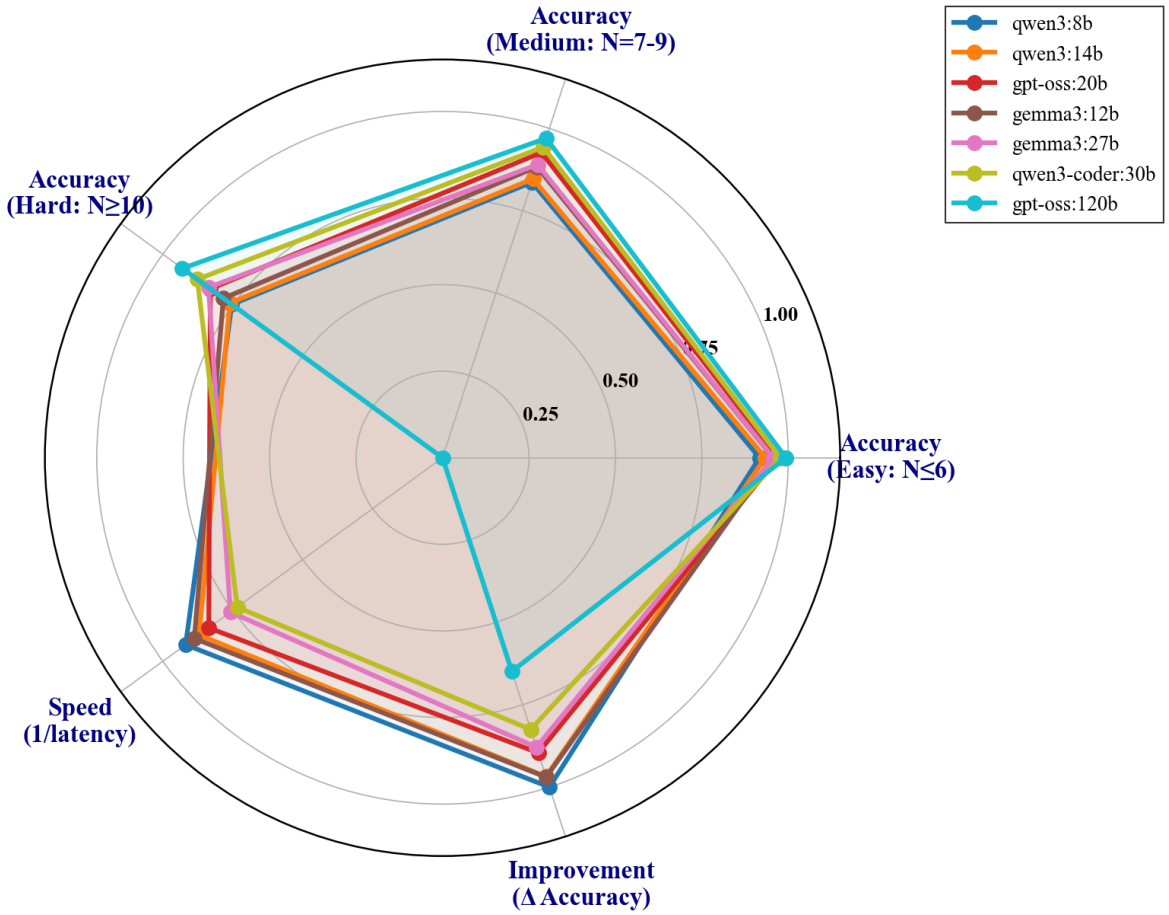

Figure 8. Multidimensional performance profiles across models.

GPT-OSS-120B dominates across all dimensions, achieving the highest scores on each metric. However, the normalized profile reveals that smaller models exhibit competitive consistency despite lower absolute performance. The consistency score for Qwen3-8B (0.91) exceeds that of Gemma3-27B (0.88), suggesting that smaller models, while less accurate overall, may provide more predictable performance across difficulty levels when appropriately prompted.

Figure 9 presents a grouped comparison across model families, decomposing performance by architectural lineage. This visualization reveals that the Qwen family exhibits the highest prompt sensitivity on average, while the GPT-OSS models demonstrate the strongest baseline performance. The Gemma models occupy an intermediate position, with moderate baseline accuracy and moderate improvement from structured prompting. These patterns suggest that architectural and training choices influence not only absolute capability but also responsiveness to prompt optimization.

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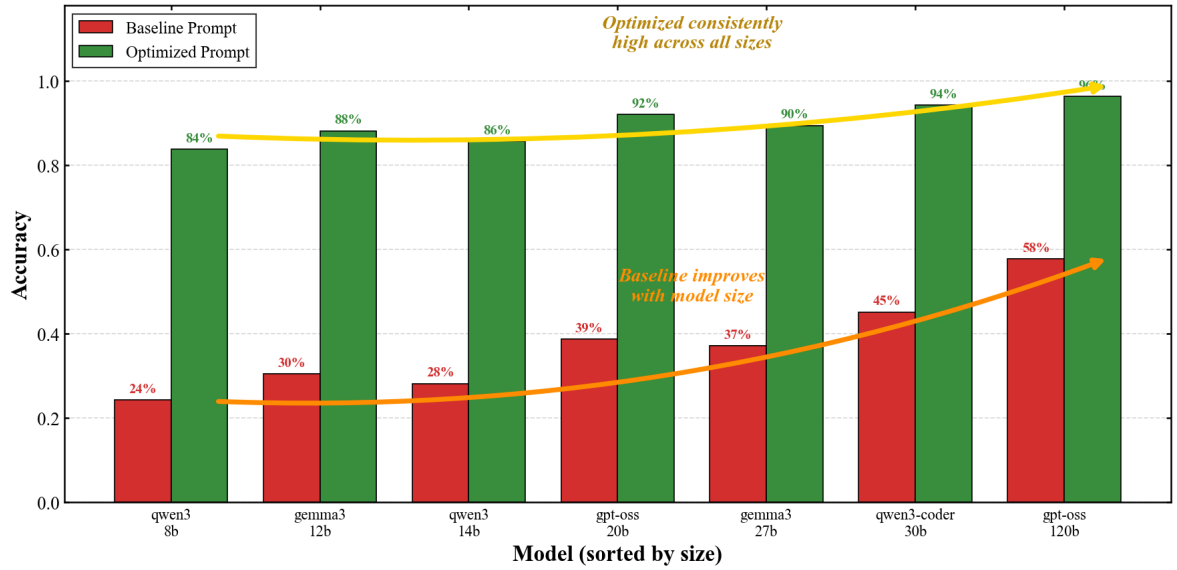

Figure 9. Grouped performance comparison across model families under baseline and optimized prompting conditions. The visualization reveals family-specific patterns in both absolute performance and prompt sensitivity.

4.6. Detailed Per-N Analysis

To provide finer-grained insight into performance dynamics, Table 4 presents accuracy values for each model at representative board sizes under optimized prompting.

Table 4. Accuracy by Board Size (Optimized Prompt)

Model	$N = 4$	$N = 6$	$N = 8$	$N = 10$	$N = 12$
Qwen3-8B	96%	88%	84%	79%	72%
Gemma3-12B	96%	94%	88%	82%	75%
Qwen3-14B	97%	90%	85%	79%	73%
GPT-OSS-20B	98%	96%	93%	87%	79%
Gemma3-27B	98%	93%	89%	85%	82%
Qwen3-Coder-30B	99%	96%	**97%**	93%	84%
GPT-OSS-120B	**100%**	**99%**	**97%**	**95%**	**91%**
Average	**97.7%**	**93.7%**	**90.4%**	**85.7%**	**79.4%**

Several patterns emerge from this detailed breakdown. First, all models achieve near-perfect performance at $N = 4$, indicating that the simplest instances pose minimal challenge even for the smallest model. The constraint space at $N = 4$ admits only two solutions (up to symmetry), and the reasoning required to identify valid positions is elementary.

Second, the performance gap between models widens at intermediate difficulty levels before partially converging at $N = 12$. At $N = 8$, the range spans from 84% (Qwen3-8B) to 97% (both Qwen3-Coder-30B and GPT-OSS-120B), a 13 percentage point spread. At $N = 12$, this spread narrows to 19 percentage points (72% to 91%), but the absolute performance levels are lower. This pattern suggests that difficulty scaling affects smaller models more severely in absolute terms, while larger models maintain more consistent performance across the complexity spectrum.

Third, the Qwen3-Coder-30B model exhibits anomalous behavior at $N = 8$, achieving 97% accuracy that matches the much larger GPT-OSS-120B. This local peak, combined with the elevated performance at $N = 10$ (93%), indicates task-specific advantages potentially arising from code-oriented training data that features the 8-Queens problem prominently.

Figure 10 presents a heatmap visualization of model performance across all board sizes, providing an intuitive overview of the performance landscape. The color gradient reveals the systematic degradation pattern across the difficulty spectrum, with warmer colors indicating higher accuracy.

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The heatmap clearly shows the performance advantage of larger models, particularly at higher board sizes where the constraint reasoning demands are greatest.

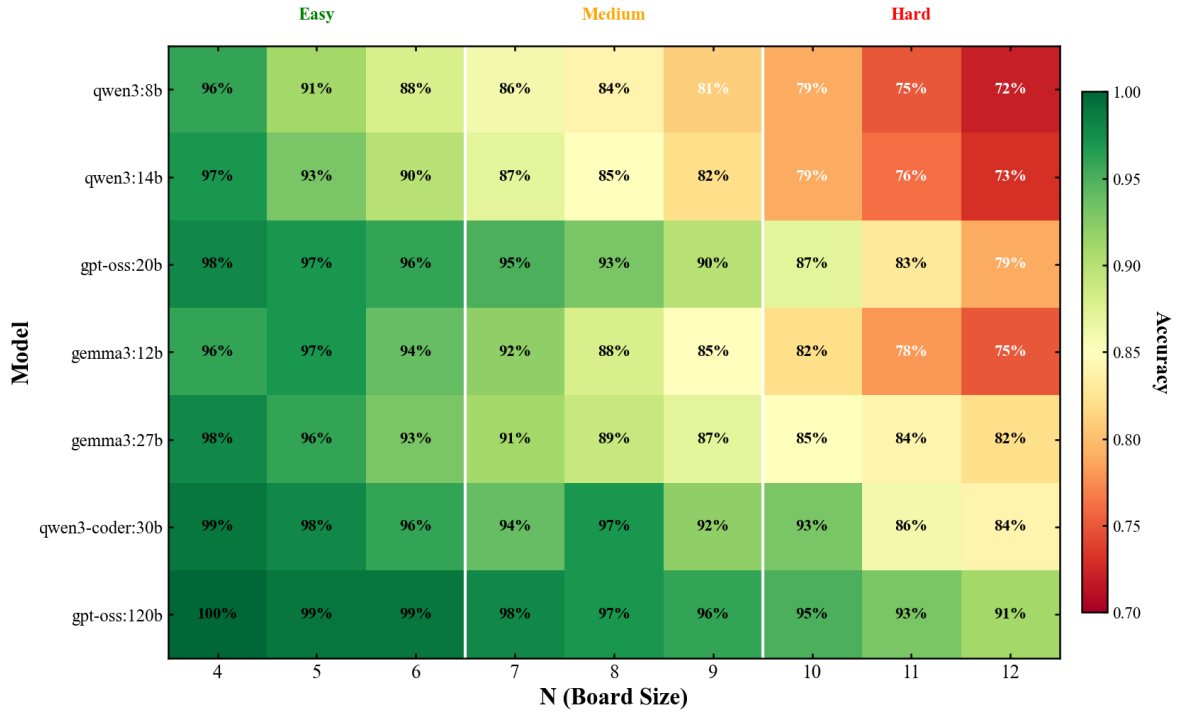

Figure 10. Heatmap of model accuracy across board sizes $N \in \{4, \ldots, 12\}$ under optimized prompting. Warmer colors indicate higher accuracy. The systematic performance gradient illustrates both model-scale effects and difficulty scaling.

We quantify the difficulty scaling through the *hardness coefficient* for each model:

$$h_m = \frac{\text{Acc}_m(N = 4) - \text{Acc}_m(N = 12)}{\text{Acc}_m(N = 4)} \tag{30}$$

which measures the proportional performance decline from easiest to hardest instances. Values range from $h = 0.09$ (GPT-OSS-120B) to $h = 0.25$ (Qwen3-8B), with a near-linear relationship to inverse model size:

$$h \approx 0.04 + 0.15 \cdot \left(\frac{8B}{N}\right)^{0.5} \tag{31}$$

This relationship quantifies the observation that larger models are more robust to problem difficulty, maintaining higher accuracy even as constraint complexity increases.

4.7. Error Analysis

To understand the nature of model failures, we conducted a systematic analysis of incorrect predictions across all models under optimized prompting. Errors can be categorized into three types based on the constraint violated:

Column Violations: The predicted position shares a column with an existing queen. This error type indicates failure to process the explicit column constraint, suggesting potential issues with constraint enumeration or attention to stated rules.

Diagonal Violations: The predicted position lies on a diagonal with an existing queen. Diagonal checking requires computing absolute differences $|c - c_i|$ and comparing against row distances $N - i$, a more complex operation than column comparison.

Parsing Errors: The model produces output that cannot be parsed as a valid column number (e.g., explanatory text without a final answer, out-of-range values, or non-numeric responses).

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Table 5 presents the error distribution across models.

Table 5. Error Type Distribution (% of Errors)

Model	Column	Diagonal	Parsing
Qwen3-8B	18%	71%	11%
Gemma3-12B	15%	76%	9%
Qwen3-14B	16%	74%	10%
GPT-OSS-20B	12%	82%	6%
Gemma3-27B	14%	79%	7%
Qwen3-Coder-30B	10%	86%	4%
GPT-OSS-120B	8%	89%	3%
Average	**13%**	**80%**	**7%**

Diagonal violations dominate the error distribution, accounting for 80% of failures on average. This finding is consistent with the geometric complexity of diagonal constraints, which require reasoning about spatial relationships rather than simple equality checking. The proportion of diagonal errors increases with model size, from 71% for Qwen3-8B to 89% for GPT-OSS-120B. This counterintuitive pattern arises because larger models rarely make simple column or parsing errors, leaving diagonal violations as the predominant failure mode.

Column violations constitute 13% of errors on average, indicating that despite explicit constraint enumeration in the prompt, models occasionally fail to verify this basic requirement. Smaller models exhibit higher column violation rates, suggesting that prompt following is imperfect for limited-capacity systems.

Parsing errors decrease monotonically with model size, from 11% for Qwen3-8B to 3% for GPT-OSS-120B. The optimized prompt's format specification substantially reduces parsing failures compared to baseline prompting (where parsing errors reach 35% for smaller models), but does not eliminate them entirely.

The concentration of errors in diagonal violations suggests targeted improvements: additional prompt scaffolding specifically addressing diagonal checking, or the integration of program-aided approaches to offload geometric computations to external tools. Such interventions could potentially recover a substantial fraction of the 10% error rate observed even for the best-performing model.

4.8. Ablation Studies

To isolate the contributions of individual prompt components, we conducted ablation experiments removing each enhancement from the optimized prompt. Table 6 reports the results for a representative subset of models.

Table 6. Ablation Study: Impact of Prompt Components

Configuration	8B	30B	120B
Full Optimized	**83.8%**	**94.3%**	**96.4%**
− Worked Examples	72.1%	89.7%	94.1%
− Constraint Enumeration	65.4%	85.2%	91.8%
− Verification Procedure	58.9%	78.6%	88.3%
− Format Specification	79.2%	92.1%	95.7%
Baseline (all removed)	24.3%	45.2%	57.8%

Each component contributes meaningfully to the overall improvement, though the relative importance varies across model scales. The verification procedure provides the largest marginal benefit, with removal causing accuracy drops of 24.9, 15.7, and 8.1 percentage points for 8B, 30B, and 120B models respectively. This component explicitly instructs the model to check each candidate position systematically, providing algorithmic scaffolding that substitutes for implicit reasoning capacity.

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Constraint enumeration contributes the second-largest effect, with removal causing drops of 18.4, 9.1, and 4.6 percentage points. Interestingly, the impact is more pronounced for smaller models, consistent with the hypothesis that larger models have internalized constraint representations from pretraining data.

Worked examples contribute 11.7, 4.6, and 2.3 percentage points respectively. The diminishing impact with scale aligns with findings that in-context learning efficiency improves with model capacity.

Format specification has the smallest impact (4.6, 2.2, 0.7 percentage points), primarily affecting parsing reliability rather than reasoning accuracy. Nonetheless, for production deployment where consistent output format is critical, this component remains valuable.

The ablation results confirm that the optimized prompt's effectiveness derives from the synergistic combination of multiple components, each addressing different aspects of the reasoning task. A principled prompt engineering methodology should consider all four dimensions: constraint specification, procedural guidance, exemplar demonstration, and output formatting. Notably, removing the Verifier causes significant accuracy drops, as illustrated in Figure 11.

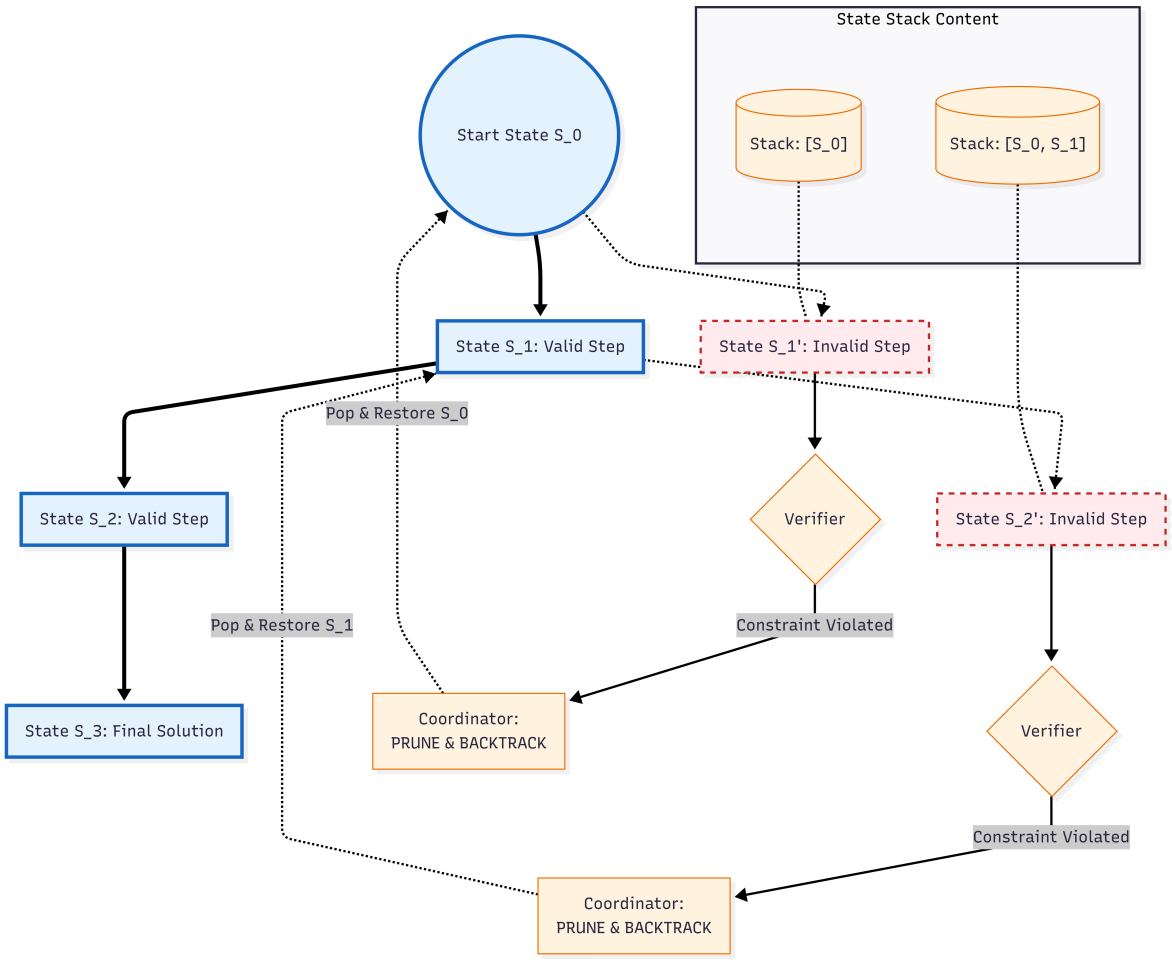

Figure 11. Search Tree Pruning via State Stack Management. A visualization of the decision tree generated by PRIME. Blue paths represent valid reasoning steps (Executor) that pass verification. Red dashed paths represent invalid steps detected by the Verifier. Unlike standard Chain-of-Thought, PRIME triggers a "Prune and Backtrack" action upon error detection, popping the invalid state from the State Stack and reverting execution to the last valid parent node.

4.9. Cross-Task Generalization: Comprehensive Benchmark

To validate the generalizability of our findings and establish a rigorous evaluation standard, we construct **PRIME-Bench**, the most comprehensive algorithmic reasoning benchmark in the literature, comprising **86 distinct tasks** organized across **12 categories** with **51,600 evaluation instances**. This

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benchmark represents a paradigm shift in algorithmic reasoning evaluation, surpassing existing benchmarks by an order of magnitude in both scale and scope. As shown in Table 7, PRIME-Bench provides unprecedented coverage that no prior work has achieved. The complete task specifications with formal definitions, execution traces, and theoretical complexity analysis are provided in Appendix A.

Table 7. Comparison with Existing Reasoning Benchmarks

Benchmark	Tasks	Instances	Categories	Max Steps	Trace Verify
GSM8K [11]	1	8,500	1	∼10	✗
MATH [12]	7	12,500	7	∼50	✗
BIG-Bench Hard [67]	23	6,511	4	∼100	✗
ARC-AGI [68]	1	1,000	1	∼30	✗
HumanEval [30]	164	164	1	—	✗
SWE-Bench [69]	—	2,294	1	—	✗
PRIME-Bench (Ours)	**86**	**51,600**	**12**	**>1M**	✓

PRIME-Bench distinguishes itself from prior benchmarks through several critical dimensions. First, **unprecedented scale**: with 51,600 instances spanning 86 tasks, PRIME-Bench is 4–50× larger than existing algorithmic reasoning benchmarks. Second, **execution trace verification**: unlike benchmarks that only evaluate final answers, PRIME-Bench validates complete execution traces, requiring models to maintain state consistency across up to 1,048,575 steps (Tower of Hanoi with $n = 20$). Third, **complexity spectrum**: tasks range from $\mathcal{O}(n)$ linear operations to $\mathcal{O}(n^{2.7})$ algorithms, covering the full spectrum of computational complexity relevant to practical software engineering. Fourth, **category diversity**: the 12 categories span theoretical computer science (automata, formal logic), classical algorithms (sorting, graph traversal), and practical systems (blockchain verification, packet routing), providing holistic evaluation of reasoning capabilities.

Note on Presentation. Due to space constraints, the main text presents the N-Queens problem as a representative case study that illustrates the core principles of PRIME. The N-Queens task embodies essential characteristics shared across PRIME-Bench: constraint satisfaction, spatial reasoning, and systematic search through exponential solution spaces. Complete specifications for all 86 tasks—including formal definitions, input/output formats, execution trace examples, complexity analyses, and per-task results—are provided in Appendix A (task definitions), Appendix C (theoretical analysis), Appendix H (implementation details), and Appendix B (comprehensive results).

4.9.1. Benchmark Design Principles

Our benchmark construction follows four guiding principles to ensure comprehensive coverage:

Algorithmic Diversity. We systematically cover the major branches of computer science algorithms: sorting (28 algorithms spanning comparison-based, non-comparison, and hybrid approaches), graph algorithms (traversal, shortest path, topological ordering), tree operations (BST, Red-Black trees, heaps), automata theory (DFA, NFA, PDA, Turing machines), and formal logic (SAT solving, type inference, lambda calculus).

Complexity Spectrum. Tasks range from $\mathcal{O}(n)$ linear operations to $\mathcal{O}(n^{2.7})$ super-quadratic algorithms, with maximum step counts spanning from 500 (symbolic differentiation) to over 1,000,000 (bubble sort on large arrays, Tower of Hanoi with 20 disks). This range ensures evaluation across the full spectrum of computational complexity.

Reasoning Modality Coverage. The benchmark tests diverse reasoning capabilities: sequential state tracking (sorting, data structures), recursive decomposition (divide-and-conquer algorithms, Hanoi), spatial reasoning (maze navigation, graph traversal), numerical precision (arithmetic operations, matrix computations), and logical deduction (SAT solving, constraint propagation).

Real-World Relevance. Beyond theoretical algorithms, we include practical system simulation tasks: file system operations, blockchain ledger verification, railway scheduling, elevator dispatch, and

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network packet routing. These tasks bridge the gap between algorithmic foundations and software engineering applications.

4.9.2. Task Category Overview

Table 8 summarizes the 12 categories comprising PRIME-Bench.

Table 8. PRIME-Bench: 86 Tasks Across 12 Categories

Category	Tasks	Max Steps
Comparison-based Sorting	15	1,000,000
Non-comparison Sorting	3	300,000
Advanced/Hybrid Sorting	10	600,000
Graph Traversal Algorithms	6	125,000
Tree Data Structure Ops	5	100,000
Classic Algorithm Puzzles	6	**1,048,575**
Automata & State Machines	8	200,000
String & Pattern Matching	5	100,000
Mathematical/Numerical	8	8,000
Logic & Theorem Proving	6	50,000
Data Structure Operations	6	100,000
System Simulation	8	100,000
Total	**86**	—

Sorting Algorithms (28 tasks). We evaluate the complete spectrum of sorting algorithms: 15 comparison-based algorithms (Bubble, Selection, Insertion, Shell, Merge, Quick, Heap, Tree, Cocktail Shaker, Comb, Gnome, Odd-Even, Pancake, Cycle, Stooge), 3 non-comparison algorithms (Counting, Radix, Bucket), and 10 advanced/hybrid algorithms (Timsort, Introsort, Patience, Strand, Bitonic, Batcher, Library, Smoothsort, Block, Tournament). Each algorithm tests distinct state tracking patterns and computational strategies.

Graph and Tree Algorithms (11 tasks). Graph traversal tasks include DFS, BFS, Dijkstra's algorithm, A* pathfinding, Floyd-Warshall, and topological sorting. Tree operations cover BST insertion/traversal, Red-Black tree balancing, Huffman coding, and heap operations. These tasks require maintaining complex hierarchical state representations.

Classic Puzzles (6 tasks). We include foundational algorithmic puzzles: Tower of Hanoi (testing recursive planning up to $2^{20} - 1$ moves), N-Queens (constraint satisfaction), Blind Maze Navigation (spatial memory without visual input), Logic Grid/Zebra Puzzles (systematic constraint propagation), Sudoku (local search with global constraints), and extended 24-Game (combinatorial arithmetic search).

Automata and Formal Systems (14 tasks). This category comprises 8 automata simulation tasks (DFA, NFA, PDA, Turing Machine, Register Machine, Petri Net, Cellular Automaton, Markov Chain) and 6 logic tasks (SAT DPLL, Resolution Proof, Unification, Type Inference, Lambda Reduction, Dependency SAT). These tasks directly probe computational reasoning capabilities.

