PBEBench: A Multi-Step Programming by Examples Reasoning Benchmark inspired by Historical Linguistics

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Abstract

Recently, long chain of thought (LCoT), Large Language Models (LLMs), have taken the machine learning world by storm with their breathtaking reasoning capabilities. However, are the abstract reasoning abilities of these models general enough for problems of practical importance? Unlike past work, which has focused mainly on math, coding, and data wrangling, we focus on a historical linguistics-inspired inductive reasoning problem, formulated as Programming by Examples. We develop a fully automated pipeline for dynamically generating a benchmark for this task with controllable difficulty in order to tackle scalability and contamination issues to which many reasoning benchmarks are subject. Using our pipeline, we generate a test set with nearly 1k instances that is challenging for all state-of-the-art reasoning LLMs, with the best model (Claude-3.7-Sonnet) achieving a mere 54% pass rate, demonstrating that LCoT LLMs still struggle with a class or reasoning that is ubiquitous in historical linguistics as well as many other domains.

1 Introduction

Students in a introductory historical linguistics course are often given problems where they are provided sets of etymologically related words from modern languages and asked to infer two things: (1) a set of reconstructed words from the hypothetical most recent shared ancestor language ($\vec{i}$), and (2) chronologically ordered string rewrite rules ($\vec{p}$) for each language to derive the modern words ($\vec{o}$) from the reconstructed words. A good deal of progress has been made towards implementing (1), which can be seen as a sequence transduction problem, computationally (Ciobanu and Dinu [2018], Meloni et al. [2021], Kim et al. [2023], Lu et al. [2024a,b]). The logic behind (2), forward reconstruction, is actually quite straightforward, but it proves challenging for contemporary ML models, including LLMs. For example, Naik et al. [2024, 2025] attempted to solve this problem for very simple cases and met with limited success. Their work is the inspiration for this study.

Consider the case of Huishu, a Tangkhulic language of Northeastern India. In this language, Proto-Tangkhulic[1] *ɨ became u everywhere (p_1 : ɨ → u) and Proto-Tangkhulic **u* became *uk* at the end of words (p_3 : u# → uk#). Proto-Tangkhulic **uk* became *uʔ* everywhere (p_2 : uk → uʔ). p_1 must have applied before p_3. Otherwise words like **nɨ* 'laugh' would have became *nu* rather than the attested *nuk* in Huishu. Linguists say that p_1 FEEDS p_3 (creates a context where it can apply). Likewise, p_2 must apply before p_3. Otherwise, words like **ru* would become *ruʔ* in Huishu, rather than the

[1] Proto-Tangkhulic is the name of the reconstructed ancestor language (or "proto-language") that is ancestral to Huishu and its linguistic siblings.

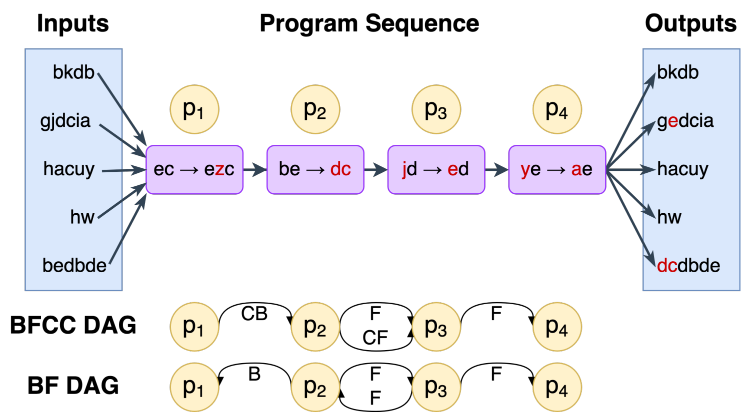

Figure 1: Structure of the <$\vec{i}, \vec{p}, \vec{o}$> triples dataset. The relations between the programs in the sequence are shown by the BFCC DAG, and the simplified BF DAG replaces the counterfactual relations with a reversed simple link.

attested *ruk*. Linguists would say that p_3 COUNTER-FEEDS p_2 (if the order of the two processes were reversed, Rule p_3 would create contexts where Rule p_2 could apply, that is, p_3 would feed p_2). The reverse of feeding is BLEEDING, in which a p_4 destroys a context in which a p_5 would apply. It also has a counterfactual version, COUNTER-BLEEDING (in which p_4 would bleed p_5 if it applied first). In the history of a language, if the order of two sound changes matters, one of these relations holds between them. More generally, since counter-feeding and counter-bleeding are simply counterfactual versions of feeding and bleeding, the chronologies of sound changes can be reasoned about by students of historical linguistics simply in terms of the potential feeding and bleeding relations between them. Since these relations can be defined algorithmically (see §3), the underlying logic is simple. The forward reconstruction problem simply involves defining the rules jointly with a multi-step plan consistent with that logic.

