

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

Terry Tong¹ Yu Feng¹ Surbhi Goel¹ Dan Roth¹

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

Consider the algorithmic task of computing arithmetic operations encoded in natural language. We wish to compute:

$$p(Y=3|X=\text{What is one plus two?})$$

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

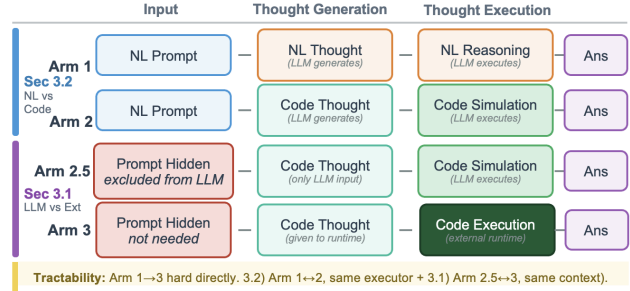


Figure 1. Bayesian Inference model showing the *three arms methodology* in Section 2. Given an algorithmic problem, we may split it into two steps (1) Translate (2) Execute. The (1) translation $\in \{\text{Code, NL}\}$. Then (2) execution $\in \{\text{LLM Reasoning, Solver Execution}\}$. We have three pairs, Arm 1: $\{\text{NL Gen, LLM Reasoning}\}$, Arm 2: $\{\text{Code Gen, LLM Reasoning}\}$, Arm 3: $\{\text{Code Gen, Solver Execution}\}$. 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.

The language model forward pass could decide (1) to generate the solution directly with natural language reasoning (Wei et al., 2022) (2) translate the problem into code and use a solver (Gao et al., 2023). This paper provides empirical evidence that Arm 1 < Arm 3 quantified by end-task accuracy. A body of work shows that this pipeline is generally effective (Lyu et al., 2023; Pan et al., 2023), further evidenced by the empirical success of tool-use¹. However, little progress has been made on explaining *why* solver-based tools lead to higher end-task accuracy than natural language reasoning.

One might be tempted to prove a statistical advantage by showing that sample complexity to learn code is less than natural language because code is structured, but will quickly find that this problem becomes intractable due to the hardness of capturing natural language under a mathematical

¹Here we primarily refer to solver-based tool-use as opposed to knowledge-intensive tool-use like RAG

Evaluation Arm Prompts			
Arm 1: Natural Language (NL)	Arm 2: Code Similarity (Sim)	Arm 2.5: Controlled Simulation (ControlSim)	Arm 3: Code Execution (Code)
Prompt: "Solve the following algorithmic problem: {question} YOU ARE NEVER ALLOWED TO USE CODE. FOLLOW THE FORMAT CAREFULLY."	Prompt: "Solve the following algorithmic problem: {question} FOLLOW THE FORMAT CAREFULLY." Response includes: • code: Python solution() function • simulation: Natural language trace	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	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: 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"}	Example: Q: "Compute: 123 + 456" A: {"code": def solution(): return 123 + 456 "simulation": "Adds 123 + 456", "Answer": "579"}	Example: Q: "Simulate: def solution(): return 123 + 456" A: {"simulation": "The function computes 123 + 456 and returns 579", "Answer": "579"}	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.

framework. The same problem arises when attempting to use approximation theory to provide evidence that DNNs can better learn compositional or structured languages (like code) than natural language. Broadly speaking, the problem is challenging because the inputs and outputs are different, one is a structured language, the other is an unstructured language. This drastically complicates comparison. Or, one might be tempted to show a computational advantage by showing that code unlocks a new level of expressivity (Merrill & Sabharwal, 2023). However, one will find that whether using a solver or not will not overcome the hardness of the problem. E.g., we can prove by contradiction that using a solver will not allow us to better solve NP-Hard problems, unless $P=NP$.

As a solution, we leverage a Bayesian Inference paradigm to reason about the two different settings (Xie et al., 2021). Doing so, enables us to break down the algorithmic reasoning pipeline into two distinct phases (1) Translation $\in \{\text{Code, NL}\}$ (2) Execution $\in \{\text{LLM Reasoning, Solver Execution}\}$ (Lyu et al., 2023; Pan et al., 2023). Enumerating the valid combinations, we obtain three pairs, Arm 1: {NL Gen, LLM Reasoning}, Arm 2: {Code Gen, LLM Reasoning}, Arm 3: {Code Gen, Solver Execution}. Introducing Arm 2 makes the problem tractable.

Empirically, this framework enables controlled comparisons. A rigorous comparison has not been instantiated because it is hard to control the experiment and determine what representation is actually being used—whether code, natural language, or something else. We overcome this by verbalizing the representation using Chain-of-Thought. We provide statistical evidence for the alternative hypothesis Arm 3 > Arm 2 > Arm 1 on (Gemma, Deepseek, Llama), we demonstrate that generating code and executing leads to 78% accuracy on (ILP, DP, Arithmetic) tasks, over 30% for code simulation and just over 20% for natural language reasoning across 5 models. Our results are computed over 5 seeds, and a Friedman Chi-square gives results a test statistic of 9277.32 and 8369.34 for deepseek and llama, enabling

us to reject the null in favor of the alternative.

