

Algorithmic Thinking Theory

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Abstract

Large language models (LLMs) have proven to be highly effective for solving complex reasoning tasks. Surprisingly, their capabilities can often be improved by iterating on previously generated solutions. In this context, a reasoning plan for generating and combining a set of solutions can be thought of as an algorithm for reasoning using a probabilistic oracle.

We introduce a theoretical framework for analyzing such reasoning algorithms. This framework formalizes the principles underlying popular techniques for iterative improvement and answer aggregation, providing a foundation for designing a new generation of more powerful reasoning methods.

Unlike approaches for understanding models that rely on architectural specifics, our model is grounded in experimental evidence. As a result, it offers a general perspective that may extend to a wide range of current and future reasoning oracles.

Keywords: LLM post-training, algorithmic reasoning, inference-time scaling

1. Introduction

The rapid advancement of large language models (LLMs) has marked a paradigm shift in artificial intelligence. Today’s models achieve strong performance across a wide range of language benchmarks and show impressive capability on complex reasoning tasks (Ahn et al., 2024; Yan et al., 2025). As a result, benchmarks that used to define the frontier, such as grade-school mathematics (GSM8k) and standard competition math (the MATH dataset), have largely been surmounted. Attention is therefore shifting toward “grand challenge” problems that demand deep insight, creativity, and rigorous proof, such as those from the International Mathematical Olympiad (IMO).

These problems also expose a striking weakness in current LLMs. While a model’s performance on a single attempt ($pass@1$) may be very low, its ability to produce a correct solution within k attempts ($pass@k$) can be substantially higher. This $pass@1$ versus $pass@k$ gap, often most pronounced when sampling at high temperature to produce diverse outputs, suggests that models possess substantial latent capability that is not reliably accessible by a single, high-confidence generation. This discrepancy has motivated a growing family of inference-time reasoning methods that leverage additional *test-time compute* to boost accuracy (Huang and Yang, 2025; Venkatraman et al., 2025).

In this article, we initiate the theoretical study of such *algorithmic thinking* procedures. Our aim is to formalize multi-call reasoning pipelines as algorithms and to understand, under explicit assumptions, what improvements are achievable with a fixed budget of model calls. Concretely, we ask: given a budget of oracal calls, what success probability is achievable, and what algorithmic structures are the most efficient?

To make these questions precise, we model a reasoning pipeline as an algorithm interacting with a probabilistic *reasoning oracle*. The oracle takes as input a context C of previously generated solutions, and outputs a new solution s . The oracle’s behavior is summarized by a *transfer function* \mathcal{F} that maps the (multi)set of solution qualities in C to a distribution over the quality of the output. This abstraction captures common empirical techniques as special cases: $pass@1$ corresponds to calling the oracle with empty context, i.e., $\mathcal{F}(\emptyset)$; the $pass@1$ versus $pass@k$ gap is captured by the improvement $\mathcal{F}(C) > \mathcal{F}(\emptyset)$ when C contains k solutions sampled from $\mathcal{F}(\emptyset)$. More complex procedures, such as Recursive Self-Aggregation (RSA) (Venkatraman et al., 2025), can be modeled as an algorithm that iteratively construct contexts from past outputs and repeatedly query the oracle.

This framework allows us to move from empirical observation to theoretical analysis. We study three families of reasoning algorithms. The Branching Algorithm (Algorithm 1) models tree-like synthesis by repeatedly combining independently generated solutions across multiple rounds. The Genetic Algorithm (Algorithm 2) is a more compute-efficient population-based variant that reuses solutions across rounds, directly mirroring the evolutionary approach of RSA (Venkatraman et al., 2025). Finally, the Random Sampling Algorithm (Algorithm 3) forms each context by reusing a random subset of all previously generated solutions.

Our central analysis is driven by a monotonicity principle (Definition 9): better contexts should (in a formal, stochastic sense) lead to better outputs. We introduce and study the class of Decaying Models (Definition 1), in which the success probability depends only on whether the context contains at least one correct solution and on the context size $|C|$, and decays as context size grows. This class captures an experimentally motivated phenomenon: providing more context can eventually hurt, as overly long contexts may degrade oracle performance. We further analyze special cases, including the Uniform Model (Definition 2) and models with explicit degradation behavior as context size increases (Definitions 3 and 4).

We believe that a theoretical understanding of reasoning algorithms can do more than explaining existing heuristics: it can yield quantitative guidance for allocating test-time compute and, ultimately, contribute to inference-time scaling laws governing the trade-offs between additional sampling, reuse, and synthesis.

1.1. Overview of contributions

Framework. We formalize inference-time reasoning as an algorithm that adaptively queries a probabilistic oracle \mathcal{A} with contexts of previously generated solutions from a solution space \mathcal{S} . The transfer function \mathcal{F} captures how context composition alters the distribution of subsequent outputs, subsuming $pass@1/pass@k$ and iterative aggregation methods within a single abstraction.

Models. We focus our initial study on Decaying Models, where success probability depends only on (i) whether the context contains a correct solution, and (ii) the context length $|C|$. For this class, we characterize the maximum success probability achievable by any reasoning algorithm and analyze convergence behavior for natural algorithm families. We additionally study concrete special cases: (1) a simple step model that success with probability $q > p$ whenever the context contains

a correct solution and $|C| \leq k$ (Definition 2); and (2) models in which the success probability is a function decaying with $|C|$, including exponential and polynomial decay (Definitions 3 and 4).

Algorithms and optimality. We analyze three reasoning algorithms: the Branching Algorithm, the Genetic Algorithm, and the Random Sampling Algorithm. We establish guarantees for their success probability under Decaying Models. In particular, we characterize the *optimal success probability* that any reasoning algorithm can achieve for a family of models, and prove that all three algorithms attain this optimal success probability in the unbounded-compute limit (Section 4 and Appendix A).

Efficiency Beyond characterizing the limit, we also perform convergence analysis on how quickly each algorithm approaches the limit (Appendix B). We study the two special cases (Uniform Model, specific Decaying Models) in (Appendices C and D). We find that in several cases, the required number of calls to achieve near-optimal success probability is of order $1/p$, where p is the baseline success probability under an empty-context call. In our basic setting, $1/p$ is also an information-theoretic lower bound on the number of calls needed to obtain even a single correct solution among all generated solutions.

1.2. Related work

To recover the full power of reasoning algorithms, it is not sufficient to simply increase k and rely on *pass@k*-style sampling: on the most difficult problems, simply sampling k times and selecting the best answer (e.g., “best-of-32”) still yields poor results. For instance, Huang and Yang (2025) report that a best-of-32 baseline on the IMO 2025 problems achieved an accuracy of only 31.6–38.1% for leading models (Huang and Yang, 2025). This paradox lies at the heart of our work: the latent capability of LLMs is not merely a matter of *selection* (finding one correct needle in a haystack of k attempts), but one of *synthesis*. While established techniques like Self-Consistency (Wang et al., 2023) leverage majority voting to improve reliability, they remain bound by the quality of individual samples. The “deep” reasoning ability of the model appears to be distributed across multiple, diverse, and often individually flawed chains of thought (Wei et al., 2022).

This shift highlights a growing focus on scaling inference-time compute—leveraging more computational resources *after* training to boost performance on hard tasks. These algorithms effectively simulate a “System 2” reasoning process atop the base model’s “System 1” generations (Kahneman, 2011), iteratively refining and synthesizing information to reach conclusions that are unreachable in a single forward pass. While empirical results show this works, we lack a formal theory governing the efficient allocation of this test-time budget. Existing theoretical work often focuses on the expressivity of standard Transformer forward passes, leaving the dynamics of these iterative, multi-call reasoning systems unexplored.

While our theoretical understanding of LLMs reasoning is still limited, the hypothesis that the ability to synthesize is a key ingredient in LLMs success is strongly backed by recent empirical breakthroughs. Work such as *Reflexion* (Shinn et al., 2023) demonstrated the value of verbal reinforcement for iterative improvement, while Huang and Yang (2025) showed that a similar model-agnostic, multi-stage “verification and refinement pipeline” can achieve a stunning 85.7% accuracy (5 out of 6 problems) on the same IMO 2025 dataset (Huang and Yang, 2025). Explicitly showing that a complex reasoning procedure—which iteratively generates, improves, verifies, and refines a solution—is able to harness the model’s latent abilities to achieve a result far beyond what simple

sampling could. Earlier structured approaches like *Tree of Thoughts* (Yao et al., 2023) attempted to harness latent reasoning by framing it as a search over intermediate steps. While effective for moderate complexity, grand challenge problems have required even more involved, iterative pipelines.

A similar, complementary approach is proposed by Venkatraman et al. (2025) with their “Recursive Self-Aggregation” (RSA) algorithm (Venkatraman et al., 2025). Inspired by evolutionary methods, RSA maintains a *population* of candidate solutions. In each step, it refines this population by “aggregating” subsets of solutions, prompting the model to combine their useful ideas and produce a new, improved generation. RSA is shown to “enable bootstrapping from partially correct intermediate steps within different chains of thought” (Venkatraman et al., 2025). Again, this demonstrates a mechanism for *synthesis*, not selection.