This "forward reconstruction" task, which combines inductive reasoning and planning, is a specific instance of a more general kind of reasoning problem, which has been a topic of discussion since the early years of artificial intelligence. It is related to all problems where it is necessary to plan a discrete series of processes $\vec{p} = [s_1 \to t_1, s_2 \to t_2, \ldots, s_n \to t_n]$ that, when applied in sequence to each element, will transform the elements of a source vector $\vec{i} = [i_1, i_2, \ldots, i_m]$ into the corresponding elements of the target vector $\vec{o} = [o_1, o_2, \ldots, o_m]$. Problems of this type appear in many domains, from computer science to cooking.

The forward reconstruction formulation of the problem, though, has a number of properties that make it particularly attractive for benchmarking language models: (1) It can be structured to largely avoid domain-specific biases, so that it is strictly a reasoning task. (2) The reasoning necessary to complete the task can be expressed via a very simple pair of logical relations between processes (feeding and bleeding). (3) The processes themselves can be expressed very simply (e.g., as string rewrite rules).

We present an automated benchmark generation procedure based on this forward reconstruction class of problems. Models are given a list of input pairs and the corresponding outputs (generated by applying a randomly sampled program $\vec{p}$ to the elements of $\vec{i} = [i_1, i_2, \ldots, i_n]$, yielding outputs $\vec{o} = [o_1, o_2, \ldots, o_n]$. The task is to infer a program $\hat{p}$ that is functionally equivalent to $\vec{p}$. Moreover, our fully automated procedure for generating challenging data allows the benchmark to **scale easily** and **avoid data leakage**. Unlike popular mathematics Balunović et al. [2025], coding Jain et al. [2024], and reasoning benchmarks Chollet et al. [2024], any contamination in the current version can be resolved by automatically generating new, harder data without any need for manual curation. The provided dataset is already challenging, with the most successful model (Claude-3.7-Sonnet) achieving a pass rate of only 54%.

Based on linguists' assessment of this problem, we hypothesized that, other things being equal, problems requiring reasoning about "opaque" rule ordering (counter-feedispng and counter-bleeding) would be more difficult than those involving "transparent" rule ordering (feeding and bleeding) since stronger surface evidence is required to infer them. This disparity, though, should diminish as the reasoning power of models goes up since the same fundamental search strategies apply to opaque orders as to transparent orders. Analysis of model outputs support this speculation, but shows that average Levenshtein distance between $\vec{i}$ and $\vec{o}$ and the number of programs in $\vec{p}$ are better predictors of difficulty than the types of programs in $\vec{p}$.

2 Related Work

Programming By Example Programming by Example (PBE) [Gulwani, 2010] is a well-known and intuitive paradigm within program synthesis research. It entails inferring programs solely from a small set of input-output pairs. Early symbolic approaches employ domain-specific languages (DSLs) and constraint solving: FlashFill uses string-transformation DSLs to automate spreadsheet tasks [Gulwani, 2011], and Syntax-Guided Synthesis (SyGuS) constrains program search via grammar specifications [Alur et al., 2013]. DeepCoder [Balog et al., 2017] uses learned function predictions to guide search, while RobustFill [Devlin et al., 2017] trains sequence-to-sequence models to emit DSL programs directly. Large Language Models [Chen et al., 2021a, Guo et al., 2024] have demonstrated few-shot learning capabilities in code generation tasks, but struggle on out-of-distribution examples, improving only after fine-tuning [Li and Ellis, 2024].