Theoretically, we first compare Arm 1 < 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 Arm 2 < 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 Arm 3 > Arm 2.

Piecing these results together, we show that Arm 1 < Arm 2 < 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:

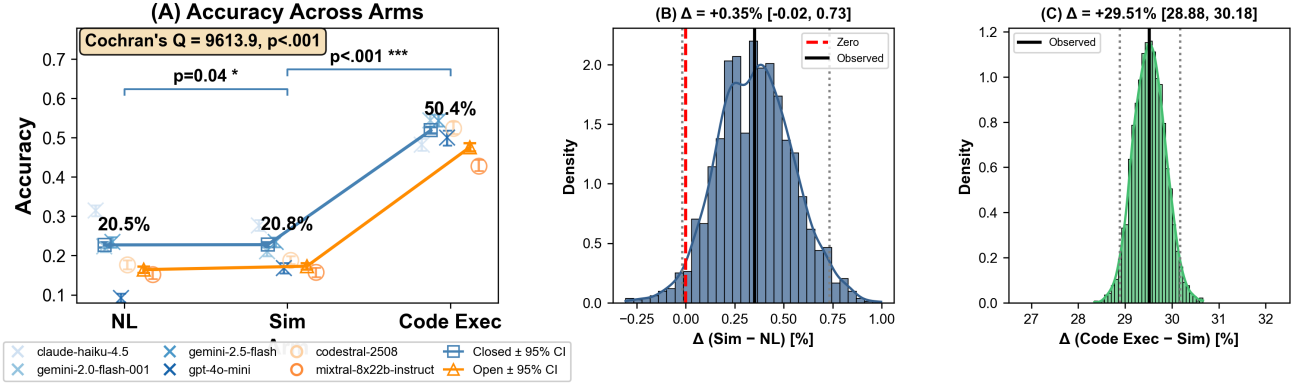


Figure 3. Average accuracy across arms for all models and tasks. Code execution (Arm 3) outperforms code simulation (Arm 2), which outperforms natural language reasoning (Arm 1) on CLRS₃₀ (n=500), NPHardEval (n=270), and Fine-Grained evaluation (n=270) benchmarks across 3 seeds. Statistical significance measured by Wilcoxon signed-rank test between adjacent arms. Error bars show bootstrapped Wilson confidence intervals at the model level.

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

2. Evaluation Framework

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

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 $(X_i) \rightarrow Y_i^{(\text{NL})}$. Likewise, Arm 2 can be written as using the same LLM to first $(X_i) \rightarrow C_i$ and then $(X_i, C_i) \rightarrow Y_i^{(\text{Sim})}$. 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

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

Arm 1 \leq Arm 2 $<$ Arm 3 Setup. We observe bernoulli outcomes $(Y_i^{(\text{NL})}, Y_i^{(\text{Sim})}, Y_i^{(\text{Exec})})$. Thus, we run Cochran's Q test across paired binary outcomes with the null $E[Y_i^{(\text{NL})}] = E[Y_i^{(\text{Sim})}] = E[Y_i^{(\text{Exec})}]$, testing whether at least one arm has a different marginal success accuracy.

Condition on failing to reject the null, following the framework, we break down the tests into Arm 1 and Arm 2 ($Y_i^{(\text{NL})}, Y_i^{(\text{Sim})}$), and Arm 2 and Arm 3 ($Y_i^{(\text{Sim})}, Y_i^{(\text{Exec})}$). For these paired bernoulli outcomes, we run the McNemar test under the null that $\Pr(Y^{(\text{Sim})} = 1, Y^{(\text{Exec})} = 0) = \Pr(Y^{(\text{Sim})} = 0, Y^{(\text{Exec})} = 1)$, that is, when pairs disagree, each one (Sim $\not\leq$ NL) and (NL $\not\leq$ Sim) occur equally as often. Similarly, this applies for the null for arm 2 and arm 3. To quantify effect size, we take paired accuracies $\Delta_{\text{Exec-Sim}} = \text{Acc}(\text{Exec}) - \text{Acc}(\text{Sim})$ and estimate its sampling distribution via cluster bootstrap resampling over instance pairs $(Y_i^{(\text{Sim})}, Y_i^{(\text{Exec})})$ corresponding to i . We do this for both Arm 1 vs Arm 2 and Arm 2 vs Arm 3.

