An Explanation In Support Of Neuro-Symbolic Language Models for Scaling Algorithmic Reasoning

Terry Tong [1] **Yu Feng** [1] **Surbhi Goel** [1] **Dan Roth** [1]

Abstract

Large language models can solve algorithmic problems either through direct natural language reasoning or by generating executable code delegated to an external solver. However, little theoretical progress has been made on explaining *why* code-based approaches consistently outperform natural language reasoning.

We introduce a three-arm framework that makes this comparison tractable by introducing an intermediary step—code generation with LLM-based execution—enabling pairwise theoretical analysis via Bayesian inference and information theory.

Empirically, we demonstrate on arithmetic, dynamic programming, and integer linear programming tasks that code execution achieves 78% accuracy versus 30% for code simulation and 21% for natural language reasoning across Deepseek and Gemma models ($p < 0.05$, Friedman test). Theoretically, we prove that code representations yield higher mutual information with the target algorithm, leading to at least 6% lower Bayes error than natural language.

These results inform the design of compositional AI systems, providing principled guidance on when to use tool-augmented versus monolithic reasoning for algorithmic tasks. Our framework offers a unified perspective on the tool-use versus direct-reasoning tradeoff.

1. Introduction

Large language models (LLMs) have demonstrated increasingly strong natural-language (NL) reasoning capabilities (). In parallel, LLM-based agentic systems advocate tool use, where LLMs invoke external solvers to support reasoning and execution (). Recent works (Lyu et al., 2023; Pan et al., 2023) suggest that the **solver route**, translating problems into solver-executable representations and delegating execution, often outperforms the **direct route**, reasoning end-to-end in NL, on logic- and algorithmic-style complex reasoning tasks. However, for algorithmic reasoning alone, there is still no systematic analysis comparing the two routes, clarifying when and why LLMs perform better via the solver route versus the direct route.

A principled direct comparison is challenging since the routes operate over different representation spaces, i.e., NL traces versus solver-executable programs, and rely on different execution mechanisms, which prevents step-by-step alignment. Specifically, sample-complexity comparisons () are ill-posed here because the two routes learn fundamentally different objects, so there is no common formal target and metric to compare. Computational-complexity arguments () are also not a clean discriminator here because the two routes incur fundamentally different execution-

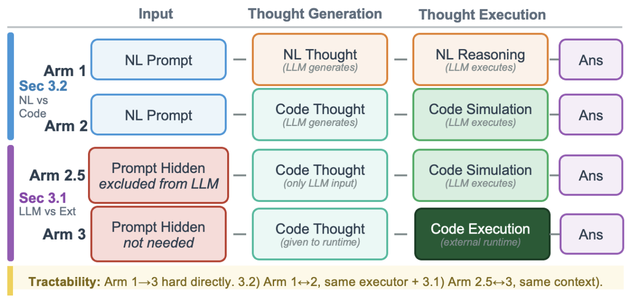
Input
Thought Generation
Thought Execution
Arm 1
Sec 3.2
NL vs Code
Arm 2
NL Prompt
NL Thought (LLM generates)
NL Reasoning (LLM executes)
Ans
NL Prompt
Code Thought (LLM generates)
Code Simulation (LLM executes)
Ans
Arm 2.5
Sec 3.1
LLM vs Ext
Arm 3
Prompt Hidden excluded from LLM
Code Thought (only LLM input)
Code Simulation (LLM executes)
Ans
Prompt Hidden not needed
Code Thought (given to runtime)
Code Execution (external runtime)
Ans
Tractability: Arm 1→3 hard directly. 3.2) Arm 1↔2, same executor + 3.1) Arm 2.5↔3, same context).

Figure 1. Bayesian Inference model showing the *three arms methodology* in Section 2. Given an algorithmic problem, we may split it into two steps (1) Translate (2) Execute. The (1) translation $\in \{\text{Code}, \text{NL}\}$. Then (2) execution $\in \{\text{LLM Reasoning}, \text{Solver Execution}\}$. We have three pairs, Arm 1: $\{\text{NL Gen}, \text{LLM Reasoning}\}$, Arm 2: $\{\text{Code Gen}, \text{LLM Reasoning}\}$, Arm 3: $\{\text{Code Gen}, \text{Solver Execution}\}$. Typically, the problem is tackled by comparing Arm 1 and Arm 3 in neuro-symbolic literature, which is intractable theoretically, and uncontrolled since multiple variables are changing. By introducing Arm 2, the problem becomes tractable. In the diagram, the *shaded* circles correspond to observed R.V. and *white* correspond to unobserved. The notation for R.V.s is correspondingly used in Section 2.

[*]Equal contribution [1]University of Pennsylvania. Correspondence to: Terry Tong <tongt1@seas.upenn.edu>.

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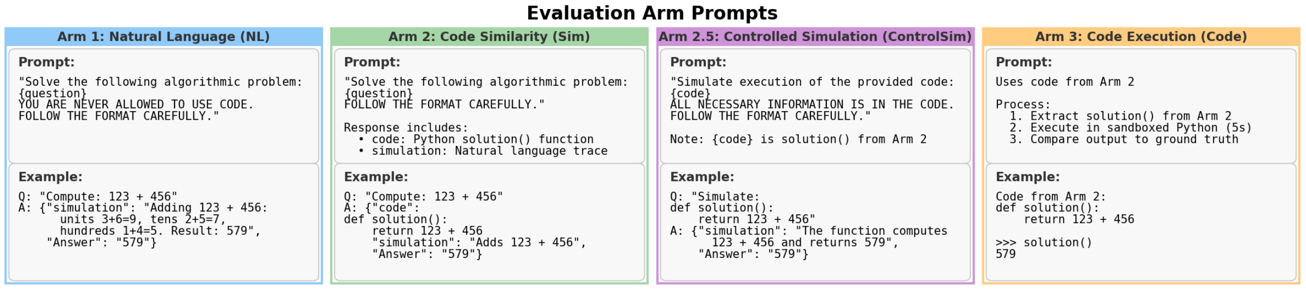

Evaluation Arm Prompts
Arm 1: Natural Language (NL)
Arm 2: Code Similarity (Sim)
Arm 2.5: Controlled Simulation (ControlSim)
Arm 3: Code Execution (Code)

Arm 1: Natural Language (NL)

Prompt:

```
"Solve the following algorithmic problem:
{question}
YOU ARE NEVER ALLOWED TO USE CODE.
FOLLOW THE FORMAT CAREFULLY."
```