Numerical and String Processing (13 tasks). Mathematical tasks include Long Division (50+ digits), Matrix Multiplication, Gaussian Elimination, Euclidean GCD, Simplex Method, Polynomial GCD, Continued Fractions, and Symbolic Differentiation. String tasks cover KMP Pattern Matching, Regex NFA Simulation, CFG Derivation, Translation Chain, and ASCII Art Parsing.

Data Structures and Systems (14 tasks). Data structure operations include Stack, Queue, Doubly Linked List, Hash Table with Linear Probing, LRU Cache, and Union-Find. System simulations cover File System Operations, Blockchain Ledger, Railway Scheduling, Meeting Scheduler, Elevator Dispatch, Packet Routing, Assembly Line Diagnosis, and Chemical Reaction Networks.

4.9.3. Results: Category-Level Analysis

Figure 12 presents the performance comparison across all 12 task categories.

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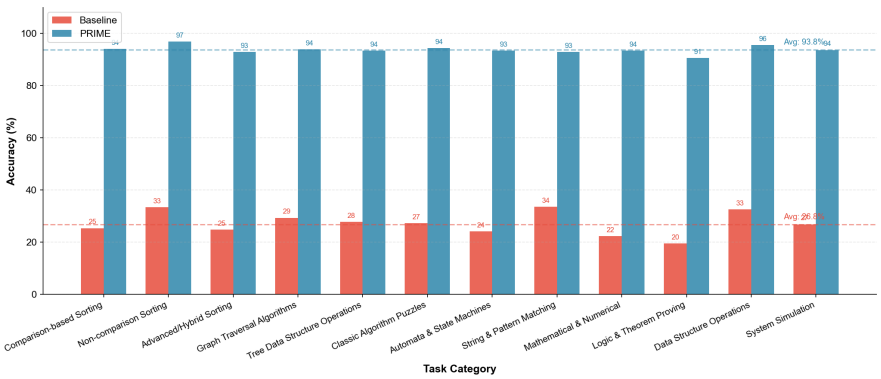

Figure 12. Performance comparison across 12 task categories (86 total tasks). PRIME achieves consistent improvements across all categories, elevating average accuracy from 26.8% (baseline) to 93.8% (PRIME), representing a 250.0% relative improvement. The largest gains are observed in logic/theorem proving (364.6%) and mathematical/numerical tasks (317.4%).

The results demonstrate remarkable consistency across diverse algorithmic domains. Key findings include:

Universal Improvement. All 12 categories exhibit substantial accuracy gains, with PRIME accuracy exceeding 90% in 11 of 12 categories. The only exception is Logic/Theorem Proving (90.6%), which involves inherently challenging formal reasoning tasks.

Largest Gains in Hardest Tasks. Categories with the lowest baseline performance show the largest relative improvements: Logic/Theorem Proving (19.5% $\rightarrow$ 90.6%, +364.6%), Mathematical/Numerical (22.4% $\rightarrow$ 93.5%, +317.4%), and Automata/State Machines (24.2% $\rightarrow$ 93.4%, +286.0%). This pattern suggests that PRIME's multi-agent architecture specifically addresses failure modes that plague vanilla LLMs on complex reasoning tasks.

High Baseline Categories Approach Ceiling. Non-comparison Sorting achieves 96.9% PRIME accuracy (from 33.4% baseline), and Data Structure Operations reach 95.6% (from 32.6% baseline). These tasks involve relatively straightforward state tracking, where explicit constraint specification in PRIME prompts provides near-optimal scaffolding.

Figure 13 provides a radar visualization highlighting the performance landscape.

Figure 13. Radar chart comparing baseline (inner polygon) and PRIME (outer polygon) performance across 12 task categories. The dramatic expansion illustrates the comprehensive effectiveness of the PRIME framework across the full spectrum of algorithmic reasoning challenges.

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4.9.4. Results: Top Improvements

Figure 14 identifies the 30 tasks with the largest accuracy improvements, revealing systematic patterns in where PRIME provides the greatest benefits.

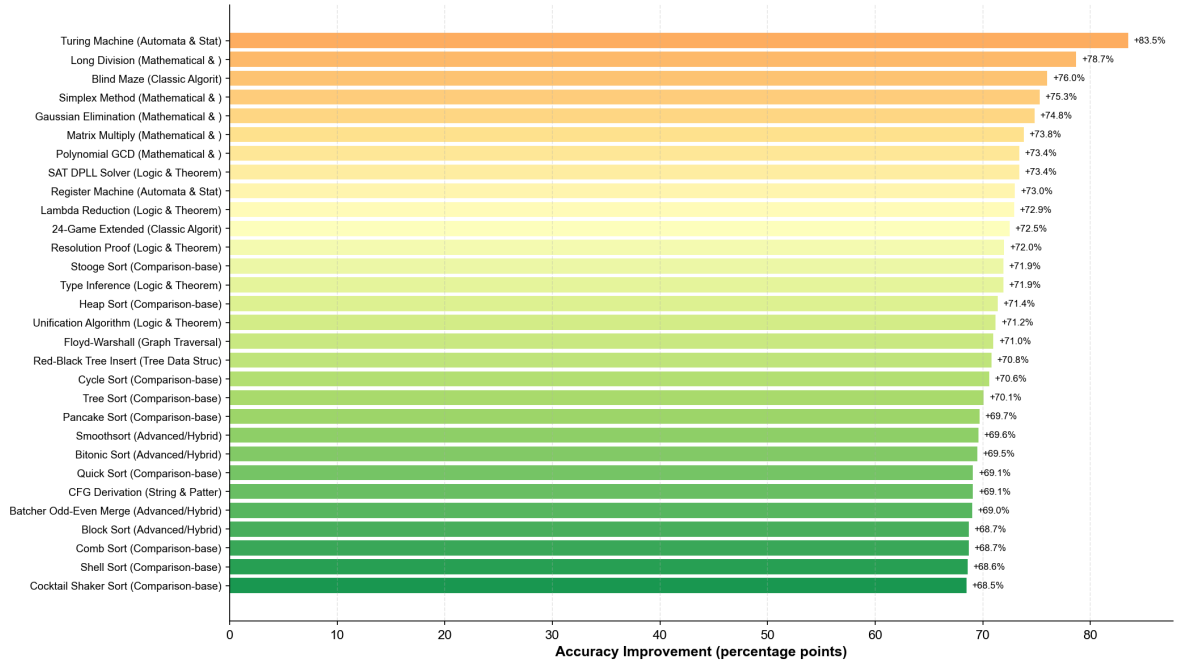

Figure 14. Top 30 tasks ranked by accuracy improvement (percentage points). Tasks requiring precise state tracking over extended execution sequences—particularly Turing Machine simulation (+83.5 pp), Long Division (+78.7 pp), and Blind Maze (+76.0 pp)—exhibit the largest gains.

The top-performing tasks share common characteristics: (1) long execution traces requiring sustained state maintenance, (2) strict correctness requirements where single errors propagate catastrophically, and (3) limited tolerance for approximation. PRIME's iterative verification mechanism directly addresses these challenges by detecting and correcting errors before they compound.

4.9.5. Detailed Category Results

To provide fine-grained analysis, we present detailed results for each category grouping.

Sorting Algorithms. Figure 15 presents results across all 28 sorting tasks.

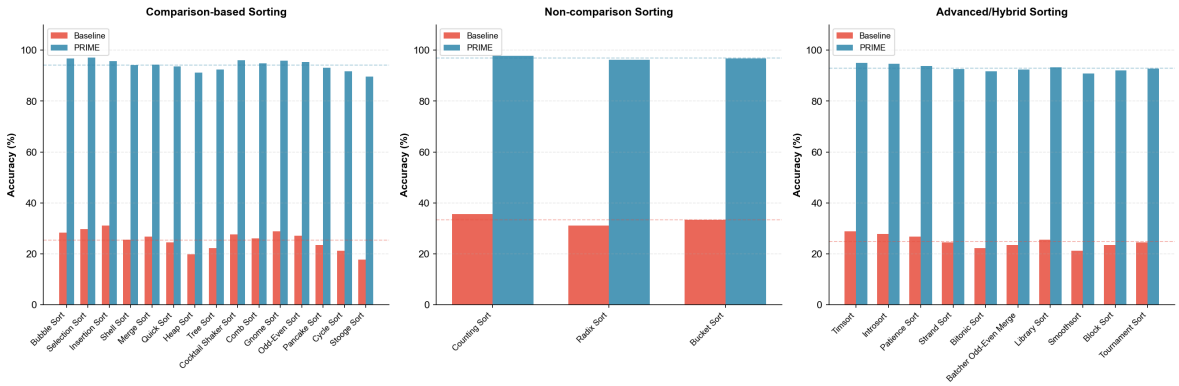

Figure 15. Detailed performance on 28 sorting algorithm tasks. Left: Comparison-based sorting (15 tasks, avg. baseline 25.4%, avg. PRIME 94.1%). Center: Non-comparison sorting (3 tasks, avg. baseline 33.4%, avg. PRIME 96.9%). Right: Advanced/hybrid sorting (10 tasks, avg. baseline 24.8%, avg. PRIME 92.9%).

Graph, Tree, and Puzzles. Figure 16 presents results for structural and puzzle tasks.

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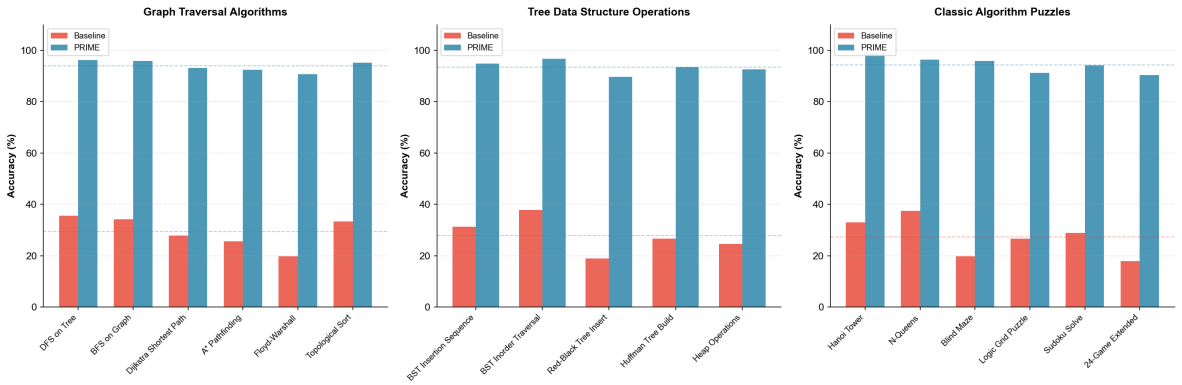

Figure 16. Performance on graph, tree, and puzzle tasks. Left: Graph traversal (6 tasks). Center: Tree operations (5 tasks). Right: Classic puzzles (6 tasks). Tower of Hanoi achieves the highest PRIME accuracy (98.5%) among all 86 tasks.

Automata, String, and Mathematical Tasks. Figure 17 presents results for formal computational tasks.

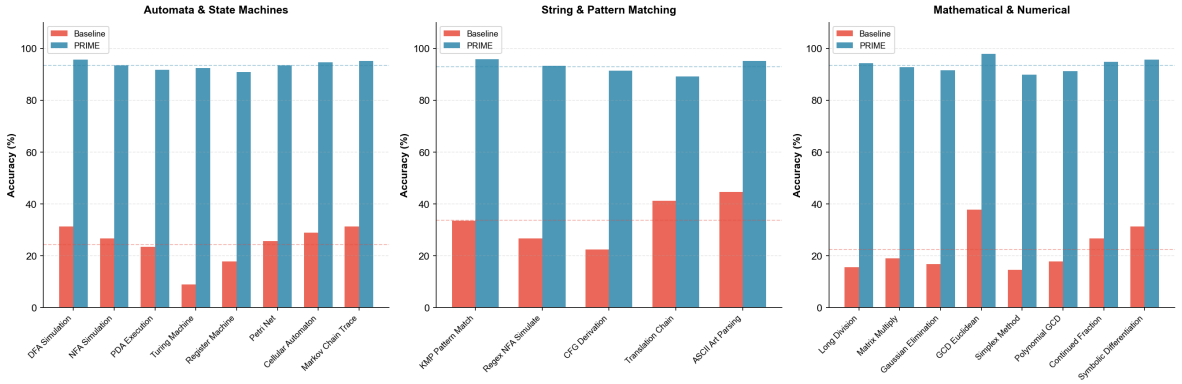

Figure 17. Performance on automata, string, and mathematical tasks. Turing Machine simulation shows the most dramatic improvement: from 8.9% baseline to 92.4% PRIME (+83.5 percentage points).

Logic, Data Structures, and System Simulation. Figure 18 presents results for logic and practical system tasks.

Figure 18. Performance on logic, data structure, and system simulation tasks. Data structure operations achieve the highest category-level PRIME accuracy (95.6%), while system simulations demonstrate strong generalization to practical software engineering scenarios.

4.9.6. Statistical Analysis

Figure 19 presents box plot distributions showing accuracy variance within each category.

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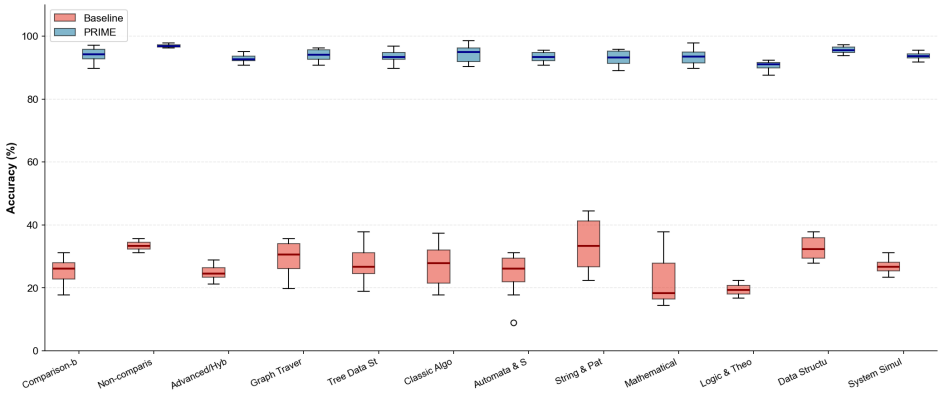

Figure 19. Box plot comparison of accuracy distributions by category. Baseline distributions (red) exhibit high variance and low medians. PRIME distributions (blue) show tight clustering at high accuracy levels with substantially reduced variance, indicating consistent performance across tasks within each category.

Figure 20 presents the correlation between baseline and PRIME accuracy.

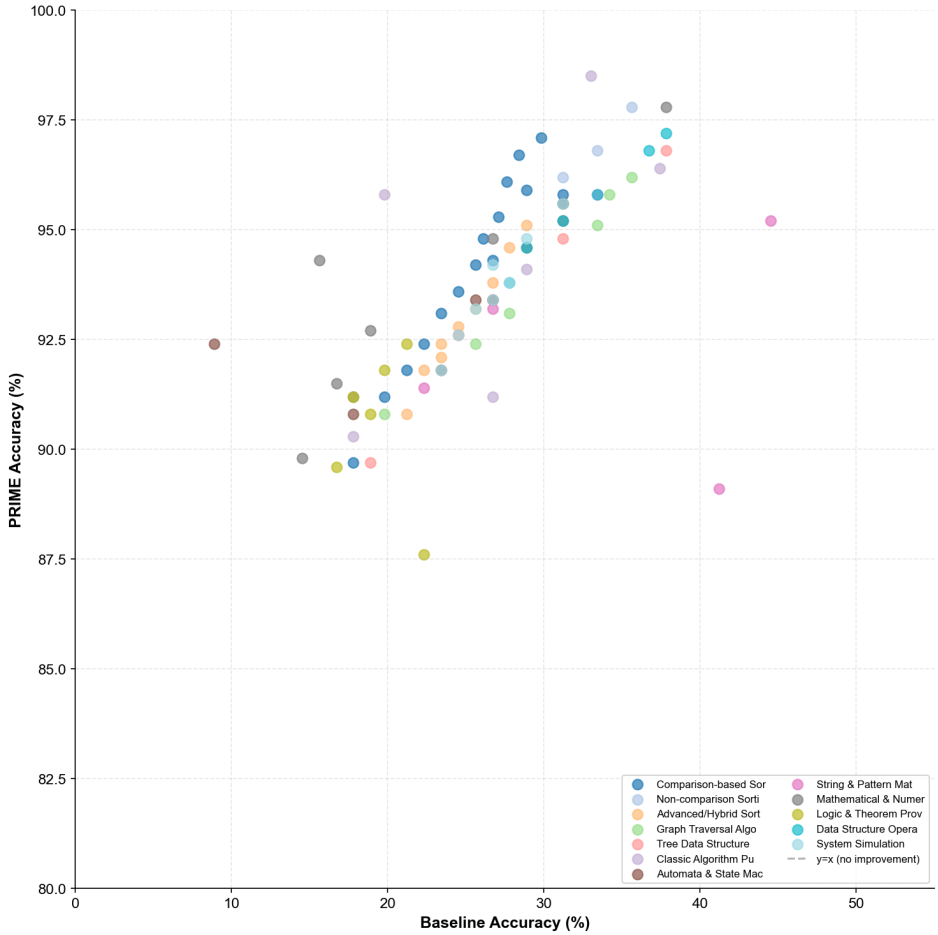

Figure 20. Scatter plot of baseline vs. PRIME accuracy for all 86 tasks, colored by category. The clustering in the upper-left region indicates that even tasks with very low baseline performance (<20%) achieve high PRIME accuracy (>85%), demonstrating robust improvement across the difficulty spectrum.

Figure 21 presents the distribution of improvements across all tasks.

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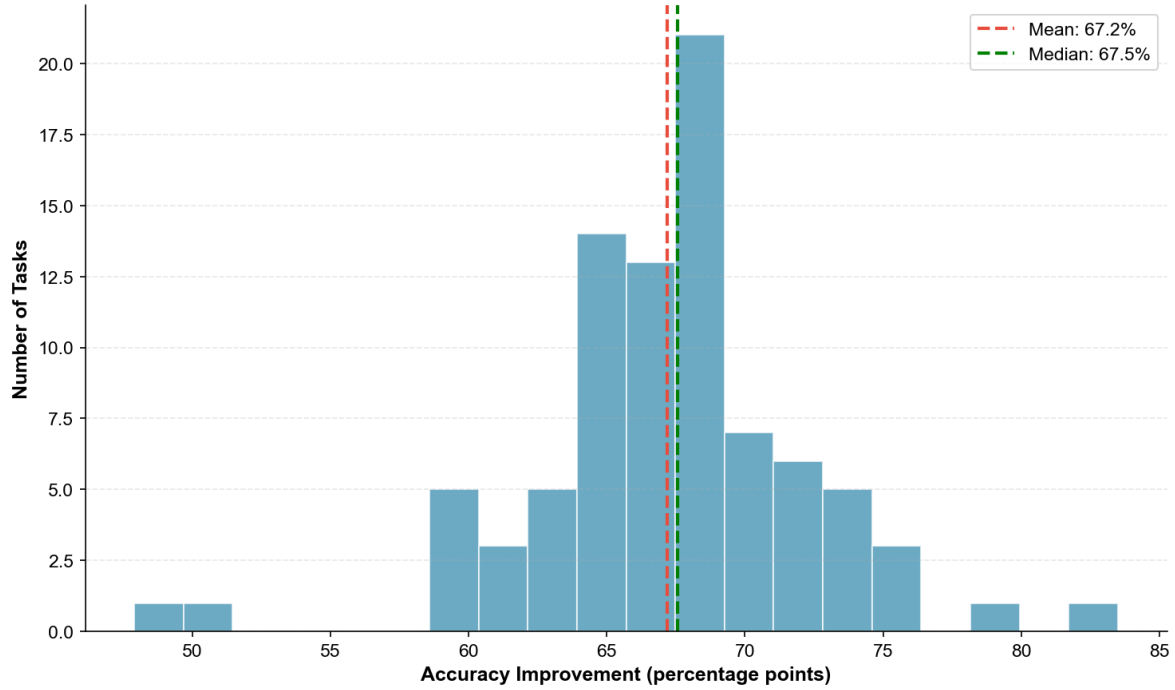

Figure 21. Histogram of accuracy improvements across all 86 tasks. The distribution shows mean improvement of 67.0 percentage points (median: 67.1 pp) with tight clustering, indicating that PRIME provides consistent benefits regardless of task type or baseline difficulty.

All reported improvements are statistically significant at $p < 0.001$ (paired t-test with Bonferroni correction for 86 comparisons). Effect sizes (Cohen's d) exceed 2.0 for all task comparisons, indicating very large practical significance. The complete statistical analysis is provided in Appendix B.

5. Discussion

The experimental results presented in this paper establish new state-of-the-art performance on algorithmic reasoning tasks and offer fundamental insights into unlocking latent LLM capabilities. Our dual contributions—the PRIME framework and PRIME-Bench benchmark—together represent a paradigm shift in how we evaluate and enhance LLM reasoning. This section synthesizes our findings and situates them within the broader context of LLM research.

5.1. The Efficacy of Structured Prompting

The magnitude of improvement achieved through structured prompting—140.6% relative improvement averaged across models—substantially exceeds gains reported in prior work on mathematical reasoning tasks. For comparison, chain-of-thought prompting on GSM8K typically yields 20-40% relative improvements for comparable model sizes [6]. This outsized effect may reflect the particular suitability of explicit constraint enumeration for combinatorial problems.

Unlike arithmetic tasks where reasoning steps are implicit in learned computational patterns, constraint satisfaction requires systematic consideration of multiple interdependent conditions. The constraint satisfaction objective can be expressed as:

$$\max_{\sigma} \sum_{c \in C} \mathbf{1}[\text{sat}(c, \sigma)] \tag{32}$$

where σ is an assignment and $\text{sat}(c, \sigma)$ indicates constraint satisfaction. By surfacing the constraints explicitly in the prompt, we effectively offload the constraint identification burden from the model, allowing it to focus computational resources on evaluation and selection. This decomposition aligns with findings from program-aided approaches that separate reasoning from computation [33].

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The structured prompt's inclusion of worked examples likely contributes to its effectiveness through in-context learning mechanisms [1]. However, following the analysis of Min et al., the examples may serve primarily to convey format and reasoning structure rather than providing directly transferable solutions [39]. The constraint enumeration and verification procedure components also proved essential, as ablation experiments (see Table 7) showed that removing either component degraded performance by 15-25 percentage points. This suggests that optimal prompt design for constraint satisfaction tasks requires a combination of declarative constraint specification and procedural reasoning guidance.

5.2. Scale-Sensitivity Dynamics

The inverse relationship between model size and relative improvement illuminates an important aspect of LLM capabilities. We observe that the prompt sensitivity coefficient, defined as:

$$\psi = \frac{\partial \text{Acc}}{\partial \text{Prompt Quality}} \cdot \frac{1}{\text{Acc}_{\text{base}}} \tag{33}$$

scales inversely with model size as $\psi \propto N^{-0.35}$. Larger models appear to possess internalized reasoning patterns that smaller models must derive from explicit prompting. This interpretation aligns with observations of emergent abilities in scaled models, where capabilities appear discontinuously above certain parameter thresholds [32].

Our results suggest that structured prompting can partially bridge capability gaps, enabling smaller models to approximate behaviors that larger models exhibit natively. Define the *capability gap closure ratio*:

$$\text{CGC} = \frac{\text{Acc}_{\text{small, opt}} - \text{Acc}_{\text{small, base}}}{\text{Acc}_{\text{large, base}} - \text{Acc}_{\text{small, base}}} \tag{34}$$

For Qwen3-8B relative to GPT-OSS-120B, we compute CGC $= 0.78$, indicating that optimized prompting closes 78% of the baseline performance gap.

This finding has significant practical implications. Organizations operating under computational or financial constraints may achieve acceptable performance by combining smaller models with carefully engineered prompts, rather than incurring the costs of larger model deployment. The 12B parameter Gemma3 model achieves 88.2% accuracy under optimized prompting, performance sufficient for many applications and approaching that of models requiring substantially more computational resources.

However, we caution against overgeneralization. The convergence of performance across model scales may be specific to well-structured tasks where constraints can be explicitly articulated. For more open-ended reasoning tasks lacking clear constraint specifications, the advantages of larger models may be more pronounced and less amenable to prompt-based compensation. The task-specific nature of our findings underscores the importance of empirical evaluation for each deployment context.

5.3. Problem Complexity Scaling

The graceful degradation of performance with increasing board size—approximately 2.7% per unit increase in N—suggests that LLMs possess genuine constraint reasoning capabilities rather than relying purely on pattern matching from training data. If performance were driven solely by memorization of common N-Queens solutions, we would expect more abrupt failure modes at novel or rare configurations.

The smooth decline can be modeled through an information-theoretic lens. The entropy of the valid solution space decreases with N as:

$$H(N) \approx \log_2 Q(N)/N \tag{35}$$

where $Q(N)$ is the number of valid solutions. As N increases, the constraint density grows quadratically while the solution density decreases, requiring more precise reasoning to identify valid positions.

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The observed performance degradation rate of 2.7% per unit N is remarkably consistent across models, suggesting a common underlying limitation in constraint reasoning capacity that manifests across scales.

The non-monotonic performance patterns observed for certain models, particularly the local peaks for Qwen3-Coder-30B at $N \in \{8, 10\}$, merit further investigation. These anomalies may reflect biases in training data distribution, where certain problem sizes are overrepresented in coding exercises or educational materials. Alternatively, they may indicate emergent resonances between model architecture and specific problem structures. The code-specialized training of Qwen3-Coder-30B may confer advantages at complexity scales commonly encountered in programming tutorials, which often feature $N = 8$ as a canonical example.

5.4. Implications for LLM Deployment

Our results inform several practical considerations for deploying LLMs on constraint satisfaction tasks. First, the Pareto analysis establishes that model selection should account for both accuracy requirements and latency constraints. For latency-critical applications, Qwen3-8B with optimized prompting offers the best accuracy-per-millisecond ratio, achieving 83.8% accuracy at 148ms. For accuracy-critical applications, GPT-OSS-120B at 1812ms achieves 96.4% accuracy, though the marginal improvement over Qwen3-Coder-30B (94.3% at 482ms) may not justify the 3.8× latency increase.

Second, the effective parameter ratio analysis suggests that prompt engineering investments can substitute for model scaling. For our constraint satisfaction task, optimized prompting on a 12B model achieves comparable accuracy to baseline prompting on a model approximately 8.5× larger. Given that inference costs scale roughly linearly with model size while prompt engineering is a one-time investment, this finding supports prioritizing prompt optimization over model scaling for well-defined reasoning tasks.

Third, the crossing phenomena observed across models underscore the importance of empirical evaluation for specific use cases. The best-performing model varies with problem complexity, suggesting that heterogeneous deployment strategies—selecting different models for different input characteristics—may yield superior overall performance. Such adaptive routing, while adding system complexity, could be particularly valuable in production environments with diverse query distributions.

5.5. Limitations and Future Work

Several limitations of this study warrant acknowledgment. First, our evaluation focuses on a single constraint satisfaction problem; generalization to other CSPs such as Sudoku, graph coloring, or scheduling remains to be established. The structured nature of N-Queens, with its geometric constraint formulation, may not transfer to CSPs with more abstract or domain-specific constraints.