Inducing Context-Sensitive Grammars in LLMs Attempts to induce string-rewrite rules from data have a long history Gildea and Jurafsky [1995]; discussions of the formal properties of these rules in linguistics go back farther, including (pivotal to this study) the discovery of feeding and bleeding relationships between such rules Kiparsky [1968]. More recently, formal language benchmarks have shown that RNNs can outperform transformers on formal language tasks involving certain classes of grammars [Butoi et al., 2025]. Morphophonological probes [Borenstein, 2024] reveal that while models fit the training data, they often default to heuristics, highlighting limitations in true rule induction. Naik et al. [2024] demonstrate that LLMs can induce low-resource sound laws, generalizing the method to full context-sensitive program synthesis [Naik et al., 2025]. However, none of these prior works have proposed provably correct algorithms for detecting feeding and bleeding relations (a unique contribution of this work).

Benchmarks A range of benchmarks test reasoning and PBE skills. Code-centric suites include HumanEval and MBPP [Chen et al., 2021a, Austin et al., 2021], while PBE-style tasks appear in FlashFill datasets [Gulwani, 2011]. Linguistic and reasoning benchmarks such as HotpotQA [Yang et al., 2018], DROP [Dua et al., 2019], and GSM8K [Cobbe et al., 2021] stress multi-step and mathematical reasoning. System-2 reasoning is evaluated in BIG-Bench Hard [Suzgun et al., 2022], where chain-of-thought prompting improves performance significantly. Compositional generalization splits like SCAN [Lake and Baroni, 2018] and CFQ [Keysers et al., 2020] reveal extrapolation gaps. Visual PBE in ARC [Chollet, 2019] is a non-language analog to our task. However, our benchmark is significantly more resistant to leakage, easily scalable, and offers a mechanism to modulate task difficulty by simple adjustment of the generation parameters. To our knowledge, no benchmark targets multi-step synthesis of string-rewriting programs; PBEBench fills this niche by unifying PBE and compositional generalization in a single benchmark.

3 Theoretical Framework

We propose the function $\mathsf{feeds}(\cdot,\cdot)$, which classifies pairs of rules as feeding or not feeding.

$$\mathsf{feeds}(s_i \to t_i, s_j \to t_j) = \begin{cases} \top & t_i = \varepsilon \wedge |s_j| > 1 \\ \top & t_i \in \mathsf{Substr}(s_j) \wedge t_i \notin \mathsf{Substr}(s_i) \\ \top & t_j \in (\mathsf{Substr}(t_i) \setminus \mathsf{Substr}(s_i)) \\ \top & \mathsf{Pref}(t_i) \setminus \mathsf{Substr}(s_i) \cap \mathsf{Suff}(s_j) \neq \emptyset \\ \top & \mathsf{Suff}(t_i) \setminus \mathsf{Substr}(s_i) \cap \mathsf{Pref}(s_j) \neq \emptyset \\ \bot & \text{otherwise} \end{cases} \tag{1}$$

where $\mathsf{Pref}(s)$, $\mathsf{Suff}(s)$, and $\mathsf{Substr}(s)$ are the multisets of prefixes, suffixes, and substrings of s, respectively.

Definition 3.1 (Feeding)**.** Feeding is a relation between pairs of rules $p_i = s_i \rightarrow t_i$ and $p_j = s_j \rightarrow t_j$, such that $\exists s, t \in \Sigma^*$ such that $s \xrightarrow{p_i} t$ and t includes a string w that meets the structural description of p_j but is not present in s.

Definition 3.2 (Bleeding)**.** Bleeding is a relation between pairs of rules $p_i = s_i \rightarrow t_i$ and $p_j = s_j \rightarrow t_j$, such that $\exists s, t' \in \Sigma^*$ such that $s_i \xrightarrow{p_i} t_i$ and s_i includes a string w that meets the structural description of p_j but is not present in t_i.

Definition 3.3 (Substr)**.** $\mathsf{Substr}(s)$ denotes the multiset of substrings of s, counting multiple occurances separately.

Lemma 1: If $\mathsf{feeds}(p_i, p_j)$ then p_i feeds p_j.