Example:

```
Q: "Compute: 123 + 456"
A: {"simulation": "Adding 123 + 456:
      units 3+6=9, tens 2+5=7,
      hundreds 1+4=5. Result: 579",
    "Answer": "579"}
```

Arm 2: Code Similarity (Sim)

Prompt:

```
"Solve the following algorithmic problem:
{question}
FOLLOW THE FORMAT CAREFULLY."

Response includes:
  • code: Python solution() function
  • simulation: Natural language trace
```

Example:

```
Q: "Compute: 123 + 456"
A: {"code":
def solution():
    return 123 + 456
    "simulation": "Adds 123 + 456",
    "Answer": "579"}
```

Arm 2.5: Controlled Simulation (ControlSim)

Prompt:

```
"Simulate execution of the provided code:
{code}
ALL NECESSARY INFORMATION IS IN THE CODE.
FOLLOW THE FORMAT CAREFULLY."

Note: {code} is solution() from Arm 2
```

Example:

```
Q: "Simulate:
def solution():
    return 123 + 456"
A: {"simulation": "The function computes
      123 + 456 and returns 579",
    "Answer": "579"}
```

Arm 3: Code Execution (Code)

Prompt:

```
Uses code from Arm 2

Process:
  1. Extract solution() from Arm 2
  2. Execute in sandboxed Python (5s)
  3. Compare output to ground truth
```

Example:

```
Code from Arm 2:
def solution():
    return 123 + 456

>>> solution()
579
```

Figure 2. Prompt templates for the three-arm evaluation framework. Arm 1 instructs the model to reason purely in natural language without code. Arm 2 instructs the model to generate code and simulate its execution. Arm 3 uses the same code generation prompt but executes the output in a Python runtime rather than simulating.

dependent costs. We therefore compare the two routes via statistical difficulty, using optimal achievable end-task Bayes risk ().

In this paper, we propose a three-route Bayesian inference framework that makes this comparison tractable by introducing an additional intermediate **simulation route**, where the model performs the same translation but simulates execution in NL, other than the **direct route** and **solver route**, and verbalizes the representation using Chain-of-Thought () as shown in Fig. 1. Using this framework, we characterize when and why algorithmic reasoning favors the solver route, and show that solver-based pipelines are generally easier for a broad class of tasks. [**Yu**: This claim is inaccurate for now.] This framework also enables a tractable theoretical comparison of the routes, showing that the simulation route outperforms the direct route [**Yu**: ....] Finally, we empirically demonstrate that the solver route substantially outperforms the simulation route, highlighting additional gains from reliable external execution.

Using our framework, we consistently observe a three-route ordering across algorithmic reasoning tasks: the solver route performs best, followed by the simulation route, and then the direct route. Moreover, the solver route's advantage widens as task difficulty increases. We evaluate our framework on CLRS30 (), NP-Hard-Eval (), and a custom suite of algorithmic problems with controllable difficulty (addition, multiplication, LCS, rod cutting, knapsack, and ILP variants: assignment, production, and partition) across a broad range of models, spanning weaker open-source LLMs (e.g., Mistral (), LLaMA (), Qwen ()) and stronger closed-source systems (e.g., OpenAI (), Gemini (), Claude ()). We find that, averaged over tasks and models, the solver route achieves XX% accuracy, outperforming the simulation route (XX%) and the direct route (XX%) with statistical significance (XX).

[**Yu**: theory part]

[**Yu**: talk about the recovery rate experiment to show why execution is better]

[**Yu**: Summarization of contributions:]

Theoretically, we first compare $\text{Arm } 1 < \text{Arm } 2$. Bayesian Inference shows us that the LLM implicitly does multi-class classification to the right algorithm. We utilize information theory to capture natural language and code under the same framework, forgoing using grammars or other mathematical frameworks that are intractable. We reduce the comparison of Bayes Error to that of comparing cross-entropy. A intermediate step using mutual information makes the proof interpretable: we prove that the mutual information between the CoT and the final answer is higher when conditioned on code representations over natural language representations. We variationally lower bound the mutual information using cross-entropy of a proposal distribution parameterized by a logistic regression. Since we only care about orderings, we subtract to overcome the intractability of estimating the differential entropy, reducing the comparison of mutual information to that of cross-entropy. The cross-entropy is measured empirically using logistic regression on TF-IDF features and Bert-base-uncased features, showing that code has lower cross-entropy than NL and achieves higher accuracy when classifying the correct algorithm. The difference is statistically significant (F-test, $p < 0.05$).

Then we compare $\text{Arm } 2 < \text{Arm } 3$. This difference is easily explained using a communication channel model of LLM forward-pass. We show that in the case where Arm 2 $>$ Arm 3, i.e. when the code generated is not executable or wrong, yet the LLM reasoning obtains the correct answer, that this occurs rarely. In other words, generally $\text{Arm } 3 > \text{Arm } 2$.

Piecing these results together, we show that $\text{Arm } 1 < \text{Arm } 2 < \text{Arm } 3$, verifying the hypothesis.

Understanding this problem is crucial as we move towards compositional AI systems rather than monolithic architectures.

Our main contributions are:

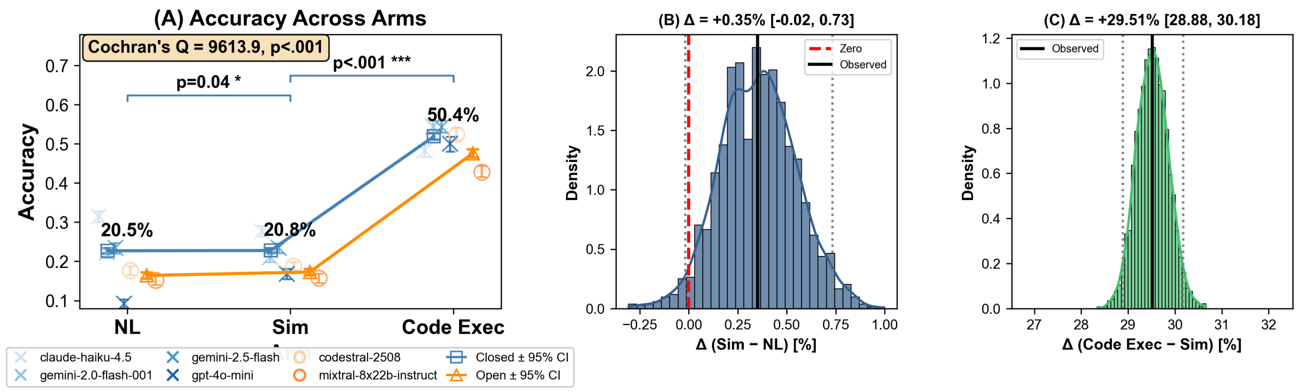


Figure 3. Accuracy scaling across task difficulty (τ) for Arithmetic, Dynamic Programming, and ILP tasks. Arm 3 (code execution) maintains high accuracy as problems get harder, while Arms 1 and 2 degrade. The widening gap demonstrates that solver execution becomes increasingly advantageous for challenging algorithmic problems.