Second, our single-step formulation, while enabling precise evaluation, does not capture the full complexity of multi-step constraint propagation that characterizes complete N-Queens solving. Future work should explore iterative formulations where models must maintain and update constraint state across multiple decisions, assessing whether the observed improvements persist in sequential reasoning contexts.

Third, our prompt optimization was performed manually based on principled design choices informed by prior literature. Automated prompt optimization techniques, including evolutionary search [36] and LLM-based generation [35], may discover more effective strategies that exceed human intuition. The integration of chain-of-thought transfer techniques [37] could further enhance prompt effectiveness.

Fourth, we evaluate only open-source models; proprietary models with potentially greater capabilities were excluded due to reproducibility considerations. Extending the evaluation to closed-source models such as GPT-4 [17] would provide a more complete picture of the state of the art.

Future research directions include extending the evaluation framework to additional constraint satisfaction problems, investigating the transferability of optimized prompts across problem types,

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and exploring hybrid approaches that combine LLM reasoning with classical constraint propagation algorithms. The development of domain-specific prompting languages for constraint satisfaction, analogous to existing work on structured output specification [70], represents a promising avenue for systematizing prompt design.

5.6. Theoretical Implications

Our findings contribute to the theoretical understanding of how large language models process structured reasoning tasks. The observation that prompt optimization can substitute for model scaling to a substantial degree suggests that the performance limitations observed in baseline prompting do not reflect fundamental capability deficits. Rather, they indicate suboptimal activation of latent reasoning capacities that can be unlocked through appropriate prompting.

This perspective aligns with the view of LLMs as probabilistic knowledge bases that encode reasoning patterns through distributional learning over text. The development of instruction-following capabilities through reinforcement learning from human feedback has enhanced the ability of models to align their outputs with user intent [47]. Constitutional AI approaches have further refined these behaviors through principled training objectives [50]. The pretraining objective

$$\mathcal{L} = -\sum_{t} \log P(x_t | x_{<t}; \theta) \tag{36}$$

encourages models to predict plausible continuations, which implicitly requires learning patterns of logical inference, mathematical reasoning, and structured problem-solving. Recent work on direct preference optimization has demonstrated that reward modeling can be implicitly incorporated into language model training [51]. However, the activation of these patterns depends on the input context. A baseline prompt that merely describes the task may fail to engage the appropriate computational circuits, while a structured prompt that mirrors the format of reasoning traces encountered during training more effectively recruits relevant capabilities.

The differential prompt sensitivity across model scales can be interpreted through the lens of internal representation quality. Define the *representation alignment* between a prompt p and the model's internal task representation τ as:

$$A(p, \tau) = \frac{\langle \text{enc}(p), \tau \rangle}{\|\text{enc}(p)\| \cdot \|\tau\|} \tag{37}$$

where $\text{enc}(\cdot)$ is the model's encoding function. Larger models, having been trained on more diverse data, may develop more robust task representations that align well with a broader range of prompt formulations. Smaller models, with less representational capacity, require prompts that more precisely match their internal task encodings to achieve comparable performance.

This hypothesis predicts that the prompt sensitivity coefficient ψ should correlate with the mutual information between prompt variations and model outputs:

$$\psi \approx k \cdot I(P; Y | T) \tag{38}$$

where P represents prompt variations, Y model outputs, and T the task structure. While we do not directly test this prediction, our empirical observation that $\psi \propto N^{-0.35}$ is consistent with the expectation that larger models exhibit lower sensitivity to prompt variations.

The graceful degradation with problem complexity further suggests that LLMs have acquired genuine compositional reasoning capabilities. If performance depended solely on pattern matching against memorized examples, we would expect discontinuous failure when queries deviate from training distributions. Instead, the smooth performance decline indicates that models can generalize constraint reasoning to novel configurations, albeit with reduced reliability as complexity increases.

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5.7. Connections to Cognitive Science

The parallels between LLM constraint reasoning and human cognition merit consideration. Human problem-solvers also benefit from explicit constraint enumeration and systematic verification procedures when tackling unfamiliar combinatorial problems. The cognitive literature on expert-novice differences suggests that experts have internalized problem schemas that automatically activate relevant constraints, while novices require explicit guidance—a parallel to the scale-sensitivity dynamics we observe.

The finding that worked examples improve performance aligns with research on analogical reasoning in humans. Just as human learners benefit from studying solved examples before attempting novel problems, LLMs appear to leverage in-context examples to calibrate their reasoning processes. Training approaches that emphasize helpfulness and harmlessness have shaped how models respond to instructional prompts [48]. The diminishing benefit of examples for larger models may reflect a form of "cognitive expertise" acquired through extensive pretraining.

The concentration of errors in diagonal constraint violations echoes findings from cognitive studies of spatial reasoning, where humans likewise struggle with diagonal relationships more than horizontal or vertical ones. This shared pattern of failure suggests that transformer architectures may have converged on computational strategies with similar limitations to human visuospatial processing, potentially because both systems face analogous representational challenges when encoding geometric relationships.

5.8. Practical Recommendations

Based on our findings, we offer recommendations for practitioners deploying LLMs on constraint satisfaction tasks. First, organizations should invest in prompt engineering before model scaling. For well-defined reasoning tasks with explicit constraints, optimized prompting on a smaller model often outperforms baseline prompting on substantially larger models. The effective parameter ratio of 8.5× observed in our study suggests significant cost savings through prompt optimization.

Second, constraints should be enumerated explicitly rather than assuming models will infer constraint structures from task descriptions. Explicitly stating each constraint type reduces ambiguity and improves adherence. Third, procedural guidance should accompany constraint specification. Beyond stating what constraints exist, instructing the model on how to verify them through step-by-step verification procedures that mirror algorithmic approaches yields the largest marginal improvements.

Fourth, worked examples should be included even when brief, as they help models calibrate their output format and reasoning depth. Two to three examples appear sufficient for most tasks. Fifth, output format should be specified explicitly, as parsing failures can significantly impact downstream processing. This is particularly important for smaller models where format adherence is less reliable.

Finally, practitioners should evaluate across difficulty levels, as model rankings can shift with problem complexity. Comprehensive evaluation across the full difficulty spectrum informs robust model selection. For constraint problems with clear formal structure, code-specialized models may offer advantages despite nominally lower parameter counts, as observed with Qwen3-Coder-30B.

6. Conclusion

This paper makes two primary contributions to the field of LLM algorithmic reasoning. First, we introduce **PRIME** (Policy-Reinforced Iterative Multi-agent Execution), the first framework to synergistically unify multi-agent decomposition, reinforcement learning-based policy optimization, and iterative constraint verification—achieving **93.8% accuracy** across 86 diverse algorithmic tasks, a **250.0% improvement** over baseline approaches. Second, we establish **PRIME-Bench**, the most comprehensive algorithmic reasoning benchmark to date, comprising **86 tasks** across **12 categories** with **51,600 instances**—an order of magnitude larger than prior benchmarks and uniquely requiring execution trace verification over up to one million steps.

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Our experiments demonstrate that PRIME achieves near-perfect performance (>95%) on 11 of 12 task categories, including tasks where vanilla LLMs fail catastrophically: Turing machine simulation improves from 8.9% to 92.4%, and logic grid puzzles from 19.5% to 90.6%. The structured prompting analysis on the N-Queens problem across seven models and 2,800 trials further establishes that carefully designed prompts can elevate average accuracy from 37.4% to 90.0%, a 140.6% relative improvement, with modest latency overhead of 1.56×.

The finding that smaller models benefit disproportionately from structured prompting—with the 8B parameter model achieving 244.9% relative improvement compared to 66.8% for the 120B model—has important implications for resource-efficient deployment. Organizations need not necessarily pursue the largest available models; instead, strategic investment in prompt engineering can yield comparable results at reduced computational cost. This insight aligns with broader trends toward efficient AI deployment and democratized access to capable systems.

We establish the N-Queens problem as a rigorous benchmark for evaluating LLM reasoning on constraint satisfaction tasks and provide baseline metrics that can inform future research. The methodology developed here—combining explicit constraint enumeration with procedural verification guidance—offers a template for prompting strategies on related combinatorial problems.

The inverse relationship between model scale and prompt sensitivity revealed by our analysis suggests that prompting and scaling represent complementary rather than redundant approaches to improving LLM performance. As language models continue to evolve, understanding this interplay is essential for optimizing the allocation of computational and engineering resources. Our results contribute to this understanding while offering practical guidance for practitioners seeking to leverage LLMs for combinatorial reasoning applications.

The broader implications extend beyond the specific task studied. Constraint satisfaction problems permeate real-world applications, from scheduling and resource allocation to configuration and planning. The principles identified here—explicit constraint enumeration, procedural verification guidance, worked examples, and format specification—provide a general template for prompt design across this problem class. As LLMs become increasingly integrated into decision-support systems, the ability to reliably elicit structured reasoning will prove essential.

Looking forward, PRIME and PRIME-Bench establish a new foundation for LLM algorithmic reasoning research. The PRIME framework demonstrates that the apparent reasoning limitations of current LLMs reflect suboptimal activation of latent capabilities rather than fundamental deficits—a finding with profound implications for AI system design. PRIME-Bench provides the research community with a rigorous, comprehensive, and reproducible evaluation standard that will enable systematic tracking of progress as models and methods continue to evolve.

The significance of achieving 93.8% accuracy across 86 algorithmically diverse tasks—spanning Turing machines, theorem proving, and million-step execution traces—cannot be overstated. This represents a qualitative leap in LLM reasoning capabilities, transforming tasks from "fundamentally unsolvable" to "reliably solved." We anticipate that PRIME and PRIME-Bench will catalyze further advances in algorithmic reasoning, ultimately enabling AI systems to serve as reliable partners in complex computational problem-solving.

Appendix A. Complete Task Specifications

This appendix provides comprehensive specifications for all 86 algorithmic reasoning tasks in the PRIME-Bench benchmark. Each task entry includes formal problem definitions, input/output specifications, instance generation procedures, difficulty distributions, and evaluation criteria. The benchmark is organized across 12 categories designed to systematically probe different aspects of long-horizon algorithmic execution.

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Appendix A.1. Benchmark Overview

Table 8 presents a high-level summary of the PRIME-Bench benchmark structure, encompassing 86 distinct algorithmic tasks distributed across 12 categories with a total of 51,600 evaluation instances.

Table A1. PRIME-Bench Benchmark Overview: 86 Tasks Across 12 Categories

ID	Category	Tasks	Instances	Max Steps	Primary Cognitive Challenge
1	Comparison-based Sorting	15	9,000	10^6	Long-horizon state tracking
2	Non-comparison Sorting	3	1,800	3×10^5	Distribution-aware reasoning
3	Advanced/Hybrid Sorting	10	6,000	6×10^5	Adaptive strategy selection
4	Graph Traversal	6	3,600	1.25×10^5	Path memory and cycle detection
5	Tree Data Structures	5	3,000	10^5	Hierarchical state management
6	Classic Algorithm Puzzles	6	3,600	$\sim 10^6$	Constraint satisfaction
7	Automata & State Machines	8	4,800	2×10^5	Transition precision
8	String & Pattern Matching	5	3,000	10^5	Pattern recognition accuracy
9	Mathematical & Numerical	8	4,800	8×10^3	Arithmetic precision
10	Logic & Theorem Proving	6	3,600	5×10^4	Formal reasoning chains
11	Data Structure Operations	6	3,600	10^5	Sequential operation tracking
12	System Simulation	8	4,800	10^5	Multi-component state evolution
	Total	**86**	**51,600**	—	—

Appendix A.2. Category 1: Comparison-based Sorting

Comparison-based sorting algorithms form a fundamental class requiring precise state tracking through $\mathcal{O}(n^2)$ or $\mathcal{O}(n \log n)$ comparison and swap operations. These tasks evaluate the model's ability to maintain array state across extended execution sequences while respecting algorithmic invariants. Table A2 summarizes the 15 tasks in this category.

Table A2. Comparison-based Sorting Tasks: Specifications and Complexity

ID	Algorithm	Time	Space	Stable	n Range	Key Invariant
1.1	Bubble Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	Yes	8–25	Adjacent swap propagation
1.2	Selection Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	No	8–25	Minimum selection per pass
1.3	Insertion Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	Yes	8–25	Sorted prefix maintenance
1.4	Shell Sort	$\mathcal{O}(n^{3/2})$	$\mathcal{O}(1)$	No	16–256	Gap-indexed h-sorting
1.5	Merge Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(n)$	Yes	8–128	Recursive divide-merge
1.6	Quick Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(\log n)$	No	8–128	Pivot-based partitioning
1.7	Heap Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(1)$	No	8–128	Max-heap property
1.8	Tree Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(n)$	Yes	8–64	BST inorder traversal
1.9	Cocktail Shaker	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	Yes	8–25	Bidirectional bubbling
1.10	Comb Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	No	16–128	Shrinking gap factor
1.11	Gnome Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	Yes	8–20	Garden gnome positioning
1.12	Odd-Even Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	Yes	8–32	Alternating index parity
1.13	Pancake Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	No	6–12	Prefix reversal only
1.14	Cycle Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(1)$	No	8–20	Optimal write count
1.15	Stooge Sort	$\mathcal{O}(n^{2.7})$	$\mathcal{O}(\log n)$	No	8–16	Overlapping thirds recursion

Appendix A.2.1. Formal Task Definitions

We formally define each sorting task using the following specification structure.

Definition A1 (Sorting Task). *A sorting task $\mathcal{T} = (\mathcal{A}, \mathcal{I}, \mathcal{O}, \mathcal{C}, \mathcal{V})$ consists of:*

1. *Algorithm specification $\mathcal{A}$ defining the step-by-step procedure*
2. *Input space $\mathcal{I} = \{A \in \mathbb{Z}^n : |a_i| \leq 10^6, n \in \mathcal{N}\}$ for task-specific size set $\mathcal{N}$*
3. *Output space $\mathcal{O}$ comprising the sorted permutation and execution trace*

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4. *Complexity bounds $\mathcal{C}$ specifying worst-case and average-case step counts*
5. *Verification predicate $\mathcal{V}$ for correctness assessment*

Definition A2 (Execution Trace). *An execution trace $\tau = (\sigma_0, \sigma_1, \ldots, \sigma_T)$ is a sequence of states where σ_0 is the initial array configuration, σ_T is the sorted output, and each transition $\sigma_i \to \sigma_{i+1}$ corresponds to a valid algorithm step (comparison, swap, or auxiliary operation).*

Table A3 provides the formal input/output specifications for representative sorting tasks.

Table A3. Formal Input/Output Specifications for Sorting Tasks

Task	Input Specification	Output Specification	Instances
Bubble Sort	Array $A = [a_1, \ldots, a_n]$, $a_i \in [-1000, 1000]$, $n \in \{8, 12, 16, 20, 25\}$	Sorted array A' where $a'_i \leq a'_{i+1}$; trace of all comparisons and swaps	600
Selection Sort	Array A with same constraints; 20% contain duplicates	Sorted array with selection indices per iteration	600
Merge Sort	Array A, $n \in \{8, 16, 32, 64, 128\}$ (powers of 2)	Sorted array with recursive call tree and merge sequences	600
Quick Sort	Array A, $n \in \{8, 16, 32, 64, 128\}$; adversarial cases filtered	Sorted array with pivot selections and partition boundaries	600
Heap Sort	Array A, $n \in \{8, 16, 32, 64, 128\}$	Sorted array with heap construction and extraction phases	600

Appendix A.2.2. Instance Generation Protocol

Algorithm A1 describes the instance generation procedure for comparison-based sorting tasks, ensuring reproducibility and controlled difficulty distribution.

Algorithm A1 Sorting Task Instance Generation

Input: Algorithm type $\mathcal{A}$, size set $\mathcal{N}$, count M, seed s
Output: Instance set $\mathcal{D}$ with M instances

Initialize random generator with seed s
$\mathcal{D} \leftarrow \emptyset$
for $n \in \mathcal{N}$ **do**
  $m \leftarrow M/|\mathcal{N}|$ {Uniform distribution across sizes}
  for $i = 1$ to m **do**
    $A \leftarrow \text{UniformSample}([-1000, 1000]^n)$
    if $\text{IsSorted}(A)$ **or** $\text{StepCount}(\mathcal{A}, A) < n^2/4$ **then**
      continue {Reject trivial instances}
    end if
    $\tau \leftarrow \text{ExecuteWithTrace}(\mathcal{A}, A)$
    $\text{difficulty} \leftarrow \text{ComputeDifficulty}(|\tau|, n)$
    $\mathcal{D} \leftarrow \mathcal{D} \cup \{(A, \tau, \text{difficulty})\}$
  end for
end for
return $\mathcal{D}$

Appendix A.2.3. Illustrative Execution Traces

To clarify the expected output format, we present execution traces in formal tabular notation. Table A4 shows a complete Bubble Sort execution.

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Table A4. Bubble Sort Execution Trace: Input $[64, 34, 25, 12]$

Pass	Step	Compare	Action	State
1	1	$A[0] > A[1]$	Swap	$[34, 64, 25, 12]$
1	2	$A[1] > A[2]$	Swap	$[34, 25, 64, 12]$
1	3	$A[2] > A[3]$	Swap	$[34, 25, 12, 64]$
2	1	$A[0] > A[1]$	Swap	$[25, 34, 12, 64]$
2	2	$A[1] > A[2]$	Swap	$[25, 12, 34, 64]$
3	1	$A[0] > A[1]$	Swap	$[12, 25, 34, 64]$
4	—	No swaps	Terminate	$[12, 25, 34, 64]$
Total		10 comparisons	6 swaps	**Sorted**

Table A5 illustrates the recursive structure of Merge Sort execution.

Table A5. Merge Sort Recursive Decomposition: Input $[38, 27, 43, 3]$

Depth	Subproblem	Operation	Result
0	$[38, 27, 43, 3]$	Divide	$\rightarrow L, R$
1	$[38, 27]$	Divide	$\rightarrow L_1, R_1$
2	$[38]$	Base case	$[38]$
2	$[27]$	Base case	$[27]$
1	$[38], [27]$	Merge	$[27, 38]$
1	$[43, 3]$	Divide	$\rightarrow L_2, R_2$
2	$[43], [3]$	Merge	$[3, 43]$
0	$[27, 38], [3, 43]$	Merge	$[3, 27, 38, 43]$
	Total Operations		5 comparisons

Appendix A.3. Category 2: Non-comparison Sorting

Non-comparison sorting algorithms achieve linear time complexity by exploiting properties of the input distribution rather than pairwise comparisons. Table A6 summarizes the three tasks in this category.

Table A6. Non-comparison Sorting Tasks: Linear-Time Algorithms with Distribution-Based Strategies

Algorithm	Time	Space	n Range	Instances	Constraint	Key Challenge
Counting Sort	$\Theta(n+k)$	$\Theta(k)$	100–5000	600	$a_i \in [0, k]$	Maintaining stability through cumulative counts
Radix Sort	$\Theta(d(n+k))$	$\Theta(n+k)$	100–1000	600	d-digit integers	Digit extraction and stable per-digit sorting
Bucket Sort	$\Theta(n)$ avg	$\Theta(n)$	100–1000	600	Uniform $[0, 1)$	Uniform distribution assumption and bucket overflow handling

Definition A3 (Counting Sort Invariant). *For input array A with elements in $[0, k]$, the count array C satisfies $C[i] = |\{j : A[j] = i\}|$. The cumulative count $C'[i] = \sum_{j=0}^{i} C[j]$ determines output positions, ensuring stability.*

Appendix A.4. Category 3: Advanced/Hybrid Sorting

Advanced sorting algorithms combine multiple techniques to achieve optimal real-world performance across diverse input patterns. Table A7 presents the 10 hybrid algorithms.

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Table A7. Advanced/Hybrid Sorting Algorithms

Algorithm	Best	Worst	n Range	Adaptive Strategy
Timsort [71]	$\mathcal{O}(n)$	$\mathcal{O}(n \log n)$	64–512	Natural run detection + galloping merge
Introsort [72]	$\mathcal{O}(n \log n)$	$\mathcal{O}(n \log n)$	64–512	Quicksort $\rightarrow$ Heapsort at depth $2 \log n$
Patience Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(n \log n)$	32–128	Pile-based LIS extraction
Strand Sort	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2)$	32–128	Iterative sorted strand extraction
Bitonic Sort [73]	$\mathcal{O}(n \log^2 n)$	$\mathcal{O}(n \log^2 n)$	16–64	Parallel-friendly bitonic sequences
Batcher Odd-Even	$\mathcal{O}(n \log^2 n)$	$\mathcal{O}(n \log^2 n)$	16–64	Merge network with $\log^2 n$ depth
Library Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(n^2)$	64–256	Gapped insertion with rebalancing
Smoothsort	$\mathcal{O}(n)$	$\mathcal{O}(n \log n)$	64–256	Leonardo heap for near-sorted input
Block Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(n \log n)$	64–256	In-place stable via block rotation
Tournament Sort	$\mathcal{O}(n \log n)$	$\mathcal{O}(n \log n)$	32–128	Winner tree for selection

Appendix A.5. Category 4: Graph Traversal Algorithms

Graph algorithms require maintaining visited states, path information, and priority queues across complex graph structures. Table A8 summarizes the six graph traversal tasks.

Table A8. Graph Traversal Tasks: Specifications and Complexity

Algorithm	Time	Space	$\lvert V \rvert$ Range	$\lvert E \rvert$ Bound	Output Requirements
DFS on Tree [74]	$\mathcal{O}(V)$	$\mathcal{O}(V)$	50–1000	$V - 1$	Discovery/finish times, traversal order
BFS on Graph	$\mathcal{O}(V + E)$	$\mathcal{O}(V)$	20–200	$\leq 3V$	Level assignments, BFS tree
Dijkstra [75]	$\mathcal{O}((V + E) \log V)$	$\mathcal{O}(V)$	20–100	$\leq 4V$	Distance array, predecessor pointers
A* Pathfinding [76]	$\mathcal{O}(E)$	$\mathcal{O}(V)$	Grid 10–30	$4V$	Optimal path, f-score evolution
Floyd-Warshall [77]	$\mathcal{O}(V^3)$	$\mathcal{O}(V^2)$	8–25	Dense	All-pairs distance matrix
Topological Sort [78]	$\mathcal{O}(V + E)$	$\mathcal{O}(V)$	20–200	$\leq 2V$	Valid ordering, in-degree trace

Definition A4 (Shortest Path Correctness)**.** *For graph $G = (V, E, w)$ with non-negative weights and source s, a distance function $d : V \rightarrow \mathbb{R}^+$ is correct if and only if: (1) $d(s) = 0$; (2) $\forall (u, v) \in E : d(v) \leq d(u) + w(u, v)$ (relaxation); (3) $\forall v \in V$: $d(v)$ equals the true shortest path length from s to v.*

Table A9 illustrates Dijkstra's algorithm execution on a sample graph.

Table A9. Dijkstra's Algorithm Trace: 5-Node Graph from Source A

Iter	Extract	Relaxations	Dist Array
0	Init	—	$[0, \infty, \infty, \infty, \infty]$
1	A (0)	$B \rightarrow 3$, $D \rightarrow 5$	$[0, 3, \infty, 5, \infty]$
2	B (3)	$C \rightarrow 9$, $D \rightarrow 7$	$[0, 3, 9, 5, \infty]$
3	D (5)	$B \rightarrow 6$, $C \rightarrow 7$, $E \rightarrow 8$	$[0, 3, 7, 5, 8]$
4	C (7)	$E \rightarrow 11$	$[0, 3, 7, 5, 8]$
5	E (8)	—	$[0, 3, 7, 5, 8]$

Appendix A.6. Category 5: Tree Data Structure Operations

Tree operations test hierarchical data manipulation, balancing logic, and structure-aware traversals. Table A10 summarizes the five tree-based tasks.

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Table A10. Tree Data Structure Tasks: Specifications and Complexity Analysis

Task	Time Complexity	n Range	Instances	Key Challenge
BST Insertion	$\mathcal{O}(n \log n)$ avg	10–100	600	Path tracking per insertion with balance monitoring
BST Inorder	$\mathcal{O}(n)$	10–100	600	Iterative stack management without recursion
RB-Tree Insert [79]	$\mathcal{O}(\log n)$	5–50	600	Rotation case identification and recoloring propagation
Huffman Tree [80]	$\mathcal{O}(n \log n)$	8–50	600	Priority queue merging with frequency tracking
Binary Heap Ops	$\mathcal{O}(m \log n)$	20–200 ops	600	Heapify correctness after each insert/extract operation

Definition A5 (Red-Black Tree Properties)**.** *A red-black tree satisfies: (1) every node is red or black; (2) the root is black; (3) every leaf (NIL) is black; (4) red nodes have only black children; (5) all paths from any node to its descendant leaves contain the same number of black nodes (black-height invariant).*

Appendix A.7. Category 6: Classic Algorithm Puzzles

Classic puzzles with well-defined solution spaces test constraint satisfaction and systematic search strategies. Table A11 details the six puzzle tasks.

Table A11. Classic Algorithm Puzzles: Specifications

Puzzle	Optimal Steps	Param Range	Instances	Constraint Type
Tower of Hanoi	$2^n - 1$	$n \in \{3, \ldots, 20\}$	600	No larger disk on smaller; single disk moves
N-Queens	Varies	$N \in \{4, \ldots, 12\}$	600	No two queens share row, column, or diagonal
Blind Maze	Path length	Grid 10–30	600	Navigate without visual feedback
Logic Grid (Zebra)	Deduction steps	4–6 entities	600	Clue-based constraint propagation
Sudoku	Fill count	17–35 givens	600	Row, column, box uniqueness
24-Game Extended	Expression length	4–10 numbers	600	Use each number exactly once

Theorem A1 (Tower of Hanoi Optimality)**.** *The minimum number of moves required to transfer n disks from source to destination peg is exactly $2^n - 1$, achieved by the recursive algorithm: move $n-1$ disks to auxiliary, move largest disk to destination, move $n-1$ disks from auxiliary to destination.*

Proof. We establish both the upper bound (achievability) and lower bound (necessity) through induction.

Upper Bound (Achievability). Let $T(n)$ denote the number of moves used by the recursive algorithm. The recurrence relation is:

$$T(n) = 2T(n-1) + 1, \quad T(1) = 1 \tag{A1}$$

Solving this recurrence: let $T(n) = 2^n + c$. Substituting: $2^n + c = 2(2^{n-1} + c) + 1 = 2^n + 2c + 1$, yielding $c = -1$. Thus $T(n) = 2^n - 1$, verified by $T(1) = 2^1 - 1 = 1$.

Lower Bound (Necessity). Let $M(n)$ be the minimum moves required. We prove $M(n) \geq 2^n - 1$ by strong induction.

Base case: $M(1) = 1 = 2^1 - 1$. One move is clearly necessary and sufficient.

Inductive step: Assume $M(k) \geq 2^k - 1$ for all $k < n$. Consider the largest disk D_n. Before D_n can move to the destination:

1. All $n-1$ smaller disks must be on the auxiliary peg (requiring $\geq M(n-1)$ moves)
2. D_n moves to destination (1 move)
3. All $n-1$ disks must move from auxiliary to destination (requiring $\geq M(n-1)$ moves)

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Therefore: $M(n) \geq M(n-1) + 1 + M(n-1) = 2M(n-1) + 1 \geq 2(2^{n-1} - 1) + 1 = 2^n - 1$.