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

We run a GLMM with fixed effects and random effects, and observe how hardness interacts with the accuracy, and

² X_i is ignored by executor, but we include it for notational symmetry

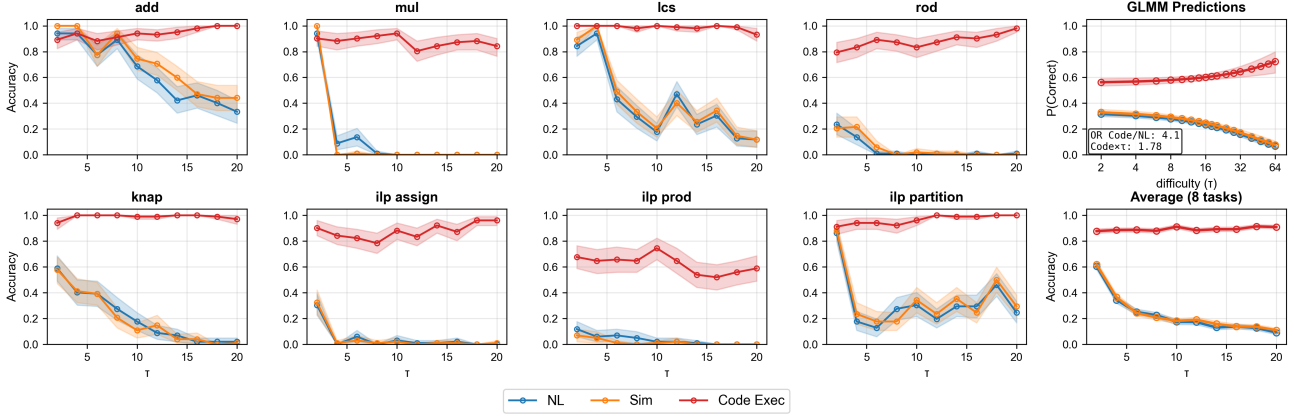


Figure 4. Accuracy scaling across task difficulty (τ) for Arithmetic, Dynamic Programming, and ILP tasks. Arm 3 (code execution) maintains high accuracy as problems get harder, while Arms 1 and 2 degrade. The widening gap demonstrates that solver execution becomes increasingly advantageous for challenging algorithmic problems.

whether code or natural language helps modulate the performance.

2.2. Experiments

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 outright 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. Similarly for Arm 2, we prompt the LLM to use code in its reasoning, generating a structured output that contains a piece of code, and an attempt at simulating the execution of that piece of code in natural language, followed by a final answer. For Arm 3, we take the generated function (no prompt), and execute it in a python3 runtime. Models have access to native python packages, and numpy, pandas, scipy, PuLP, and pytorch. Figure 2 illustrates the prompt templates used across all three arms.

Arm 1 \leq Arm 2 < Arm 3 Results. Across 6 different

types of models, and 44 algorithmic tasks spanning the CLRS 30 benchmark, NPHardEval benchmark and a custom suite of evals (Appendix), we strongly reject the null hypothesis, observing ($p \leq 0.001$) and that 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.

we run 30,000+ samples total and reject the null ($p=0.04$). However, the results are inconclusive since, under the cluster bootstrap, we see that the distribution’s confidence interval overlaps with 0.0, meaning that natural language reasoning and code simulation are approximately equal, with code simulation occasionally being better (not strict inequality). For the purposes of our framework, instrict inequality is ok.

Conclusive across both open and closed models.

Advantages of Arm 3 emerge as tasks get harder. Figure 4

3. Evaluating Translated NL and NL Distributional Similarity.

One key hypothesis is that natural language reasoning follows a deeper algorithmic procedure encoded in its representations. If this is the case, it would make sense to surface the code and send it to an executor. 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.

(a) Translator Prompt	(b) Discriminator Prompt
<p>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.</p> <hr/> <p>GUIDELINES</p> <ul style="list-style-type: none"> • 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) <hr/> <p>10 IN-CONTEXT EXAMPLES</p> <p>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, ...)</p> <hr/> <p>TEST INPUT</p> <pre>def solution(): # [Code to translate]</pre>	<p>You are analyzing an explanation of how to solve an algorithmic problem.</p> <p>TASK: Determine whether this was written by someone solving naturally ("Native NL") or translating/simulating code ("Translated").</p> <hr/> <p>INPUT FORMAT</p> <p>PROBLEM: {Algorithmic problem description} EXPLANATION: {Reasoning trace to classify}</p> <hr/> <p>OUTPUT FORMAT</p> <p>PREDICTION: [NATIVE or TRANSLATED] CONFIDENCE: [HIGH, MEDIUM, or LOW] REASONING: [1-2 sentence justification]</p>

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.

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 function across tasks and models. For each task instance x drawn from a held-out test distribution over 21 different algorithmic problems in CLRS, we consider two conditional distributions: Arm 1: $p_{NL}(\cdot | x)$, original NL traces generated by an LLM (Gemini 2.0 Flash in our case) and Arm 2 Translated: $p_{Translated}(\cdot | x)$, NL traces obtained by first generating code by an LLM, then translating that code into natural language using a fixed translator.