These empirical successes present a clear theoretical gap. We have powerful, practical examples of “reasoning algorithms”—like the IMO pipeline or RSA—that unlock performance far exceeding a model’s baseline. Yet, we lack a formal theory to understand *why* they work and *how* to design them. What properties of an LLM (as a “reasoning oracle”) make aggregation and refinement effective? How do we model the trade-off between parallel branching (like RSA) and sequential depth (like the IMO pipeline)? Early theoretical work focused on the expressivity of the architecture, proving that Transformers are universal approximators of sequence-to-sequence functions, meaning they can theoretically model any such function as the number of parameters approaches infinity (Yun et al., 2020). Since then, there have been various proposals for understanding the experimentally observed benefit of providing context.

A leading theoretical approach explains in-context learning (ICL) as an algorithmic mechanism called “Induction Heads.” These are 2-layer circuits that allow the model to copy and complete patterns from the context (Olsson et al., 2022). Another major theoretical angle formalizes ICL as an algorithm learning problem, where the Transformer implicitly constructs a hypothesis function at inference time (Li et al., 2023). Theoretical work has shown that Transformers trained by gradient flow can provably learn classes of linear models in-context (Garg et al., 2022).

Recent work has moved beyond showing Chain-of-Thought (CoT) helps to proving it is theoretically required for certain classes of problems. A recent, pivotal study proved rigorous separation results, showing that bounded-depth Transformers cannot directly solve basic arithmetic or linear equations unless their size grows super-polynomially. However, with CoT (autoregressive intermediate steps), they can solve these, effectively allowing them to handle problems up to P-complete (like dynamic programming) (Feng et al., 2024). Newer theoretical frameworks have derived scaling laws for an “optimal” CoT length, proving that while CoT is necessary, excessively long chains are susceptible to noise and error accumulation (“overthinking”) (Zhang et al., 2025). In our model, we explain this behavior as the context becoming increasingly correlated and therefore providing less value.

Another line of complexity theoretic work established that both Transformers and SSMs generally fall into the TC0 computational complexity class (Sarraf et al., 2024). Despite being in the same broad class, they have distinct theoretical strengths. Transformers are provably better at state tracking and copying from long history (due to their ability to attend to any previous state), while SSMs excel at different types of structured state tracking without needing a full history cache.

Finally, recent work models grokking as a phase transition where the network shifts from a high-complexity “memorization” phase to a low-complexity “generalization” phase, effectively compressing the data (Kumar and Nanda, 2024). More recent studies have begun linking this strictly

to internal mechanisms, such as the evolution of routing pathways in Mixture of Experts (MoE) models during pretraining (Li et al., 2025).

1.3. Roadmap

Section 2 introduces notation and formalizes our framework, including the Decaying Model family. Section 3 presents the reasoning algorithms studied in this article: Branching Algorithm, Genetic Algorithm, and Random Sampling Algorithm. Section 4 characterizes the optimal success probability achievable by any reasoning algorithm for a large family of models satisfying suitable monotonicity assumptions, and show that our algorithm attains the optimum (except for the Random Sampling algorithm, which is deferred to Appendix A). Section 5 discusses directions for extending the framework beyond binary correctness to leverage partial solutions.

Appendix B establishes the convergence rate for the algorithms to achieve the optimal success probability. In Appendices C and D, we further study the Uniform Model and specific Decaying Models, respectively. Appendix E provides experimental evidence to ground our modeling choices.

2. Preliminaries

Notations. We let $\log(\cdot)$ refer to the natural logarithm and $[n] = \{1, \dots, n\}$. $\mathbb{N} = \mathbb{Z}_{\geq 0}$ denotes the set of non-negative integers.

Question. Throughout the article, we fix a question Q which we seek to answer.

Solution space and quality. Let \mathcal{S} be the space of possible solutions of question Q and $\mathcal{V} \subseteq \mathbb{R}$ denote the space of possible quality scores. We associate with \mathcal{S} a scoring function $\text{score} : \mathcal{S} \rightarrow \mathcal{V}$. For every solution $s \in \mathcal{S}$, the value $\text{score}(s)$ assesses to what extent solution s answers question Q . A reasoning algorithm does not have access to the function score . In this article, we will focus on $\mathcal{V} = \{0, 1\}$, i.e., the scoring function where every solution has a binary score.¹

Reasoning oracle. To produce answers to question Q , we will exclusively use an oracle \mathcal{A} . This oracle is a randomized algorithm that given context $C \subseteq \mathcal{S}$ samples a solution $s \in \mathcal{S}$. The distribution from which the oracle samples depends only on the quality of the solutions in C .

We assume that the distribution of the score of the output of the oracle depends only on the multiset of scores in the context C , in the following way. Let $\mathcal{M}(\mathcal{V})$ denote the set of all finite multisets with elements in \mathcal{V} , and $\mathcal{P}(\mathcal{V})$ denote the set of distributions over \mathcal{V} . We assume there exists a transfer function $\mathcal{F} : \mathcal{M}(\mathcal{V}) \rightarrow \mathcal{P}(\mathcal{V})$ such that the distribution of the score of the output of the oracle on context C is given by $\mathcal{F}(\{\text{score}(s) : s \in C\}_{\text{multiset}})$. In particular, $\mathcal{F}(\emptyset)$ denotes the distribution of scores when the oracle is called with an empty context. We further assume that the probability of obtaining a correct solution monotonically increases with the number of correct solutions in a fixed-size multiset.

We remark that the transfer function depending only on the correctness of solutions is an abstraction of reality for the sake of simplicity. While it is interesting to study transfer functions that depend on more complicated properties of solutions, we believe that many phenomena can already be studied in this simple case.

1. While we adopt a binary scoring function to enable a simple convergence analysis and experiments, we acknowledge that this is a simplification of complex reasoning tasks where ‘partial credit’—reflecting valid intermediate lemmas or correct methodology despite a wrong final answer—often drives the discovery process.

Reasoning algorithm. An (\mathcal{A}, n) -reasoning algorithm is a procedure that calls the oracle \mathcal{A} at most n times to output a solution s . The goal is to maximize the expected score $\mathbb{E}[\text{score}(s)]$ of the final output s . If $\mathcal{V} = \{0, 1\}$, then we say a reasoning algorithm succeeds if $\text{score}(s) = 1$.

In general, a reasoning algorithm has the form (S_1, \dots, S_n) , where $S_k \subseteq [k-1]$ indicates the previous outputs used as context for the k -th oracle call. That is, for $k = 1, \dots, n$, the algorithm calls the oracle \mathcal{A} with context $\{s_i : i \in S_k\}_{\text{multiset}}$ to obtain s_k . We remark that reasoning oracles can (and often will) be randomized. Therefore, the inputs S_i should be viewed as random variables.

We can represent a reasoning algorithm as a DAG with n nodes, where each node corresponds to an oracle call, and there is a directed edge from node i to node j if $i \in S_j$. The n -th node corresponds to the final output of the algorithm. We define the *depth* of an algorithm as the length (number of edges) of the longest paths in its DAG representation. The depth captures the inference time of the reasoning algorithm, assuming infinite parallelism.

Answer population. If the image of the score function is $\{0, 1\}$, then we call a subset $S \subset \mathcal{S}$ a p -correct answer population if at least a p fraction of the elements in S have score 1. For the rest of the article, we let $\mathcal{V} = \{0, 1\}$.²

Decaying Model. Most of our results focus on a class of models called the decaying model, defined as follows.

Definition 1 (Decaying Model) Let $\mathcal{V} = \{0, 1\}$. Let $f : \mathbb{N} \rightarrow [0, 1]$ and $g : \mathbb{N} \rightarrow [0, 1]$ be two functions satisfying $f(k) \geq g(k)$ for all $k \in \mathbb{N}$. The decaying model $\mathcal{A}^{(f,g)}$ is defined as the oracle satisfying for any context $C \subseteq \mathcal{S}$:

$$\Pr[\text{score}(\mathcal{A}^{(f,g)}(C)) = 1] = \begin{cases} f(|C|), & \text{if } \sum_{s \in C} \text{score}(s) \geq 1, \\ g(|C|), & \text{if } \sum_{s \in C} \text{score}(s) = 0. \end{cases}$$

We note that the functions f and g are typically monotonically decreasing, which motivates the nomenclature. For this decaying model, we are able to give a precise characterization of the optimal success probability achievable by reasoning algorithms (see [Section 4](#)).

Next, we introduce several special cases of the decaying model.

Uniform Model. The uniform model is the special case of the decaying model where $f(i) = q$ and $g(i) = p$ for all $i \in \mathbb{N}$ such that $i \leq k$.

Definition 2 (Uniform Model) Let $0 \leq p \leq q \leq 1$ and integer $k \geq 1$. For the uniform model $\mathcal{A}_u^{(p,q,k)}$, each call has $\text{score}(\mathcal{A}_u^{(p,q,k)}(C)) = 1$ independently with probability

$$p + (q - p) \mathbb{1} \left\{ \sum_{s \in C} \text{score}(s) \geq 1 \text{ and } |C| \leq k \right\}$$

and $\text{score}(\mathcal{A}_u^{(p,q,k)}) = 0$ otherwise.

If we remove the constraint $|C| \leq k$ in the definition, then the optimal strategy is to use all previous answers as context. We therefore limit the context size $|C|$ to be at most k in the definition of the uniform model.

2. We remark that some of the general results presented in [Section 4](#) apply to general sets \mathcal{V} .

Exponentially and Polynomially Decaying Models. When implementing the oracle with a large language model, we experimentally observe a slow decay in model accuracy as the context size increases. We therefore study models that capture this decay more explicitly.