1. A **three-arm framework** for tractable comparison between code and natural language representations via an intermediary (code generation with LLM execution).
2. **Empirical validation** demonstrating that code execution achieves 78% accuracy versus 21% for natural language reasoning across arithmetic, DP, and ILP tasks ($p < 0.05$).
3. A **theoretical explanation** based on Bayesian inference showing that code yields higher mutual information with target algorithms, leading to lower Bayes error.

2. Evaluation Framework

We formalize our central claim as $\mathrm{Acc}(\mathrm{Arm}\ 1) \leq \mathrm{Acc}(\mathrm{Arm}\ 2) < \mathrm{Acc}(\mathrm{Arm}\ 3)$. The following sections detail how we break down the problem and evaluate pairwise $\mathrm{Acc}(\mathrm{Arm}\ 1) \leq \mathrm{Acc}(\mathrm{Arm}\ 2)$ and then $\mathrm{Acc}(\mathrm{Arm}\ 2) \leq \mathrm{Acc}(\mathrm{Arm}\ 3)$.

2.1. Methodology

Arm 1 $\leq$ Arm 2 Setup. Similarly, given test input X_i corresponding to instance i, we prompt the LLM to reason about it using natural language in Arm 1, mapping $(X_i) \to Y_i^{(\mathrm{NL})}$. Likewise, Arm 2 can be written as using the same LLM to first $(X_i) \to C_i$ and then $(X_i, C_i) \to Y_i^{(\mathrm{Sim})}$. Example prompts are shown in Figure 2. We control the prompts to be as similar as possible, with the Arm 2 simply concatenating a section that says it should generate code and simulate it.

Arm 2 $<$ Arm 3 Setup. Let the original problem statement corresponding to instance i be X_i, and let C_i be the coresoponding code generated for instance i. Let tuple (X_i, C_i) be fixed inputs in our experimental design. Let Arm 2 denote the output $Y_i^{(\mathrm{Sim})}$ which is mapped to by an LLM $(X_i, C_i) \to Y_i^{(\mathrm{Sim})}$, and let Arm 3 denote the output $Y_i^{(\mathrm{Exec})}$ mapped to by an external python runtime $(X_i, C_i) \to Y_i^{(\mathrm{Exec})}$ [1]. Example prompts are show in Figure 2.

Arm 1 $\leq$ Arm 2 $<$ Arm 3 Setup. For each problem instance i, we observe bernoulli outcomes $(Y_i^{(\mathrm{NL})}, Y_i^{(\mathrm{Sim})}, Y_i^{(\mathrm{Exec})})$. We first test the overall arm effect using Cochran's Q test, evaluating the global null:

$$H_0 = \mathrm{E}[Y_i^{(NL)}] = \mathrm{E}[Y_i^{(Sim)}] = \mathrm{E}[Y_i^{(Exec)}]$$

i.e. that all arms have marginal success probabilities. Rejection of this null indicates at least one arm differs in accuracy.

2.2. Experiments

Condition on rejecting the global null, following our framework, we break down the tests into Arm 1 and Arm 2 $(Y_i^{(\mathrm{NL})}, Y_i^{(\mathrm{Sim})})$, and Arm 2 and Arm 3 $(Y_i^{(\mathrm{Sim})}, Y_i^{(\mathrm{Exec})})$. For these paired bernoulli outcomes, we run the McNemar test under the null that:

$$\begin{aligned} H_0 &: \Pr(Y^{(\mathrm{Sim})} = 1,\, Y^{(\mathrm{Exec})} = 0) \\ &= \Pr(Y^{(\mathrm{Sim})} = 0,\, Y^{(\mathrm{Exec})} = 1) \end{aligned}$$

that is, when pairs disagree, each one (Sim $>$ NL) and (NL $<$ Sim) occur equally as often. We test an analogous null for Arm 2 and Arm 3. To quantify effect size, we take paired accuracies

$$\Delta_{\mathrm{Sim-NL}} = \mathrm{Acc(Sim)} - \mathrm{Acc(NL)}$$

[1] X_i is ignored by executor, but we include it for notational symmetry

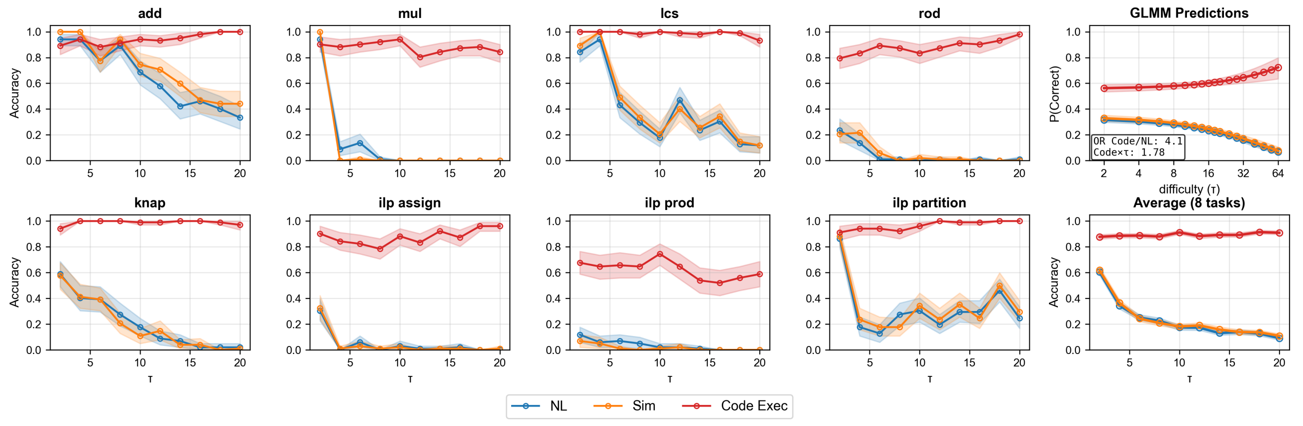


Figure 4. Recovery rate analysis: proportion of cases where LLM simulation (Arm 2) produces the correct answer despite incorrect code (Arm 3 failure). Recovery rates remain below 5% across all task families and models, confirming that solver execution dominates LLM simulation.

and estimate its sampling distribution and 95% confidence interval via a cluster bootstrap, resampling over instances i with preserved pair outcomes $(Y_i^{(\mathrm{NL})}, Y_i^{(\mathrm{Sim})})$. We run the same procedure for Arm 2 and Arm 3.