Evaluation Setup We formulate a binary classification task in which a powerful judge model (Claude Opus 4.5) is given a problem instance x , and a single reasoning trace z , and must predict whether z was generated by Arm 1, or the translated Arm 2. This setup corresponds to discriminating between the joint distributions $p(x)p_{NL}(z | x)$ and $p(x)p_{Translated}(z | x)$. For each evaluation task x , we construct two samples (x, z_{NL}) , where $z_{NL} \sim p_{NL}(\cdot | X)$, labelled Original, and (x, \hat{z}_{NL}) where $\hat{z}_{NL} \sim p_{Translated}(\cdot | x)$, labelled Translated. The label counts are balanced on the test set, and the judge’s accuracy, and AUC are computed on held-out tasks (disjoint from any in-context prompting examples).

In the evaluation, all generation parameters are fixed, model, prompt, and decoding hyperparameters, and the only variability is the seed for both the original Arm 1 and translated Arm 2, i.e. we compare samples from two fixed conditionals given a task instance.

We ensure the judge has enough discriminative power by asking it to classify between raw code and the native NL reasoning. High accuracy would indicate that the performance results on the main evaluation is not due to an underpowered judge. We prompt the judge zero-shot, instructing it that there are original natural language reasoning traces and translated ones that it must distinguish.

The translator, gemini-2.0 flash, is given 10 in-context pairs between code in Arm 2 and original natural language reasoning in Arm 1, and asked to learn the mapping and apply on new instances. The 10 in-context examples are 10 different tasks, which are disjoint from the 21 other tasks in CLRS benchmark that we evaluate on.

Results. Across 2000 samples, we find that the accuracy of the prompt is 49.4% $\in [47.2\%.51.5\%]$ Wilson CI, obtaining a 0.479 AUC. The control accuracy is 79.0% so the discriminator is calibrated. We include per-task analysis in the appendix. We see that this is generally true across different models with only a few exceptions between rod cutting and the kruskal algorithm problems.

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 (gemini) 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 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.

Results. We fail to reject the null hypothesis on 1000 samples, and see that using the original Arm 1 and the translated Arm 2 concatenated to the same original task prompt yield the same results.

Qualitative Analysis In observing the LLM responses, we notice the model's have a propensity to follow similar reasoning. This happens across individual models, but problem solving methodology is surprisingly similar across models. Show figure here.

4. Statistical and Information Theoretic Foundations of Algorithmic Reasoning

We claim that natural language reasoning is a garbling of code (Blackwell, 1953) under a noisy channel paradigm of inference, leading code reasoning to be at least as good as NL reasoning.

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 $\ell : \mathcal{Y} \times X \rightarrow [0, 1]$ be a bounded and measurable loss function (0–1 binary loss). In Arm 1 and Arm 2, each arm corresponds to an intermediate representation Z (e.g. CoT) produced by channel $p(z | x)$ (e.g. LLM), and then choosing an output Y via a randomized decision rule $\delta(y | x, z)$ (i.e. LLM test-time reasoning).

For any CoT observation Z , define the Bayes risk:

$$R^*(Z) := \inf_{\delta} \mathbb{E}[\ell(Y, X)],$$

$$X \sim p, Z \sim p(\cdot | X), Y \sim \delta(\cdot | X, Z).$$

In the first arm, we observe $Z_{NL} \sim p_{NL}(\cdot | X)$. For the second arm, we have $Z_{Code} \sim p_{Code}(\cdot | X)$.

We show that $R^*(Z_{Code}) \leq R^*(Z_{NL}) + O(\varepsilon)$ for some negligible ε .

4.1. Assumptions

Assumption 1. We assume there exists a stochastic kernel T such that the Markov chain $X \rightarrow Z_{Code} \rightarrow \hat{Z}_{NL}$ is representative of CoT, with the final decision stage being

$\delta(y | X, \hat{Z}_{NL})$. That is,

$$\hat{Z}_{NL} \sim p_{translation}(\cdot | x), p_{translation}(z | X) := \int T(z | z_{Code}) p_{Code}(z_{Code} | x) dz_{Code}.$$

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 $p_{translated}(\cdot | x)$ be the translated NL channel. Assume an average conditional TV bound:

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

where

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

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 (Markov kernel).

4.2. Proof

Proof. Under Assumptions 1–2, for the bounded loss $\ell \in [0, 1]$,

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

Step 1: Simulate NL from code via translation. Here we first translate the input problem into CoT, then execute the CoT:

$$\delta_{Code}(y | x, z_{Code}) := \int \underbrace{\delta_{NL}(y | x, z)}_{\text{Execute}} \underbrace{T(z | z_{Code})}_{\text{Translate}} dz.$$

Let $Y_{Code} \sim \delta_{Code}(\cdot | X, Z_{Code})$. Let $\hat{Y}_{translated} \sim \delta_{NL}(\cdot | X, \hat{Z}_{NL})$, where \hat{Z}_{NL} is produced from Z_{Code} via the translator kernel T .