We are particularly interested in two natural decay functions, exponential decay and polynomial decay.

Definition 3 (Exponential Decay) *Let $0 < p \leq q \leq 1$. The exponential decaying model is the decaying model $\mathcal{A}^{(f,g)}$ where $f(k) = q^{k-1}$ and $g(k) = p\mathbb{1}_{\{k=0\}}$.*

Definition 4 (Polynomial Decay) *Let $0 < p \leq q \leq 1$. The polynomial decaying model is the decaying model $\mathcal{A}^{(f,g)}$ where $f(k) = \frac{1}{k^q}$ and $g(k) = p\mathbb{1}_{\{k=0\}}$.*

3. Reasoning Algorithms

In this section, we introduce the reasoning algorithms we study in this article:

1. **Branching Algorithm (Algorithm 1):** A simple algorithm that merges independently generated solutions in a tree-like fashion. It achieves optimal success probability for a broad class of oracles.
2. **Genetic Algorithm (Algorithm 2):** A more efficient version of the branching algorithm that re-uses solutions to reduce the number of oracle calls. It approaches the branching algorithm as the population sizes grow.
3. **Random Sampling Algorithm (Algorithm 3):** An algorithm that generates new solutions by randomly sampling from all previously generated solutions. It also achieves the optimal success probability, and has better convergence rate in certain settings.

Branching algorithm. The branching algorithm assembles a solution by initially generating a set of $pass@1$ solutions without providing any context. We call such solutions level 0 solutions. Then, it builds a tree obtaining a set of level i solutions via combining groups of k_i solutions from level $i - 1$ until it creates a single level L solution. See Algorithm 1 for pseudocode of this algorithm.

Algorithm 1: BRANCHINGALGORITHM($\mathcal{A}, L, (k_1, \dots, k_L)$)

```

if  $L = 0$  then
  | return  $\mathcal{A}(\emptyset)$ 
end
 $C \leftarrow \emptyset$ 
for  $j \in 1, \dots, k_L$  do
  |  $C \leftarrow C \cup \{\text{BRANCHINGALGORITHM}(\mathcal{A}, L - 1, (k_1, \dots, k_{L-1}))\}$ 
end
return  $\mathcal{A}(C)$ 

```

From this construction, we observe that all solutions generated by this algorithm are completely independent, and that therefore the solutions at level i also have to have the same guarantees. We conclude that all the solutions at level i have the same success probability, and that any reasonable algorithm increases the success probability of the solutions over time (See Section 4).

Genetic Algorithm. While the branching algorithm achieves the best possible success probability for a broad class of oracles (Proposition 14), it exponentially grows the number of solutions with the depth L . This quickly blows up the necessary computational resources. Therefore, genetic algorithms are often used in practice (Venkatraman et al., 2025). These follow the template from Algorithm 1, but reuse solutions from level $i - 1$ to avoid branching. Concretely, they have a fixed population size for layer i , and each solution at layer $i > 0$ is created by sampling k_i solutions from layer $i - 1$ uniformly at random with replacement. See Algorithm 2 for pseudocode of the algorithm and note that the population sizes (s_1, \dots, s_L) are an additional input. We observe that this algorithm approaches the branching algorithm as the population sizes go towards infinity.

Observation 5 *The genetic algorithm (Algorithm 2) approaches the branching algorithm (Algorithm 1) when $s_1, \dots, s_L \rightarrow \infty$ and $\frac{s_i}{s_{i+1}} \rightarrow \infty$ for $i = 1, \dots, L - 1$.*

Algorithm 2: GENETICALGORITHM($\mathcal{A}, L, (s_1, \dots, s_L), (k_1, \dots, k_L)$)

```

 $S_0 \leftarrow \emptyset$ 
for  $j = 1, \dots, s_1$  do
    |  $S_0 \leftarrow S_0 \cup \{\mathcal{A}(\emptyset)\}$ 
end
for  $i = 1, \dots, L - 1$  do
    |  $S_i \leftarrow \emptyset$ 
    | for  $j = 1, \dots, s_{i+1}$  do
    | | Let  $C$  consist of  $k_i$  i.i.d. uniformly sampled items from  $S_{i-1}$ 
    | |  $S_i \leftarrow S_i \cup \{\mathcal{A}(C)\}$ 
    | end
end
Let  $C$  consist of  $k_L$  i.i.d. uniformly sampled items from  $S_{L-1}$ 
return  $\mathcal{A}(C)$ 

```

In the following, we show that any branching algorithm can be turned into a genetic algorithm given access to a slightly stronger oracle in the case where every solution is either wrong or correct (i.e., $\mathcal{V} = \{0, 1\}$).

Recall the following standard Chernoff bound.

Theorem 6 (Chernoff bound, see e.g. (Mitzenmacher and Upfal, 2005)) *Suppose that X_1, \dots, X_n are i.i.d. random variables taking values in $\{0, 1\}$. Let $X = \sum_{i=1}^n X_i$ and $\mu = \mathbb{E}[X]$. Then*

$$\Pr[X \leq (1 - \epsilon)\mu] \leq e^{-\epsilon^2\mu/2}.$$

Definition 7 *We say oracle $\mathcal{A}'(\cdot)$ α -dominates oracle $\mathcal{A}(\cdot)$ if the success probability of $\mathcal{A}'(\cdot)$ is at least α times the success probability of oracle \mathcal{A} for some α and for all inputs to \mathcal{A} .*

Lemma 8 *Suppose an oracle $\mathcal{A}(\cdot)$, a parameter L and a vector (k_1, \dots, k_L) are given such that BRANCHINGALGORITHM($\mathcal{A}, i, (k_1, \dots, k_i)$) returns a solution s that is correct with probability p_i for each $1 \leq i \leq L$. Then, given an oracle \mathcal{A}' that $\frac{1}{1-\epsilon}$ dominates the oracle \mathcal{A} , GENETICALGORITHM($\mathcal{A}', L, (s_1, \dots, s_L), (k_1, \dots, k_L)$) returns a solution s' that is correct with probability at least p_L , provided that $s_i \geq -2 \log(\epsilon/L)/(p_{i-1}\epsilon^2)$ for each $1 \leq i \leq L$.*

Proof Next, we prove by induction that for each $0 \leq i \leq L$, the set S_i is a p_{i-1} -correct answer population with probability at least $1 - i \cdot \epsilon/L$.

For S_0 , we sample directly from an oracle which guarantees that the solutions are correct with probability $\frac{1}{1-\epsilon}p_0$. Therefore, $s_1 = -2 \log(\epsilon/L)/(p_0\epsilon^2)$ samples suffice with probability $1 - \epsilon/L$ by [Theorem 6](#). This concludes the base case.

Then, in the inductive step, we have that if S_{i-1} is a p_{i-2} -correct answer population with probability $1 - (i-1)\epsilon/L$ by induction. We assume that it is in fact a p_{i-2} -correct answer population, and then obtain that S_i is a p_{i-1} -correct answer population with probability $1 - \epsilon/L$ by [Theorem 6](#). The inductive step follows by a union bound.

From this, we obtain that S_L is a p_{L-1} -correct answer population with probability $1 - \epsilon$. If it is, then the output is correct with probability $\frac{1}{1-\epsilon}p_L$. The lemma follows. \blacksquare

Random Sampling Algorithm. The genetic algorithm samples solutions from the previous layer only. An alternative is to sample solutions from all previously generated solutions. This is the idea behind the random sampling algorithm, whose pseudocode is given in [Algorithm 3](#). We refer to [Appendix A](#) for the analysis of this algorithm.

Algorithm 3: RANDOMSAMPLINGALGORITHM(\mathcal{A}, n, k)

```

 $s_1 \leftarrow \mathcal{A}(\emptyset)$ 
for  $j = 2, \dots, n$  do
    | Let  $C$  consist of  $k$  i.i.d. uniformly sampled items from  $\{s_1, \dots, s_{j-1}\}$ 
    |  $s_j \leftarrow \mathcal{A}(C)$ 
end
return  $s_n$ 
    
```

4. Optimal Success Probability

In this section, we study the optimal success probability achievable by reasoning algorithms (without restrictions on the number of calls). We show that for decaying models, the algorithms introduced in [Section 3](#) achieve the optimal success probability as the number of calls goes to ∞ .

4.1. Monotonicity

In this section, we establish some general properties of reasoning oracles and algorithms. We study two versions of monotonicity and show that they have interesting consequences for the structure of an optimal algorithm.

Definition 9 (Monotonicity) *An oracle \mathcal{A} is called*

- weakly monotone if for any two multisets $A = \{a_1, \dots, a_k\}$, $B = \{b_1, \dots, b_k\}$ satisfying $a_i \leq b_i$ for all $i \in [k]$, we have $\mathcal{F}(A) \preceq \mathcal{F}(B)$, where \preceq denotes (first order) stochastic dominance (i.e., there is a monotone coupling between $\mathcal{F}(A)$ and $\mathcal{F}(B)$);
- strongly monotone if it is weakly monotone and for any two multisets A and B satisfying $A \subseteq B$ (as multisets), we have $\mathcal{F}(A) \preceq \mathcal{F}(B)$.

The following result shows that weak monotonicity implies an FKG inequality for the joint distribution of scores of solutions (Fortuin et al., 1971).