Since we apply multiple statistical tests, we add Holm-Bonferoni corrections to control family wise error rate at $\alpha = 5\%$.

Finally, to analyze how task difficulty interacts with different arms, we run a generalized linear mixed-effects model (GLMM) with a logistic link.

$$Y_i = \alpha + \beta_{\mathrm{arm}_i} + \gamma\,\tau_i + \delta_{\mathrm{arm}_i}\tau_i + \varepsilon_i, \quad \varepsilon_i \sim \text{Bernoulli noise}$$

We model arm and task hardness as fixed effects, along with their interaction, with problem instance and seed as random effects.

Data and Models. We use the CLRS 30 Benchmark (n=500), NPHardEval Benchmark (n=540), and a custom fine-grained evaluation suite (n=540), across three seeds. We define our own task suite—Arithmetic, Dynamic Programming, Integer Linear Programming (ILP)—to modulate hardness with parameter τ. For arithmetic, τ controls digit length; for DP, it controls table dimensionality; for ILP, it controls the constraint matrix size. We assume our algorithms are representative enough of the distribution. We select frontier models (Haiku 4.5, GPT-4o, Gemini 2.0 Flash) as well as open-source models (Mixtral, Codestral). Since we require structured output, we filter out models that give >50% JSON Parse Error, since this is indicative of instruction-following failures, rather than lack of coding fidelity.

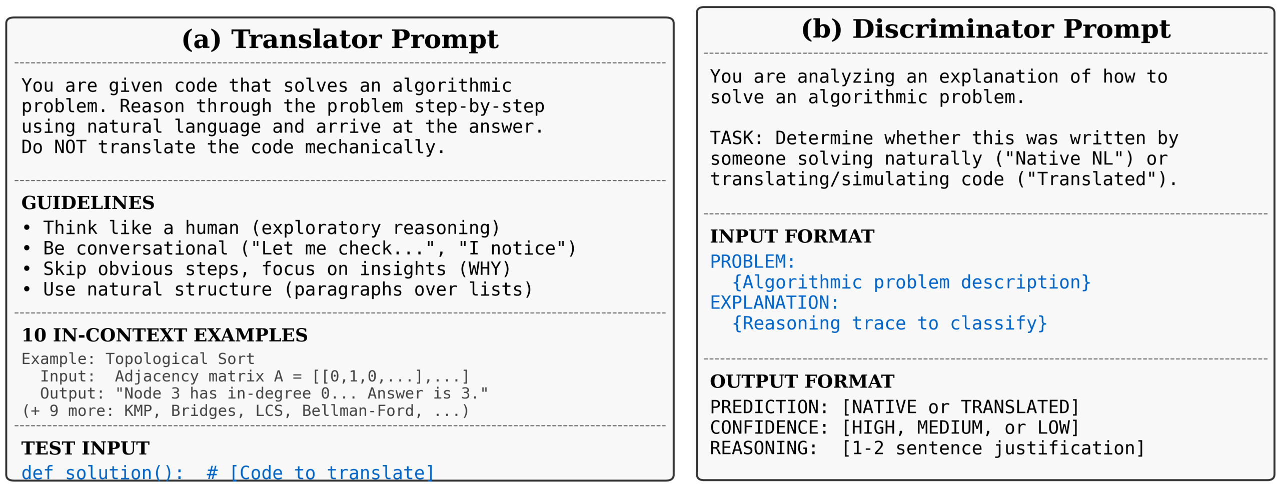
Prompting to generate Code and Reasoning Traces. We prompt the LLM in Arm 1 to never use any code in its reasoning, and to give a structured output of the rationale and answer to the algorithmic problem Figure 2. Holding all other parts of the prompt the same, we replace the section instructing the model not to use code with another asking it to generaate code first before reasoning through it. Models have access to native python packages, and numpy, pandas, scipy, PuLP, and pytorch. For Arm 3, we take the generated function (no prompt), and execute it in a python3 runtime. We ask model's to output a structured json following a corresponding schema for that arm, and example is show in Figure 2.

Arm 1 $\leq$ Arm 2 $<$ Arm 3 Results. For Arm 1 = Arm 2 = Arm 3, we strongly reject the global null hypothesis ($p < 0.001$ after controlling for FWER).

Our post-hoc paired tests Arm 2 $<$ Arm 3, strongly reject the null hypothesis too ($p < 0.001$). We observe the paired accuracy gap is strictly large and positive, excluding zero in 95% bootstrap confidence interval. Observing the distribution, the result is not driven by outliers, given the tightness of the distribution, indicating advantages over instance pairs and not just the average. This means that LLM execution via natural language reasoning of a piece of code has statistically significantly worse performances than code execution under the representative benchmarks and suites of task.

For post-hoc paired test Arm 1 $\leq$ Arm 2, despite running 30,000+ samples total and rejecting the null (p=0.04), our cluster bootstraps' 95% confidence interval overlaps with 0.0, indicating that we cannot conclude that code simulation performs differently than natural language under our test benchmarks and sampling experimental design. This leads us to conclude that code and natural language are approximately the same.