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

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

This is because conditional on $X = x$, sampling $Z_{code} \sim p_{code}(\cdot | x)$, then $\hat{Z}_{nl} \sim T(\cdot | Z_{code})$, then $Y \sim \delta_{NL}(\cdot | x, \hat{Z}_{NL})$ induces the same conditional distribution over Y as $Y \sim \delta_{code}(\cdot | x, Z_{code})$.

Step 2: Substitute translated NL and original NL via TV lemma.

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

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

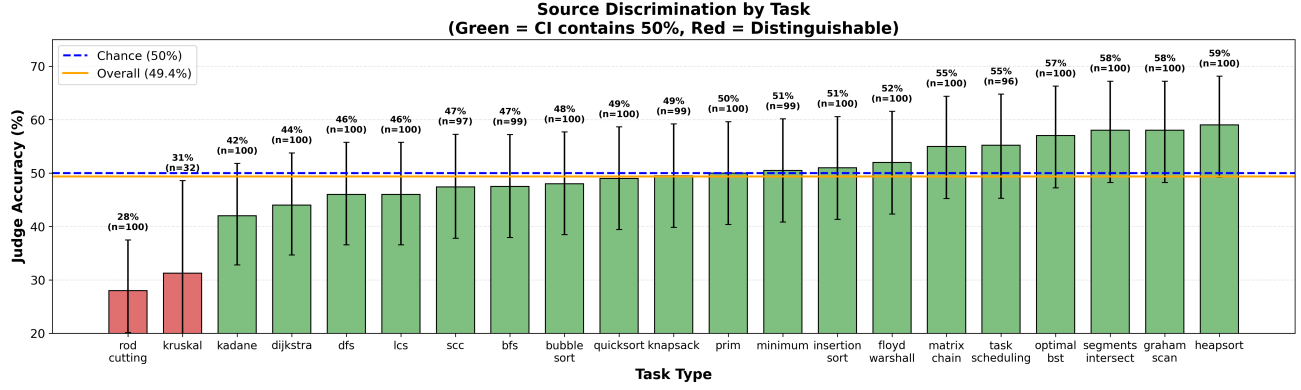


Figure 6. Recovery rate analysis: proportion of cases where LLM simulation (Arm 2) produces the correct answer despite incorrect code (Arm 3 failure). Recovery rates remain below 5% across all task families and models, confirming that solver execution dominates LLM simulation.

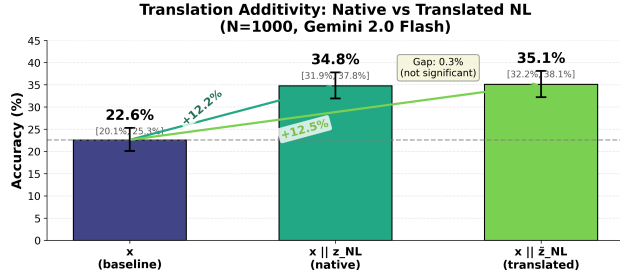


Figure 7. Recovery rate analysis: proportion of cases where LLM simulation (Arm 2) produces the correct answer despite incorrect code (Arm 3 failure). Recovery rates remain below 5% across all task families and models, confirming that solver execution dominates LLM simulation.

Suppose we have $Y_{NL} \sim \delta_{NL}(\cdot \mid Z_{NL})$ under the actual channel $p_{NL}(\cdot \mid x)$. For each x and trace z , define $g(x, z) := \mathbb{E}_{y \sim \delta(\cdot \mid z)}[\ell(y, x)]$.

Then $g(x, z) \in [0, 1]$. Note that

$$\begin{aligned} \mathbb{E}[\ell(Y_{NL}, X)] &= \mathbb{E}[g(X, Z_{NL})], \\ \mathbb{E}[\ell(\hat{Y}_{\text{translated}}, X)] &= \mathbb{E}[g(X, \hat{Z}_{NL})]. \end{aligned}$$

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

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

Therefore, rearranging gives

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

Thus,

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

Since this holds for arbitrary NL rule δ_{NL} , taking the infimum over δ_{NL} on the right-hand side yields $R^*(Z_{\text{Code}}) \leq R^*(Z_{NL}) + \varepsilon$. \square

4.3. Arm 2 < Arm 3

We model the comparison between LLM simulation (Arm 2) and solver execution (Arm 3) under the following assumptions:

1. **Solver correctness.** Given correct code Z , the solver deterministically produces the ground-truth answer: $Y_3 = g(X, Z) = Y^*(X)$.
2. **Noisy simulation.** LLM simulation adds stochastic noise: $Y_2 \sim N(\cdot \mid Y_3, X, Z)$ for some noise kernel N .
3. **0-1 loss.** We evaluate under $\ell(y, x) = \mathbf{1}\{y \neq Y^*(x)\}$.

Under these assumptions, 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. Therefore, $R_3 < R_2$.

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).