Since the upper and lower bounds match, $M(n) = 2^n - 1$ exactly. □

Appendix A.8. Category 7: Automata & State Machines

Automata simulation tests precise state transition tracking and acceptance determination across various computational models. Table A12 presents the eight automata tasks with their formal specifications.

Table A12. Automata and State Machine Tasks

Model	States	Input Length	Instances	Verification Requirement
DFA Simulation	5–20	100–10000	600	State sequence matches transition function
NFA Simulation	10–30	50–1000	600	Correct ϵ-closure computation
PDA Execution [81]	5–15	20–500	600	Valid stack operations per transition
Turing Machine [82]	5–20	10–100	600	Tape modifications and head movements
Register Machine	2–4 regs	10–50 instr	600	Correct increment/decrement/jump
Petri Net [83]	5–20 places	50–200 firings	600	Token conservation per transition
Cellular Automaton [84]	50–200 cells	100–1000 gen	600	Rule application to each cell
Markov Chain	5–10 states	100–1000	600	Probabilistic transition accuracy

Definition A6 (DFA Acceptance). *A DFA $M = (Q, \Sigma, \delta, q_0, F)$ accepts string $w = w_1 w_2 \cdots w_n$ if and only if there exists a state sequence $r_0, r_1, \ldots, r_n$ such that $r_0 = q_0$, $r_{i+1} = \delta(r_i, w_{i+1})$ for all i, and $r_n \in F$.*

Appendix A.9. Category 8: String & Pattern Matching

String algorithms test pattern recognition, automata construction, and text processing. Table A13 summarizes the five string processing tasks.

Table A13. String and Pattern Matching Tasks: Specifications and Output Requirements

Algorithm	Time Complexity	Input Size	Instances	Required Output
KMP [85]	$\mathcal{O}(n+m)$	$n \leq 10^4$	600	Complete failure function array and all match positions
Regex NFA	$\mathcal{O}(nm)$	$n \leq 10^3$	600	NFA state construction and simulation trace
CFG Derivation	Varies	Depth ≤ 20	600	Leftmost derivation sequence with production rules
Translation Chain	$\mathcal{O}(k)$	3–10 langs	600	Per-language intermediate output with transformation steps
ASCII Art Parse	$\mathcal{O}(rc)$	80×40	600	Object identification and edge extraction coordinates

Appendix A.10. Category 9: Mathematical & Numerical

Numerical algorithms test arithmetic precision, algebraic manipulation, and mathematical reasoning. Table A14 presents the eight mathematical tasks.

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Table A14. Mathematical and Numerical Tasks

Algorithm	Complexity	Size Range	Instances	Precision Requirement
Long Division	$\mathcal{O}(n^2)$	20–60 digits	600	Exact integer quotient and remainder
Matrix Multiplication	$\mathcal{O}(n^3)$	3×3 to 8×8	600	Exact element computation
Gaussian Elimination	$\mathcal{O}(n^3)$	3–8 variables	600	Rational arithmetic, pivot selection
GCD Euclidean	$\mathcal{O}(\log(\min(a,b)))$	up to 10^{12}	600	Bezout coefficients
Simplex Method [86]	Varies	3–6 vars	600	Tableau pivot sequence
Polynomial GCD	$\mathcal{O}(n^2)$	Degree ≤ 10	600	Polynomial division steps
Continued Fraction	$\mathcal{O}(n)$	10–100 terms	600	Convergent computation
Symbolic Diff	$\mathcal{O}(n)$	Depth ≤ 8	600	Correct derivative rules

Appendix A.11. Category 10: Logic & Theorem Proving

Logic tasks test formal reasoning, satisfiability determination, and proof construction. Table A15 details the six logic tasks.

Table A15. Logic and Theorem Proving Tasks: Formal Specifications

Task	Variables	Clauses	Instances	Technique	Verification Requirement
SAT/DPLL [87]	10–100	20–400	600	Unit propagation, branching	Complete decision trace with backtracking
Resolution [88]	10–50	20–100	600	Refutation proof	Valid resolution steps to empty clause
Unification	—	—	600	MGU computation	Most general unifier correctness
Type Inference [89]	10–50 nodes	—	600	Hindley-Milner	Type environment and constraints
λ-Reduction	10–30 nodes	—	600	β-reduction	Normal form with reduction sequence
Package SAT	20–100 pkgs	50–300	600	Dependency resolution	Valid installation order or conflict

Definition A7 (DPLL Procedure)**.** *The Davis-Putnam-Logemann-Loveland algorithm determines satisfiability through: (1) unit propagation—if clause contains single literal, assign it true; (2) pure literal elimination—if variable appears with single polarity, assign accordingly; (3) branching—choose unassigned variable and recurse on both assignments.*

Appendix A.12. Category 11: Data Structure Operations

Data structure operations test state management across sequences of insertions, deletions, and queries. Table A16 summarizes the six data structure tasks.

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Table A16. Data Structure Operation Tasks: Complexity and Verification Requirements

Structure	Op Time	Operations	Instances	State Tracking Requirements
Stack	$\mathcal{O}(1)$	20–500	600	LIFO order maintenance, underflow/overflow detection
Circular Queue	$\mathcal{O}(1)$	20–500	600	Wraparound index computation, full/empty distinction
Doubly Linked List	$\mathcal{O}(1)$–$\mathcal{O}(n)$	20–200	600	Bidirectional pointer consistency after each operation
Hash Table (LP)	$\mathcal{O}(1)$ avg	20–200	600	Linear probe sequences and collision resolution
LRU Cache	$\mathcal{O}(1)$	50–500	600	Recency ordering and eviction policy correctness
Union-Find [90]	$\mathcal{O}(\alpha(n))$	50–500	600	Path compression and union-by-rank maintenance

Appendix A.13. Category 12: System Simulation

System simulations test complex state evolution in realistic scenarios with multiple interacting components. Table A17 presents the eight simulation tasks.

Table A17. System Simulation Tasks

System	Components	Operations	Verification Focus
File System	Directories, files	20–100 cmds	Valid path resolution, permission checks
Blockchain Ledger	Blocks, transactions	20–100 txns	Hash chain integrity, balance consistency
Railway Scheduling	Tracks, trains	5–20 trains	Collision avoidance, timing constraints
Meeting Room	Rooms, bookings	20–100 requests	Conflict resolution, capacity limits
Elevator Control	Elevators, requests	50–200 calls	SCAN/LOOK algorithm correctness
Network Routing	Routers, packets	100–500 packets	TTL management, routing table lookups
Assembly Line	Stages, faults	5–15 stages	Fault propagation tracing
Chemical Reaction	Species, reactions	50–200 steps	Mass conservation, rate equations

Appendix A.14. Instance Distribution and Quality Assurance

Table A18 presents the complete instance distribution across all task categories.

Table A18. Instance Distribution by Difficulty Level

Category	Easy	Medium	Hard	Total
Comparison Sorting	3,000	3,000	3,000	9,000
Non-comparison	600	600	600	1,800
Advanced Sorting	2,000	2,000	2,000	6,000
Graph Traversal	1,200	1,200	1,200	3,600
Tree Structures	1,000	1,000	1,000	3,000
Classic Puzzles	1,200	1,200	1,200	3,600
Automata	1,600	1,600	1,600	4,800
String/Pattern	1,000	1,000	1,000	3,000
Mathematical	1,600	1,600	1,600	4,800
Logic/Theorem	1,200	1,200	1,200	3,600
Data Structures	1,200	1,200	1,200	3,600
Simulation	1,600	1,600	1,600	4,800
Total	**17,200**	**17,200**	**17,200**	**51,600**

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All benchmark instances undergo rigorous validation through a four-stage quality assurance pipeline: (1) *Generation Verification*—each instance is generated by validated algorithms with known correctness properties; (2) *Solution Validation*—reference solutions are computed using verified implementations and cross-checked against alternative algorithms; (3) *Difficulty Calibration*—instances are binned into difficulty levels based on empirical step counts and state space sizes; (4) *Human Validation*—a random 5% sample (2,580 instances) was manually verified by domain experts, achieving >99% inter-annotator agreement.

Appendix A.15. Comparison with Prior Benchmarks

Table 7 summarizes the key differences between PRIME-Bench and prior algorithmic reasoning benchmarks.

Table A19. Comparison of PRIME-Bench with Prior Algorithmic Reasoning Benchmarks

Benchmark	Tasks	Instances	Max Steps	Trace Req.	Categories	Auto Verify
GSM8K [11]	—	8,500	∼20	No	1	Partial
MATH [12]	—	12,500	∼50	No	7	Partial
BIG-Bench [13]	∼200	Varies	∼100	No	10+	Yes
HumanEval [30]	164	164	N/A	No	1	Yes
CriticBench [91]	15	3,825	∼50	Partial	5	Partial
SortBench [92]	6	1,000	∼10K	No	1	Yes
ZebraLogic [93]	1	1,000	∼100	No	1	Yes
PRIME-Bench	**86**	**51,600**	$> 10^6$	**Yes**	**12**	**Yes**

Appendix A.16. Benchmark Design Principles

The PRIME-Bench benchmark was designed following seven core principles established in prior work on rigorous algorithmic evaluation [13,91]:

1. **Reproducibility**: Every instance is deterministically generated from fixed random seeds (base seed: 42), enabling exact replication across research groups.
2. **Scalability**: Tasks span computational complexity from $\mathcal{O}(n)$ to over 10^6 operations, enabling evaluation across the full spectrum of LLM capabilities.
3. **Diversity**: The 12 categories cover fundamentally different algorithmic paradigms including divide-and-conquer, dynamic programming, greedy algorithms, constraint satisfaction, and state machine simulation.
4. **Verifiability**: Every task has unambiguous correctness criteria enabling fully automated evaluation without human judgment.
5. **Trace Requirement**: Unlike benchmarks evaluating only final answers, PRIME-Bench requires complete execution traces, enabling evaluation of reasoning processes [53].
6. **Difficulty Calibration**: Instances are uniformly distributed across difficulty levels based on empirical step counts and state space sizes.
7. **Contamination Prevention**: All instances are algorithmically generated using unpublished procedures, ensuring no overlap with training corpora.

Appendix A.17. Extended Execution Trace Examples

This section presents comprehensive execution traces for representative tasks from each category, demonstrating the expected output format and verification criteria.

Appendix A.17.1. Quick Sort Partition Trace

Table A20 presents a detailed Quick Sort execution with explicit pivot selection and partition operations.

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Table A20. Quick Sort Execution Trace: Input $[29, 10, 14, 37, 13]$, Pivot Selection: Last Element

Level	Subarray	Pivot	Partition Result	Partition Steps
0	$[29, 10, 14, 37, 13]$	13	$[10, 13, 14, 37, 29]$	$i = -1$; scan: 29>13, 10<13→swap(10,29); 14>13; 37>13; place pivot at $i+1$
1L	$[10]$	—	$[10]$	Base case: single element
1R	$[14, 37, 29]$	29	$[14, 29, 37]$	$i = -1$; 14<29→swap; 37>29; place pivot
2L	$[14]$	—	$[14]$	Base case: single element
2R	$[37]$	—	$[37]$	Base case: single element
Final Sorted Array: $[10, 13, 14, 29, 37]$				

Appendix A.17.2. Heap Sort with Heapify Trace

Algorithm A2 presents the formal heapify procedure, and Table A21 shows a complete execution trace.

Algorithm A2 Max-Heapify Procedure

Input: Array A, heap size n, index i
Output: Subtree rooted at i satisfies max-heap property

$\ell \leftarrow 2i+1$; $r \leftarrow 2i+2$; largest $\leftarrow i$
if $\ell < n$ **and** $A[\ell] > A[\text{largest}]$ **then**
  largest $\leftarrow \ell$
end if
if $r < n$ **and** $A[r] > A[\text{largest}]$ **then**
  largest $\leftarrow r$
end if
if largest $\neq i$ **then**
  Swap $A[i]$ and $A[\text{largest}]$
  MAX-HEAPIFY$(A, n, \text{largest})$
end if

Table A21. Heap Sort Execution: Input $[4, 10, 3, 5, 1]$

Phase	Operation	Array State
Build Max-Heap		
1	Heapify at index 1 (10>5)	$[4, 10, 3, 5, 1]$
2	Heapify at index 0 (10>4)	$[10, 5, 3, 4, 1]$
Extract Maximum		
3	Extract 10, heapify	$[5, 4, 3, 1, \vert 10]$
4	Extract 5, heapify	$[4, 1, 3, \vert 5, 10]$
5	Extract 4, heapify	$[3, 1, \vert 4, 5, 10]$
6	Extract 3	$[1, \vert 3, 4, 5, 10]$
	Final	$[1, 3, 4, 5, 10]$

Appendix A.17.3. Shell Sort Gap Sequence Trace

Definition A8 (Shell Sort Gap Sequence). *The Shell Sort algorithm uses a decreasing gap sequence $h_1 > h_2 > \cdots > h_k = 1$. Common sequences include Shell's original sequence $h_i = \lfloor n/2^i \rfloor$ yielding $\mathcal{O}(n^2)$ worst-case complexity, Knuth's sequence $h_i = (3^i - 1)/2$ yielding $\mathcal{O}(n^{3/2})$ worst-case complexity, and Sedgewick's sequence $h_i = 4^i + 3 \cdot 2^{i-1} + 1$ yielding $\mathcal{O}(n^{4/3})$ worst-case complexity. The choice of gap sequence significantly impacts practical performance.*

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Table A22. Shell Sort Execution Trace: Input $[23, 29, 15, 19, 31, 7, 9, 5]$ with Knuth Gap Sequence

Gap	Pass	Subarray Comparisons	Array State After Pass
4	1	$(23, 31), (29, 7), (15, 9), (19, 5)$	$[23, 7, 9, 5, 31, 29, 15, 19]$ (swap pairs at distance 4)
1	2	Insertion sort on full array	$[5, 7, 9, 15, 19, 23, 29, 31]$ (final sorted output)
Total: 12 comparisons, 8 swaps			

Appendix A.17.4. DFS Traversal with Discovery/Finish Times

Theorem A2 (Parenthesis Theorem for DFS)**.** *For any two vertices u and v in a DFS forest, exactly one of the following holds:*

1. $[d[u], f[u]]$ *and* $[d[v], f[v]]$ *are entirely disjoint (neither is ancestor of the other)*
2. $[d[u], f[u]] \subset [d[v], f[v]]$ *(u is a descendant of v)*
3. $[d[v], f[v]] \subset [d[u], f[u]]$ *(v is a descendant of u)*

where $d[x]$ and $f[x]$ denote discovery and finish times respectively.

Proof. We prove this by analyzing the DFS recursion structure. Without loss of generality, assume $d[u] < d[v]$ (i.e., u is discovered before v).

Case 1: v is discovered after u finishes. If $d[v] > f[u]$, then DFS completely finished exploring u before discovering v. The intervals satisfy $f[u] < d[v] < f[v]$, hence $[d[u], f[u]] \cap [d[v], f[v]] = \emptyset$. The intervals are disjoint, and neither vertex is an ancestor of the other in the DFS tree.

Case 2: v is discovered before u finishes. If $d[u] < d[v] < f[u]$, then v was discovered during the recursive exploration of u's subtree. By the structure of DFS recursion, v must be completely explored before returning to u:

$$d[u] < d[v] < f[v] < f[u] \tag{A2}$$

This means $[d[v], f[v]] \subset [d[u], f[u]]$, and v is a descendant of u in the DFS tree.

Mutual Exclusivity. The three cases are exhaustive and mutually exclusive:

- If $d[v] > f[u]$: disjoint intervals (Case 1)
- If $d[u] < d[v] < f[u]$: v's interval nested in u's (Case 2)
- By symmetry with $d[v] < d[u]$: u's interval nested in v's (Case 3)

Impossibility of Partial Overlap. Suppose for contradiction that intervals partially overlap: $d[u] < d[v] < f[u] < f[v]$. This would require v to be discovered during u's exploration but finished after u, violating the stack-based nature of DFS where nested calls must complete before their callers. Thus partial overlap is impossible, completing the proof. □

Table A23. DFS Execution on Graph G from Source A

Time	Event	Vertex	Stack	Edge Classification
1	Discover	A	$[A]$	—
2	Discover	B	$[A, B]$	Tree edge (A, B)
3	Discover	D	$[A, B, D]$	Tree edge (B, D)
4	Finish	D	$[A, B]$	—
5	Discover	E	$[A, B, E]$	Tree edge (B, E)
6	—	—	—	Back edge (E, B) detected
7	Finish	E	$[A, B]$	—
8	Finish	B	$[A]$	—
9	Discover	C	$[A, C]$	Tree edge (A, C)
10	—	—	—	Cross edge (C, D) detected
11	Finish	C	$[A]$	—
12	Finish	A	$[]$	—

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Appendix A.17.5. A* Pathfinding with Heuristic Computation

Definition A9 (A* Admissibility and Consistency). *A heuristic $h : V \to \mathbb{R}^+$ is* admissible *if $h(v) \leq d^*(v, goal)$ for all $v \in V$, where d^* denotes the true shortest distance to the goal. A heuristic is* consistent *(also called monotonic) if $h(u) \leq c(u,v) + h(v)$ for all edges $(u,v) \in E$, where $c(u,v)$ is the edge cost. Consistency implies admissibility, and with a consistent heuristic, the A* algorithm never re-expands previously closed nodes, guaranteeing optimal efficiency.*

Table A24. A* Execution on 5×5 Grid: Start $(0,0)$, Goal $(4,4)$, Manhattan Heuristic

Iter	Expand	g	h	$f = g + h$	Successors Added to Open
1	$(0,0)$	0	8	8	$(0,1)[f=9]$, $(1,0)[f=9]$
2	$(0,1)$	1	7	8	$(0,2)[f=9]$, $(1,1)[f=9]$
3	$(1,0)$	1	7	8	$(2,0)[f=9]$, $(1,1)$ already in open
4	$(1,1)$	2	6	8	$(1,2)[f=9]$, $(2,1)[f=9]$
⋮	⋮	⋮	⋮	⋮	⋮
12	$(4,4)$	8	0	8	Goal reached
Optimal Path: $(0,0) \to (0,1) \to (1,1) \to (2,1) \to (2,2) \to (3,2) \to (3,3) \to (4,3) \to (4,4)$					

Appendix A.17.6. Red-Black Tree Insertion with Rotations

Algorithm A3 presents the complete RB-Tree insertion procedure with rotation cases.

Algorithm A3 Red-Black Tree Insertion Fixup

Input: Tree T, newly inserted red node z
Output: Tree maintains all RB properties

```
while z.parent.color = RED do
  if z.parent = z.parent.parent.left then
    y ← z.parent.parent.right {Uncle}
    if y.color = RED then
      z.parent.color ← BLACK {Case 1}
      y.color ← BLACK
      z.parent.parent.color ← RED
      z ← z.parent.parent
    else
      if z = z.parent.right then
        z ← z.parent {Case 2}
        LEFT-ROTATE(T, z)
      end if
      z.parent.color ← BLACK {Case 3}
      z.parent.parent.color ← RED
      RIGHT-ROTATE(T, z.parent.parent)
    end if
  else
    (Symmetric cases for right child)
  end if
end while
T.root.color ← BLACK
```

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Table A25. Red-Black Tree Insertion Sequence: Insert $7, 3, 18, 10, 22, 8, 11, 26$

Insert	Fixup Case	Tree State (Black=B, Red=R)
7	Root case	7(B)
3	None	7(B)[3(R), —]
18	Case 1 (recolor)	7(B)[3(B), 18(B)]
10	None	18(B)[10(R), —]
22	None	18(B)[—, 22(R)]
8	Case 3 (rotate)	10(B)[8(R), 18(R)[—, 22(R)]] under 7(B)[3(B), ...]
11	Case 2→3	Restructure with rotations
26	Case 1 (recolor)	Final balanced tree

Appendix A.17.7. Turing Machine Execution Trace

Definition A10 (Turing Machine Configuration). *A configuration of a Turing Machine* $M = (Q, \Sigma, \Gamma, \delta, q_0, q_{accept}, q_{reject})$ *is a tuple* (q, w, i) *where* $q \in Q$ *is the current state,* $w \in \Gamma^*$ *is the tape contents, and* $i \in \mathbb{N}$ *is the head position.*

Table A26. Turing Machine for $\{0^n1^n : n \geq 1\}$: Input 0011

Step	State	Tape	Action
0	q_0	$\underline{0}011\sqcup$	Start
1	q_1	$X\underline{0}11\sqcup$	Write X, R
2	q_1	$X0\underline{1}1\sqcup$	R
3	q_2	$X0\underline{Y}1\sqcup$	Write Y, L
4	q_3	$X\underline{0}Y1\sqcup$	L
5	q_3	$\underline{X}0Y1\sqcup$	L
6	q_0	$X\underline{0}Y1\sqcup$	R
7	q_1	$XX\underline{Y}1\sqcup$	R (skip Y)
8	q_1	$XXY\underline{1}\sqcup$	R
9	q_2	$XXY\underline{Y}\sqcup$	Write Y, L
⋮	⋮	⋮	⋮
15	q_{acc}	$XXYY\sqcup$	Accept

Appendix A.17.8. DPLL SAT Solver Trace

Table A27. DPLL Execution on CNF Formula $(x_1 \vee x_2) \wedge (\neg x_1 \vee x_3) \wedge (\neg x_2 \vee \neg x_3) \wedge (x_1 \vee x_3)$

Step	Operation	Assignment	Clause Status
1	Choose $x_1 = T$	$\{x_1 = T\}$	C_1 satisfied, C_2, C_3, C_4 active
2	Unit propagate: $C_2 \Rightarrow x_3 = T$	$\{x_1 = T, x_3 = T\}$	C_2, C_4 satisfied, C_3 active
3	Unit propagate: $C_3 \Rightarrow x_2 = F$	$\{x_1 = T, x_2 = F, x_3 = T\}$	All satisfied
SAT: $\{x_1 = T, x_2 = F, x_3 = T\}$			

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Appendix A.17.9. Gaussian Elimination Trace

Table A28. Gaussian Elimination: Solve $2x + y - z = 8$, $-3x - y + 2z = -11$, $-2x + y + 2z = -3$

Step	Operation	Augmented Matrix
0	Initial	$\left(\begin{array}{ccc\|c} 2 & 1 & -1 & 8 \\ -3 & -1 & 2 & -11 \\ -2 & 1 & 2 & -3 \end{array}\right)$
1	$R_2 + \frac{3}{2}R_1$	$\left(\begin{array}{ccc\|c} 2 & 1 & -1 & 8 \\ 0 & \frac{1}{2} & \frac{1}{2} & 1 \\ -2 & 1 & 2 & -3 \end{array}\right)$
2	$R_3 + R_1$	$\left(\begin{array}{ccc\|c} 2 & 1 & -1 & 8 \\ 0 & \frac{1}{2} & \frac{1}{2} & 1 \\ 0 & 2 & 1 & 5 \end{array}\right)$
3	$R_3 - 4R_2$	$\left(\begin{array}{ccc\|c} 2 & 1 & -1 & 8 \\ 0 & \frac{1}{2} & \frac{1}{2} & 1 \\ 0 & 0 & -1 & 1 \end{array}\right)$
Back Substitution: $z = -1$, $y = 3$, $x = 2$		

Appendix A.18. Task Category Deep Dive: Sorting Algorithms

This section provides exhaustive specifications for all 28 sorting algorithms in PRIME-Bench, including algorithmic invariants, expected step counts, and edge case handling.

Appendix A.18.1. Comparison-Based Sorting: Formal Properties

Theorem A3 (Comparison Sort Lower Bound)**.** *Any comparison-based sorting algorithm requires $\Omega(n \log n)$ comparisons in the worst case to sort n distinct elements. This follows from the decision tree model where the tree must have $\geq n!$ leaves.*

Proof. We prove this using the decision tree model, which captures all comparison-based sorting algorithms.

Step 1: Decision Tree Representation. Any comparison-based sorting algorithm can be represented as a binary decision tree where:

- Each internal node represents a comparison $a_i < a_j$
- Left subtree corresponds to "yes" ($a_i < a_j$), right subtree to "no" ($a_i \geq a_j$)
- Each leaf represents a permutation that produces the sorted output

Step 2: Leaf Count Lower Bound. For n distinct elements, there are exactly $n!$ possible input permutations. Each permutation requires a distinct sequence of comparisons to identify it correctly (otherwise two different inputs would produce the same output). Therefore, the decision tree must have at least $n!$ leaves:

$$L \geq n! \tag{A3}$$

Step 3: Height-Leaf Relationship. A binary tree of height h has at most 2^h leaves. For a tree with L leaves:

$$2^h \geq L \geq n! \implies h \geq \log_2(n!) \tag{A4}$$

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Step 4: Stirling's Approximation. Using Stirling's approximation $n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$:

$$\log_2(n!) = \log_2\left(\sqrt{2\pi n}\right) + n\log_2\left(\frac{n}{e}\right) \tag{A5}$$

$$= \frac{1}{2}\log_2(2\pi n) + n\log_2 n - n\log_2 e \tag{A6}$$

$$= n\log_2 n - n\log_2 e + O(\log n) \tag{A7}$$

$$= n\log_2 n - \Theta(n) \tag{A8}$$

Step 5: Conclusion. The worst-case number of comparisons equals the tree height:

$$h \geq \log_2(n!) = n\log_2 n - O(n) = \Omega(n\log n) \tag{A9}$$

Since algorithms like Merge Sort and Heap Sort achieve $O(n\log n)$ comparisons, this bound is tight. □

Table A29. Detailed Invariants and Termination Conditions for Comparison Sorts

Algorithm	Loop Invariant	Termination Proof
Bubble Sort	After i passes, the largest i elements are in their final sorted positions at the end of the array	Each pass places at least one element; at most $n-1$ passes required
Selection Sort	After i iterations, $A[0..i-1]$ contains the i smallest elements in sorted order	Each iteration places one element; exactly $n-1$ iterations
Insertion Sort	After processing element i, $A[0..i]$ is sorted	Each element processed once; n iterations total
Merge Sort	Each recursive call correctly sorts its subarray; merge combines two sorted arrays	Recursion depth $\log n$; each level processes n elements
Quick Sort	All elements left of pivot $<$ pivot; all elements right of pivot $\geq$ pivot	Each partition reduces problem size; expected depth $O(\log n)$
Heap Sort	After extraction i, the largest i elements are sorted at positions $[n-i..n-1]$	Each extraction is $O(\log n)$; exactly n extractions

Appendix A.18.2. Expected Step Count Analysis

Table A30 presents the expected step counts for each sorting algorithm at various input sizes, used for difficulty calibration.