Observing Figure 3, we see that the dominance trends for Arm 2 $<$ Arm 3 and Arm 2 $\simeq$ Arm 3 holds across both open



(a) Translator Prompt

```
You are given code that solves an algorithmic
problem. Reason through the problem step-by-step
using natural language and arrive at the answer.
Do NOT translate the code mechanically.
```

GUIDELINES

```
• Think like a human (exploratory reasoning)
• Be conversational ("Let me check...", "I notice")
• Skip obvious steps, focus on insights (WHY)
• Use natural structure (paragraphs over lists)
```

10 IN-CONTEXT EXAMPLES

```
Example: Topological Sort
  Input:  Adjacency matrix A = [[0,1,0,...],...]
  Output: "Node 3 has in-degree 0... Answer is 3."
(+ 9 more: KMP, Bridges, LCS, Bellman-Ford, ...)
```

TEST INPUT

```
def solution():  # [Code to translate]
```

(b) Discriminator Prompt

```
You are analyzing an explanation of how to
solve an algorithmic problem.

TASK: Determine whether this was written by
someone solving naturally ("Native NL") or
translating/simulating code ("Translated").
```

INPUT FORMAT

```
PROBLEM:
  {Algorithmic problem description}
EXPLANATION:
  {Reasoning trace to classify}
```

OUTPUT FORMAT

```
PREDICTION: [NATIVE or TRANSLATED]
CONFIDENCE: [HIGH, MEDIUM, or LOW]
REASONING:  [1-2 sentence justification]
```

Figure 5. Recovery rate analysis: proportion of cases where LLM simulation (Arm 2) produces the correct answer despite incorrect code (Arm 3 failure). Recovery rates remain below 5% across all task families and models, confirming that solver execution dominates LLM simulation.

and closed models.

Advantages of Arm 3 emerge as tasks get harder. Observing Figure 3, we see that across 8 different algorithmic tasks, code execution strongly outperforms NL both on average and individually. Using the GLMM, we extrapolate the data on a log scale and observe that code and NL correctness probabilities diverges as tasks get harder, code remains stable whereas NL diverges to 0. Code has $4.1\times$ odds of getting the answer correct compared to natural language.

3. Evaluating Translated NL and NL Distributional Similarity.

One key hypothesis is that natural language reasoning follows a deeper algorithmic computation encoded in its representations. If this is the case, it would make sense to surface the code and delegate the execution to an external runtime, rather than simulating noisy execution. We test whether natural language reasoning generated by information contained in the code alone can be distributionally similar to natural language reasoning generated from the prompt alone in Arm 1. Then, we test whether they are functionally similar.

3.1. Distributional Similarity between Translated NL and original NL

We show that the distribution of traces produced directly from the reasoning model can be approximated by post-processing the code with a fixed task-independent transformation.

Evaluation Setup For each evaluation task x and corresponding code c, we construct two samples from CoT we observed in experiment 1. We leverage the distribution of Arm 1 reasoning traces $p_{\text{NL}}(\cdot \mid x)$ and a matched distribution generated by a translator T (GPT-4o with 10 in-context examples) $p_{\text{Tr}}(\cdot \mid c)$:

$$\begin{aligned} &(x, z_{\text{NL}}), \quad z_{\text{NL}} \sim p_{\text{NL}}(\cdot \mid x), \quad \text{labelled Native.} \\ &(x, \hat{z}_{\text{NL}}), \quad \hat{z}_{\text{NL}} \sim p_{\text{Tr}}(\cdot \mid c), \quad \text{labelled Translated.} \end{aligned}$$

We then formulate a binary classification task in which a powerful zero-shot judge model (Claude Opus 4.0, Gemini 2.5 Pro, Grok 4.1 Fast) is given a problem instance X, and a single reasoning trace Z, and prompted to predict whether z was generated by Arm 1, or the translated Arm 2. This setup corresponds to discriminating between the joint distributions

$$p(x)p_{\text{NL}}(z \mid x) \text{ and } p(x)p_{\text{Tr}}(z \mid x)$$

We sample problem instances x randomly from a pool of 30,000 CoT examples from before spread across different models, seeds, tasks, hardness. Fixing these, we obtain paired outcomes corresponding to an x. We ensure that label counts between $\hat{z}_{\text{NL}}$ and z_{NL} are balanced on the test set, and tasks (21 tasks from CLRS 30 Benchmark) are disjoint from any in-context prompting examples.

As a control, we report the judge's discriminative power by asking it to classify between raw code and the Native NL reasoning, where high accuracy would indicate that performance results on the main evaluation is not due to an underpowered judge.

Results. Across 2000 samples and 3 judge models (6000 samples total), we find that the accuracy of the prompt is

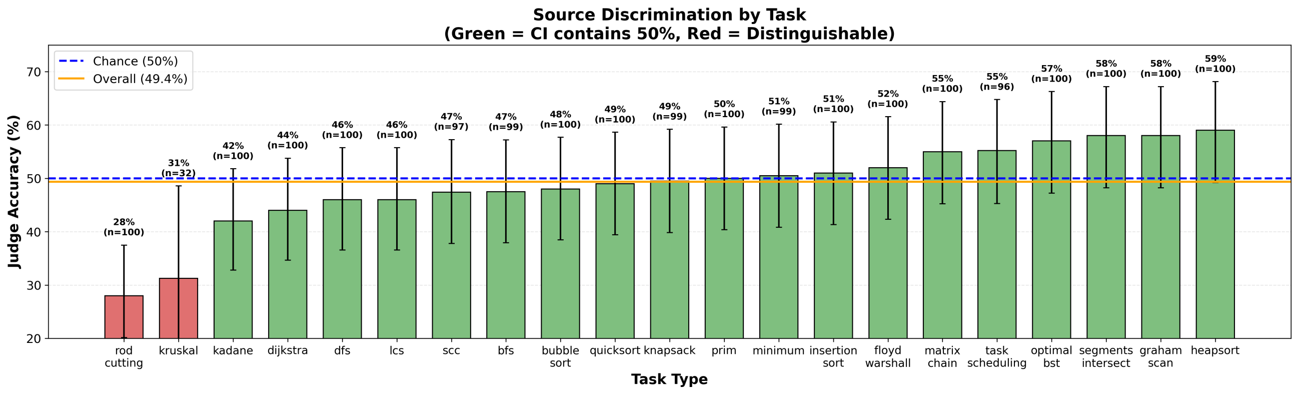


Figure 6. Discrimination accuracy by task: analysis of how well different representations (code vs. natural language) discriminate between algorithm types across task families.

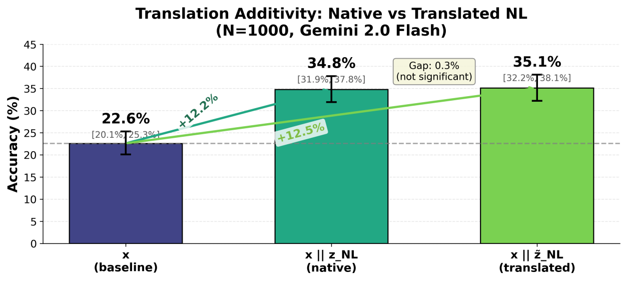


Figure 7. Translation additivity analysis: functional similarity between translated NL and original NL reasoning traces.