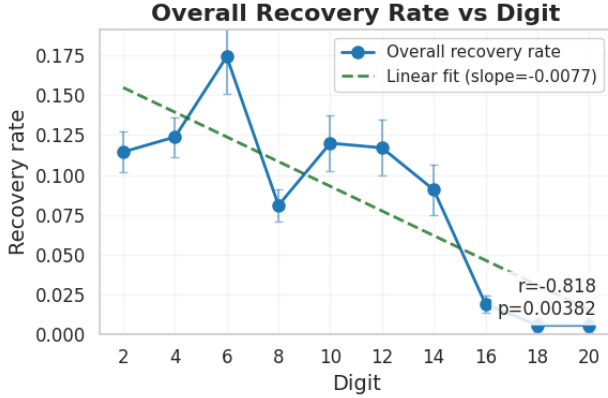


Figure 8. Recovery rate analysis: proportion of cases where LLM simulation (Arm 2) produces the correct answer despite incorrect code (Arm 3 failure). Recovery rates remain below 5% across all task families and models, confirming that solver execution dominates LLM simulation.

Figure 5 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 in-

ference, 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.

References

Akyürek, E., Schuurmans, D., Andreas, J., Ma, T., and Zhou, D. What learning algorithm is in-context learn-

- ing? investigations with linear models. *arXiv preprint arXiv:2211.15661*, 2022.
- Alon, U., Zilberstein, M., Levy, O., and Yahav, E. code2vec: learning distributed representations of code. *Proceedings of the ACM on Programming Languages*, 3(POPL): 1–29, January 2019. ISSN 2475-1421. doi: 10.1145/3290353. URL <https://dl.acm.org/doi/10.1145/3290353>.
- Altabaa, A., Montasser, O., and Lafferty, J. Cot information: Improved sample complexity under chain-of-thought supervision. *arXiv preprint arXiv:2505.15927*, 2025a.
- Altabaa, A., Montasser, O., and Lafferty, J. CoT Information: Improved Sample Complexity under Chain-of-Thought Supervision, May 2025b. URL <http://arxiv.org/abs/2505.15927>. arXiv:2505.15927 [stat].
- Anderson, M. L. Neural reuse: A fundamental organizational principle of the brain. *Behavioral and Brain Sciences*, 33(4):245–266, August 2010. ISSN 0140-525X, 1469-1825. doi: 10.1017/S0140525X10000853. URL https://www.cambridge.org/core/product/identifier/S0140525X10000853/type/journal_article.
- Andreas, J., Rohrbach, M., Darrell, T., and Klein, D. Neural Module Networks, July 2017. URL <http://arxiv.org/abs/1511.02799>. arXiv:1511.02799 [cs].
- Berant, J., Chou, A., Frostig, R., and Liang, P. Semantic Parsing on Freebase from Question-Answer Pairs. In Yarowsky, D., Baldwin, T., Korhonen, A., Livescu, K., and Bethard, S. (eds.), *Proceedings of the 2013 Conference on Empirical Methods in Natural Language Processing*, pp. 1533–1544, Seattle, Washington, USA, October 2013. Association for Computational Linguistics. URL <https://aclanthology.org/D13-1160/>.
- Blackwell, D. Equivalent comparisons of experiments. *The Annals of Mathematical Statistics*, 24(2):265–272, 1953.
- Chen, Q. and Zhou, M. A neural framework for retrieval and summarization of source code. In *Proceedings of the 33rd ACM/IEEE International Conference on Automated Software Engineering*, pp. 826–831, Montpellier France, September 2018. ACM. ISBN 978-1-4503-5937-5. doi: 10.1145/3238147.3240471. URL <https://dl.acm.org/doi/10.1145/3238147.3240471>.
- Dietterich, T. G. Hierarchical Reinforcement Learning with the MAXQ Value Function Decomposition. *Journal of Artificial Intelligence Research*, 13:227–303, November 2000. ISSN 1076-9757. doi: 10.1613/jair.639. URL <https://www.jair.org/index.php/jair/article/view/10266>.
- Dong, L. and Lapata, M. Language to Logical Form with Neural Attention, June 2016. URL <http://arxiv.org/abs/1601.01280>. arXiv:1601.01280 [cs].
- Gao, L., Madaan, A., Zhou, S., Alon, U., Liu, P., Yang, Y., Callan, J., and Neubig, G. Pal: Program-aided language models. In *International Conference on Machine Learning*, pp. 10764–10799. PMLR, 2023.
- Garg, S., Tsipras, D., Liang, P. S., and Valiant, G. What can transformers learn in-context? a case study of simple function classes. *Advances in neural information processing systems*, 35:30583–30598, 2022.
- Graves, A., Wayne, G., and Danihelka, I. Neural Turing Machines, December 2014. URL <http://arxiv.org/abs/1410.5401>. arXiv:1410.5401 [cs].
- Graves, A., Wayne, G., Reynolds, M., Harley, T., Danihelka, I., Grabska-Barwińska, A., Colmenarejo, S. G., Grefenstette, E., Ramalho, T., Agapiou, J., Badia, A. P., Hermann, K. M., Zwols, Y., Ostrovski, G., Cain, A., King, H., Summerfield, C., Blunsom, P., Kavukcuoglu, K., and Hassabis, D. Hybrid computing using a neural network with dynamic external memory. *Nature*, 538(7626):471–476, October 2016. ISSN 0028-0836, 1476-4687. doi: 10.1038/nature20101. URL <https://www.nature.com/articles/nature20101>.
- Han, S., Schoelkopf, H., Zhao, Y., Qi, Z., Riddell, M., Zhou, W., Coady, J., Peng, D., Qiao, Y., Benson, L., Sun, L., Wardle-Solano, A., Szabo, H., Zubova, E., Burtell, M., Fan, J., Liu, Y., Wong, B., Sailor, M., Ni, A., Nan, L., Kasai, J., Yu, T., Zhang, R., Fabbri, A. R., Kryscinski, W., Yavuz, S., Liu, Y., Lin, X. V., Joty, S., Zhou, Y., Xiong, C., Ying, R., Cohan, A., and Radev, D. FOLIO: Natural Language Reasoning with First-Order Logic, October 2024. URL <http://arxiv.org/abs/2209.00840>. arXiv:2209.00840 [cs].
- Hudson, D. A. and Manning, C. D. Compositional Attention Networks for Machine Reasoning, April 2018. URL <http://arxiv.org/abs/1803.03067>. arXiv:1803.03067 [cs].
- Hupkes, D., Dankers, V., Mul, M., and Bruni, E. Compositionality decomposed: how do neural networks generalise?, February 2020. URL <http://arxiv.org/abs/1908.08351>. arXiv:1908.08351 [cs].
- Ibarz, B., Kurin, V., Papamakarios, G., Nikiforou, K., Ben-nani, M., Csordás, R., Dudzik, A. J., Bošnjak, M., Vitvitskiy, A., Rubanova, Y., Deac, A., Bevilacqua, B., Ganin, Y., Blundell, C., and Veličković, P. A Generalist Neural Algorithmic Learner. In *Proceedings of the First Learning on Graphs Conference*, pp. 2:1–2:23. PMLR, December 2022. URL <https://proceedings.mlr.press/v198/ibarz22a.html>. ISSN: 2640-3498.