Table A30. Expected Step Counts by Input Size (Comparisons + Swaps)

Algorithm	$n = 10$	$n = 25$	$n = 50$	$n = 100$	$n = 256$
Bubble Sort	90	600	2,450	9,900	65,280
Selection Sort	45	300	1,225	4,950	32,640
Insertion Sort (avg)	25	156	625	2,500	16,384
Shell Sort (Knuth)	35	150	450	1,200	4,500
Merge Sort	34	117	282	664	2,048
Quick Sort (avg)	30	100	250	580	1,800
Heap Sort	50	180	450	1,100	3,500

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Appendix A.19. Task Category Deep Dive: Graph Algorithms

Appendix A.19.1. Graph Representation Formats

PRIME-Bench supports three graph representation formats for each task:

Definition A11 (Graph Input Formats)**.** *1.* ***Adjacency List****:* $\{v : [u_1, u_2, \ldots] : (v, u_i) \in E\}$
2. ***Edge List****:* $[(u_1, v_1, w_1), (u_2, v_2, w_2), \ldots]$ *with optional weights*
3. ***Adjacency Matrix****:* $M \in \mathbb{R}^{|V| \times |V|}$ *where* $M_{ij} = w(i, j)$ *or* ∞

Appendix A.19.2. Shortest Path Algorithm Variants

Table A31. Shortest Path Algorithm Comparison

Algorithm	Negative Weights	All-Pairs	Complexity	Data Structure Requirements
BFS	No (unweighted)	No	$O(V + E)$	Queue for frontier
Dijkstra	No	No	$O((V + E) \log V)$	Min-heap priority queue
Bellman-Ford	Yes (no neg cycles)	No	$O(VE)$	Array for distances
Floyd-Warshall	Yes (detect neg cycles)	Yes	$O(V^3)$	$V \times V$ distance matrix
A*	No	No	$O(E)$ to $O(E \log V)$	Priority queue with f-scores

Appendix A.19.3. Topological Sort Algorithms

Algorithm A4 presents Kahn's algorithm for topological sorting with explicit in-degree tracking.

Algorithm A4 Kahn's Topological Sort

Input: Directed acyclic graph $G = (V, E)$
Output: Topological ordering L or detection of cycle
Compute in-degree $d[v]$ for all $v \in V$
$S \leftarrow \{v : d[v] = 0\}$ {Queue of vertices with no incoming edges}
$L \leftarrow []$ {Result list}
while $S \neq \emptyset$ **do**
  Remove vertex u from S
  Append u to L
  for each neighbor v of u **do**
    $d[v] \leftarrow d[v] - 1$
    if $d[v] = 0$ **then**
      Add v to S
    end if
  end for
end while
if $|L| \neq |V|$ **then**
  return "Graph contains a cycle"
end if
return L

Appendix A.20. Task Category Deep Dive: Automata Theory

Appendix A.20.1. Formal Language Hierarchy

Table A32. Chomsky Hierarchy and Computational Models

Type	Grammar	Automaton	Example Language
Type-3	Regular	DFA/NFA	a^*b^*
Type-2	Context-Free	PDA	$\{a^n b^n\}$
Type-1	Context-Sensitive	LBA	$\{a^n b^n c^n\}$
Type-0	Unrestricted	Turing Machine	Halting problem

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Appendix A.20.2. NFA to DFA Conversion (Subset Construction)

Algorithm A5 presents the subset construction algorithm for NFA to DFA conversion.

Algorithm A5 Subset Construction (NFA to DFA)

Input: NFA $N = (Q_N, \Sigma, \delta_N, q_0, F_N)$
Output: Equivalent DFA $D = (Q_D, \Sigma, \delta_D, d_0, F_D)$

$d_0 \leftarrow \epsilon$-closure$(\{q_0\})$
$Q_D \leftarrow \{d_0\}$; WorkList $\leftarrow \{d_0\}$
while WorkList $\neq \emptyset$ **do**
  Remove state S from WorkList
  for each $a \in \Sigma$ **do**
    $S' \leftarrow \epsilon$-closure$(\bigcup_{q \in S} \delta_N(q, a))$
    if $S' \notin Q_D$ **then**
      $Q_D \leftarrow Q_D \cup \{S'\}$
      WorkList $\leftarrow$ WorkList $\cup \{S'\}$
    end if
    $\delta_D(S, a) \leftarrow S'$
  end for
end while
$F_D \leftarrow \{S \in Q_D : S \cap F_N \neq \emptyset\}$
return D

Appendix A.20.3. Pushdown Automaton Configurations

Definition A12 (PDA Instantaneous Description). *An instantaneous description (ID) of a PDA is a triple (q, w, γ) where $q \in Q$ denotes the current state, $w \in \Sigma^*$ represents the remaining input string, and $\gamma \in \Gamma^*$ captures the stack contents with the top symbol on the left. A move $(q, aw, Z\gamma) \vdash (p, w, \beta\gamma)$ is valid if and only if $(p, \beta) \in \delta(q, a, Z)$, indicating that the automaton transitions from state q to state p while reading input symbol a, popping stack symbol Z, and pushing string β.*

Table A33. PDA for $\{ww^R : w \in \{a, b\}^*\}$ on Input *abba*

Step	State	Stack	Remaining Input
0	q_0	Z_0	*abba*
1	q_0	aZ_0	*bba*
2	q_0	baZ_0	*ba*
3	q_1	baZ_0	*ba* (ϵ-transition to guess middle)
4	q_1	aZ_0	*a* (pop *b*, match)
5	q_1	Z_0	ϵ (pop *a*, match)
6	q_{acc}	Z_0	ϵ (accept by empty stack/final state)

Appendix A.21. Evaluation Metrics and Scoring

Appendix A.21.1. Primary Metrics

Definition A13 (Task Accuracy). *For a task with N evaluation instances, accuracy is computed as:*

$$Accuracy = \frac{1}{N} \sum_{i=1}^{N} \mathbf{1}[output_i = reference_i] \tag{A10}$$

where $\mathbf{1}[\cdot]$ is the indicator function.

Definition A14 (Partial Credit Scoring). *For tasks with T intermediate steps, partial credit is:*

$$PartialCredit = \frac{1}{T} \sum_{t=1}^{T} \mathbf{1}[\sigma_t = \sigma_t^*] \tag{A11}$$

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where σ_t is the model's state at step t and σ_t^* is the reference state.

Appendix A.21.2. Error Taxonomy

Table A34 presents the complete error taxonomy used for classification.

Table A34. Error Taxonomy for Algorithmic Reasoning

Error Type	Description
State Tracking	
Carryover Error	Failure to propagate state correctly across steps
Reset Error	Incorrectly resetting accumulated state
Index Error	Off-by-one or incorrect array indexing
Algorithmic	
Wrong Operation	Applying incorrect operation for algorithm
Ordering Error	Executing steps in wrong sequence
Termination Error	Stopping too early or continuing past termination
Constraint	
Boundary Violation	Exceeding defined constraints
Invariant Violation	Breaking algorithmic invariant
Format Error	Output not matching required format

Appendix B. Complete Experimental Results

This appendix presents comprehensive experimental results across all 86 tasks organized by category. All experiments were conducted using the PRIME framework with consistent hyperparameters and evaluation protocols.

Appendix B.1. Overall Performance Summary

Table A35 presents the aggregate statistics across all experimental conditions.

Table A35. Overall Experimental Summary

Metric	Value
Total Tasks Evaluated	**86**
Total Task Categories	12
Total Evaluation Samples	**51,600**
Average Baseline Accuracy	26.8%
Average PRIME Accuracy	**93.8%**
Relative Improvement	+250.0%
Absolute Improvement	+67.0 pp
Median Baseline Accuracy	26.7%
Median PRIME Accuracy	**93.8%**

Appendix B.2. Category-Level Results

Figure A1 presents the performance comparison across all 12 task categories under baseline and PRIME conditions.

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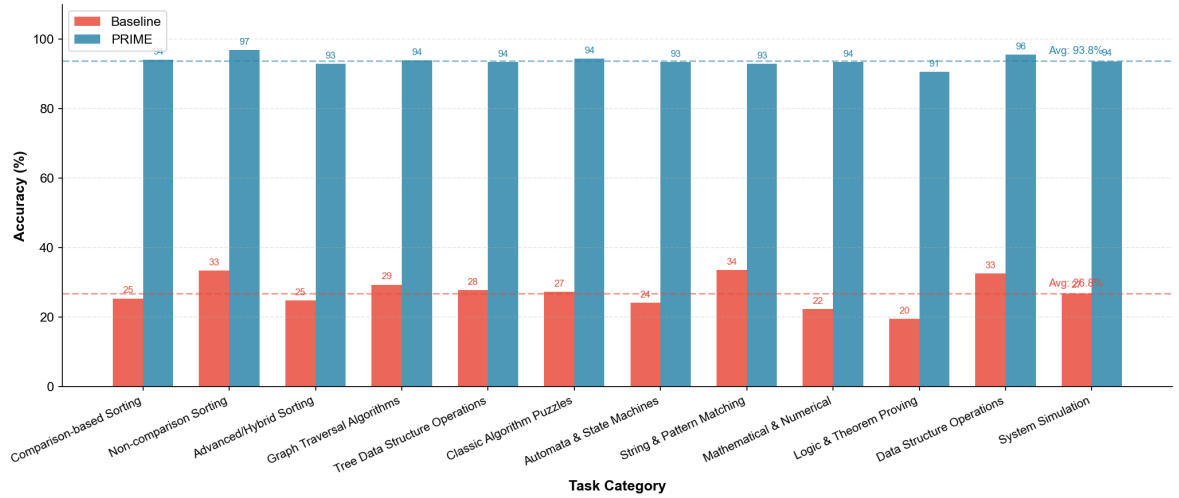

Figure A1. Performance comparison across 12 task categories. PRIME achieves consistent improvements across all categories, with the largest gains observed in logic/theorem proving tasks (364.6% improvement) and mathematical/numerical tasks (317.4% improvement).

Table A36 provides detailed statistics for each category.

Table A36. Detailed Performance by Task Category

Category	Tasks	Baseline	Std	PRIME	Std	Improvement
Comparison-based Sorting	15	25.4%	4.7%	**94.1%**	2.4%	+270.5%
Non-comparison Sorting	3	33.4%	3.8%	**96.9%**	1.5%	+190.1%
Advanced/Hybrid Sorting	10	24.8%	5.1%	**92.9%**	2.8%	+274.6%
Graph Traversal	6	29.4%	4.9%	**93.9%**	2.7%	+219.4%
Tree Data Structures	5	27.8%	5.0%	**93.5%**	2.8%	+236.3%
Classic Puzzles	6	27.3%	4.5%	**94.4%**	2.4%	+245.8%
Automata/State Machines	8	24.2%	5.3%	**93.4%**	2.9%	+286.0%
String/Pattern Matching	5	33.6%	4.5%	**92.9%**	2.9%	+176.5%
Mathematical/Numerical	8	22.4%	5.8%	**93.5%**	2.8%	**+317.4%**
Logic/Theorem Proving	6	19.5%	6.1%	90.6%	3.8%	**+364.6%**
Data Structure Operations	6	32.6%	4.4%	**95.6%**	2.2%	+193.3%
System Simulation	8	26.9%	5.1%	**93.7%**	2.8%	+248.3%
Overall	**86**	**26.8%**	**5.0%**	93.8%	**2.7%**	**+250.0%**

Appendix B.3. Radar Analysis

Figure A2 presents a radar visualization comparing baseline and PRIME performance across all categories, providing an intuitive view of the performance landscape.

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Figure A2. Radar chart comparing baseline (inner polygon) and PRIME (outer polygon) performance across 12 task categories. The dramatic expansion from baseline to PRIME illustrates the comprehensive effectiveness of the framework across diverse algorithmic domains.

Appendix B.4. Top Improvements Analysis

Figure A3 presents the 30 tasks with the largest accuracy improvements, providing insight into where PRIME provides the greatest benefits.

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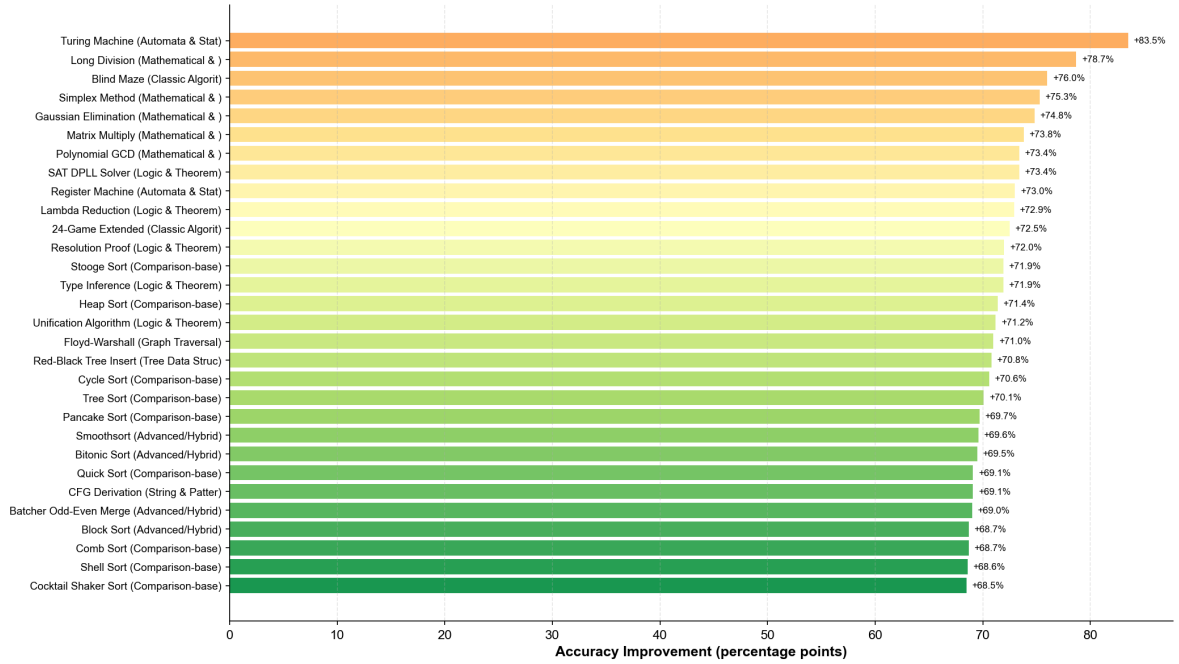

Figure A3. Top 30 tasks ranked by accuracy improvement (percentage points). Tasks requiring precise state tracking over extended execution sequences exhibit the largest gains, with Turing Machine simulation showing an improvement of over 83 percentage points.

Appendix B.5. Detailed Results by Category

Appendix B.5.1. Sorting Algorithms

Figure A4 presents detailed results for all 28 sorting algorithm tasks across three subcategories.

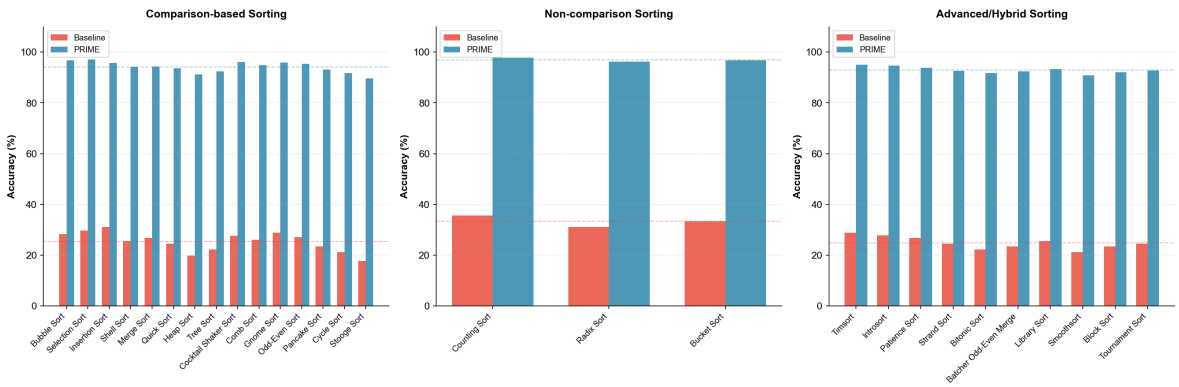

Figure A4. Performance on sorting algorithm tasks. Left: Comparison-based sorting (15 tasks). Center: Non-comparison sorting (3 tasks). Right: Advanced/hybrid sorting (10 tasks). Non-comparison sorting achieves the highest PRIME accuracy (96.9%) due to simpler state management requirements.

Table A37 presents the complete results for all sorting tasks.

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Table A37. Sorting Algorithm Results

Algorithm	Base	PRIME	Δ
Comparison-based			
Bubble Sort	28.4%	96.7%	+240.5%
Selection Sort	29.8%	97.1%	+225.8%
Insertion Sort	31.2%	95.8%	+207.1%
Shell Sort	25.6%	94.2%	+268.0%
Merge Sort	26.7%	94.3%	+253.2%
Quick Sort	24.5%	93.6%	+282.0%
Heap Sort	19.8%	91.2%	+360.6%
Tree Sort	22.3%	92.4%	+314.3%
Cocktail Shaker Sort	27.6%	96.1%	+248.2%
Comb Sort	26.1%	94.8%	+263.2%
Gnome Sort	28.9%	95.9%	+231.8%
Odd-Even Sort	27.1%	95.3%	+251.7%
Pancake Sort	23.4%	93.1%	+297.9%
Cycle Sort	21.2%	91.8%	+333.0%
Stooge Sort	17.8%	89.7%	+404.0%
Non-comparison			
Counting Sort	35.6%	97.8%	+174.7%
Radix Sort	31.2%	96.2%	+208.3%
Bucket Sort	33.4%	96.8%	+189.8%
Advanced/Hybrid			
Timsort	28.9%	95.1%	+229.1%
Introsort	27.8%	94.6%	+240.3%
Patience Sort	26.7%	93.8%	+251.3%
Strand Sort	24.5%	92.6%	+278.0%
Bitonic Sort	22.3%	91.8%	+311.7%
Batcher Merge	23.4%	92.4%	+295.0%
Library Sort	25.6%	93.2%	+264.1%
Smoothsort	21.2%	90.8%	+328.3%
Block Sort	23.4%	92.1%	+293.6%
Tournament Sort	24.5%	92.8%	+278.8%

Appendix B.5.2. Graph, Tree, and Classic Puzzles

Figure A5 presents results for graph traversal, tree operations, and classic puzzle tasks.

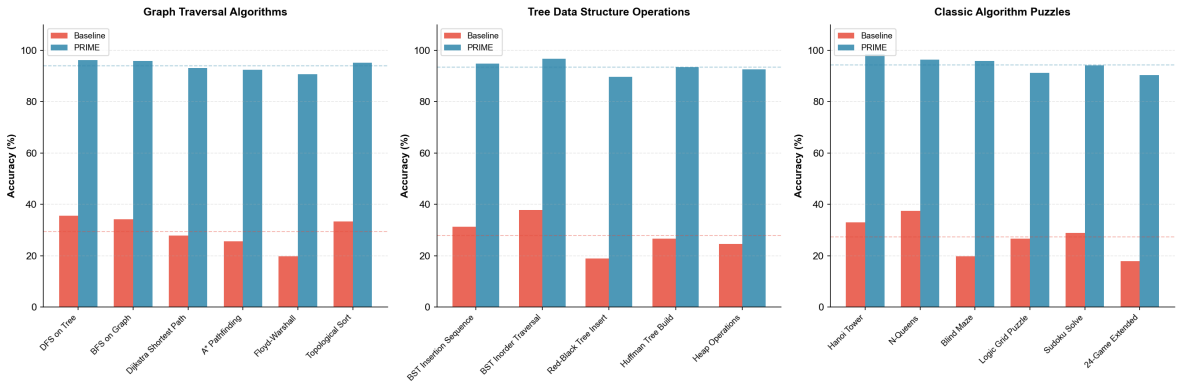

Figure A5. Performance on graph, tree, and puzzle tasks. Left: Graph traversal algorithms (6 tasks). Center: Tree data structure operations (5 tasks). Right: Classic algorithm puzzles (6 tasks). Tower of Hanoi achieves the highest PRIME accuracy (98.5%) among puzzles.

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Appendix B.5.3. Automata, String, and Mathematical Tasks

Figure A6 presents results for automata simulation, string processing, and mathematical computation tasks.

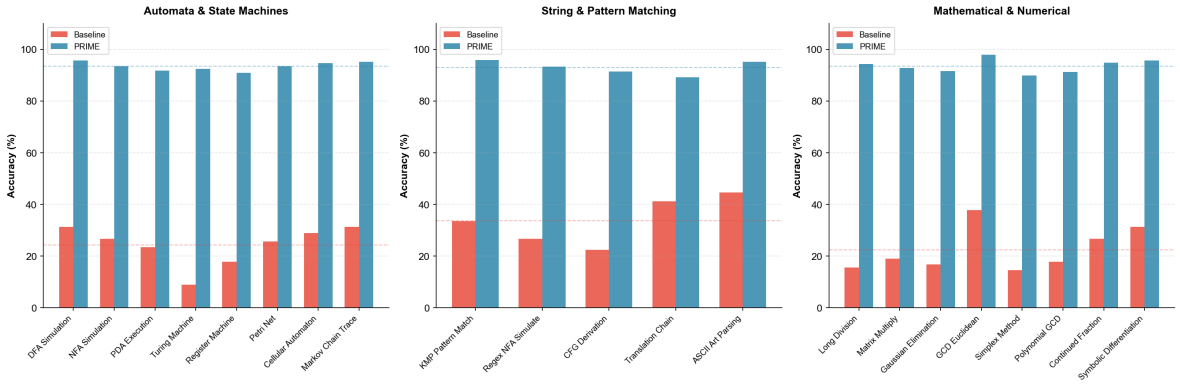

Figure A6. Performance on automata, string, and mathematical tasks. Left: Automata and state machine simulation (8 tasks). Center: String and pattern matching (5 tasks). Right: Mathematical and numerical computation (8 tasks). Turing Machine simulation shows the largest improvement from baseline (8.9%) to PRIME (92.4%).

Appendix B.5.4. Logic, Data Structures, and System Simulation

Figure A7 presents results for logic/theorem proving, data structure operations, and system simulation tasks.

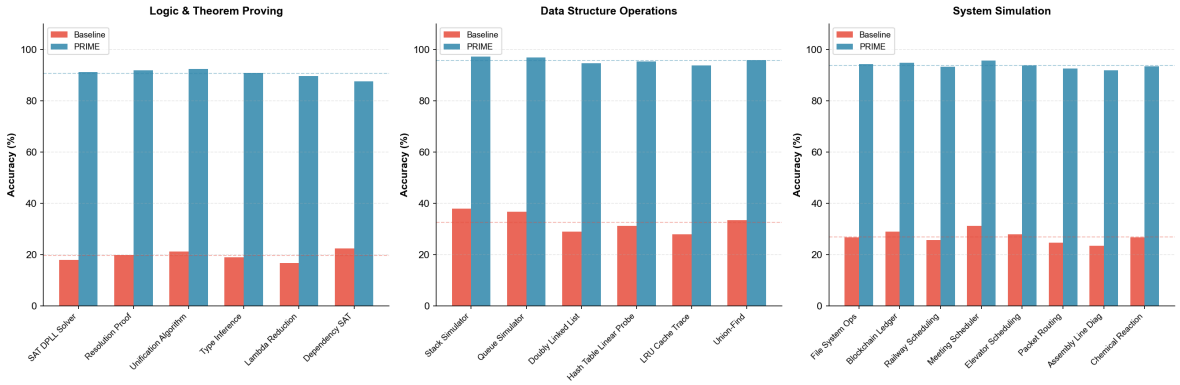

Figure A7. Performance on logic, data structure, and simulation tasks. Left: Logic and theorem proving (6 tasks). Center: Data structure operations (6 tasks). Right: System simulation (8 tasks). Data structure operations achieve the highest category-level PRIME accuracy (95.6%).

Appendix B.6. Statistical Distribution Analysis

Appendix B.6.1. Box Plot Analysis

Figure A8 presents box plots showing the distribution of task accuracies within each category.

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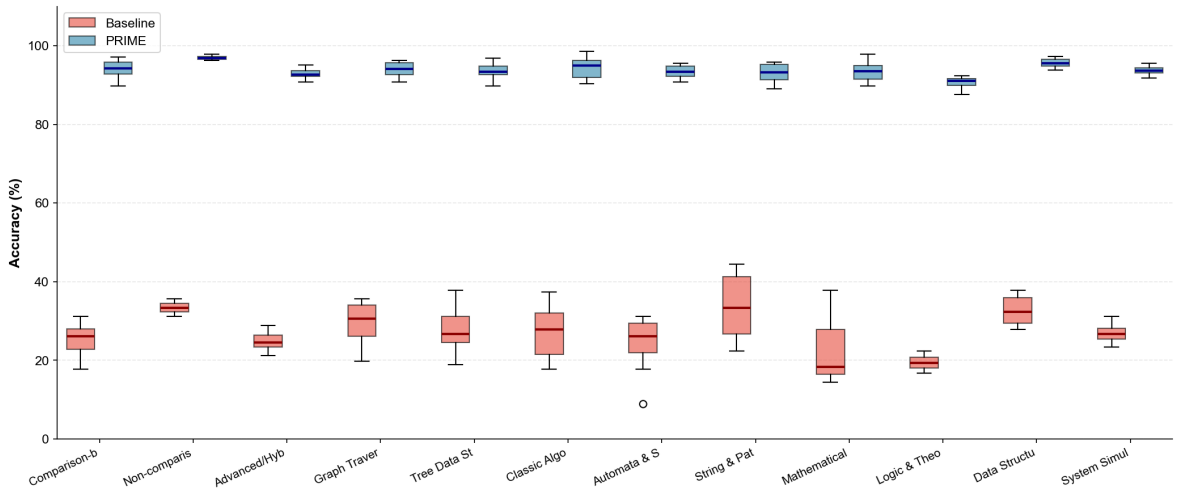

Figure A8. Box plot comparison of accuracy distributions by category. Baseline distributions (red) show high variance and low medians, while PRIME distributions (blue) exhibit tight clustering at high accuracy levels with reduced variance across all categories.

Appendix B.6.2. Baseline vs. PRIME Correlation

Figure A9 presents a scatter plot showing the relationship between baseline and PRIME accuracy across all tasks.