Proof. Given $u, v, o, s_i, t_i, s_j, t_j \in \Sigma^*$, $s_i \xrightarrow{p_i} t_i$, and $s_j \xrightarrow{p_j} t_j$ there are four types of transformations of u by applying p_i that will yield v such that $s_j \sqsubseteq v$ (where $\sqsubseteq$ indicates "is a substring of"). (1) **Deletion.** Assume that $t_i = \varepsilon$. $\exists wx \in \Sigma^+$ such that $ws_ix \xrightarrow{p_i} xw$. If $s_j = xw$ then p_i feeds p_j. (2) **Containment.** $t_i \sqsubseteq s_j \wedge t_i \not\sqsubseteq s_i$, $\exists w, x \in \Sigma+$ such that $w \xrightarrow{p_i} x \wedge s_j \sqsubseteq x \wedge s_j \not\sqsubseteq x$. (3) **Subsumption.** Assume that $s_j \in \mathsf{Substr}(t_i) \setminus \mathsf{Substr}(s_i)$. Given $s_i \xrightarrow{p_i} t_i$, t_i will always contain instances of s_j not present in s_i, entailing that p_i feeds p_j. (4) **Completion.** Assume that $t_i = uo$ and $s_j = ov$ (so that o is a suffix of t_i and a prefix of s_j). $s_iov \xrightarrow{p_i} t_iov = uov = us_j$, entailing that p_i feeds p_j (as with $t_i = ou$ and $s_j = vo$, *mutatis mutandis*). $\square$

Lemma 2: If $\neg\mathsf{feeds}(p_i, p_j)$ then p_i does not feed p_j

Proof. Given $s_i, t_i, s_j, t_ju \in \Sigma^*$, assume for the sake of contradiction two rewrite rules $s_i \xrightarrow{p_i} t_i$ and $s_j \xrightarrow{t}_j$ such that p_i feeds p_j but s_i, t_i, and s_j do not satisfy any of the following conditions: **Deletion.** $s_i \neq \varepsilon \vee s_j \neq wx \forall w, x \in \Sigma^+$, **Containment.** $t\neg \sqsubseteq s_j \vee t_i \sqsubseteq s_i$ **Subsumption.** s_j does not occur in t_i except where it occurs in s_i. **Completion.** $\nexists u, o, v$ such that$(t_i = ou \wedge s_j = vo) \vee t_i = uo \wedge s_j = ov$. Either t_i is a non-empty string neither containing nor being contained by s_j and sharing no prefix or suffix with s_j or replacing s_i with t_i derives no instances of s_j. The first case must be false, since the conditions exhaust the transformations that could yield a string containing s_j. The second case must be false, because it contradicts the definition of feeding. $\square$

Theorem 3 (Feeding)**:** A rule $s_i \rightarrow t_i$ feeds a rule $s_j \rightarrow t_j$ iff $\mathsf{feeds}(s_i \rightarrow t_i, s_j \rightarrow t_j)$

Proof. Given two rules $p_i = s_i \rightarrow t_i$ and $s_j \rightarrow t_j$, Lemma 1 proves by enumerating cases that each of the conditions defined for $\mathsf{feed}(p_i, p_j)$ are sufficient for establishing that p_i feeds p_j. Lemma 2 proves by enumerating cases than p_i does not feed p_j if none of these conditions are satisfied. $\square$

Theorem 4 (Bleeding)**:** A rule $p_i = s_i \rightarrow t_i$ bleeds a rule $p_j = s_j \rightarrow t_j$ iff $\mathsf{feeds}(t_i \rightarrow s_i, s_j \rightarrow t_j)$

Proof. if $\exists u, v \in \Sigma^*, u \xrightarrow{t_i \rightarrow s_i} v$ such that $s_j \sqsubseteq v \wedge s_j \not\sqsubseteq u$, it follows that mapping $s_i \xrightarrow{p_i} t_i$ bleeds p_j (where $s_j \xrightarrow{p_j} t_j$). $\square$

4 Methodology

4.1 Benchmark Generation

We construct our benchmark programmatically by sampling from an input distribution $\mathcal{I}$ and program distribution $\mathcal{P}$ and applying the programs $\vec{p} = \{p_1, \ldots p_m\} \in \mathcal{P}$ on the inputs $\vec{i} = \{i_1, \ldots i_n\} \in \mathcal{I}$ to obtain the outputs $\vec{o} = \{p_m(\ldots p_1(i_1)), \ldots p_m(\ldots p_1(i_n))\}$ (we use $\vec{o} = \vec{p}(\vec{i})$ as a notational shorthand). The inputs, outputs and program sequence $<\vec{i},\vec{p},\vec{o}>$ together constitute a single instance of our benchmark dataset. Our data generation algorithm takes $n(= 5)$ (number of input and output pairs) and $m(= 5)$ (maximum number of transformation rules or programs) as input parameters. Additionally we also store information like the relationships or interactions (e.g. BLEEDING, FEEDING, etc.) between all pairs of programs.