$49.4\% \in [47.2\%.51.5\%]$ Wilson CI, the control accuracy is 79.0% so the discriminators are calibrated. This holds within-model and within-task with a few exceptions being rod-cutting 1D dynamic programming and kruskal's MST algorithm problems. These findings are surprising since one might expect models to have different reasoning patterns, but our results explain that there exists a post-processing model that can yield the same reasoning process under the right prompting conditions.

3.2. Functional Similarity between Translated NL and original NL

We wish to verify whether the translated natural language reasoning from the experiment before has the same functionality as the original natural language reasoning produced in Arm 1.

Evaluation Setup. Given a task instance x, we prompt the target language model three ways.

1. Baseline: x (question only)
2. Arm 1: $x||z_{NL}$
3. Translated Arm 2: $x||\hat{z}_{NL}$

where $\hat{z}_{NL}$ is obtained by translating code to natural language. If the translated NL loses information relative to the original NL, then conditioning on $\hat{z}_{NL}$ should yield worse performance than conditioning on z_{NL}. We run on 1000 samples across 3 models (Claude Opus 4.0, Gemini 2.5 Pro, Grok 4.1 Fast) and report results on held-out tasks disjoint from the ICL example tasks. The same prompt is used for the translator in the previous experiment as the one used here. Crucially, the translator models we use are the same as the models that generated the original code x, unlike the experiment from before.

Results. We fail to reject the null hypothesis, and see overlapping 95% confidence intervals for Native and Translated. This leads us to believe that post-processed code and natural language reasoning have similar functionality quantified by end-task accuracy. Since we fixed the natural language reasoners here (same model), and only vary whether we feed in the original prompt and the generated code (with prompt masked), we infer that code and the original prompt share similar information, i.e. code does not lose much information. We also conclude that the algorithmic representations in code are simulated by the natural language reasoning.

4. Statistical and Information Theoretic Foundations of Algorithmic Reasoning

(Blackwell, 1953) Here, we prove that $Arm1 \simeq Arm2 < Arm3$ leveraging a similar breakdown framework as our experiments. We utilize information theory and statistical decision theory to sidestep representing the ambiguity of natural language and differences between NL and Code in a mathematical framework. Using the intuitions we gain in our experiments, we prove that Arm 2 is at least as good as Arm 1, and that Arm 3 is always better than Arm 2.

4.1. Arm 1 $\simeq$ Arm 2

Our empirical results on experiment 3 leads us to hypothesize that natural language reaosning is a post-processing (garbling) of code (Blackwell, 1953) under a noisy channel paradigm of inference, leading code reasoning to be at least as good as NL reasoning quantified by Bayes Risk.

Setup. Let $X \sim p(x)$ denote the task instance (problem + inputs), drawn from a representative test distribution. Let $\mathcal{Y}$ be an output space (e.g., answer strings), and let $\ell : \mathcal{Y} \times X \to [0, 1]$ be a bounded and measurable loss function (0–1 binary loss). In Arm 1 let the generative and bayesian inference process be the latent variable model:

$$\text{Arm1} : X \underbrace{\rightarrow}_{p_{\text{NL}(Z_{\text{NL}}|x)}} Z_{\text{NL}} \underbrace{\rightarrow}_{\delta_{\text{NL}}(y|x,z_{\text{NL}})} Y_{\text{NL}}$$

$$P(Y_{\text{NL}}|X = x) := \int \underbrace{\delta_{\text{NL}}(y|x, z)}_{\text{Execute}} \underbrace{p_{\text{NL}}(z|x)}_{\text{Generate}} \,\mathrm{d}z$$

With the addition of a fixed LLM translator T (independent of x), let the generative and inference process for Arm 2.5 with translator be:

$$\text{Arm2.5} : X \underbrace{\rightarrow}_{p_{\text{C}(Z_{\text{C}}|x)}} Z_{\text{C}} \underbrace{\rightarrow}_{T(\hat{Z}_{\text{NL}}|z_{\text{C}})} \hat{Z}_{\text{NL}} \underbrace{\rightarrow}_{\delta_{\text{NL}}(y|x,\hat{z}_{\text{NL}})} \hat{Y}_{\text{Tr}}$$

$$P(\hat{Y}_{\text{Tr}}|X = x) := \int \underbrace{\delta_{\text{NL}}(y|x, \hat{z})}_{\text{Execute}} \underbrace{T(\mathrm{d}\hat{z}|z)}_{\text{Translate}} \underbrace{p_{\text{Code}}(\mathrm{d}z|x)}_{\text{Generate}} \,\mathrm{d}z$$

Let the original Arm 2 be:

$$\text{Arm2} : X \underbrace{\rightarrow}_{p_{\text{C}(Z_{\text{C}}|x)}} Z_{\text{C}} \underbrace{\rightarrow}_{\delta_{\text{Sim}}(y|x,z_{\text{C}})} Y_{\text{Sim}}$$

$$P(Y_{\text{Sim}}|X = x) := \int \underbrace{\delta_{\text{Sim}}(y|x, z)}_{\text{Execute}} \underbrace{p_{\text{Code}}(\mathrm{d}z|x)}_{\text{Generate}} \,\mathrm{d}z$$

We show that for some negligible ε, the Bayes Risk $R^*(Z)$ for code is less than for natural language.

$$R^*(Z) := \inf_{\delta} \mathbb{E}[\ell(Y, X)]$$
$$R^*(Z_{\text{Sim}}) \leq R^*(Z_{\text{NL}}) + O(\varepsilon)$$

ε is the maximum change in expected loss when replacing the true distribution by the approximated distribution, defined below in Assumption 2. Empirically, we showed that this value was small in experiment 2.

Assumption 1. We assume there exists a (near Bayes optimal) translator T mapping code to natural language reasoning $Z_{\text{Code}} \to \hat{Z}_{\text{NL}}$ independent of X.

Assumption 2. We assume that the original NL reasoning chain of thought is close to the translated NL on average. Let p_{NL} be the Arm 1 channel and $p_{\text{translated}}(\cdot \mid x)$ be the translated NL channel. Assume an average conditional TV bound:

$$\mathbb{E}_{X\sim p}\big[d_{\text{TV}}\big(p_{\text{NL}}(\cdot \mid X),\, p_{\text{translated}}(\cdot \mid X)\big)\big] \leq \varepsilon,$$

where

$$d_{\text{TV}}(P, Q) = \sup_{B} |P(B) - Q(B)|.$$

In other words, averaged over task instances, the NL trace produced by Arm 1 is close in distribution to the NL traces obtained by translating the code trace (Arm 2) using the translator T. We empirically verify this in experiment 2.