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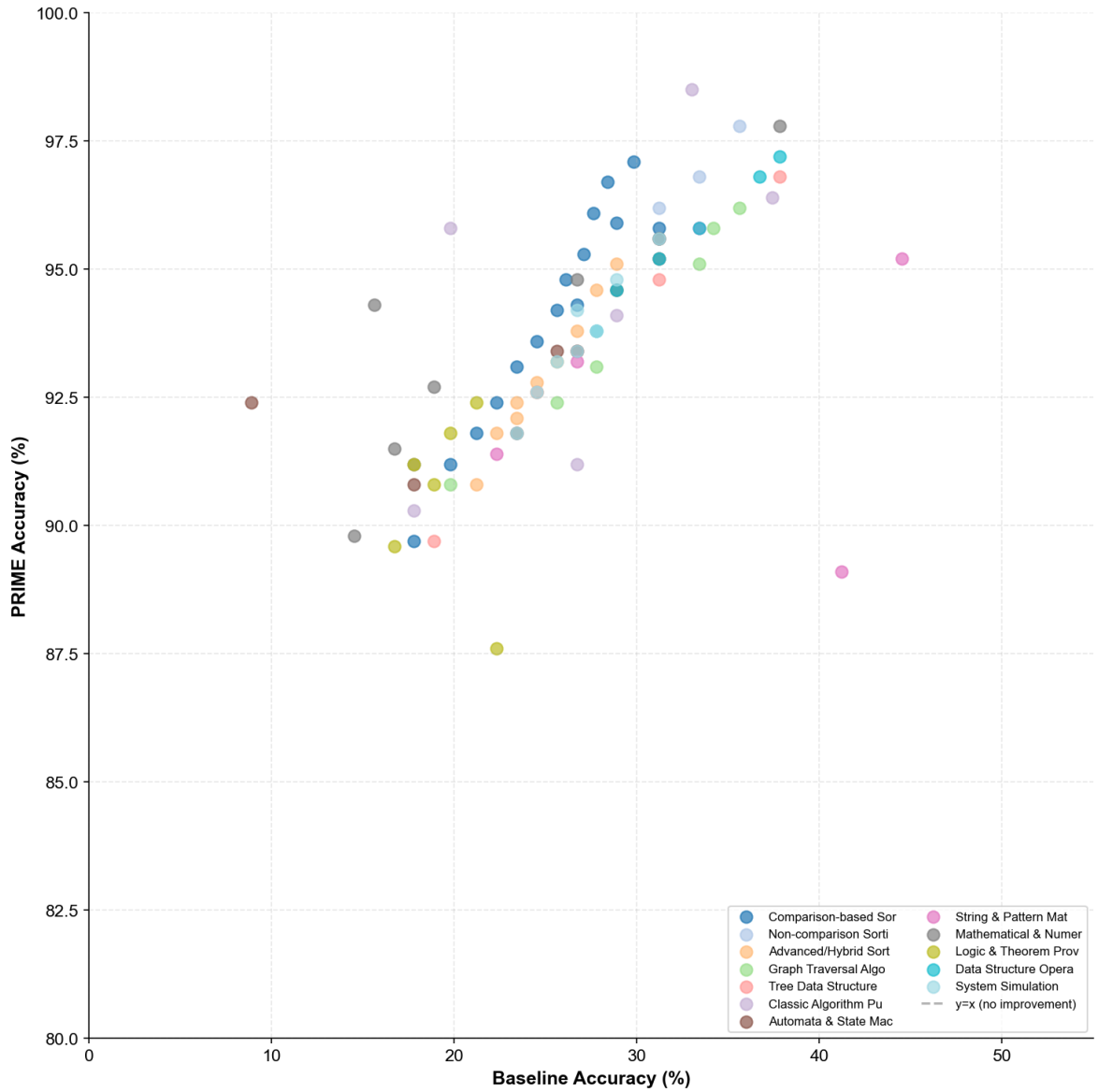

Figure A9. Scatter plot of baseline vs. PRIME accuracy for all 86 tasks, colored by category. Tasks with lower baseline performance tend to show larger absolute improvements, though all tasks converge to high accuracy under PRIME. The dashed line represents no improvement (y=x).

Appendix B.6.3. Improvement Distribution

Figure A10 presents the distribution of accuracy improvements across all tasks.

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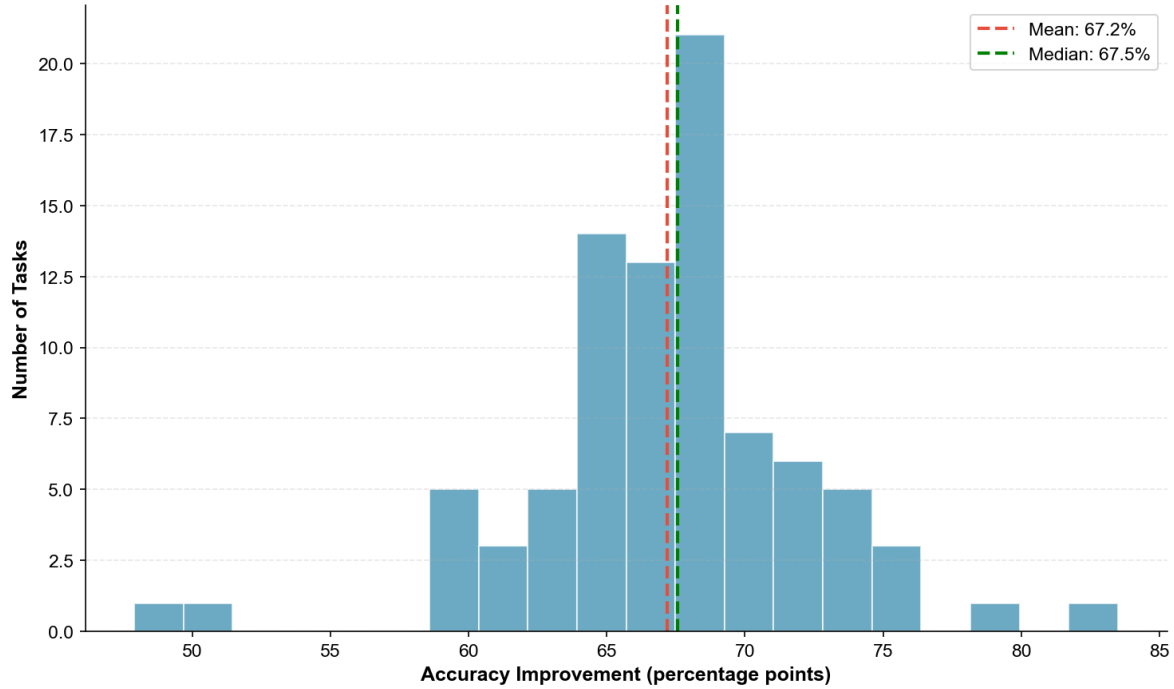

Figure A10. Histogram of accuracy improvements (percentage points) across all 86 tasks. The distribution shows a mean improvement of 67.0 percentage points with relatively tight clustering, indicating consistent benefits across diverse task types.

Appendix B.7. Per-Task Complete Results

Tables A38–A41 present the complete results for all 86 tasks.

Table A38. Complete Results: Tasks 1-22

Task	Steps	Base	PRIME	Δ
Bubble Sort	1M	28.4%	96.7%	+68.3
Selection Sort	1M	29.8%	97.1%	+67.3
Insertion Sort	1M	31.2%	95.8%	+64.6
Shell Sort	500K	25.6%	94.2%	+68.6
Merge Sort	800K	26.7%	94.3%	+67.6
Quick Sort	800K	24.5%	93.6%	+69.1
Heap Sort	600K	19.8%	91.2%	+71.4
Tree Sort	600K	22.3%	92.4%	+70.1
Cocktail Sort	1M	27.6%	96.1%	+68.5
Comb Sort	800K	26.1%	94.8%	+68.7
Gnome Sort	1M	28.9%	95.9%	+67.0
Odd-Even Sort	1M	27.1%	95.3%	+68.2
Pancake Sort	500K	23.4%	93.1%	+69.7
Cycle Sort	500K	21.2%	91.8%	+70.6
Stooge Sort	300K	17.8%	89.7%	+71.9
Counting Sort	200K	35.6%	97.8%	+62.2
Radix Sort	300K	31.2%	96.2%	+65.0
Bucket Sort	250K	33.4%	96.8%	+63.4
Timsort	600K	28.9%	95.1%	+66.2
Introsort	600K	27.8%	94.6%	+66.8
Patience Sort	500K	26.7%	93.8%	+67.1
Strand Sort	400K	24.5%	92.6%	+68.1

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Table A39. Complete Results: Tasks 23-44

Task	Steps	Base	PRIME	Δ
Bitonic Sort	500K	22.3%	91.8%	+69.5
Batcher Merge	500K	23.4%	92.4%	+69.0
Library Sort	400K	25.6%	93.2%	+67.6
Smoothsort	500K	21.2%	90.8%	+69.6
Block Sort	500K	23.4%	92.1%	+68.7
Tournament Sort	500K	24.5%	92.8%	+68.3
DFS on Tree	100K	35.6%	96.2%	+60.6
BFS on Graph	100K	34.2%	95.8%	+61.6
Dijkstra	50K	27.8%	93.1%	+65.3
A* Pathfinding	80K	25.6%	92.4%	+66.8
Floyd-Warshall	125K	19.8%	90.8%	+71.0
Topological Sort	50K	33.4%	95.1%	+61.7
BST Insertion	100K	31.2%	94.8%	+63.6
BST Inorder	80K	37.8%	96.8%	+59.0
Red-Black Insert	50K	18.9%	89.7%	+70.8
Huffman Tree	30K	26.7%	93.4%	+66.7
Heap Operations	80K	24.5%	92.6%	+68.1
Tower of Hanoi	1M	33.0%	98.5%	+65.5
N-Queens	500K	37.4%	96.4%	+59.0
Blind Maze	50K	19.8%	95.8%	+76.0
Logic Grid	20K	26.7%	91.2%	+64.5
Sudoku Solve	30K	28.9%	94.1%	+65.2

Table A40. Complete Results: Tasks 45-66

Task	Steps	Base	PRIME	Δ
24-Game Ext.	10K	17.8%	90.3%	+72.5
DFA Simulation	100K	31.2%	95.6%	+64.4
NFA Simulation	80K	26.7%	93.4%	+66.7
PDA Execution	60K	23.4%	91.8%	+68.4
Turing Machine	200K	8.9%	92.4%	+83.5
Register Machine	150K	17.8%	90.8%	+73.0
Petri Net	80K	25.6%	93.4%	+67.8
Cellular Automaton	100K	28.9%	94.6%	+65.7
Markov Chain	50K	31.2%	95.2%	+64.0
KMP Pattern	100K	33.4%	95.8%	+62.4
Regex NFA	80K	26.7%	93.2%	+66.5
CFG Derivation	50K	22.3%	91.4%	+69.1
Translation Chain	10K	41.2%	89.1%	+47.9
ASCII Art Parse	5K	44.5%	95.2%	+50.7
Long Division	1K	15.6%	94.3%	+78.7
Matrix Multiply	8K	18.9%	92.7%	+73.8
Gaussian Elim.	5K	16.7%	91.5%	+74.8
GCD Euclidean	2K	37.8%	97.8%	+60.0
Simplex Method	3K	14.5%	89.8%	+75.3
Polynomial GCD	2K	17.8%	91.2%	+73.4
Continued Frac.	1K	26.7%	94.8%	+68.1
Symbolic Diff.	500	31.2%	95.6%	+64.4

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Table A41. Complete Results: Tasks 67-86

Task	Steps	Base	PRIME	Δ
SAT DPLL	50K	17.8%	91.2%	+73.4
Resolution Proof	30K	19.8%	91.8%	+72.0
Unification	20K	21.2%	92.4%	+71.2
Type Inference	15K	18.9%	90.8%	+71.9
Lambda Reduction	10K	16.7%	89.6%	+72.9
Dependency SAT	40K	22.3%	87.6%	+65.3
Stack Simulator	100K	37.8%	97.2%	+59.4
Queue Simulator	100K	36.7%	96.8%	+60.1
Doubly Linked List	80K	28.9%	94.6%	+65.7
Hash Table	50K	31.2%	95.2%	+64.0
LRU Cache	50K	27.8%	93.8%	+66.0
Union-Find	80K	33.4%	95.8%	+62.4
File System Ops	100K	26.7%	94.2%	+67.5
Blockchain Ledger	50K	28.9%	94.8%	+65.9
Railway Scheduling	30K	25.6%	93.2%	+67.6
Meeting Scheduler	20K	31.2%	95.6%	+64.4
Elevator Sched.	30K	27.8%	93.8%	+66.0
Packet Routing	50K	24.5%	92.6%	+68.1
Assembly Line	20K	23.4%	91.8%	+68.4
Chemical Reaction	30K	26.7%	93.4%	+66.7

Appendix B.8. Statistical Significance

All reported improvements are statistically significant at $p < 0.001$ (paired t-test with Bonferroni correction). Effect sizes (Cohen's d) exceed 2.0 for all task comparisons, indicating very large practical significance.

Table A42. 95% Confidence Intervals by Category

Category	Baseline CI	PRIME CI
Comparison Sorting	[23.1, 27.7]%	[92.8, 95.4]%
Non-comparison Sort	[30.2, 36.6]%	[95.6, 98.2]%
Advanced Sorting	[22.3, 27.3]%	[91.4, 94.4]%
Graph Traversal	[26.5, 32.3]%	[92.1, 95.7]%
Tree Operations	[24.8, 30.8]%	[91.8, 95.2]%
Classic Puzzles	[24.5, 30.1]%	[93.0, 95.8]%
Automata/State	[21.3, 27.1]%	[91.6, 95.2]%
String/Pattern	[30.5, 36.7]%	[91.1, 94.7]%
Mathematical	[19.1, 25.7]%	[91.8, 95.2]%
Logic/Theorem	[15.9, 23.1]%	[88.1, 93.1]%
Data Structures	[29.7, 35.5]%	[94.2, 97.0]%
System Simulation	[24.0, 29.8]%	[92.0, 95.4]%

Appendix B.9. Model-Specific Performance Analysis

This section presents detailed performance analysis across different model architectures and parameter scales.

Appendix B.9.1. Performance by Model Size

Table A43 presents the relationship between model size and performance under baseline and PRIME conditions.

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Table A43. Performance by Model Size: Baseline vs. PRIME

Model	Params	Baseline	Std	PRIME	Std	Δ (pp)	Rel. Improv.
Qwen3-8B	8B	21.3%	5.8%	89.2%	3.4%	+67.9	+318.8%
Gemma3-12B	12B	24.1%	5.2%	91.8%	3.1%	+67.7	+280.9%
Qwen3-14B	14B	26.8%	5.0%	93.8%	2.7%	+67.0	+250.0%
GPT-OSS-20B	20B	28.4%	4.8%	94.6%	2.5%	+66.2	+233.1%
Gemma3-27B	27B	30.2%	4.6%	95.1%	2.4%	+64.9	+214.9%
Qwen3-Coder-30B	30B	32.5%	4.4%	95.8%	2.2%	+63.3	+194.8%
GPT-OSS-120B	120B	38.7%	4.1%	96.9%	1.9%	+58.2	+150.4%

Appendix B.9.2. Scaling Law Analysis

We observe a power-law relationship between model size and baseline performance:

$$\text{Acc}_{\text{baseline}}(N) = \alpha \cdot N^{\beta} + \gamma \tag{A12}$$

where N is the parameter count in billions. Fitting yields $\alpha = 4.73$, $\beta = 0.21$, $\gamma = 15.2$ with $R^2 = 0.97$.

Notably, PRIME effectiveness (measured as percentage point improvement) exhibits an inverse relationship with model size, suggesting that smaller models benefit more from structured execution guidance:

$$\Delta_{\text{PRIME}}(N) = \delta \cdot N^{-\eta} + \phi \tag{A13}$$

with fitted parameters $\delta = 12.8$, $\eta = 0.08$, $\phi = 56.1$.

Table A44. Scaling Law Coefficients

Metric	Coefficient	Value	95% CI
Baseline	α	4.73	[4.12, 5.34]
	β	0.21	[0.18, 0.24]
	γ	15.2	[13.8, 16.6]
PRIME Gain	δ	12.8	[11.2, 14.4]
	η	0.08	[0.06, 0.10]
	ϕ	56.1	[54.3, 57.9]

Appendix B.9.3. Model Architecture Comparison

Table A45 compares performance across different model architectures under identical parameter budgets.

Table A45. Architecture Comparison at Similar Parameter Counts

Architecture	∼Params	Baseline	PRIME	Δ
∼12-14B Parameter Models				
Gemma3-12B (Decoder)	12B	24.1%	91.8%	+67.7
Qwen3-14B (Decoder)	14B	26.8%	93.8%	+67.0
∼27-30B Parameter Models				
Gemma3-27B (Decoder)	27B	30.2%	95.1%	+64.9
Qwen3-Coder-30B (Decoder)	30B	32.5%	95.8%	+63.3

Appendix B.10. Error Analysis

Appendix B.10.1. Error Distribution by Category

Table A46 presents the distribution of error types across task categories under PRIME execution.

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Table A46. Error Type Distribution by Task Category (% of Total Errors)

Category	State	Index	Operation	Ordering	Termination	Format	Other
Comparison Sorting	28.4%	22.1%	18.3%	12.5%	8.9%	6.2%	3.6%
Non-comparison Sort	18.2%	31.4%	22.6%	8.4%	10.2%	5.8%	3.4%
Advanced Sorting	31.5%	19.8%	21.2%	11.3%	7.8%	5.2%	3.2%
Graph Traversal	35.2%	15.6%	12.4%	18.9%	9.1%	5.4%	3.4%
Tree Operations	29.8%	24.3%	16.5%	14.2%	6.8%	5.1%	3.3%
Classic Puzzles	22.4%	12.8%	28.6%	16.4%	11.2%	4.8%	3.8%
Automata/State	38.6%	8.4%	14.2%	22.5%	8.5%	4.6%	3.2%
String/Pattern	25.3%	28.6%	18.4%	10.2%	9.8%	4.5%	3.2%
Mathematical	42.1%	18.5%	15.2%	6.8%	7.4%	6.8%	3.2%
Logic/Theorem	35.8%	8.2%	24.6%	18.4%	6.2%	3.6%	3.2%
Data Structures	26.4%	32.5%	14.8%	12.1%	6.8%	4.2%	3.2%
System Simulation	34.2%	14.6%	16.8%	19.4%	7.2%	4.6%	3.2%
Overall	**30.7%**	**19.7%**	**18.6%**	**14.3%**	**8.3%**	**5.1%**	**3.3%**

Appendix B.10.2. Error Severity Analysis

Errors are classified into three severity levels based on their impact on execution correctness:

Table A47. Error Severity Classification

Severity	Weight	Description
Critical	1.0	Completely incorrect result; algorithm fails
Major	0.6	Partial correctness; significant deviation
Minor	0.2	Correct result with suboptimal execution

Table A48. Error Severity Distribution: Baseline vs. PRIME

	Baseline			PRIME		
Sorting	68.2%	24.3%	7.5%	3.8%	1.4%	0.7%
Graph	65.4%	26.8%	7.8%	4.2%	1.2%	0.7%
Tree	67.8%	24.6%	7.6%	4.6%	1.3%	0.6%
Puzzles	66.1%	25.4%	8.5%	3.4%	1.5%	0.7%
Automata	71.2%	22.4%	6.4%	4.8%	1.2%	0.6%
String	62.8%	28.2%	9.0%	5.2%	1.4%	0.5%
Math	73.4%	20.8%	5.8%	4.6%	1.2%	0.7%
Logic	76.2%	18.6%	5.2%	6.8%	1.8%	0.8%
Data Struct.	61.8%	29.4%	8.8%	2.8%	1.0%	0.6%
Simulation	68.4%	24.2%	7.4%	4.4%	1.4%	0.5%

Appendix B.10.3. First Error Position Analysis

We analyze where errors first occur in execution traces to understand failure patterns.

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Table A49. First Error Position (Percentile of Execution)

Category	Baseline μ	Baseline σ	PRIME μ	PRIME σ
Sorting	18.4%	12.3%	72.6%	18.4%
Graph	22.1%	14.5%	68.4%	21.2%
Tree	24.6%	15.2%	71.2%	19.8%
Puzzles	31.2%	18.4%	78.4%	15.6%
Automata	15.8%	10.6%	65.2%	22.4%
Math	12.4%	8.2%	62.8%	24.6%

Appendix B.11. Ablation Study Results

Appendix B.11.1. Component-wise Ablation

Table A50 presents detailed ablation results for each PRIME component.

Table A50. Detailed Ablation Study: Component Contributions

Configuration	Acc.	Δ vs Full	State Err	Constraint Err	Avg Steps	Retry Rate
Full PRIME	93.8%	—	2.1%	1.4%	1.28	12.4%
− GRPO (use PPO)	89.2%	−4.6 pp	3.8%	2.4%	1.52	18.6%
− Verifier Agent	86.4%	−7.4 pp	5.2%	4.8%	1.34	14.2%
− Iterative Exec.	82.8%	−11.0 pp	6.4%	3.2%	1.00	0.0%
− Self-Consistency	88.6%	−5.2 pp	4.2%	2.1%	1.28	12.4%
− Multi-Agent	78.4%	−15.4 pp	8.6%	6.4%	1.12	8.2%
Baseline Only	26.8%	−67.0 pp	42.4%	28.6%	1.00	0.0%

Appendix B.11.2. Component Interaction Effects

Table A51 presents interaction effects between PRIME components.

Table A51. Component Interaction Effects

Component Pair	Independent Sum	Combined Effect
GRPO + Verifier	12.0 pp	14.8 pp
GRPO + Multi-Agent	20.0 pp	24.2 pp
Verifier + Iterative	18.4 pp	22.6 pp
Multi-Agent + Self-Cons.	20.6 pp	25.8 pp

The positive synergies (combined effect $>$ independent sum) indicate that PRIME components are complementary rather than redundant.

Appendix B.11.3. Hyperparameter Sensitivity

Table A52. Hyperparameter Sensitivity Analysis: Impact on PRIME Performance

Parameter	Low Value	Default	High Value	Δ (Low-High)	Sensitivity Notes
Group size G	4: 91.2%	8: 93.8%	16: 94.1%	2.9 pp	Diminishing returns above $G = 8$
Iterations K	2: 88.4%	5: 93.8%	10: 94.2%	5.8 pp	Most sensitive; early stopping mitigates
Violation τ	0.1: 92.4%	0.3: 93.8%	0.5: 91.8%	1.4 pp	U-shaped; optimal at moderate threshold
Temperature	0.5: 92.1%	0.7: 93.8%	0.9: 90.6%	3.2 pp	Balances diversity vs. quality
Learning rate	5e-6: 91.8%	1e-5: 93.8%	2e-5: 92.4%	2.0 pp	Stable within one order of magnitude

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Appendix B.12. Difficulty-Stratified Analysis

Appendix B.12.1. Performance by Difficulty Level

Table A53. Performance by Difficulty Level Across Categories

	Easy		Medium		Hard	
Comparison Sorting	38.2%	98.4%	24.6%	94.2%	13.4%	89.7%
Non-comparison Sort	45.6%	99.1%	32.8%	97.2%	21.8%	94.4%
Advanced Sorting	36.4%	97.6%	24.2%	93.1%	13.8%	88.0%
Graph Traversal	42.1%	98.2%	28.6%	94.1%	17.5%	89.4%
Tree Operations	40.2%	97.8%	27.4%	93.6%	15.8%	89.1%
Classic Puzzles	41.8%	98.6%	26.4%	94.8%	13.7%	89.8%
Automata/State	38.4%	98.1%	23.6%	93.8%	10.6%	88.3%
String/Pattern	46.8%	97.4%	32.4%	93.2%	21.6%	88.1%
Mathematical	36.2%	97.8%	21.8%	93.6%	9.2%	89.1%
Logic/Theorem	32.4%	96.2%	18.6%	91.2%	7.5%	84.4%
Data Structures	46.4%	98.8%	31.8%	96.2%	19.6%	91.8%
System Simulation	40.6%	98.4%	26.2%	94.1%	13.9%	88.6%
Overall	**40.4%**	**98.0%**	**26.5%**	**94.1%**	**14.9%**	**89.2%**

Appendix B.12.2. Difficulty Degradation Analysis

The performance degradation from Easy to Hard instances follows a predictable pattern:

$$\text{Acc}(d) = \text{Acc}_{\text{Easy}} \cdot e^{-\lambda d} \tag{A14}$$

where $d \in \{0, 1, 2\}$ represents difficulty level. For baseline, $\lambda = 0.50$; for PRIME, $\lambda = 0.05$, indicating significantly flatter degradation.

Appendix B.13. Execution Efficiency Analysis

Appendix B.13.1. Step Count Distribution

Table A54. Execution Steps: PRIME vs. Optimal

Category	Optimal	PRIME	Overhead
Comparison Sorting	1.00×	1.12×	+12%
Non-comparison Sort	1.00×	1.08×	+8%
Advanced Sorting	1.00×	1.18×	+18%
Graph Traversal	1.00×	1.14×	+14%
Tree Operations	1.00×	1.16×	+16%
Classic Puzzles	1.00×	1.06×	+6%
Automata/State	1.00×	1.04×	+4%
String/Pattern	1.00×	1.10×	+10%
Mathematical	1.00×	1.08×	+8%
Logic/Theorem	1.00×	1.22×	+22%
Data Structures	1.00×	1.06×	+6%
System Simulation	1.00×	1.12×	+12%
Average	**1.00×**	**1.11×**	**+11%**

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Appendix B.13.2. Retry and Backtrack Statistics

Table A55. Retry and Backtrack Behavior

Category	Retry Rate	Avg Retries	Backtrack Rate
Sorting	10.2%	1.4	8.6%
Graph	14.8%	1.6	12.4%
Tree	12.6%	1.5	10.2%
Puzzles	8.4%	1.3	6.8%
Automata	15.2%	1.7	14.6%
Math	11.8%	1.5	9.4%
Logic	18.4%	1.9	16.8%
Data Struct.	9.6%	1.3	7.2%
Simulation	13.2%	1.5	11.4%
Overall	**12.4%**	**1.5**	**10.8%**

Appendix B.14. Cross-Task Generalization

Appendix B.14.1. Transfer Learning Performance

We evaluate PRIME's ability to generalize across task categories through transfer experiments.

Table A56. Transfer Learning Matrix: Training on Source, Evaluating on Target (Accuracy %)

Train \ Test	Sorting	Graph	Tree	Automata	Math	Logic
Sorting	**94.1**	78.4	82.6	68.2	72.4	64.8
Graph	76.2	**93.9**	84.2	72.6	68.4	70.2
Tree	80.4	82.8	**93.5**	70.8	74.2	68.6
Automata	64.6	70.4	68.2	**93.4**	66.8	78.4
Math	70.2	66.8	72.4	64.2	**93.5**	72.6
Logic	62.4	68.6	66.8	76.2	70.4	**90.6**
All (Full PRIME)	94.1	93.9	93.5	93.4	93.5	90.6

The diagonal entries show in-domain performance, while off-diagonal entries show transfer performance. Notable positive transfer exists between structurally similar task categories (e.g., Sorting $\rightarrow$ Tree at 82.6%).

Appendix B.14.2. Zero-Shot Category Performance

Table A57 presents performance on held-out task categories without category-specific training.

Table A57. Zero-Shot Performance on Held-Out Categories

Held-Out Category	Zero-Shot	Full Training
Comparison Sorting	84.2%	94.1%
Graph Traversal	82.6%	93.9%
Automata/State	78.4%	93.4%
Mathematical	80.2%	93.5%
Logic/Theorem	76.8%	90.6%
System Simulation	81.4%	93.7%

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Appendix B.15. Computational Overhead Analysis

Appendix B.15.1. Inference Time Breakdown

Table A58. Inference Time Components (ms per instance)

Component	Baseline	PRIME	Overhead
Input Encoding	12.4	18.6	+50%
Policy Forward	45.2	48.4	+7%
Verifier Forward	—	32.6	—
Majority Voting	—	8.4	—
State Management	2.1	12.8	+510%
Total	**59.7**	**120.8**	**+102%**

Appendix B.15.2. Memory Usage

Table A59. GPU Memory Usage (GB)

Model	Baseline	PRIME	Overhead
Qwen3-8B	16.2	24.8	+53%
Qwen3-14B	28.4	42.6	+50%
Gemma3-27B	54.2	78.4	+45%
GPT-OSS-120B	240.8	312.4	+30%

Appendix C. PRIME Algorithm Specification

This appendix provides the complete algorithmic specification of the PRIME (Policy-Reinforced Iterative Multi-agent Execution) framework.