Lemma 10 *If an oracle \mathcal{A} is weakly monotone, then for any (\mathcal{A}, n) -reasoning algorithm (S_1, \dots, S_n) and any functions $f, g : \mathcal{V}^n \rightarrow \mathbb{R}$ that are both non-decreasing (or both non-increasing), we have*

$$\mathbb{E}[fg] \geq \mathbb{E}[f] \mathbb{E}[g].$$

Proof Let $v_i = \text{score}(s_i)$ for $i \in [n]$. Let (X_1, \dots, X_n) be i.i.d. samples from $\text{Unif}([0, 1])$. For every $j \in [n]$ and every possible combination of values $(v_i : i \in S_j)$, we can couple $\text{Unif}([0, 1])$ with $P_{v_j | (v_i : i \in S_j)}$ in an order-preserving way. In this way, we can construct an order-preserving coupling between (v_1, \dots, v_n) and (X_1, \dots, X_n) . So f, g can be lifted to non-decreasing (or non-increasing) functions $\tilde{f}, \tilde{g} : [0, 1]^n \rightarrow \mathbb{R}$ such that $f(v_1, \dots, v_n) = \tilde{f}(X_1, \dots, X_n)$ and $g(v_1, \dots, v_n) = \tilde{g}(X_1, \dots, X_n)$. The FKG inequality (Fortuin et al., 1971) implies that

$$\mathbb{E}[fg] = \mathbb{E}[\tilde{f}\tilde{g}] \geq \mathbb{E}[\tilde{f}] \mathbb{E}[\tilde{g}] = \mathbb{E}[f] \mathbb{E}[g].$$

■

Strong monotonicity, in addition to the above, implies that an optimal algorithm must use all available context size.

Lemma 11 *If an oracle \mathcal{A} is strongly monotone, then for any (\mathcal{A}, n) -reasoning algorithm, adding more solutions to the context of any oracle call never decreases the expected score of the final output.*

Proof For two (\mathcal{A}, n) -reasoning algorithms operating on contexts (S_1, \dots, S_n) and (S'_1, \dots, S'_n) respectively satisfying $S_i \subseteq S'_i$, we can construct a monotone coupling step by step between the distributions of $(\text{score}(s_1), \dots, \text{score}(s_n))$ and $(\text{score}(s'_1), \dots, \text{score}(s'_n))$. So adding more solutions to the context never hurts. ■

For the binary quality model considered in this article (i.e., $\mathcal{V} = \{0, 1\}$), the transfer function \mathcal{F} can be compactly represented by a function $F : \mathbb{N} \times \mathbb{N} \rightarrow [0, 1]$, where $F(a, b)$ is the probability that the oracle outputs a correct solution when the context contains a correct solutions and b incorrect solutions. With minor abuse of notation, we call F the transfer function as well.

A binary quality model is weakly monotone if and only if F satisfies $F(a+1, b) \geq F(a, b+1)$ for all $a, b \geq 0$. A binary quality model is strongly monotone if and only if F satisfies $F(a+1, b) \geq F(a, b+1) \geq F(a, b)$ for all $a, b \geq 0$. So we have the following corollary.

Corollary 12 (Monotonicity for binary quality models) *Consider a binary quality model with transfer function F .*

If $F(a+1, b) \geq F(a, b+1)$ for all $a, b \geq 0$, then for any (\mathcal{A}, n) -reasoning algorithm (S_1, \dots, S_n) and any functions $f, g : \{0, 1\}^n \rightarrow \mathbb{R}$ that are both non-decreasing (or both non-increasing), we have $\mathbb{E}[fg] \geq \mathbb{E}[f] \mathbb{E}[g]$.

If $F(a+1, b) \geq F(a, b+1) \geq F(a, b)$ for all $a, b \geq 0$, then for any (\mathcal{A}, n) -reasoning algorithm, adding more solutions to the context of any oracle call never decreases the expected score of the final output.

Proof Directly follows from Lemma 10 and Lemma 11. ■

4.2. Optimality of the branching algorithm

In the following, we show that for all decaying models, the branching algorithm achieves the maximum achievable success probability. The next lemma discusses solutions to a class of polynomial equations which arise in this study.

Lemma 13 *Let $p, q \in [0, 1]$ and $k \in \mathbb{N}$. Consider the equation $x = q - (1 - x)^k(q - p)$ and its solutions in $[0, 1]$.*

- When $k = 0$, the equation has a unique solution $x = p$.
- When $k = 1$ and $(p, q) \neq (0, 1)$, the equation has a unique solution $x = \frac{p}{1-q+p}$. If $k = 1$ and $(p, q) = (0, 1)$, every $x \in [0, 1]$ is a solution.
- When $k \geq 2$ and $p \geq q$, the equation has a unique solution in $[0, 1]$. When $k \geq 2$ and $0 < p < q$, the equation has a unique solution in $[0, 1]$. When $k \geq 2$, $p = 0$, and $kq \leq 1$, the equation has a unique solution 0 in $[0, 1]$. When $k \geq 2$, $p = 0$, and $kq > 1$, the equation has two solutions in $[0, 1]$, one of which is 0 and the other is in $(0, 1]$.

Proof Let $f(x) = x - q + (1 - x)^k(q - p)$. Then $f(0) = -p \leq 0$, and $f(1) = 1 - q \geq 0$. The $k = 0, 1$ cases follow directly. We therefore assume $k \geq 2$.

Suppose $p \geq q$. Then f is strictly increasing in $[0, 1]$, and there is a unique root in $[0, 1]$.

Suppose $p < q$. Then f is strictly convex in $[0, 1]$. When $p > 0$, there is a unique root in $[0, 1]$. When $p = 0$, 0 is a root, and $f'(0) = 1 - kq$. So when $kq \leq 1$, there is no root in $(0, 1]$; when $kq > 1$, there is a unique root in $(0, 1]$. ■

A decaying model is a binary quality model whose transfer function F satisfies $F(a + 1, b) = F(a, b + 1)$ for all $a \geq 1, b \geq 0$. We have $f(k) = F(k, 0)$ and $g(k) = F(0, k)$ for all $k \in \mathbb{N}$.

Proposition 14 (Optimality of branching algorithm) *Consider a decaying model.*

Let x_k^ be the largest solution in $[0, 1]$ to the equation $x = f(k) - (1 - x)^k(f(k) - g(k))$ (c.f. Lemma 13).*

Then the success probability of any (\mathcal{A}, n) -reasoning algorithm is at most $x^ = \sup_{k \geq 0} x_k^*$.*

Furthermore, if $g(0) > 0$, then for any $\epsilon > 0$, a branching algorithm (Algorithm 1) achieves success probability at least $x^ - \epsilon$.*

Proof We prove lower and upper bounds separately.

Upper bound. We let (S_1, \dots, S_n) be a given (\mathcal{A}, n) -reasoning algorithm. Further, let $v_i = \text{score}(s_i)$ for $i \in [n]$. Next, we prove by induction that $\Pr[v_i = 1] \leq x^*$ for all $i \in [n]$.

Fix any $m \in [n]$ and let $k_m = |S_m|$. We apply the induction hypothesis, and obtain that $\Pr[v_i = 0] \geq 1 - x^*$ for each $i \in S_m$. By Corollary 12, we obtain

$$\Pr[v_i = 0 \text{ for all } i \in S_m] = \mathbb{E} \left[\prod_i (1 - v_i) \right].$$

and conclude that $\Pr[v_i = 0 \text{ for all } j \in S_i] \geq (1 - x^*)^{k_m}$.

Then $\Pr[v_i] \leq f(k_m) - (1 - x^*)^{k_m}(f(k_m) - g(k_m)) \leq x^*$, where last step follows from the definition of x^* .

Lower bound. Choose k such that $x_k^* > x^* - \epsilon$. Consider the branching algorithm [Algorithm 1](#) with fan-in $k_i = k$ for all $i \in 1, \dots, L$. Since all the generated solutions at a particular level are independent, the success probability evolves according to the function whose fixed point we are searching. Then, it is easy to observe that the success probability monotonically increases across levels, and goes to x_k^* in the limit. ■

In fact, the branching algorithm achieves optimal success probability not only in the limit, but also among algorithms with fixed depth.

Proposition 15 (Optimality of branching algorithm for fixed-depth algorithms) *Work under the setting of [Proposition 14](#). Among algorithms with a fixed depth L , a branching algorithm with L levels achieves the maximum success probability.*

Proof Let $a_0 = g(0)$ and $a_i = \max_k (f(k) - (1 - a_{i-1})^k (f(k) - g(k)))$ for $i \geq 1$. Clearly, a depth- L branching algorithm can achieve success probability a_L . Furthermore, using the same induction as in the proof of [Proposition 14](#), we can show that any depth- L algorithm has success probability at most a_L . ■

These optimality results can be understood as meaning that independence between solutions is favored. In [Appendix C](#), we show that the natural algorithm that always passes the most recently generated solutions is not optimal because of these dependencies.

4.3. Optimality of the genetic algorithm

Via [Lemma 8](#), [Proposition 14](#) implies that the genetic algorithm also achieves optimal success probability.