4.1.1 Input Sampling

For sampling the inputs $\vec{i} = \{i_1, \dots i_n\}$ we sample each input $i_j, j \in \{1, \dots n\}$ independently from each other by first sampling the length of each i_j, from a uniform discrete distribution $p_{\text{length}} = \frac{1}{5}\mathbf{1}_{\mathcal{L}}$ ($\mathcal{L} = \{2, 3, 4, 5, 6\}$) or $|i_j| \sim p_{\text{length}}$. Then given the length we sample $|i_j|$ characters from a uniform character distribution $p_{\text{char}} = \frac{1}{14}\mathbf{1}_{\Sigma}$ over the restricted set of characters $\Sigma =$`abcdefghijkxyz`).

4.1.2 Program Sampling and Output Generation

We sample a sequence of m string rewrite programs: $\vec{p} = \{p_1, \dots p_m\}$ of the form $p_i = \text{replace}(a_i, b_i)$ where replace is identical to the Python builtin `replace()` function for strings and a_i and b_i are substrings, where a_i is replaced by b_i. To sample each program p_i we simply sample a_i and b_i independently similar to how the inputs are sampled: 1) first sample the lengths $|a_i|, |b_i| \sim p_{length}$ where the length distribution is $p_{\text{length}} = \frac{1}{3}\mathbf{1}_{\mathcal{L}}$ ($\mathcal{L} = \{1, 2, 3\}$) and 2) sample $|a_i|$ and $|b_i|$ characters from the same uniform character distribution $p_{\text{char}} = \frac{1}{14}\mathbf{1}_{\Sigma}$ over the restricted set of characters $\Sigma =$`abcdefghijkxyz`).

Such a simple sampling procedure might not produce meaningful string rewrite transformations (e.g., none of the sampled inputs may be transformed). To ensure meaningful transformations and control their complexity, we perform careful rejection sampling that analyzes the sampled program sequences and also analyzes the effect of applying it to the inputs. Any sequences that 1) fail to transform any inputs or 2) do not meet the desired level of complexity are discarded.

4.1.3 Measuring Instance Complexity

We describe how complex an instance or $\langle \vec{i}, \vec{p}, \vec{o} \rangle$ triple is based on the types of relations between all pairs of programs in the program sequence $\vec{p}$. An important contribution of our work is provably correct and automatic classification of the types of relations between any given pair of string rewrite programs (section 3). For a given pair of programs p_i and p_j in the program sequence $\vec{p}$:

Feeding (F): p_i creates substrings that enable p_j to apply.
Bleeding (B): p_i removes substrings that p_j requires.
Counter-Feeding (CF): p_i could have fed p_j, but p_j precedes p_i.
Counter-Bleeding (CB): p_i could have bled p_j, but p_j precedes p_i.
No Relation: p_i and p_j can be ordered in any way possible.

We do not store or identify the counterfactuals separately, instead incorporating them by classifying and storing the relationship between the pair (p_i, p_j) and (p_j, p_i), where (p_i, p_j) indicates a scenario where p_i is applied before p_j and (p_j, p_i) indicates a scenario where p_j is applied before p_i. We can also visualize the relationships between the rules using a Directed Acyclic Graph (DAG) as shown in Figure 1. We show both the actual DAG with all relations and a simplified DAG that indirectly captures counterfactual relations by reversing them.

4.1.4 Controlling Instance Complexity

To ensure that we can control the distribution of relation types and hence the complexity of the $<\vec{i}, \vec{p}, \vec{o}>$ triples, we apply rejection sampling as mentioned in 4.1.2. Each example is categorized into a complexity bucket based on the presence or absence of at least one relation of each type (B, F, CF, or CB), which can be expressed as a 4-bit vector. Based on these categories, we generate the data to roughly balance instances of each of the possible $2^4 = 16$ complexity buckets. We start discarding $<\vec{i}, \vec{p}, \vec{o}>$ triples if any of the complexity buckets is overrepresented. This procedure is designed to likely yield a dataset balanced both in the complexity and diversity of BFCC relations between program pairs.