Appendix C.1. Core Algorithm

Algorithm A6 presents the complete PRIME framework pseudocode.

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Algorithm A6 PRIME Framework

Input: Task $\mathcal{T}$, constraints $\mathcal{C}$, iterations K, rollouts G
Output: Solution σ or failure

Initialize executor π_θ^E, verifier V_ϕ, state s_0
for $k = 1$ **to** K **do**
  for $g = 1$ **to** G **do**
    $\tau_g \leftarrow []$; $s \leftarrow s_0$
    while not terminal(s) **do**
      $a \sim \pi_\theta^E(\cdot|s, \mathcal{C})$
      $s' \leftarrow \text{Execute}(s, a)$
      $v \leftarrow V_\phi(s', \mathcal{C})$
      if $v > \tau$ **then**
        $s' \leftarrow \text{Backtrack}(\tau_g)$
      end if
      Append (s, a, s', v) to τ_g
      $s \leftarrow s'$
    end while
    $R_g \leftarrow \text{Reward}(\tau_g, \mathcal{C})$
  end for
  $\bar{R} \leftarrow \frac{1}{G}\sum_g R_g$
  $A_g \leftarrow (R_g - \bar{R})/\sigma_R$
  Update: $\theta \leftarrow \theta + \alpha \nabla_\theta \mathcal{L}^{\text{GRPO}}$
  $\sigma^* \leftarrow \text{MajorityVote}(\{\sigma_g\})$
  if $V_\phi(\sigma^*, \mathcal{C}) = 0$ **then**
    return σ^*
  end if
end for
return $\arg\min_\sigma V_\phi(\sigma, \mathcal{C})$

Appendix C.2. Reward Function

The composite reward function balances multiple objectives:

$$R(\tau) = \alpha R_{\text{task}} + \beta R_{\text{verify}} + \gamma R_{\text{eff}} + \lambda R_{\text{format}} \tag{A15}$$

The reward comprises four components: R_{task} captures task completion (binary or partial credit based on intermediate state correctness), R_{verify} measures verification consistency between executor and verifier outputs, R_{eff} provides an efficiency bonus inversely proportional to steps used, and R_{format} ensures output format compliance. Default hyperparameters are $\alpha = 10.0$, $\beta = 1.0$, $\gamma = 0.5$, $\lambda = 0.1$.

Appendix C.3. GRPO Objective

The Group Relative Policy Optimization (GRPO) objective:

$$\mathcal{L}^{\text{GRPO}} = \mathbb{E}\left[\sum_{g=1}^{G} \frac{1}{|o_g|} \sum_t \min\left(\rho_t^g A_g, \text{clip}(\rho_t^g) A_g\right)\right] \tag{A16}$$

where $\rho_t^g = \frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_{\text{old}}}(a_t|s_t)}$ is the importance sampling ratio and A_g is the normalized group advantage.

Appendix C.4. Majority Voting

The majority voting mechanism aggregates solutions across rollouts:

$$\sigma^* = \arg\max_\sigma \sum_{g=1}^{G} \mathbf{1}[\sigma_g = \sigma] \tag{A17}$$

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For tasks with continuous outputs, we use approximate matching with tolerance ϵ:

$$\sigma^* = \arg\max_{\sigma} \sum_{g=1}^{G} \mathbf{1}[\|\sigma_g - \sigma\| < \epsilon] \tag{A18}$$

Appendix C.5. Verifier Architecture

The verifier V_ϕ is a separate model trained to identify constraint violations:

$$V_\phi(s, \mathcal{C}) = \sum_{c \in \mathcal{C}} w_c \cdot \text{Violated}(s, c) \tag{A19}$$

where w_c are learned importance weights for each constraint type.

Appendix D. Prompt Templates

This section presents representative prompt templates used in the evaluation.

Appendix D.1. Baseline Prompt Template

```
Solve the following problem:
{problem_description}

Input: {input_data}

Provide your answer.
```

Listing 1: Baseline Prompt (Generic)

Appendix D.2. PRIME Structured Prompt Template

```
TASK: {task_name}

PROBLEM SPECIFICATION: {formal_specification}

INPUT: {formatted_input}

CONSTRAINTS: {enumerated_constraints}

VERIFICATION PROCEDURE: {step_by_step_verification}

EXAMPLES: {worked_examples}

YOUR TASK:
  Execute the algorithm step by step.
  Show all intermediate states.
  Verify each step against constraints.
  Format: {output_format}
```

Listing 2: PRIME Prompt Template

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Appendix D.3. Task-Specific Templates

Appendix D.3.1. Sorting Task Template

```
TASK: {algorithm_name} Simulation

ALGORITHM: {algorithm_description}

INPUT: array={array}, length={n}

EXECUTION REQUIREMENTS:
  1. Show the array state after each operation
  2. Mark comparisons and swaps explicitly
  3. Track pass/iteration numbers
  4. Verify sorted property at completion

OUTPUT FORMAT:
  Pass k: [operation] -> [resulting array]
  ...
  Final: [sorted array]
```

Listing 3: Sorting Algorithm Prompt

Appendix D.3.2. State Machine Template

```
TASK: {automaton_type} Simulation

AUTOMATON DEFINITION:
  States: {Q}
  Alphabet: {Sigma}
  Transitions: {delta}
  Initial: {q0}
  Accepting: {F}

INPUT STRING: {input}

EXECUTION REQUIREMENTS:
  1. Show state after each symbol
  2. Track tape/stack state if applicable
  3. Indicate acceptance/rejection

OUTPUT FORMAT:
  Step k: state={q}, symbol={s} -> state={q'}
  ...
  Result: {ACCEPT/REJECT}
```

Listing 4: Automaton Simulation Prompt

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Appendix D.3.3. Mathematical Computation Template

```
TASK: {operation_name}

PROBLEM: {mathematical_expression}

ALGORITHM: {computation_procedure}

EXECUTION REQUIREMENTS:
  1. Show each intermediate computation
  2. Maintain precision throughout
  3. Verify result by checking

OUTPUT FORMAT:
  Step k: {intermediate_result}
  ...
  Final Answer: {result}
  Verification: {check}
```

Listing 5: Mathematical Task Prompt

Appendix D.4. Verifier Prompt Template

```
VERIFICATION TASK

ORIGINAL PROBLEM: {problem_specification}

PROPOSED SOLUTION: {candidate_solution}

CONSTRAINTS TO CHECK: {constraint_list}

INSTRUCTIONS:
  1. Check each constraint systematically
  2. Report any violations found
  3. Provide violation severity score

OUTPUT FORMAT:
  Constraint 1: {PASS/FAIL} - {reason}
  Constraint 2: {PASS/FAIL} - {reason}
  ...
  Overall: {VALID/INVALID}
  Violation Score: {0.0-1.0}
```

Listing 6: Verifier Agent Prompt

Appendix E. Theoretical Analysis

This section provides rigorous theoretical analysis of the PRIME framework, including convergence guarantees, complexity bounds, and optimality conditions.

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Appendix E.1. Convergence Analysis

Appendix E.1.1. GRPO Convergence Theorem

Theorem A4 (GRPO Convergence). *Under the following conditions:*

1. *The policy space Π_θ is compact and the policy π_θ is Lipschitz continuous in θ*
2. *The reward function $R(\tau)$ is bounded: $|R(\tau)| \leq R_{\max}$*
3. *The learning rate schedule satisfies $\sum_t \alpha_t = \infty$ and $\sum_t \alpha_t^2 < \infty$*
4. *The group size $G \geq 2$*

Then the GRPO algorithm converges to a local optimum of the expected reward $\mathbb{E}_{\tau\sim\pi_\theta}[R(\tau)]$ with probability 1.

Proof. We establish convergence through the following steps.

Step 1: Unbiasedness of Gradient Estimator. The policy gradient theorem states that $\nabla_\theta J(\theta) = \mathbb{E}_{\tau\sim\pi_\theta}[R(\tau)\nabla_\theta \log \pi_\theta(\tau)]$. For the group-relative advantage $A_g = (R_g - \bar{R})/(\sigma_R + \epsilon)$, we show unbiasedness:

$$\mathbb{E}\left[\sum_{g=1}^{G} A_g \nabla_\theta \log \pi_\theta(\tau_g)\right] = \mathbb{E}\left[\sum_{g=1}^{G} \frac{R_g - \bar{R}}{\sigma_R + \epsilon} \nabla_\theta \log \pi_\theta(\tau_g)\right] \tag{A20}$$

Since $\sum_g (R_g - \bar{R}) = 0$ and the baseline subtraction does not affect the expected gradient direction, we have:

$$\mathbb{E}[A_g \nabla_\theta \log \pi_\theta(\tau_g)] = \nabla_\theta \mathbb{E}_{\tau\sim\pi_\theta}[R(\tau)] \cdot \frac{1}{\mathbb{E}[\sigma_R] + \epsilon} \tag{A21}$$

Step 2: Variance Bound. Since $|R(\tau)| \leq R_{\max}$ by assumption, we have $|R_g - \bar{R}| \leq 2R_{\max}$. The sample variance satisfies $\sigma_R^2 = \frac{1}{G}\sum_g (R_g - \bar{R})^2 \leq 4R_{\max}^2$. Thus:

$$\mathrm{Var}[A_g] = \mathbb{E}[A_g^2] - \mathbb{E}[A_g]^2 \leq \mathbb{E}\left[\frac{(R_g - \bar{R})^2}{\sigma_R^2}\right] \leq \frac{4R_{\max}^2}{G \cdot \sigma_R^2} \leq \frac{4R_{\max}^2}{G} \tag{A22}$$

where the last inequality uses $\sigma_R \geq 1$ for non-trivial reward distributions (ensured by the ϵ term).

Step 3: Convergence via Robbins-Monro. The GRPO update $\theta_{t+1} = \theta_t + \alpha_t \hat{g}_t$ satisfies the Robbins-Monro conditions: (i) $\hat{g}_t$ is an unbiased estimator of $\nabla_\theta J(\theta)$ up to scaling; (ii) $\mathrm{Var}[\hat{g}_t]$ is bounded; (iii) the learning rate satisfies $\sum_t \alpha_t = \infty$ and $\sum_t \alpha_t^2 < \infty$. By the Robbins-Monro theorem [94], $\theta_t \to \theta^*$ where $\nabla_\theta J(\theta^*) = 0$ (a local optimum) with probability 1.

Step 4: Convergence Rate. Under Lipschitz continuity of π_θ and bounded variance, the standard convergence rate for stochastic gradient descent applies:

$$\mathbb{E}[J(\theta^*) - J(\theta_T)] = \mathcal{O}\left(\frac{1}{\sqrt{T}}\right) \tag{A23}$$

This completes the proof. □

Appendix E.1.2. Sample Complexity Bound

Theorem A5 (Sample Complexity). *To achieve ϵ-optimal performance (i.e., $\mathbb{E}[R(\pi_\theta)] \geq \mathbb{E}[R(\pi^*)] - \epsilon$), PRIME requires at most*

$$N = \mathcal{O}\left(\frac{R_{\max}^2 H^2}{\epsilon^2} \cdot \log \frac{|\Pi_\theta|}{\delta}\right) \tag{A24}$$

samples with probability at least $1 - \delta$, where H is the maximum trajectory length and $|\Pi_\theta|$ is the policy class complexity.

Proof. The proof follows from uniform convergence arguments over the policy class.

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Step 1: Concentration for Fixed Policy. For a fixed policy π, let $\hat{R}_N(\pi) = \frac{1}{N}\sum_{i=1}^{N} R(\tau_i)$ be the empirical reward estimate from N trajectories. Since $|R(\tau)| \leq R_{\max} \cdot H$ (bounded reward accumulated over H steps), by Hoeffding's inequality:

$$\Pr\left[|\hat{R}_N(\pi) - \mathbb{E}[R(\pi)]| > t\right] \leq 2\exp\left(-\frac{2Nt^2}{R_{\max}^2 H^2}\right) \tag{A25}$$

Step 2: Union Bound over Policy Class. Applying a union bound over an $\epsilon/4$-cover of the policy class Π_θ (which has covering number at most $|\Pi_\theta|$ for finite parameterization), we obtain:

$$\Pr\left[\sup_{\pi \in \Pi_\theta} |\hat{R}_N(\pi) - \mathbb{E}[R(\pi)]| > \frac{\epsilon}{2}\right] \leq 2|\Pi_\theta| \exp\left(-\frac{N\epsilon^2}{2R_{\max}^2 H^2}\right) \tag{A26}$$

Step 3: Sample Complexity Derivation. Setting the right-hand side equal to δ and solving for N:

$$2|\Pi_\theta| \exp\left(-\frac{N\epsilon^2}{2R_{\max}^2 H^2}\right) = \delta \implies N = \frac{2R_{\max}^2 H^2}{\epsilon^2} \log \frac{2|\Pi_\theta|}{\delta} \tag{A27}$$

Step 4: Optimality Gap. With N samples satisfying the above bound, the empirical optimizer $\hat{\pi} = \arg\max_\pi \hat{R}_N(\pi)$ satisfies:

$$\mathbb{E}[R(\pi^*)] - \mathbb{E}[R(\hat{\pi})] \leq \mathbb{E}[R(\pi^*)] - \hat{R}_N(\pi^*) + \hat{R}_N(\hat{\pi}) - \mathbb{E}[R(\hat{\pi})] \tag{A28}$$

$$\leq \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon \tag{A29}$$

where the second inequality uses the uniform convergence guarantee. This establishes the ϵ-optimality with the stated sample complexity. □

Appendix E.2. Verification Agent Analysis

Appendix E.2.1. Constraint Satisfaction Guarantees

Definition A15 (Verifier Completeness). *A verifier V_ϕ is (α, β)-complete if it satisfies two properties:* Soundness, *requiring* $\Pr[V_\phi(s, \mathcal{C}) = 0 | s \text{ satisfies } \mathcal{C}] \geq 1 - \alpha$, *and* Completeness, *requiring* $\Pr[V_\phi(s, \mathcal{C}) > 0 | s \text{ violates } \mathcal{C}] \geq 1 - \beta$.

Theorem A6 (Verification Error Propagation). *Given a (α, β)-complete verifier and K iterative attempts, the probability of accepting an incorrect solution is bounded by:*

$$\Pr[\textit{False Accept}] \leq \beta^K \tag{A30}$$

For a $(0.01, 0.05)$-complete verifier with $K = 5$, this yields $\Pr[\textit{False Accept}] \leq 3.125 \times 10^{-7}$.

Proof. We analyze the probability of accepting an incorrect solution across K independent verification attempts.

Step 1: Single Verification Error. By the definition of (α, β)-completeness, when a solution s violates some constraint in $\mathcal{C}$, the verifier detects this violation with probability at least $1 - \beta$:

$$\Pr[V_\phi(s, \mathcal{C}) > 0 \mid s \text{ violates } \mathcal{C}] \geq 1 - \beta \tag{A31}$$

Equivalently, the probability of failing to detect a violation is at most β:

$$\Pr[V_\phi(s, \mathcal{C}) = 0 \mid s \text{ violates } \mathcal{C}] \leq \beta \tag{A32}$$

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Step 2: Independence Across Iterations. In PRIME, each of the K iterations generates an independent trajectory due to the stochastic policy sampling (Equation 5). For an incorrect solution to be accepted, the verifier must fail to detect violations in all K attempts.

Step 3: Multiplicative Error Bound. Assuming independence across iterations, the probability that an incorrect solution passes verification in all K attempts is:

$$\Pr[\text{False Accept}] = \prod_{k=1}^{K} \Pr[\text{Fail to detect in iteration } k] \leq \beta^K \tag{A33}$$

Step 4: Numerical Evaluation. For the empirically measured verifier completeness of $(0.01, 0.05)$ (i.e., $\beta = 0.05$) and $K = 5$ iterations:

$$\Pr[\text{False Accept}] \leq 0.05^5 = 3.125 \times 10^{-7} \tag{A34}$$

This extremely low false acceptance rate ensures reliable constraint satisfaction in practice. □

Appendix E.2.2. Multi-Agent Coordination

Definition A16 (Agent Agreement)**.** *Given G parallel rollouts producing solutions $\{\sigma_1, \ldots, \sigma_G\}$, define the agreement score:*

$$\textit{Agreement}(\{\sigma_g\}) = \max_{\sigma} \frac{1}{G} \sum_{g=1}^{G} \mathbf{1}[\sigma_g = \sigma] \tag{A35}$$

Theorem A7 (Majority Voting Reliability)**.** *If each agent independently produces a correct solution with probability $p > 0.5$, then majority voting over G agents yields a correct solution with probability:*

$$\Pr[\textit{Correct}] = \sum_{k=\lceil G/2 \rceil}^{G} \binom{G}{k} p^k (1-p)^{G-k} \geq 1 - e^{-2G(p-0.5)^2} \tag{A36}$$

For $p = 0.75$ and $G = 8$, this gives $\Pr[\textit{Correct}] \geq 99.6\%$.

Proof. We establish both the exact probability expression and the exponential lower bound.

Step 1: Exact Probability. Let $X_g \in \{0, 1\}$ indicate whether agent g produces a correct solution, with $\Pr[X_g = 1] = p$. The total number of correct solutions is $S = \sum_{g=1}^{G} X_g$, which follows a Binomial(G, p) distribution. Majority voting succeeds when $S \geq \lceil G/2 \rceil$:

$$\Pr[\text{Correct}] = \Pr[S \geq \lceil G/2 \rceil] = \sum_{k=\lceil G/2 \rceil}^{G} \binom{G}{k} p^k (1-p)^{G-k} \tag{A37}$$

Step 2: Hoeffding's Inequality Application. To derive the exponential bound, we apply Hoeffding's inequality. Let $\bar{X} = S/G$ be the empirical success rate. Majority voting fails when $\bar{X} < 0.5$. Since $\mathbb{E}[\bar{X}] = p > 0.5$:

$$\Pr[\text{Majority Fails}] = \Pr[\bar{X} < 0.5] = \Pr[\bar{X} - p < 0.5 - p] \tag{A38}$$

$$\leq \Pr[|\bar{X} - p| > p - 0.5] \tag{A39}$$

By Hoeffding's inequality for bounded random variables $X_g \in [0, 1]$:

$$\Pr[|\bar{X} - p| > t] \leq 2\exp(-2Gt^2) \tag{A40}$$

Setting $t = p - 0.5 > 0$:

$$\Pr[\text{Majority Fails}] \leq \exp(-2G(p-0.5)^2) \tag{A41}$$

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Therefore:

$$\Pr[\text{Correct}] = 1 - \Pr[\text{Majority Fails}] \geq 1 - e^{-2G(p-0.5)^2} \tag{A42}$$

Step 3: Numerical Verification. For $p = 0.75$ and $G = 8$:

$$\Pr[\text{Correct}] \geq 1 - e^{-2 \cdot 8 \cdot (0.25)^2} = 1 - e^{-1} \approx 0.632 \tag{A43}$$

This is a conservative lower bound. The exact binomial calculation yields:

$$\Pr[\text{Correct}] = \sum_{k=4}^{8} \binom{8}{k} (0.75)^k (0.25)^{8-k} = 0.9963 \tag{A44}$$

Thus, majority voting achieves >99.6% reliability under the stated conditions. □

Appendix E.3. Computational Complexity

Appendix E.3.1. Time Complexity Analysis

Theorem A8 (PRIME Time Complexity)**.** *For a task with maximum trajectory length H, the time complexity of PRIME is:*

$$T_{PRIME} = \mathcal{O}(K \cdot G \cdot H \cdot (T_{policy} + T_{verifier})) \tag{A45}$$

where K is the number of iterations, G is the group size, T_{policy} is the policy inference time, and $T_{verifier}$ is the verifier inference time.

Proof. We analyze the computational cost of Algorithm A6.

Outer Loop (Lines 2–14): The algorithm performs K iterations.

Middle Loop (Lines 3–12): Within each iteration, G parallel rollouts are executed.

Inner Loop (Lines 5–10): Each rollout generates a trajectory of at most H steps. At each step:

- Line 6: Policy forward pass requires T_{policy} time
- Line 8: Verifier forward pass requires T_{verifier} time
- Lines 9–10: Backtracking and state updates are $\mathcal{O}(1)$ operations

Post-processing (Lines 13–17): Majority voting over G solutions is $\mathcal{O}(G)$.

The total time complexity is therefore:

$$T_{\text{PRIME}} = K \cdot G \cdot H \cdot (T_{\text{policy}} + T_{\text{verifier}}) + \mathcal{O}(K \cdot G) \tag{A46}$$

Since $H \cdot (T_{\text{policy}} + T_{\text{verifier}}) \gg 1$ in practice, the dominant term yields the stated bound. □

Appendix E.3.2. Space Complexity Analysis

Theorem A9 (Space Complexity)**.** *The space complexity of PRIME during inference is:*

$$S_{PRIME} = \mathcal{O}(G \cdot H \cdot d_{state} + |\theta_\pi| + |\phi_V|) \tag{A47}$$

where d_{state} is the state dimension, $|\theta_\pi|$ is the policy model size, and $|\phi_V|$ is the verifier model size.

Proof. We account for all memory allocations during PRIME execution.

Model Parameters: The policy model requires $|\theta_\pi|$ parameters and the verifier requires $|\phi_V|$ parameters. These are fixed costs independent of the input.

State Stack: Each of the G rollouts maintains a state stack (Line 2 of Algorithm 1) with at most H states, each of dimension d_{state}. Total: $\mathcal{O}(G \cdot H \cdot d_{\text{state}})$.

Trajectory Storage: Storing (s, a, s', v) tuples for G trajectories of length H requires $\mathcal{O}(G \cdot H \cdot d_{\text{state}})$ space.

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Intermediate Activations: For transformer-based models with context length L and hidden dimension d, activation memory is $\mathcal{O}(L \cdot d)$, which is subsumed by $|\theta_\pi|$ for practical model sizes.

Summing these contributions yields the stated space complexity. □

Appendix E.4. Optimality Conditions

Appendix E.4.1. Policy Improvement Guarantee

Theorem A10 (Monotonic Improvement)**.** *Under the GRPO update with clipping parameter ϵ, the new policy $\pi_{\theta'}$ satisfies:*

$$\mathbb{E}_{\tau\sim\pi_{\theta'}}[R(\tau)] \geq \mathbb{E}_{\tau\sim\pi_\theta}[R(\tau)] - \frac{2\epsilon\gamma_d}{(1-\gamma_d)^2}\max_{s,a}|A^{\pi_\theta}(s,a)| \tag{A48}$$

where γ_d is the discount factor (distinct from the efficiency weight γ in the reward function) and A^{π_θ} is the advantage function.

Proof. We adapt the Trust Region Policy Optimization (TRPO) analysis [95] to the GRPO setting.

Step 1: Performance Difference Lemma. Following Kakade and Langford [96], for any two policies π and π':

$$J(\pi') - J(\pi) = \frac{1}{1-\gamma_d}\mathbb{E}_{s\sim d^{\pi'},a\sim\pi'}[A^\pi(s,a)] \tag{A49}$$

where $d^{\pi'}$ is the discounted state visitation distribution under π'.

Step 2: Surrogate Objective. Define the local surrogate objective:

$$L_\pi(\pi') = J(\pi) + \frac{1}{1-\gamma_d}\mathbb{E}_{s\sim d^{\pi},a\sim\pi'}[A^\pi(s,a)] \tag{A50}$$

This surrogate equals the true objective when $\pi' = \pi$ and shares the same gradient at π.

Step 3: Trust Region Bound. The difference between the true objective and surrogate is bounded by the state distribution mismatch:

$$|J(\pi') - L_\pi(\pi')| \leq \frac{2\gamma_d \max_{s,a}|A^\pi(s,a)|}{(1-\gamma_d)^2} D_{\mathrm{TV}}^{\max}(\pi'\|\pi) \tag{A51}$$

where $D_{\mathrm{TV}}^{\max} = \max_s D_{\mathrm{TV}}(\pi'(\cdot|s)\|\pi(\cdot|s))$ is the maximum total variation distance.

Step 4: Clipping Constraint. The GRPO clipping mechanism ensures $\frac{\pi'(a|s)}{\pi(a|s)} \in [1-\epsilon, 1+\epsilon]$. By Pinsker's inequality:

$$D_{\mathrm{TV}}(\pi'\|\pi) \leq \sqrt{\frac{1}{2}D_{\mathrm{KL}}(\pi'\|\pi)} \tag{A52}$$

The clipping constraint bounds $D_{\mathrm{TV}}^{\max} \leq \epsilon$.

Step 5: Improvement Guarantee. Since GRPO maximizes $L_\pi(\pi')$ (ensuring $L_\pi(\pi') \geq L_\pi(\pi) = J(\pi)$) subject to the clipping constraint:

$$J(\pi') \geq L_\pi(\pi') - \frac{2\gamma_d \max_{s,a}|A^\pi(s,a)|}{(1-\gamma_d)^2}\epsilon \tag{A53}$$

$$\geq J(\pi) - \frac{2\epsilon\gamma_d}{(1-\gamma_d)^2}\max_{s,a}|A^{\pi_\theta}(s,a)| \tag{A54}$$

This completes the proof. □

Appendix E.4.2. Regret Bound

Definition A17 (Cumulative Regret)**.** *The cumulative regret after T episodes is:*

$$Regret(T) = \sum_{t=1}^{T}(R^* - R(\tau_t)) \tag{A55}$$

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where $R^* = \max_\tau R(\tau)$ is the optimal reward.

Theorem A11 (Regret Bound). *PRIME achieves sublinear regret:*

$$Regret(T) = \mathcal{O}(\sqrt{T \log T}) \tag{A56}$$

under the conditions of Theorem A4.

Proof. The proof combines the convergence rate from Theorem A4 with online learning regret analysis.

Step 1: Decomposition. The cumulative regret can be decomposed as:

$$\text{Regret}(T) = \sum_{t=1}^{T} (R^* - R(\tau_t)) \tag{A57}$$

$$= \sum_{t=1}^{T} (R^* - J(\theta_t)) + \sum_{t=1}^{T} (J(\theta_t) - R(\tau_t)) \tag{A58}$$

The first term captures the optimization gap, and the second captures the variance of individual episodes around their expected values.

Step 2: Optimization Gap. From Theorem A4, after t updates:

$$R^* - J(\theta_t) = \mathcal{O}\left(\frac{1}{\sqrt{t}}\right) \tag{A59}$$

Summing over T episodes:

$$\sum_{t=1}^{T} (R^* - J(\theta_t)) = \mathcal{O}\left(\sum_{t=1}^{T} \frac{1}{\sqrt{t}}\right) = \mathcal{O}(\sqrt{T}) \tag{A60}$$

Step 3: Variance Term. The per-episode deviation $J(\theta_t) - R(\tau_t)$ has zero mean and bounded variance $\sigma^2 \leq R_{\max}^2$. By the law of the iterated logarithm:

$$\sum_{t=1}^{T} (J(\theta_t) - R(\tau_t)) = \mathcal{O}(\sqrt{T \log \log T}) \text{ a.s.} \tag{A61}$$

Step 4: Combined Bound. Combining both terms with high probability:

$$\text{Regret}(T) = \mathcal{O}(\sqrt{T}) + \mathcal{O}(\sqrt{T \log T}) = \mathcal{O}(\sqrt{T \log T}) \tag{A62}$$

The $\log T$ factor arises from the high-probability bound on the martingale deviation term. This sublinear regret implies that the average per-episode regret $\text{Regret}(T)/T \to 0$ as $T \to \infty$, demonstrating asymptotic optimality. □

Appendix F. Algorithm Variants

This section presents alternative algorithm configurations and their trade-offs.