Proposition 16 *Work under the setting of [Proposition 14](#). Fix $k \geq 1$ and $\epsilon > 0$. The Genetic Algorithm ([Algorithm 2](#)) with k -way branching achieves success probability at least $x_k^* - \epsilon$ for large enough L , where x_k^* is the unique solution of $x = f(k) - (f(k) - g(k))(1 - x)^k$ in $[0, 1]$.*

Proof Let \mathcal{A} denote the given oracle. Choose $\epsilon_1 > 0$ small enough such that the unique solution to $x(1 - \epsilon_1) = f(k) - (f(k) - g(k))(1 - x)^k$ in $[0, 1]$ is at least $x_k^* - \epsilon$. This means that there is a decaying model that is $1/(1 - \epsilon_1)$ dominated by \mathcal{A} such that the optimal success probability is at least $x_k^* - \epsilon$. Then [Lemma 8](#) shows that there is a genetic algorithm that achieves success probability at least $x_k^* - \epsilon$. ■

5. Discussion

This work takes a first step toward a theory of inference-time scaling by introducing an oracle-based framework. The framework is intentionally stylized, and the limitations point to natural next steps.

Limitations. Our analysis focuses on a binary notion of solution quality (correct/incorrect). This is restrictive for the hardest problems, where useful outputs are often partial progress that must be composed. Our models also compress the effect of context into a simple dependence on whether a correct solution is present and on context length; real systems likely depend on finer properties such as diversity of intermediate steps. Finally, our theory measures only success probability under a fixed number of oracle calls, and does not explicitly model costs such as wall-clock latency.

Future work. A primary direction is to extend the framework beyond binary correctness to graded quality measures and to explicit notions of diversity/complementarity, so that combining two partially correct solutions can be modeled and analyzed. Another direction is to incorporate cost models and study optimal allocations of a test-time budget across depth, branching, and reuse, including adaptive strategies that react to intermediate outcomes. More realistic oracle models should also be grounded empirically, for example by measuring how accuracy varies with context composition (not only length) and by isolating regimes where longer contexts help versus hurt. Ultimately, we hope this line of work contributes to inference-time scaling laws that predict how additional test-time compute should be spent for reliable reasoning.

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Appendix A. Optimality of the random sampling algorithm

In this section, we additionally show that the random sampling algorithm converges to the optimal success probability. The analysis of the random sampling algorithm relies on the theory of stochastic approximation [Duflo \(2013\)](#). We use the following classic result.

Theorem 17 ([\(Duflo, 2013, Theorem 2.2.12\)](#)) *Suppose $(X_n)_{n \geq 1}$ and $(Y_n)_{n \geq 1}$ are two sequences of random variables in \mathbb{R} that are adapted to a filtration $(\mathcal{F}_n)_{n \geq 1}$ and linked by the equation $X_{n+1} = X_n + \frac{1}{n}Y_{n+1}$. Suppose*

$$\begin{aligned}\mathbb{E}[Y_{n+1}|\mathcal{F}_n] &= f(X_n), \\ \mathbb{E}[(Y_{n+1} - f(X_n))^2|\mathcal{F}_n] &= \Gamma(X_n).\end{aligned}$$

In addition, suppose that the following holds for a finite constant K :

1. *f is a function of class C^2 such that*

$$\begin{aligned}f(x)^2 &\leq K(1 + x^2), \\ f(x^*) &= 0 \text{ and for } x \neq x^*, f(x)(x - x^*) < 0;\end{aligned}$$

2. *Γ is continuous in a neighborhood of x^* and $\Gamma(x) \leq K(1 + x^2)$;*
3. *There exists an $a > 0$ such that $\sup_n \mathbb{E}[|Y_{n+1} - f(X_n)|^{2+a}|\mathcal{F}_n] < \infty$.*

Then we have the following.

1. *$(X_n)_{n \geq 1}$ converges to x^* almost surely.*
2. *Let $\tau = -f'(x^*)$ and $\Gamma^* = \Gamma(x^*)$.*
 - (a) *If $\tau > 1/2$, then $\sqrt{n}(X_n - x^*)$ converges in distribution to $\mathcal{N}(0, \Gamma^*/(2\tau - 1))$.*
 - (b) *If $\tau = 1/2$, then $\sqrt{n/\log n}(X_n - x^*)$ converges in distribution to $\mathcal{N}(0, \Gamma^*)$.*
 - (c) *If $0 < \tau < 1/2$, then $n^\tau(X_n - x^*)$ converges almost surely to a finite random variable.*

Proposition 18 *Work under the setting of [Proposition 14](#). Fix $k \geq 1$ and $\epsilon > 0$. If $g(k) > 0$, then the Random Sampling Algorithm ([Algorithm 3](#)) with context size k achieves success probability at least $x_k^* - \epsilon$ for large enough n , where x_k^* is the unique solution of $x = f(k) - (f(k) - g(k))(1 - x)^k$ in $[0, 1]$.*

Proof Define X_t as the fraction of correct solutions in $\{s_1, \dots, s_t\}$. Then we have

$$X_{t+1} = X_t + \frac{1}{t+1}(-X_t + Y_t)$$

where $Y_t = 1$ with probability $f(k) + (f(k) - g(k))(1 - X_t)^k$ and $Y_t = 0$ otherwise. Define $h(x) = f(k) - (f(k) - g(k))(1 - x)^k - x$. Then we have

$$X_{t+1} = X_t + \frac{1}{t+1}(h(X_t) + Z_t)$$

where $Z_t = Y_t - \mathbb{E}[Y_t|X_t]$ is a martingale difference sequence with bounded variance.

To apply [Theorem 17](#), we need to verify that $h(x)(x - x_k^*) < 0$ for $x \neq x_k^*$. Note that $h(x)$ is concave on $[0, 1]$ and $h(0) = g(k) > 0$. So $h(x) > 0$ for $0 \leq x < x_k^*$ and $h(x) < 0$ for $x_k^* < x \leq 1$. Thus the condition holds.

By [Theorem 17](#), X_t converges almost surely to the unique root of $h(x) = 0$, which is exactly x_k^* . \blacksquare

Appendix B. Convergence Analysis

In this section, we analyze the convergence rate of different reasoning algorithms. For simplicity, we focus on uniform models, but our analysis can be extended to general decaying models as well.

We fix a uniform model $\mathcal{A}_u^{(p,q,k)}$ as defined in [Definition 2](#), where $0 < p < q < 1$ and integer $k \geq 1$. Let x^* be the unique solution in $[0, 1]$ of the equation $x = q - (q - p)(1 - x)^k$. By [Proposition 14](#), the optimal success probability of any reasoning algorithm using the oracle $\mathcal{A}_u^{(p,q,k)}$ converges to x^* as the number of steps goes to infinity.

B.1. Convergence analysis of the branching algorithm

Proposition 19 *The success probability of the branching algorithm ([Algorithm 1](#)) with L levels of k -way branching is $x^* - \left(k \frac{q-x^*}{1-x^*} \pm o(1)\right)^L$.*

In terms of the number of calls $n = k^L$, the success probability is $x^ - \epsilon_n$ where*

$$\lim_{n \rightarrow \infty} \frac{\log(1/\epsilon_n)}{\log n} = \frac{-\log\left(k \frac{q-x^*}{1-x^*}\right)}{\log k}.$$

Proof Define $f(x) = q - (q - p)(1 - x)^k$. Let x_j be the success probability after j levels of branching. We have $x_0 = p$ and $x_{j+1} = f(x_j)$ for all $j \geq 0$.

We have shown in [Proposition 14](#) that $x_j \rightarrow x^*$ as $j \rightarrow \infty$. The convergence rate is governed by $f'(x^*) = k(q - p)(1 - x^*)^{k-1} = k \frac{q-x^*}{1-x^*}$. By the proof of [Proposition 18](#), we have $0 < f'(x^*) < 1$. So $\lim_{j \rightarrow \infty} \frac{|x_{j+1} - x^*|}{|x_j - x^*|} = f'(x^*)$. Therefore, $|x_L - x^*| = (f'(x^*) \pm o(1))^L$. \blacksquare

B.2. Convergence analysis of the genetic algorithm

Proposition 20 *There exists a Genetic Algorithm ([Algorithm 2](#)) with k -way branching whose success probability $x^* - \epsilon_n$ (where n is the number of calls to the oracle) satisfies*

$$\lim_{n \rightarrow \infty} \frac{\log(1/\epsilon_n)}{\log n} = \frac{1}{2}.$$

Proof In the proof of [Proposition 16](#), we can take $\epsilon_1 = \Theta(\epsilon)$. Then by [Lemma 8](#), the number of calls in the genetic algorithm (which achieves error probability $x^* - \epsilon$) is $\epsilon_1^{-2 \pm o(1)} = \epsilon^{-2 \pm o(1)}$. \blacksquare

B.3. Convergence analysis of the random sampling algorithm

Proposition 21 *The success probability of the Random Sampling Algorithm (Algorithm 3) with context size k after n steps is $x^* - \epsilon_n$, where*

$$\lim_{n \rightarrow \infty} \frac{\log(1/\epsilon_n)}{\log n} = \min \left\{ 1/2, 1 - k \frac{q - x^*}{1 - x^*} \right\}.$$

Proof The result essentially follows from [Theorem 17](#).

Let $h(x) = q - (q - p)(1 - x)^k - x$ as in the proof of [Proposition 18](#). Then $\tau = -h'(x^*) = 1 - k \frac{q - x^*}{1 - x^*}$. We have $0 < \tau < 1$ by the proof of [Proposition 18](#). By [Theorem 17](#), the error decays polynomially in n with exponent $-\min\{1/2, \tau\}$. ■

Appendix C. Uniform Model

In this section, we consider the uniform model. We first recall its definition.