- Kolter, J., Abbeel, P., and Ng, A. Hierarchical Apprenticeship Learning with Application to Quadruped Locomotion. In *Advances in Neural Information Processing Systems*, volume 20. Curran Associates, Inc., 2007. URL https://proceedings.neurips.cc/paper_files/paper/2007/hash/54a367d629152b720749e187b3ea11b-Abstract.html.
- Krishnamurthy, J., Dasigi, P., and Gardner, M. Neural Semantic Parsing with Type Constraints for Semi-Structured Tables. In Palmer, M., Hwa, R., and Riedel, S. (eds.), *Proceedings of the 2017 Conference on Empirical Methods in Natural Language Processing*, pp. 1516–1526, Copenhagen, Denmark, September 2017. Association for Computational Linguistics. doi: 10.18653/v1/D17-1160. URL <https://aclanthology.org/D17-1160/>.
- Lyu, Q., Havaladar, S., Stein, A., Zhang, L., Rao, D., Wong, E., Apidianaki, M., and Callison-Burch, C. Faithful chain-of-thought reasoning. In *The 13th International Joint Conference on Natural Language Processing and the 3rd Conference of the Asia-Pacific Chapter of the Association for Computational Linguistics (IJCNLP-AACL 2023)*, 2023.
- Mahdavi, S., Swersky, K., Kipf, T., Hashemi, M., Thrampoulidis, C., and Liao, R. Towards Better Out-of-Distribution Generalization of Neural Algorithmic Reasoning Tasks, March 2023. URL <http://arxiv.org/abs/2211.00692>. arXiv:2211.00692 [cs].
- Marra, G., Giannini, F., Diligenti, M., and Gori, M. Integrating Learning and Reasoning with Deep Logic Models, January 2019. URL <http://arxiv.org/abs/1901.04195>. arXiv:1901.04195 [cs].
- Merrill, W. and Sabharwal, A. The expressive power of transformers with chain of thought. *arXiv preprint arXiv:2310.07923*, 2023.
- Merrill, W. and Sabharwal, A. The Expressive Power of Transformers with Chain of Thought, April 2024. URL <http://arxiv.org/abs/2310.07923>. arXiv:2310.07923 [cs].
- Olausson, T. X., Gu, A., Lipkin, B., Zhang, C. E., Solar-Lezama, A., Tenenbaum, J. B., and Levy, R. LINC: A Neurosymbolic Approach for Logical Reasoning by Combining Language Models with First-Order Logic Provers. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pp. 5153–5176, 2023. doi: 10.18653/v1/2023.emnlp-main.313. URL <http://arxiv.org/abs/2310.15164>. arXiv:2310.15164 [cs].
- Pan, L., Albalak, A., Wang, X., and Wang, W. Y. Logiclm: Empowering large language models with symbolic solvers for faithful logical reasoning. *arXiv preprint arXiv:2305.12295*, 2023.
- Parisi, A., Zhao, Y., and Fiedel, N. TALM: Tool Augmented Language Models, May 2022. URL <http://arxiv.org/abs/2205.12255>. arXiv:2205.12255 [cs].
- Poggio, T., Mhaskar, H., Rosasco, L., Miranda, B., and Liao, Q. Why and when can deep-but not shallow-networks avoid the curse of dimensionality: a review. *International Journal of Automation and Computing*, 14(5):503–519, 2017.
- Puri, R., Kung, D. S., Janssen, G., Zhang, W., Domeniconi, G., Zolotov, V., Dolby, J., Chen, J., Choudhury, M., Decker, L., Thost, V., Buratti, L., Pujar, S., Ramji, S., Finkler, U., Malaika, S., and Reiss, F. CodeNet: A Large-Scale AI for Code Dataset for Learning a Diversity of Coding Tasks, August 2021. URL <http://arxiv.org/abs/2105.12655>. arXiv:2105.12655 [cs].
- Qin, Y., Liang, S., Ye, Y., Zhu, K., Yan, L., Lu, Y., Lin, Y., Cong, X., Tang, X., Qian, B., Zhao, S., Hong, L., Tian, R., Xie, R., Zhou, J., Gerstein, M., Li, D., Liu, Z., and Sun, M. ToolLLM: Facilitating Large Language Models to Master 16000+ Real-world APIs, October 2023. URL <http://arxiv.org/abs/2307.16789>. arXiv:2307.16789 [cs].
- Reed, S. and Freitas, N. d. Neural Programmer-Interpreters, February 2016. URL <http://arxiv.org/abs/1511.06279>. arXiv:1511.06279 [cs].
- Risko, E. F. and Gilbert, S. J. Cognitive Offloading. *Trends in Cognitive Sciences*, 20(9):676–688, September 2016. ISSN 13646613. doi: 10.1016/j.tics.2016.07.002. URL <https://linkinghub.elsevier.com/retrieve/pii/S1364661316300985>.
- Schick, T., Dessì, J. D.-Y. R., Raileanu, R., Lomeli, M., Zettlemoyer, L., Cancedda, N., and Scialom, T. Toolformer: Language Models Can Teach Themselves to Use Tools.
- Schneider, W. and Chein, J. M. Controlled & automatic processing: behavior, theory, and biological mechanisms. *Cognitive Science*, 27(3): 525–559, May 2003. ISSN 0364-0213, 1551-6709. doi: 10.1207/s15516709cog2703.8. URL https://onlinelibrary.wiley.com/doi/10.1207/s15516709cog2703_8.
- Shen, Z. LLM With Tools: A Survey, September 2024. URL <http://arxiv.org/abs/2409.18807>. arXiv:2409.18807 [cs].