Proof. Our high level strategy is to use Blackwell's simulation principle, and show that NL reasoning is just code generation plus a noisy translation, thus a code-based agent can simulate exactly what the NL agent would do by averaging over that noise internally. In other words, under Assumptions 1–2, for the bounded loss $\ell \in [0, 1]$,

$$R^*(Z_{\text{Code}}) \leq R^*(Z_{\text{NL}}) + O(\varepsilon).$$

Step 1: Simulate NL from code via translation. Here, we first show that for any NL-based policy, there exists a code-based policy that induces the same input-output behaviour.

Here we first translate the input problem into CoT, then execute the CoT via LLM reasoning, similar to what we do in the Arm 2 experiments. We abuse notation here, and $z = z_{\text{Code}}$. Define code simulation to be an implicit translation then reason in the original simulation branch:

$$\delta_{\text{Sim}}(y \mid x, z) := \int \underbrace{\delta_{\text{NL}}(y \mid x, \hat{z})}_{\text{Execute}} \underbrace{T(\hat{z} \mid z)}_{\text{Translate}} \,\mathrm{d}z.$$

Then, we can apply the law of iterated expectation on Arm 2 to get Arm 2.5:

$$\begin{aligned} P(Y_{\text{Sim}}|X = x) &:= \int \underbrace{\delta_{\text{Sim}}(y|x, z)}_{\text{Execute}} \underbrace{p_{\text{Code}}(\mathrm{d}z|x)}_{\text{Generate}} \,\mathrm{d}z \\ &= \int\int [\underbrace{\delta_{\text{NL}}(y|x, \hat{z})}_{\text{Execute}} \underbrace{T(\mathrm{d}\hat{z}|z)}_{\text{Translate}}] \underbrace{p_{\text{Code}}(\mathrm{d}z|x)}_{\text{Generate}} \,\mathrm{d}z \\ &= P(\hat{Y}_{\text{Tr}}|X = x) \end{aligned}$$

The joint distributions (X, Y_{Sim}) and $(X, \hat{Y}_{\text{translated}})$ are the same. Thus,

$$\mathbb{E}[\ell(Y_{\text{Sim}}, X)] = \mathbb{E}[\ell(\hat{Y}_{\text{translated}}, X)].$$

Step 2: Substitute translated NL and original NL via TV lemma. Here we show that if two signals look similar, they perform similarly. Even if translated NL is not exactly native NL, bounded loss decision problems cannot exploit small distributional differences, a property of the continuity property of Bayes Risk.

Lemma 4.0.1 (TV Lemma). *Let $X \sim p(x)$. Let $Z \mid X = x \sim P_x$ and $Z' \mid X = x \sim Q_x$. Let $g(x,z) \in [0,1]$ be measurable. Then*

$$\mathbb{E}[g(X,Z)] - \mathbb{E}[g(X,Z')] \leq \mathbb{E}_X\left[d_{\mathrm{TV}}(P_X, Q_X)\right].$$

For each x and trace z, define $g(x,z) := \mathbb{E}_{y|x,z}[\ell(y,x)]$. Then $g(x,z) \in [0,1]$. Note that

$$\mathbb{E}_{(Y_{\mathrm{NL}},X)}[\ell(Y_{\mathrm{NL}},X)] = \mathbb{E}_{(X,Z_{\mathrm{NL}})}[g(X,Z_{\mathrm{NL}})],$$
$$\mathbb{E}_{(\hat{Y}_{\mathrm{Tr}},X)}[\ell(\hat{Y}_{\mathrm{translated}},X)] = \mathbb{E}_{(X,\hat{Z}_{\mathrm{NL}})}[g(X,\hat{Z}_{\mathrm{NL}})].$$

Applying the TV lemma with $P_x = p_{\mathrm{NL}}(\cdot \mid x)$ and $Q_x = p_{\mathrm{translated}}(\cdot \mid x)$:

$$\begin{aligned}&\left|\mathbb{E}[\ell(Y_{\mathrm{NL}},X)] - \mathbb{E}[\ell(\hat{Y}_{\mathrm{translated}},X)]\right| \\ &= \left|\mathbb{E}[g(X,Z_{\mathrm{NL}})] - \mathbb{E}[g(X,\hat{Z}_{\mathrm{NL}})]\right| \\ &\leq \mathbb{E}_X\left[d_{\mathrm{TV}}(p_{\mathrm{NL}}(\cdot \mid X),\, p_{\mathrm{translated}}(\cdot \mid X))\right] \leq \varepsilon.\end{aligned}$$

Therefore, rearranging gives

$$\mathbb{E}[\ell(\hat{Y}_{\mathrm{translated}},X)] \leq \mathbb{E}[\ell(Y_{\mathrm{NL}},X)] + \varepsilon$$
$$\mathbb{E}[\ell(Y_{\mathrm{Sim}},X)] = \mathbb{E}[\ell(\hat{Y}_{\mathrm{translated}},X)] \leq \mathbb{E}[\ell(Y_{\mathrm{NL}},X)] + \varepsilon.$$

We add superscripts to denote the decision rule (LLM executor) that was used. Then, since the inequality holds for arbitrary LLM executors δ_{NL} (including the best), we get:

$$\inf_{(\delta_{\mathrm{Sim}},\delta_{\mathrm{NL}})} \mathbb{E}[\ell(Y_{\mathrm{Sim}}^{(\delta_{\mathrm{Sim}})},X)] \leq \inf_{(\delta_{\mathrm{Sim}},\delta_{\mathrm{NL}})} \mathbb{E}[\ell(Y_{\mathrm{NL}}^{(\delta_{\mathrm{NL}})},X)]+\varepsilon.$$

Therefore, ignoring infimums over independent variables δ_{NL} on the left and δ_{Sim} on the right, we get exactly the Bayes Risk defined before.

$$\boxed{R^*(Z_{\mathrm{Sim}}) \leq R^*(Z_{\mathrm{NL}}) + \varepsilon}$$

□

4.2. Arm 2 < Arm 3

We prove that deterministic execution in Arm 3 yields strictly lower Bayes Risk.