Definition 22 (Uniform Model) *Let $0 \leq p \leq q \leq 1$ and integer $k \geq 1$. For the uniform model $\mathcal{A}_u^{(p,q,k)}$, each call has $\text{score}(\mathcal{A}_u^{(p,q,k)}(C)) = 1$ independently with probability*

$$p + (q - p) \mathbb{1} \left\{ \sum_{s \in C} \text{score}(s) \geq 1 \text{ and } |C| \leq k \right\}$$

and $\text{score}(\mathcal{A}_u^{(p,q,k)}) = 0$ otherwise.

We remark that this corresponds to a very simple special case of the decaying model where $f(k)$ is a step function. Clearly, it is best to pass exactly k solutions to the context whenever k solutions are available. We first observe that the uniform model is strongly monotone, and therefore [Lemma 11](#) applies. Therefore, it is always better to add some extra solution that has been generated previously instead of passing less than k solutions to the oracle.

Observation 23 *In the uniform model with $q \geq p$, it is always beneficial to add k solutions to the context.*

Proof Follows directly from [Lemma 11](#) since the uniform oracle is strongly monotone [Definition 9](#). ■

From this, we immediately obtain that the maximum achievable success probability is the fixed point achieved when always adding k independently generated solutions.

Corollary 24 *The maximum achievable success probability of a $(\mathcal{A}_u^{(p,q)}, n)$ -reasoning algorithm with $q \geq p$ and maximum context length k is the unique solution of*

$$x = q + (p - q)(1 - x)^k$$

as $n \rightarrow \infty$.

Proof Directly follows from [Observation 23](#) and [Proposition 14](#) by reformulating. ■

The algorithm for achieving this probability may be quite inefficient in terms of the number of oracle calls for achieving a fixed probability. In the following, we show that introducing dependencies to reduce the number of oracle calls in fact reduces the achieved success probability. A very natural way to do so is to only consider recently generated solutions since any reasonable reasoning algorithm improves the quality of solutions over time.

First, we show that this is the case for $k = 2$ as a warm-up in [Claim 25](#). This proof can be seamlessly generalized to larger k , which we show in [Proposition 26](#).

Claim 25 (Warm-up) *The sliding window approach where the oracle is always called on the k most recently generated solutions achieves suboptimal performance for $k = 2$.*

Proof We can imagine this process as generating a sequence of solutions $\{s_i\}_{i=1,\dots,n}$, and we let $v_i = \text{score}(s_i)$. Then imagine being at some stage n . The only quantities that matter for the transfer function describing the distribution of v_{n+1} are v_n and v_{n-1} . We distinguish three states. The state is the smallest number i such that $v_{n-i} = 1$. If no such i exists, or $i \geq k$, the state is k . We then obtain the following transition matrix from the definition of the oracle.

$$W = \begin{pmatrix} q & q & p \\ 1 - q & 0 & 0 \\ 0 & 1 - q & 1 - p \end{pmatrix}^\top$$

We then compute the stationary distribution of this matrix. Solving the system $W^T \pi = \pi$ yields

$$\pi = \frac{1}{N} \begin{pmatrix} p \\ (1 - q)p \\ (1 - q)^2 \end{pmatrix}$$

where $N = p + (1 - q)p + (1 - q)^2$. We output the correct solution whenever we are in state 0, so the probability of returning a correct solution is given by p/N .

Now, given [Theorem 24](#) we aim to show that $p/N < q + (p - q)(1 - p/N)^2$. Reformulating yields

$$(p - q)^2(1 - q)^2 > 0$$

which is true whenever $q < 1$ and $p \neq q$. ■

Next, we generalize the previous claim to all k .

Proposition 26 *The sliding window approach where the oracle is always called on the k most recently generated solutions achieves suboptimal performance.*

Proof We again consider a sequence of solutions $\{s_i\}_{i=1,\dots,n}$ and let $v_i = \text{score}(s_i)$ for $i \in 1, \dots, n$. Then, for $0 \leq i \leq n$, $0 \leq j \leq n$, we let $x_{i,j}$ denote the probability that

$$j = \min\{k, \max\{a : v_i = \dots = v_{i-a+1} = 0\}\}.$$

Then, we have $x_{0,j} = \mathbb{1}_{j=k}$ and $x_{i+1,*} = x_{i,*}W$ where the transition matrix W is given by $W(k,0) = p$, $W(k,k) = 1 - p$, $W(i,0) = q$, $W(i,i+1) = 1 - q$ for $0 \leq i \leq k-1$ and W contains 0 entries everywhere else. So $x_{n,*} = x_{0,*}W^n$. We remark that this transition matrix is completely analogous to the warm-up for $k = 2$ presented in [Claim 25](#).

The stationary distribution π is given by $\pi(j) = C(1-q)^j$ for $0 \leq j \leq k-1$, $\pi(k) = C(1-q)^k/p$, where $C^{-1} = \sum_{0 \leq j \leq k-1} (1-q)^j + (1-q)^k/p = (1 - (1-q)^k)/q + (1-q)^k/p$. Since the algorithm succeeds whenever it is in state 0, the limiting success probability of the sliding window algorithm is equal to

$$\pi(0) = \left((1 - (1-q)^k)/q + (1-q)^k/p \right)^{-1}.$$

In general, this is not a solution to the equation $x = q + (p-q)(1-x)^k$. So the sliding window algorithm is not optimal for general k . ■

Therefore, even in this extremely simple model, correlations between the solutions are an issue, which motivates considering the branching and geometric algorithm. We remark that for certain decaying models (such as the exponential decaying model and the polynomial decaying model), the success probability of a sliding window algorithm goes to 0 as the number of steps goes to infinity because the context will eventually only contain wrong solutions. After this point, the oracle never generates a correct solution again. This can be seen as modeling the “overthinking” phenomenon observed in practice ([Zhang et al., 2025](#)).

Appendix D. Exponentially and Polynomially Decaying Models

Next, we analyze the exponentially and polynomially decaying models $\mathcal{A}_d^{(p,f)}$, which are a more realistic model that introduces a non-trivial dependency on the context size (See [Appendix E](#) for experimental results). We first recall the general model definition and then the exponentially and polynomially decaying special cases.

Definition 27 (Decaying Model) *Let $\mathcal{V} = \{0, 1\}$. Let $f : \mathbb{N} \rightarrow [0, 1]$ and $g : \mathbb{N} \rightarrow [0, 1]$ be two functions satisfying $f(k) \geq g(k)$ for all $k \in \mathbb{N}$. The decaying model $\mathcal{A}^{(f,g)}$ is defined as the oracle satisfying for any context $C \subseteq \mathcal{S}$:*

$$\Pr[\text{score}(\mathcal{A}^{(f,g)}(C)) = 1] = \begin{cases} f(|C|), & \text{if } \sum_{s \in C} \text{score}(s) \geq 1, \\ g(|C|), & \text{if } \sum_{s \in C} \text{score}(s) = 0. \end{cases}$$

Definition 28 (Exponential Decay) *Let $0 < p \leq q \leq 1$. The exponential decaying model is the decaying model $\mathcal{A}^{(f,g)}$ where $f(k) = q^{k-1}$ and $g(k) = p\mathbb{1}_{\{k=0\}}$.*

Definition 29 (Polynomial Decay) *Let $0 < p \leq q \leq 1$. The polynomial decaying model is the decaying model $\mathcal{A}^{(f,g)}$ where $f(k) = \frac{1}{k^q}$ and $g(k) = p\mathbb{1}_{\{k=0\}}$.*

Unlike the uniform setting, where it is always beneficial to pass as many solutions as possible in the context, a non-constant decay function $f(k)$ realizes a non-trivial trade-off. In the following, we explore the two decay functions that are arguably most natural, exponential and polynomial decay (See [Definition 3](#) and [Definition 4](#)). We sometimes write $\mathcal{A}^{(f,p)}$ when referring to the exponential and polynomial decay model with $g(k) = p\mathbb{1}_{\{k=0\}}$.

D.1. Exponential Decay

In this section, we examine exponential decay functions $e_q(k) = q^{k-1}$ (See [Definition 3](#)). These already lead to a non-trivial trade-off when selecting the context size. Due to the quick reduction in success probability, they encourage only combining a small amount of solutions.

A two-stage process. We first show how this trade-off is realized by examining the simple two-stage process $pass@k$. In the first stage, we assume we are given an algorithm that samples an arbitrarily sized collection of solutions, each of which is correct independently with some probability x . Then, we aim to select an optimal number of such solutions to put into the context for a single oracle call to maximize the probability of correctness of the generated solution. This corresponds to maximizing the success probability that a $pass@k$ algorithm can obtain.

Claim 30 *The optimal amount of independent solutions that are correct with probability x to pass to the oracle $\mathcal{A}_d^{(e_q, p)}$ for $x \geq p$ is*

$$\arg \max_{k \in \mathbb{N}_{\geq 0}} q^{k-1}(1 - (1 - x)^k) = \max \left(1, \left\lceil 1 + \frac{\log \left(\frac{1-q}{1-(1-x)q} \right)}{\log(1-x)} \right\rceil \right).$$

Proof Since passing a single solution yields success probability $x \geq p$ it is never beneficial to pass 0 solutions. We now analyze the function $g(k) \stackrel{\text{def}}{=} q^{k-1}(1 - (1 - x)^k)$ that we aim to maximize. We examine how this function changes as we increase k .