- Shin, R. and Durme, B. V. Few-Shot Semantic Parsing with Language Models Trained On Code, May 2022. URL <http://arxiv.org/abs/2112.08696>. arXiv:2112.08696 [cs].
- Tang, Q., Deng, Z., Lin, H., Han, X., Liang, Q., Cao, B., and Sun, L. ToolAlpaca: Generalized Tool Learning for Language Models with 3000 Simulated Cases, September 2023. URL <http://arxiv.org/abs/2306.05301>. arXiv:2306.05301 [cs].
- Veličković, P. and Blundell, C. Neural algorithmic reasoning. *Patterns*, 2(7):100273, July 2021. ISSN 26663899. doi: 10.1016/j.patter.2021.100273. URL <https://linkinghub.elsevier.com/retrieve/pii/S2666389921000994>.
- Wei, J., Wang, X., Schuurmans, D., Bosma, M., Xia, F., Chi, E., Le, Q. V., Zhou, D., et al. Chain-of-thought prompting elicits reasoning in large language models. *Advances in neural information processing systems*, 35:24824–24837, 2022.
- Xie, S. M., Raghunathan, A., Liang, P., and Ma, T. An explanation of in-context learning as implicit bayesian inference. *arXiv preprint arXiv:2111.02080*, 2021.
- Yan, Y., Swersky, K., Koutra, D., Ranganathan, P., and Hashemi, M. Neural Execution Engines: Learning to Execute Subroutines, October 2020. URL <http://arxiv.org/abs/2006.08084>. arXiv:2006.08084 [cs].
- Zelikman, E., Wu, Y., Mu, J., and Goodman, N. D. STaR: Bootstrapping Reasoning With Reasoning, May 2022. URL <http://arxiv.org/abs/2203.14465>. arXiv:2203.14465 [cs].
- Zhang, R., Frei, S., and Bartlett, P. L. Trained transformers learn linear models in-context. *Journal of Machine Learning Research*, 25(49):1–55, 2024.