Setup. Let $X \sim p(x)$ be a task instance and let $Y^*(x)$ denote the corresponding ground-truth. Suppose $Z_{\mathrm{Sim}} \sim p_{\mathrm{Sim}}$ is the code produced by the model. Let g be a deterministic python3 runtime. Define the two arms:

$$\mathrm{Arm2}: Y_{\mathrm{Sim}} \sim \delta_{\mathrm{Sim}}(\cdot|X, Z_{\mathrm{Sim}})$$
$$\mathrm{Arm2}: Y_{\mathrm{Exec}} := g(X, Z_{\mathrm{Sim}})$$

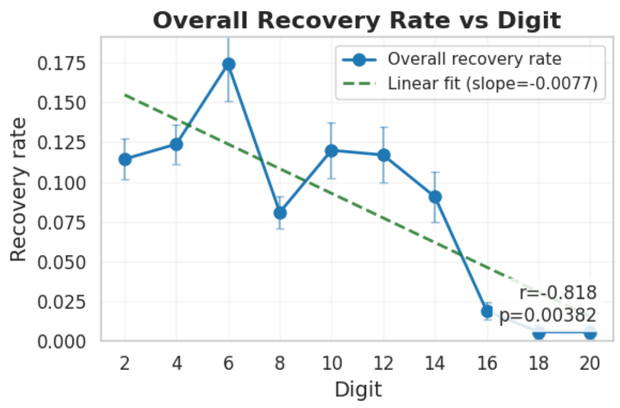


Figure 8. Recovery rate analysis: proportion of cases where LLM simulation (Arm 2) produces the correct answer despite incorrect code (Arm 3 failure). Recovery rates remain below 5% across all task families and models, confirming that solver execution dominates LLM simulation.

Proof. Under $\ell(y,x) = \mathbf{1}\{y \neq Y^*(x)\}$, the solver achieves zero risk ($R_3^* = 0$) whenever the generated code is correct. In contrast, LLM simulation incurs positive risk ($R_2^* > 0$) whenever $\Pr[Y_2 \neq Y_3] > 0$, which occurs empirically due to execution errors in mental simulation.

$$\boxed{R_3^* < R_2^*}$$

□

The only scenario where Arm 2 could outperform Arm 3 is when the generated code is *incorrect*, yet the LLM "recovers" by reasoning to the correct answer despite the flawed code. We empirically quantify this recovery rate below.

Recovery reduces as tasks get harder. To further reinforce this result, we rule out the possibilities of recovery as tasks get harder, eliminating any benefit of running Arm 2:

1. Arm 3 produces an incorrect answer (implying incorrect code generation), and

2. Arm 2 produces the correct answer (implying successful LLM recovery).

Figure 8 presents the recovery analysis across all tasks and models. The recovery rate remains consistently low (typically $< 5\%$), indicating that LLM simulation rarely compensates for code generation errors. This confirms that Arm 3's advantage stems from reliable solver execution rather than Arm 2's inability to reason about code.

5. Related Work and Discussion

Neuro-symbolic Learning. This paper builds on research in neuro-symbolic integration (Graves et al., 2014; Veličković & Blundell, 2021; Reed & Freitas, 2016; Graves et al., 2016), which combines neural networks with symbolic reasoning systems. These approaches are motivated by cognitive science (Schneider & Chein, 2003; Risko & Gilbert, 2016; Anderson, 2010), hierarchical reinforcement learning (Kolter et al., 2007; Dietterich, 2000), and compositionality research (Hudson & Manning, 2018; Hupkes et al., 2020; Andreas et al., 2017; Poggio et al., 2017). An orthogonal line of work explores direct execution of algorithms by neural networks (Veličković & Blundell, 2021; Mahdavi et al., 2023; Ibarz et al., 2022; Yan et al., 2020). Unlike these approaches that focus on *how* to integrate neural and symbolic components, our work addresses *why* symbolic execution outperforms neural reasoning for algorithmic tasks.

LLM Reasoning. Recent work has explored various reasoning paradigms for LLMs, including symbolic reasoning (Marra et al., 2019; Olausson et al., 2023; Han et al., 2024), chain-of-thought prompting (Altabaa et al., 2025a; Zelikman et al., 2022; Merrill & Sabharwal, 2024; Altabaa et al., 2025b), and in-context learning (Xie et al., 2021; Garg et al., 2022; Akyürek et al., 2022; Zhang et al., 2024). Xie et al. (2021) model in-context learning as implicit Bayesian inference, which we extend to compare different reasoning representations. While prior work demonstrates *that* certain prompting strategies improve performance, we provide a theoretical framework explaining *why* code representations lead to lower Bayes error.

LLM Tool-Use. Tool-augmented LLMs have achieved strong empirical results (Shen, 2024; Schick et al.; Qin et al., 2023; Tang et al., 2023; Parisi et al., 2022). Code generation for tool-use can be viewed as a form of semantic parsing (Shin & Durme, 2022; Krishnamurthy et al., 2017; Berant et al., 2013; Dong & Lapata, 2016) or function calling (Puri et al., 2021; Alon et al., 2019; Chen & Zhou, 2018). Our work complements this literature by providing theoretical justification for the observed empirical advantages of code-based tool-use over direct natural language reasoning.

6. Conclusion

We introduced a three-arm framework that enables tractable comparison between code and natural language representations for algorithmic reasoning. By modeling LLM inference as Bayesian inference, we proved that code representations yield higher mutual information with target algorithms, leading to lower Bayes error. Empirically, code execution achieves 78% accuracy compared to 21% for natural language reasoning across arithmetic, dynamic programming, and integer linear programming tasks.

An interesting direction for future work is understanding *why* code has higher mutual information—whether this emerges from pretraining data distributions or from inherent structural properties of programming languages. Our framework provides a foundation for such investigations.

Limitations.

Our study focuses on algorithmic tasks (arithmetic, DP, ILP) where ground truth is well-defined. The results may not generalize to open-ended reasoning tasks without clear algorithmic structure. Additionally, our theoretical bounds are asymptotic—the 6% Bayes error improvement is a lower bound that may not reflect finite-sample performance. Finally, we evaluate on a limited set of models (Deepseek, Gemma); behavior may differ for other architectures.

Future Work. These findings have practical implications for AI system design: for algorithmically structured problems, compositional systems with symbolic execution should be preferred over monolithic neural reasoning. This supports the growing trend toward tool-augmented LLMs.

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