We have $f(k+1)/g(k) = q \frac{1-(1-x)^{k+1}}{1-(1-x)^k}$. Since the term $\frac{1-(1-x)^{k+1}}{1-(1-x)^k}$ is monotonically decreasing with k , we have to find the largest k for which $q \frac{1-(1-x)^{k+1}}{1-(1-x)^k} \geq 1$ which is equivalent to

$$(1-x)^k \geq \frac{1-q}{1-q(1-x)}. \quad (1)$$

We then solve for the continuous k' for which (1) holds with equality by taking the logarithm of both sides. We obtain that $(1-x)^{k'} = \frac{1-q}{1-q(1-x)}$ for

$$k' = \frac{\log \left(\frac{1-q}{1-(1-x)q} \right)}{\log(1-x)}.$$

Since this shows there is still an increase when going from k' to $k' + 1$ in this case, we obtain that the optimal discrete solution is as claimed. \blacksquare

We observe that whenever progress is possible for some k , setting $k = 2$ also makes progress. This property of the exponential decay model enables us to derive a closed form solution of the maximum achievable success probability.

Corollary 31 *Whenever $\arg \max_{k \in \mathbb{N}_{\geq 0}} q^{k-1}(1 - (1 - x)^k) > k$, then $q(1 - x)^2 \geq x$.*

Proof As observed in the proof of [Claim 30](#), the function $g(k) = q^{k-1}(1 - x)^k$ first monotonically increases until it reaches the optimal step k , and then monotonically decreases. Since $g(1) = x$, we are guaranteed that $g(2) > x$ whenever the optimal k is at least 2. This proves the corollary. \blacksquare

The maximum achievable success probability. Similar to the case of the uniform model, we study the maximum achievable success probability with the exponential decay function.

Lemma 32 *The maximum achievable success probability of a $(\mathcal{A}_d^{(e_q,p)}, n)$ -reasoning algorithm with $q \geq p$ is*

$$\max\left(p, 2 - \frac{1}{q}\right).$$

Proof We start with the same observations as in the proof of [Section 4](#), namely that all solutions generated by a reasoning algorithm are either positively correlated or independent, and that it is always optimal to pass independent solutions with as high correctness probability as possible. We therefore obtain from [Proposition 14](#) that the solution has to be a fixed point of the function $f(x) = q(1 - (1 - x)^2)$ because the largest fixed point is achieved at $k = 2$ by [Corollary 31](#). This function has only one fixed point $x = 2 - \frac{1}{q}$. \blacksquare

We remark that it is never useful to pass more than one solution as context to $\mathcal{A}_d^{(e_q,p)}$ when $q \leq \frac{1}{2}$, as in this case the model performs worse than randomly sampling a solution from the context. Therefore, we have $q \geq 1/2$ for all boostable models.

Convergence analysis. In the following, we analyze the speed of convergence. In contrast to [Appendix B](#), we focus on the behavior when the initial success probability approaches 0. This corresponds to the setting where boosting is the most useful.

Here, we assume $k = 2$ throughout to achieve a lower bound. Furthermore, we will artificially weaken the oracle by a factor $(1 - \epsilon)$. This allows us to immediately apply [Lemma 8](#) to obtain a genetic algorithm and will not significantly change the convergence analysis.

We consider the branching algorithm that starts by generating a first generation of solutions with success probability $p_0 = p$, and then iteratively generates the next generation of solutions with success probability p_i by combining two fresh solutions from the previous generation. Formally, this is equivalent to the branching algorithm (See [Algorithm 1](#)) with $k_i = 2$ for all i .

Lemma 33 *Let $p_{\max} = 2 - \frac{1}{q} > p$. Then we obtain a solution with success probability $p_{\max} - \epsilon$ after $L = O(\frac{1}{\epsilon} \log(1/p))$ generations. This also holds if the success probability of the oracle is decreased by a multiplicative factor $1 - \epsilon/8$.*

Proof We have $p_{i+1} = q(1 - (1 - p_i)^2)$. We will show that $p_{i+1} \geq p_i(1 + \frac{\epsilon}{4})$, or equivalently

$$p_i(1 + \frac{\epsilon}{4}) \leq (1 - \epsilon/8) \cdot q(1 - (1 - p_i)^2)$$

which is implied by

$$p_i(1 + \frac{\epsilon}{2}) \leq q(1 - (1 - p_i)^2) \tag{2}$$

as long as $p_i \leq p_{\max} - \epsilon$. Reformulating (2) yields

$$p_i \leq 2 - \frac{1 + \frac{\epsilon}{2}}{q}.$$

Since $q \in [\frac{1}{2}, 1]$, this condition always holds when $p_i \leq p_{\max} - \epsilon$. Therefore, the success probability increases by at least a multiplicative factor $(1 + \frac{\epsilon}{4})$ in each iteration. ■

Corollary 34 *There is a genetic algorithm (See [Algorithm 2](#)) with $O(\log(1/\epsilon) \log(1/p)/(p\epsilon^3))$ oracle calls that achieves success probability $p_{\max} - \epsilon$. The sequential depth of the algorithm is $O(\log(1/p)/\epsilon)$.*

Proof Directly follows from [Theorem 33](#) and [Lemma 8](#). ■

In our proof, we merely focus on context sizes equal to 2. For very large q , there can, however, be substantial gains in the number of rounds when combining more answers at a time. In particular, for $q = (1 - p)$ we can get rid of the dependence on $\log(1/p)$ in the number of rounds entirely by initially combining approximately $1/p$ solutions. For most practical settings where q should be thought of as a constant close to 1, the studied setting captures the behavior.

D.2. Polynomial Decay

In this section, we examine polynomial decay functions (See [Definition 4](#)). Since these functions drop off much slower than the exponential decay we examined in the previous section, they allow much faster boosting. In particular, we can show that approximately $\log \log 1/p$ iterations suffice to boost to constant success probability with a simple algorithm.

A simple algorithm. We describe a simple algorithm that automatically scales k and quickly increases the success probability to a small constant. Given access to independent solutions with correctness probability at least p , the algorithm samples $k = \lfloor 1/p \rfloor$ such solutions as context C and passes them to the oracle $\mathcal{A}_d^{(p,q,p)}(C)$. Then, the oracle generates a solution that is correct with probability p' bounded by

$$p' \geq \frac{1}{k^q} (1 - (1 - p)^k) \geq p^q (1 - (1 - p)^{1/p-1}).$$

For $p \leq 1/2$, we obtain

$$p' \geq p^q (1 - 2/e).$$

For a constant $q < 1$, this series will recover a squaring type behavior. We next show that this series increases very quickly for a general constant c . This then allows us to replace $(1 - 2/e)$ with $(1 - 2/e)(1 - \epsilon')$ to weaken the oracle and obtain convergence guarantees for the genetic algorithm via [Lemma 8](#).

Claim 35 *Consider $p_0 = p$, and $p_i = p_{i-1}^q \cdot c$ for $i \geq 1$. Then, $p_n = p^{q^n} \cdot c^{\frac{1-q^n}{1-q}}$ for $n \geq 1$.*

Proof The proof is by induction. The base case $n = 1$ directly follows from the definition of p_1 .

Now, we assume the recurrence holds for n and aim to show it for $n + 1$. We have

$$\begin{aligned} p_{n+1} &= p_n^q \cdot c \\ &= \left(p^{q^n} \cdot c^{\frac{1-q^n}{1-q}} \right)^q \cdot c \\ &= p^{q^{n+1}} \cdot c^{1+q \frac{1-q^n}{1-q}} = p^{q^{n+1}} c^{\frac{1-q^{n+1}}{1-q}}. \end{aligned}$$

■

From [Claim 35](#), we observe that this simple algorithm converges to a success probability of $c^{\frac{1}{1-q}}$. For constant q and c , this corresponds to a constant success probability.

Claim 36 *We have $p_n \geq (1 - \epsilon)c^{\frac{1}{1-q}}$ for some $n = O(\log \log(1/p)/q + \log(\epsilon^{-1})/q)$.*

Proof We have $p_n = p^{q^n} c^{\frac{1-q^n}{1-q}} = p^{q^n} c^{\frac{1}{1-q}} c^{\frac{-q^n}{1-q}}$. We first show that $c^{\frac{-q^n}{1-q}} \geq (1 - \epsilon/2)$ for $n = O(\log \log(1/p) + \log(\epsilon^{-1}/q))$. We take the logarithm on both sides.

$$\begin{aligned} \frac{-q^n}{1-q} \log(c) &\leq \log(1 - \epsilon/2) \\ q^n &\geq -(1-q) \frac{\log(1 - \epsilon/2)}{\log(c)} \end{aligned}$$

We then approximate $\log(1 - \epsilon) \approx -\epsilon$ and collect the constant terms into C obtaining the condition

$$n \geq C' \log(1/\epsilon)/q$$

for some constant C' .

Next, we show that $p^{q^n} \geq (1 - \epsilon/2)$. We have

$$\begin{aligned} p^{q^n} &\geq (1 - \epsilon/2) \\ q^n \log(p) &\geq \log(1 - \epsilon/2) \\ n &\geq C(\log(\epsilon^{-1}) + \log \log(1/p))/q \end{aligned}$$

for some large constant C . This concludes the proof. ■

From [Claim 36](#), we obtain that this algorithm indeed converges very quickly. Furthermore, it does so even when c is slightly smaller. This allows it to pair very well with the genetic algorithm described in [Algorithm 2](#). We therefore derive a genetic algorithm.