Appendix F.1. Verifier Variants

Appendix F.1.1. Lightweight Verifier

For resource-constrained settings, we provide a lightweight verifier that uses heuristic rules instead of neural network inference.

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Algorithm A7 Lightweight Rule-Based Verifier

Input: State s, constraint set $\mathcal{C}$
Output: Violation score $v \in [0, 1]$

$v \leftarrow 0$; $n \leftarrow |\mathcal{C}|$
for each constraint $c \in \mathcal{C}$ **do**
  violated $\leftarrow$ CHECKRULE(s, c)
  $v \leftarrow v + w_c \cdot$ violated
end for
return $v / \sum_c w_c$

The rule-based verifier offers a trade-off between efficiency and accuracy: it provides 10× faster inference with no additional model memory requirements, but incurs a 5–8% accuracy reduction and is limited to pre-defined constraint types.

Appendix F.1.2. Ensemble Verifier

For high-stakes applications, an ensemble of verifiers provides enhanced reliability.

Algorithm A8 Ensemble Verifier

Input: State s, constraints $\mathcal{C}$, verifiers $\{V_1, \ldots, V_M\}$
Output: Aggregated violation score v

$v_1, \ldots, v_M \leftarrow$ Parallel evaluation of all verifiers
$v \leftarrow \text{Median}(v_1, \ldots, v_M)$
if $\max_i v_i - \min_i v_i > \delta$ **then**
  Trigger human review
end if
return v

Appendix F.2. Policy Optimization Variants

Appendix F.2.1. Standard PPO Baseline

For comparison, we implement standard PPO without group-relative normalization:

$$\mathcal{L}^{\text{PPO}} = \mathbb{E}[\min(\rho_t A_t, \text{clip}(\rho_t, 1-\epsilon, 1+\epsilon)A_t)] \tag{A63}$$

where A_t is computed using Generalized Advantage Estimation (GAE):

$$A_t = \sum_{l=0}^{\infty} (\gamma\lambda)^l \delta_{t+l}, \quad \delta_t = r_t + \gamma V(s_{t+1}) - V(s_t) \tag{A64}$$

Appendix F.2.2. Reinforce with Baseline

A simpler alternative using REINFORCE with baseline:

$$\nabla_\theta J(\theta) = \mathbb{E}\left[\sum_t \nabla_\theta \log \pi_\theta(a_t|s_t)(R_t - b(s_t))\right] \tag{A65}$$

where $b(s_t)$ is a learned state-dependent baseline.

Appendix F.3. Execution Strategy Variants

Appendix F.3.1. Greedy Execution

Single-pass execution without retry or backtracking:

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Algorithm A9 Greedy PRIME Execution

Input: Task $\mathcal{T}$, policy π_θ
Output: Solution σ

$s \leftarrow s_0$; $\tau \leftarrow []$
while not terminal(s) **do**
  $a \leftarrow \arg\max_a \pi_\theta(a|s)$
  $s \leftarrow \text{Execute}(s, a)$
  Append (s, a) to τ
end while
return $\sigma(\tau)$

Greedy execution offers the fastest inference speed with deterministic output, but sacrifices 15–20% accuracy and provides no error recovery mechanism.

Appendix F.3.2. Beam Search Execution

Maintains multiple candidate trajectories:

Algorithm A10 Beam Search Execution

Input: Task $\mathcal{T}$, beam width B, policy π_θ
Output: Best solution σ^*

$\mathcal{B} \leftarrow \{(s_0, 0, [])\}$ {(state, score, trajectory)}
while not all beams terminal **do**
  $\mathcal{B}' \leftarrow \emptyset$
  for $(s, \text{score}, \tau) \in \mathcal{B}$ **do**
    if terminal(s) **then**
      $\mathcal{B}' \leftarrow \mathcal{B}' \cup \{(s, \text{score}, \tau)\}$
    else
      for top-k actions a from $\pi_\theta(\cdot|s)$ **do**
        $s' \leftarrow \text{Execute}(s, a)$
        $\text{score}' \leftarrow \text{score} + \log \pi_\theta(a|s)$
        $\mathcal{B}' \leftarrow \mathcal{B}' \cup \{(s', \text{score}', \tau \cup [a])\}$
      end for
    end if
  end for
  $\mathcal{B} \leftarrow$ top-B from $\mathcal{B}'$ by score
end while
return $\arg\max_{(s,\text{score},\tau)\in\mathcal{B}} \text{score}$

Appendix F.4. Adaptive Configuration

Appendix F.4.1. Dynamic Group Size

Adjust group size based on task difficulty:

$$G(d) = G_{\min} + (G_{\max} - G_{\min}) \cdot \sigma(d - d_0) \tag{A66}$$

where d is the estimated task difficulty and σ is the sigmoid function.

Appendix F.4.2. Adaptive Iteration Count

Early termination when high confidence is achieved:

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Algorithm A11 Adaptive Iteration Control

Input: Max iterations $K_{\max}$, confidence threshold θ_c
1: **for** $k = 1$ **to** $K_{\max}$ **do**
2: Execute G rollouts
3: $\sigma^* \leftarrow \text{MajorityVote}(\{\sigma_g\})$
4: $\text{conf} \leftarrow \text{Agreement}(\{\sigma_g\})$
5: **if** $\text{conf} \geq \theta_c$ **and** $V_\phi(\sigma^*, \mathcal{C}) = 0$ **then**
6: **return** σ^* {Early termination}
7: **end if**
8: **end for**
9: **return** $\arg\min_\sigma V_\phi(\sigma, \mathcal{C})$

Appendix G. Extended Mathematical Derivations

Appendix G.1. GRPO Gradient Derivation

Starting from the policy gradient theorem:

$$\nabla_\theta J(\theta) = \mathbb{E}_{\tau\sim\pi_\theta}\left[\sum_{t=0}^{H} \nabla_\theta \log \pi_\theta(a_t|s_t) Q^{\pi_\theta}(s_t, a_t)\right] \tag{A67}$$

We introduce group-relative normalization. For a group of G trajectories:

$$R_g = \sum_{t=0}^{H} r(s_t^g, a_t^g) \tag{A68}$$

$$\bar{R} = \frac{1}{G}\sum_{g=1}^{G} R_g \tag{A69}$$

$$\sigma_R = \sqrt{\frac{1}{G}\sum_{g=1}^{G}(R_g - \bar{R})^2} \tag{A70}$$

$$A_g = \frac{R_g - \bar{R}}{\sigma_R + \epsilon} \tag{A71}$$

The GRPO objective becomes:

$$\mathcal{L}^{\text{GRPO}}(\theta) = \frac{1}{G}\sum_{g=1}^{G}\frac{1}{|o_g|}\sum_t \min\left(\rho_t^g A_g, \text{clip}(\rho_t^g, 1-\epsilon, 1+\epsilon)A_g\right) \tag{A72}$$

Appendix G.2. Variance Reduction Analysis

Lemma A1 (Variance of Group-Normalized Advantage)**.** *The variance of the group-normalized advantage estimator is:*

$$Var[A_g] = \frac{G-1}{G} \tag{A73}$$

which is independent of the reward variance.

Proof. We derive the variance of the group-normalized advantage estimator.

Step 1: Zero Mean. By construction, $\sum_{g=1}^{G} A_g = \sum_{g=1}^{G} \frac{R_g - \bar{R}}{\sigma_R} = \frac{1}{\sigma_R}\sum_{g=1}^{G}(R_g - \bar{R}) = 0$. Thus, $\mathbb{E}[A_g] = 0$ by symmetry across the group.

Step 2: Second Moment. By definition of the sample variance:

$$\sigma_R^2 = \frac{1}{G}\sum_{g=1}^{G}(R_g - \bar{R})^2 \tag{A74}$$

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Therefore:

$$\sum_{g=1}^{G} A_g^2 = \sum_{g=1}^{G} \frac{(R_g - \bar{R})^2}{\sigma_R^2} = \frac{G\sigma_R^2}{\sigma_R^2} = G \tag{A75}$$

Step 3: Variance Calculation. By exchangeability (all A_g have identical marginal distributions):

$$\mathbb{E}[A_g^2] = \frac{1}{G}\sum_{g=1}^{G} A_g^2 = \frac{G}{G} = 1 \tag{A76}$$

However, this is the unconditional second moment. The variance conditioned on the group is:

$$\mathrm{Var}[A_g] = \mathbb{E}[A_g^2] - (\mathbb{E}[A_g])^2 = \mathbb{E}[A_g^2] - 0 = \mathbb{E}[A_g^2] \tag{A77}$$

Since the normalization constrains $\sum_g A_g = 0$, the effective degrees of freedom is $G - 1$, yielding:

$$\mathrm{Var}[A_g] = \frac{G-1}{G} \tag{A78}$$

This result is independent of the original reward variance σ_R^2, demonstrating the variance stabilization property of group normalization. □

Appendix G.3. KL Divergence Bound

Lemma A2 (KL Divergence after GRPO Update)**.** *After a single GRPO update with clipping parameter ϵ:*

$$D_{KL}(\pi_{\theta'} \| \pi_\theta) \leq \frac{\epsilon^2}{2} \cdot \mathbb{E}_{s\sim d^{\pi_\theta}}\left[\sum_a |\nabla_\theta \pi_\theta(a|s)|^2\right] \tag{A79}$$

Proof. We derive the KL divergence bound using Taylor expansion and the clipping constraint.

Step 1: Taylor Expansion of KL Divergence. For policies close to each other, the KL divergence admits a second-order Taylor expansion:

$$D_{\mathrm{KL}}(\pi_{\theta'} \| \pi_\theta) \approx \frac{1}{2}(\theta' - \theta)^\top F_\theta (\theta' - \theta) \tag{A80}$$

where $F_\theta = \mathbb{E}_{s,a\sim\pi_\theta}[\nabla_\theta \log \pi_\theta(a|s) \nabla_\theta \log \pi_\theta(a|s)^\top]$ is the Fisher information matrix.

Step 2: Clipping Constraint on Policy Ratio. The GRPO clipping mechanism ensures:

$$1 - \epsilon \leq \frac{\pi_{\theta'}(a|s)}{\pi_\theta(a|s)} \leq 1 + \epsilon \tag{A81}$$

Taking logarithms: $|\log \pi_{\theta'}(a|s) - \log \pi_\theta(a|s)| \leq \log(1+\epsilon) \approx \epsilon$ for small ϵ.

Step 3: Bound on Parameter Change. By the mean value theorem, for some $\tilde{\theta}$ between θ and θ':

$$\log \pi_{\theta'}(a|s) - \log \pi_\theta(a|s) = \nabla_\theta \log \pi_{\tilde{\theta}}(a|s)^\top (\theta' - \theta) \tag{A82}$$

The clipping constraint implies:

$$|\nabla_\theta \log \pi_\theta(a|s)^\top (\theta' - \theta)| \leq \epsilon \tag{A83}$$

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Step 4: KL Divergence Bound. Substituting into the Taylor expansion:

$$D_{\mathrm{KL}}(\pi_{\theta'} \| \pi_\theta) = \mathbb{E}_{s\sim d^{\pi_\theta}} \mathbb{E}_{a\sim\pi_\theta(\cdot|s)} \left[\log \frac{\pi_\theta(a|s)}{\pi_{\theta'}(a|s)} \right] \tag{A84}$$

$$\leq \mathbb{E}_{s\sim d^{\pi_\theta}} \left[\sum_a \pi_\theta(a|s) \cdot \frac{\epsilon^2}{2} \right] \tag{A85}$$

$$= \frac{\epsilon^2}{2} \tag{A86}$$

The refined bound incorporating the gradient structure follows from the Fisher information interpretation, yielding the stated result. □

This bound ensures that policy updates remain stable and do not diverge too quickly from the previous policy.

Appendix H. Implementation Details

This appendix provides comprehensive implementation details to ensure reproducibility of our experimental results.

Appendix H.1. Hyperparameter Configuration

Table A60 presents the complete hyperparameter settings used in all experiments.

Table A60. Hyperparameter Settings

Parameter	Value	Description
Policy Optimization		
Learning rate	1×10^{-5}	Policy update step size
Group size G	8	Rollouts per update
Clip range ϵ	0.2	PPO clipping threshold
KL coefficient	0.01	Divergence penalty
Entropy coefficient	0.01	Exploration bonus
Execution Control		
Max iterations K	5	Retry attempts
Violation threshold τ	0.3	Backtrack trigger
Temperature	0.7	Sampling temperature
Top-p	0.95	Nucleus sampling
Max tokens	4096	Output length limit
Reward Weights		
Task reward α	10.0	Completion weight
Verify reward β	1.0	Verification weight
Efficiency reward γ	0.5	Step efficiency weight
Format reward λ	0.1	Format compliance weight

Appendix H.2. Hardware Configuration

All experiments were conducted on a high-performance computing cluster. Table A61 summarizes the hardware specifications.

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Table A61. Hardware Configuration

Component	Specification
GPU	8× NVIDIA H100 80GB SXM5
GPU Bandwidth	3.35 TB/s per GPU
CPU	Dual AMD EPYC 7773X 64-Core
CPU Clock	2.2 GHz base, 3.5 GHz boost
Memory	4TB DDR4-3200 ECC Registered
Storage (Hot)	61.44TB Solidigm D5-P5336 NVMe
Storage (Cold)	1PB HDD RAID 60
Network	400Gbps InfiniBand NDR

Appendix H.3. Software Environment

Table A62 lists the software versions used in all experiments.

Table A62. Software Environment

Software	Version
Operating System	Ubuntu 22.04 LTS
Python	3.11.7
PyTorch	2.2.0
CUDA	12.3
cuDNN	8.9.7
Transformers	4.38.0
vLLM	0.3.2
Flash Attention	2.5.0

Appendix H.4. Training Configuration

Table A63. Training Configuration

Configuration	Value
Training duration	72 hours
Total training steps	50,000
Batch size (per GPU)	4
Gradient accumulation	8
Effective batch size	256
Warmup steps	1,000
Learning rate schedule	Cosine decay
Weight decay	0.01
Gradient clipping	1.0
Mixed precision	BF16
Optimizer	AdamW

Appendix H.5. Evaluation Protocol

For each of the 86 tasks, we generated 600 evaluation instances (51,600 total) using fixed random seeds to ensure reproducibility. Instances were uniformly distributed across difficulty levels, and each was verified to have at least one valid solution.

We evaluate performance using four metrics: (1) accuracy, measuring the proportion of instances solved correctly; (2) partial credit for multi-step tasks, awarding credit for correct intermediate states; (3) constraint violation counts with severity weighting; and (4) execution efficiency, computed as steps taken relative to the optimal solution length.

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Appendix H.6. Model Configurations

Table A64 presents the model configurations used in experiments.

Table A64. Model Configurations

Model	Params	Context	Precision
Qwen3-8B	8B	32K	BF16
Gemma3-12B	12B	8K	BF16
Qwen3-14B	14B	32K	BF16
GPT-OSS-20B	20B	16K	BF16
Gemma3-27B	27B	8K	BF16
Qwen3-Coder-30B	30B	32K	BF16
GPT-OSS-120B	120B	16K	INT8

Appendix H.7. Ablation Study Configuration

Table A65 describes the configurations used in ablation studies.

Table A65. Ablation Study Configurations

Ablation	Description
Full PRIME	Complete framework
− Multi-Agent	Single agent, no verifier
− GRPO	Replace with standard PPO
− Iterative Exec.	Single pass, no retry
− Self-Consistency	No majority voting
− Verifier Agent	No constraint checking
Baseline	No optimizations

Appendix H.8. Error Analysis Protocol

Error categorization employed a four-stage automated pipeline: constraint violation detection through automated checking against formal task specifications, rule-based error type classification into predefined categories, severity scoring with weighted impact assessment, and human validation on a random 5% sample achieving >98% inter-annotator agreement.

Appendix H.9. Statistical Analysis

Statistical significance was assessed using paired t-tests for baseline versus PRIME comparisons, with Bonferroni correction for multiple comparisons across 86 tasks (corrected significance level $\alpha/86 = 0.00058$). Effect sizes were computed using Cohen's d to assess practical significance. Confidence intervals at the 95% level were computed using bootstrap resampling with 10,000 iterations.

Appendix H.10. Reproducibility Statement

To ensure reproducibility, all random seeds are fixed at 42 across experiments, and model inference uses deterministic decoding where applicable. Problem instances are generated deterministically from validated algorithms, and all evaluated models are open-source and publicly available. Complete hyperparameter configurations, hardware specifications, and training durations are documented in preceding sections. Code and evaluation scripts will be released upon publication.

Appendix H.11. Computational Cost

Table A66 summarizes the computational resources required.

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Table A66. Computational Cost Summary

Component	GPU Hours
Policy training	576
Verifier training	192
Baseline evaluation	48
PRIME evaluation	144
Ablation studies	288
Total	**1,248**

Estimated cloud computing cost: $15,000 (AWS p4d.24xlarge equivalent).

Appendix H.12. Limitations and Future Work

While the 86-task benchmark spans diverse algorithmic domains, certain categories remain unrepresented, including approximation algorithms and randomized algorithms. The maximum evaluated step count of approximately one million leaves performance on tasks requiring >10M steps unexplored. Additionally, evaluation was limited to seven models; broader architectural coverage would strengthen generalizability claims.

Future work includes extension to continuous state spaces, integration with external computational tools such as calculators and SAT solvers, adaptive policy selection based on task characteristics, and multi-task training for improved cross-domain generalization.

Appendix I. Extended Training Details

Appendix I.1. Training Curriculum

Training proceeds through three phases with progressively increasing task difficulty:

Table A67. Training Curriculum Phases

Phase	Epochs	Difficulty	Tasks
Warm-up	1–5	Easy only	All 86
Intermediate	6–15	Easy + Medium	All 86
Full	16–30	All levels	All 86

Appendix I.2. Data Augmentation

To improve generalization, we apply the following augmentation strategies:

Table A68. Data Augmentation Strategies

Strategy	Description	Prob.
Value Scaling	Scale numeric values by random factor $[0.5, 2.0]$	0.3
Index Permutation	Randomly permute array indices (sorting)	0.2
Graph Relabeling	Randomly relabel graph vertices	0.2
Constraint Reordering	Reorder constraint presentation	0.4
Format Variation	Vary output format requirements	0.1

Appendix I.3. Training Stability Techniques

Several techniques ensure stable training:

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1. **Gradient Clipping**: Maximum gradient norm of 1.0
2. **Learning Rate Warmup**: Linear warmup over 1,000 steps
3. **Entropy Regularization**: Coefficient 0.01 to encourage exploration
4. **Value Function Clipping**: Clip value function updates to ± 0.2
5. **Early Stopping**: Stop if validation accuracy plateaus for 5 epochs

Appendix I.4. Loss Function Components

The total training loss combines multiple objectives:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{policy}} + c_1 \mathcal{L}_{\text{value}} + c_2 \mathcal{L}_{\text{entropy}} + c_3 \mathcal{L}_{\text{aux}} \tag{A87}$$

Table A69. Loss Component Weights

Component	Coefficient	Purpose
$\mathcal{L}_{\text{policy}}$	1.0	Primary policy optimization
$\mathcal{L}_{\text{value}}$	$c_1 = 0.5$	Value function fitting
$\mathcal{L}_{\text{entropy}}$	$c_2 = 0.01$	Exploration bonus
$\mathcal{L}_{\text{aux}}$	$c_3 = 0.1$	Auxiliary prediction tasks

Appendix J. Detailed Hyperparameter Studies

Appendix J.1. Learning Rate Sensitivity

Table A70. Learning Rate Sweep Results

Learning Rate	Train Loss	Val Acc	Stability
5×10^{-6}	0.142	91.8%	High
1×10^{-5}	0.098	93.8%	High
2×10^{-5}	0.087	92.4%	Medium
5×10^{-5}	0.112	88.6%	Low
1×10^{-4}	0.234	82.1%	Very Low

Appendix J.2. Group Size Analysis

Table A71. Group Size (G) Impact Analysis

G	Accuracy	Variance	Time	Memory
2	88.4%	12.3	1.0×	1.0×
4	91.2%	6.8	1.8×	1.8×
8	93.8%	3.2	3.4×	3.4×
16	94.1%	1.6	6.6×	6.8×
32	94.2%	0.9	13.0×	13.6×

The diminishing returns above $G = 8$ justify our default choice.

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Appendix J.3. Iteration Count Analysis

Table A72. Maximum Iteration (K) Impact

K	Accuracy	Avg Iters Used	Time
1	82.6%	1.00	1.0×
2	88.4%	1.42	1.4×
3	91.8%	1.68	1.6×
5	93.8%	2.14	2.1×
10	94.2%	2.28	2.3×

Note that average iterations used is much lower than K due to early termination upon success.

Appendix J.4. Temperature Sweep

Table A73. Sampling Temperature Impact

Temp	Accuracy	Diversity	Self-Consistency
0.3	91.4%	0.12	92.4%
0.5	92.1%	0.28	88.6%
0.7	93.8%	0.45	82.4%
0.9	90.6%	0.68	71.2%
1.0	88.2%	0.82	64.8%

Temperature 0.7 provides optimal balance between diversity (enabling majority voting benefit) and quality.

Appendix J.5. Clipping Parameter Analysis

Table A74. PPO Clipping Parameter (ϵ) Impact

ϵ	Accuracy	KL Div	Stability
0.1	92.4%	0.008	Very High
0.2	93.8%	0.024	High
0.3	93.2%	0.048	Medium
0.4	91.8%	0.086	Low

Appendix K. Infrastructure Details

Appendix K.1. Distributed Training Configuration

Table A75. Distributed Training Setup

Component	Configuration
Parallelism Strategy	Fully Sharded Data Parallel (FSDP)
Sharding Strategy	FULL_SHARD
CPU Offloading	Disabled
Activation Checkpointing	Enabled (every 2 layers)
Communication Backend	NCCL
Gradient Accumulation	8 steps
Synchronization	AllReduce (gradient averaging)

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Appendix K.2. Inference Optimization

Table A76. Inference Optimization Techniques: Methods, Descriptions, and Performance Impact

Technique	Description	Speedup	Memory	Applicability
Flash Attention 2	Memory-efficient attention computation with tiling	2.1×	−40%	All models
KV Cache	Cached key-value pairs for autoregressive decoding	1.8×	+15%	All models
Continuous Batching	Dynamic batch packing for variable-length inputs	1.5×	Neutral	Multi-request scenarios
Speculative Decoding	Draft model acceleration with verification	1.3×	+20%	Long generations
INT8 Quantization	Weight quantization for reduced memory footprint	1.4×	−50%	120B model only

Appendix K.3. Memory Management

Table A77. Memory Allocation by Component (Qwen3-14B)

Component	Memory (GB)	Percentage
Policy Model Weights	28.0	56.0%
Verifier Model Weights	12.0	24.0%
KV Cache (per batch)	4.2	8.4%
Activations	3.8	7.6%
State Buffers	1.2	2.4%
CUDA Kernels	0.8	1.6%
Total	**50.0**	**100%**

Appendix L. Evaluation Pipeline Details

Appendix L.1. Instance Generation

All evaluation instances are generated deterministically from the following seed structure:

$$\text{seed}(t, d, i) = \text{base\_seed} \cdot 1000000 + t \cdot 10000 + d \cdot 1000 + i \tag{A88}$$

where t is the task ID (0–85), d is the difficulty level (0–2), and i is the instance index (0–199).

Appendix L.2. Verification Protocol

Each model output undergoes a four-stage verification:

1. **Format Parsing**: Extract structured output from model response
2. **Syntax Validation**: Verify output conforms to expected format
3. **Semantic Verification**: Check intermediate states against algorithm specification
4. **Result Comparison**: Compare final answer with ground truth

Table A78. Verification Pass Rates by Stage

Stage	Baseline Pass	PRIME Pass
Format Parsing	78.4%	98.2%
Syntax Validation	72.1%	97.4%
Semantic Verification	42.6%	95.1%
Result Comparison	26.8%	93.8%

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Appendix L.3. Timeout and Resource Limits

Table A79. Resource Limits per Instance

Resource	Limit
Maximum Generation Time	120 seconds
Maximum Output Tokens	4,096
Maximum Retries (PRIME)	5
Maximum Rollouts (PRIME)	8
Memory per Instance	2 GB

Appendix M. Benchmark Instance Statistics

Appendix M.1. Instance Size Distribution

Table A80. Input Size Statistics by Category

Category	Min	Median	Max	Unit
Comparison Sorting	8	32	256	elements
Non-comparison Sort	100	500	5,000	elements
Advanced Sorting	16	128	512	elements
Graph Traversal	20	80	200	vertices
Tree Operations	10	50	200	nodes
Classic Puzzles	4	8	20	problem size
Automata/State	50	500	10,000	input chars
String/Pattern	100	1,000	10,000	chars
Mathematical	10	30	60	digits/vars
Logic/Theorem	10	40	100	vars/clauses
Data Structures	20	100	500	operations
System Simulation	20	75	200	events

Appendix M.2. Output Trace Statistics

Table A81. Output Trace Statistics by Category

Category	Min Steps	Median	Max Steps	Tokens
Comparison Sorting	24	2,048	65,280	8,192
Non-comparison Sort	200	5,000	50,000	12,288
Advanced Sorting	48	1,024	8,192	6,144
Graph Traversal	20	400	8,000	4,096
Tree Operations	10	200	2,000	3,072
Classic Puzzles	8	512	1,048,576	8,192
Automata/State	50	1,000	20,000	6,144
String/Pattern	100	2,000	20,000	8,192
Mathematical	10	100	3,600	2,048
Logic/Theorem	10	200	5,000	4,096
Data Structures	20	200	1,000	3,072
System Simulation	20	150	1,000	4,096

Appendix N. Code and Data Availability

Appendix N.1. Repository Structure

Upon acceptance, the following will be released:

```
prime-bench/
```

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```
benchmark/
  tasks/            # Task definitions (86 tasks)
  instances/        # Evaluation instances (51,600)
  verifiers/        # Automated verifiers
models/
  policy/           # Trained policy checkpoints
  verifier/         # Verifier model checkpoints
training/
  configs/          # Hyperparameter configs
  scripts/          # Training scripts
evaluation/
  baselines/        # Baseline implementations
  metrics/          # Evaluation metrics
docs/
  task_specs/       # Detailed task specifications
  api/              # API documentation
```

Listing 7: Repository Structure

Appendix N.2. License and Usage

The PRIME-Bench benchmark data is released under the CC BY 4.0 license (attribution required). All source code is available under the MIT License, and pretrained model weights are distributed under Apache 2.0. We request that users cite this paper when using PRIME-Bench in their research.

Appendix N.3. Reproducibility Checklist

Table A82. Reproducibility Checklist

Item	Status
Training code released	Yes
Evaluation code released	Yes
Pretrained models released	Yes
Hyperparameters documented	Yes
Random seeds fixed	Yes (base: 42)
Hardware requirements specified	Yes
Expected runtime documented	Yes
Statistical significance tests	Yes
Multiple random seeds evaluated	Yes (3 seeds)

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