In the following, we focus on the behavior when the initial success probability approaches 0. Once a reasonably high (e.g. constant) success probability is achieved, the type of convergence analysis from [Appendix B](#) could be applied to obtain the speed of convergence for the final bit.

Lemma 37 *There is a genetic algorithm that uses the model $\mathcal{A}_d^{(p_q, p)}$ and finds a solution that is correct with probability at least $(1/16)^{1/(1-q)}$ in $O(\frac{1}{pq} \log \log 1/p)$ oracle calls.*

Proof Directly follows from [Claim 36](#) and [Lemma 8](#) and $1 - (1-p)^{1/p-1} \geq (1-2/e)$ for $p \geq 1/2$. ■

The maximum achievable success probability. To characterize the maximum achievable success probability we resort to [Proposition 14](#) since there does not appear to be an obvious simpler characterization.

Appendix E. Experiments

In this section, we verify some of our theoretical assumptions with the AIME 2025 math dataset and the Gemini 2.5 Pro model. The dataset became available after the model, which helps us avoid test set contamination. AIME 2025 has 30 questions, and we plot the average accuracy for each question across independent model calls in Figure 1. The prompt consists only of the question. As expected, Gemini 2.5 Pro has a strong performance on many of the questions.

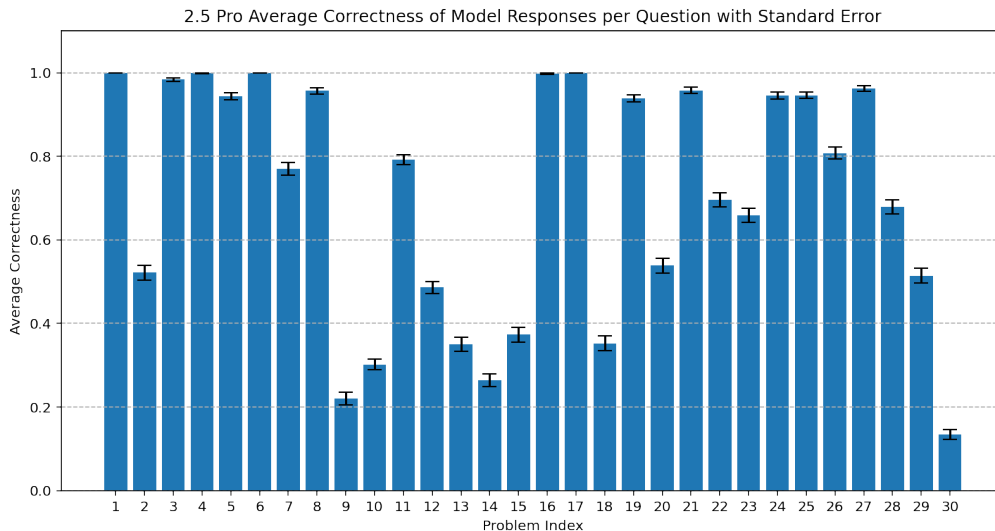


Figure 1: Average AIME 2025 accuracy per question for Gemini 2.5 Pro. We use 780 model calls per question. The error bars represent standard error.

Next, we saved the outputs and picked questions 10 and 12 to examine model accuracy when solutions are provided in context. These are questions for which the model struggled but occasionally generated correct answers. We study two settings below.

E.1. Fixing one correct solution and increasing incorrect solutions

We start by investigating model accuracy when only one of the solutions is correct, and the number of incorrect solutions grows from 0 to 12. For each of the configurations, we make 30 calls with Gemini 2.5 Pro and make sure none of the solutions are repeated across any of the calls. The solutions are also shuffled before placing them in context. Our results are in Figure 2, and we observe a decaying accuracy as the number of incorrect questions increases. This motivates our theoretical models with decay.

E.2. Fixing total number of solutions and varying correct solutions

Finally, we move to a setting where instead of fixing one correct answer, we fix the total number of solutions and vary the number of correct versus incorrect answers. We show results in Figure 3. We

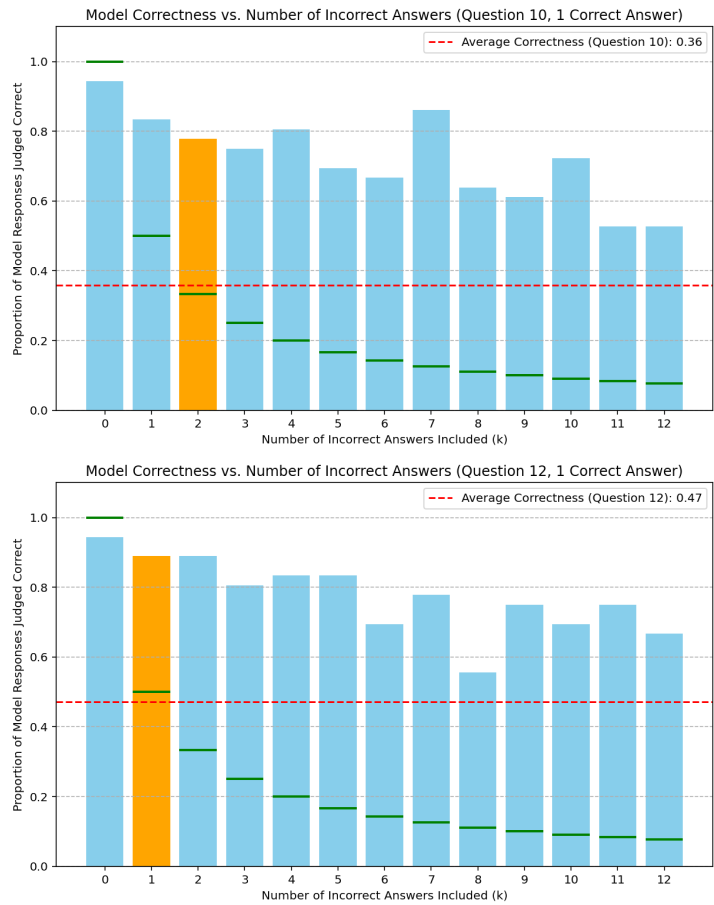


Figure 2: Gemini 2.5 Pro accuracy when providing 1 correct solution answer and $k = 0$ to 12 incorrect solutions. The red line represents base accuracy of Pro on the question without any solutions. The green lines represent $1/(k + 1)$, the accuracy when returning a solution in the context uniformly at random. The orange bar is the most likely configuration according to the base accuracy (the k for which $1/(k + 1)$ is closest to base accuracy).

again used 30 calls per configuration, did not reuse solutions across any model calls, and shuffled the order of the solutions.

We observe a very smoothly increasing accuracy as the number of correct solutions increases. We also note that the performance of this setup—sampling 5 solution answers and providing them as context for a final model call—always improves over the base accuracy of the model on average. On the two questions we examined for Pro, the gap is about 40%, suggesting that it is a particularly strong verifier.

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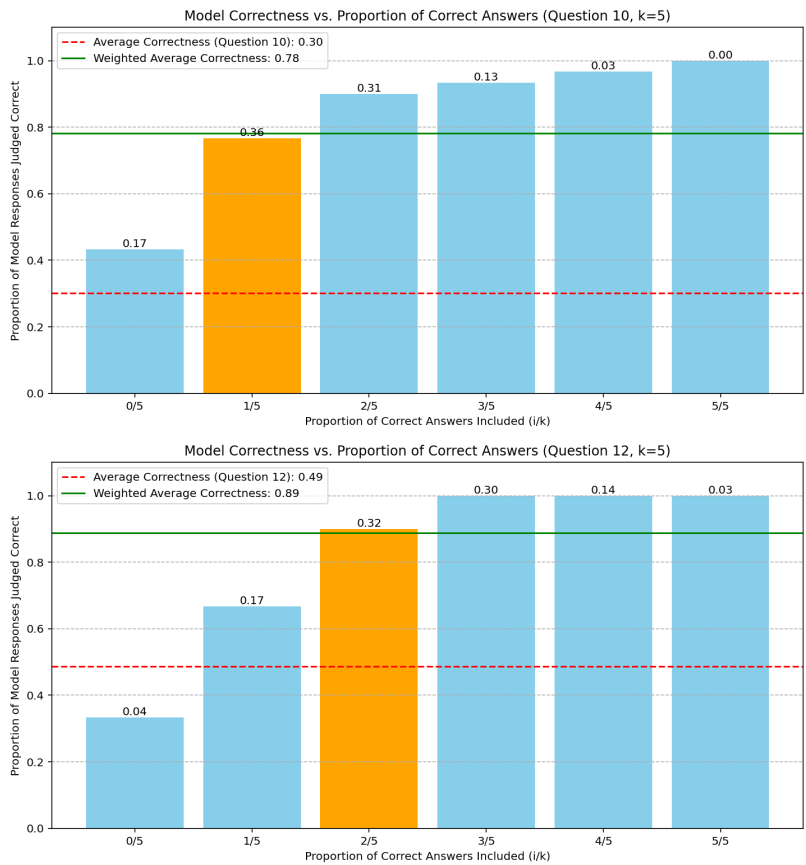


Figure 3: Gemini 2.5 Pro accuracy when providing 5 total solutions and varying the number of correct versus incorrect answers. The red line represents base accuracy of Pro on the question without any solutions. The numbers on top of each bar represent the probability of that configuration according to the average correctness. The orange bar highlights the most likely configuration. The green line uses these weights to give the accuracy when sampling 5 solutions and using them as context for a final model call.