4.2 Program Induction

4.2.1 Prompting

Once we have generated the $<\vec{i}, \vec{p}, \vec{o}>$ using the procedure described in the section above, we evaluate each model M by prompting them to generate a likely program sequence $\hat{\vec{p}} = M(\vec{i}, \vec{o})$ that can map the inputs $\vec{i}$ to the outputs $\vec{o}$. The LLM is prompted (as shown in section B.2) to generate at most $m(=5)$ programs in the predicted sequence $\hat{\vec{p}}$ for each problem (the ground truth program sequence $\vec{p}$ may have $\leq m$ programs) with the constraints that for each predicted program $\hat{p}_i$ must be of the form $\text{replace}(a_i, b_i)$, and for each substring a_i, b_i the length $|a_i| \leq 3$ and $|b_i| \leq 3$. Additionally, the substrings a_i and b_i must only contain characters from the reduced character set Σ. If any of the constraints are violated, the program $\hat{p}_i$ is rejected and replaced by a special "placeholder" or "identity" program p^I which doesn't transform any inputs (lets all inputs pass as it is). Finally given the predicted program sequence $\hat{\vec{p}}$ we can obtain a predicted output sequence $\hat{\vec{o}}$ as: $\hat{\vec{o}} = \hat{\vec{p}}(\vec{i})$. We describe the details of extracting the program sequence from the LLM response in section B.1.

5 Experiments

5.1 Benchmark

Using the benchmark generation process described in section 4.1, we generate an evaluation set $\mathcal{D}_T$ with 992 instances ($|\mathcal{D}_T| = 992$) ($<\vec{i}, \vec{p}, \vec{o}>$ triples). While ideally the rejection sampling described in section 4.1.4, should yield roughly equal examples for each complexity bucket, we observe that some programs p_i in the program sequence $\vec{p}$ do not affect any inputs (even though the program sequence $\vec{p}$ as a whole does) we remove these "degenerate" programs p_i from the program sequence. This yields a skewed data distribution with only 10.6% data having at least one BFCC relation and 2.4% data having two or more relations. While this is less complex than expected, our results show that this is still challenging for state-of-the-art reasoning LLMs. We give detailed statistics about the generated benchmark and the feature distribution in A.2.

5.2 Model Selection

We evaluate a representative set of state-of-the-art LLMs (output token budget in brackets):
General-Purpose: Qwen2.5-32B-Instruct Team [2024], Qwen3-32B-Instruct Team [2025], and Claude-3.5-Sonnet Anthropic [2024], which perform well on diverse coding tasks.
Code-Specific: Codestral-22B AI [2024], trained on 80+ languages, and Qwen2.5Coder-32B-Instruct Team [2024], with GPT-4o-level coding abilities.
Reasoning-Focused: QwQ-32B, DeepSeek-R1-Distill-Qwen-32B, o3-mini OpenAI [2024], o4-mini OpenAI [2025], Gemini 2.5 Flash Preview 04-17, and Claude-3.7-Sonnet Anthropic [2025].
MoE: Qwen3-30B-A3B Team [2025] and DeepSeek-R1.
We mention the sampling parameters used to do inference with each of these models in Table 4

5.3 Evaluation Metrics

Since a given set of inputs ($\vec{i}$) could be transformed into the outputs ($\vec{o}$) by multiple program sequences $\vec{p}$ we utilize metrics based on functional correctness that execute the model generated solution $\hat{\vec{p}}$ on the inputs and outputs, treating them like test cases. We compare the predicted outputs $\hat{\vec{o}} = \hat{\vec{p}}(\vec{i})$ with the ground truth outputs $\vec{o}$ at two levels of granularity: 1) coarse-grained evaluation (pass@1 or exact match) and 2) fine-grained evaluation (normalized edit similarity). Both metrics do element-wise comparisons on the strings in the output vectors:
Coarse-grained Metric (Pass@1): This metric is pass@1 from Chen et al. [2021b].

$$\text{pass@1} = \frac{1}{|\mathcal{D}_T|} \sum_{\vec{o}, \vec{i} \in \mathcal{D}_T} 1_{\hat{\vec{p}}(\vec{i}) = \vec{o}}$$

Here 1_X is an indicator variable which is 1 when X is true and 0 if it is false.
Fine-grained Metric (Edit Sim): This metric is the same as reward@1 used by Naik et al. [2025].

$$\text{edit\_sim} = \frac{1}{|\mathcal{D}_T|} \sum_{\vec{o}, \vec{i} \in \mathcal{D}_T} 1 - \frac{\text{dist}(\hat{\vec{p}}(\vec{i}), \vec{o})}{\text{dist}(\vec{i}, \vec{o})}$$

Here dist denotes the total Levenshtein edit distance summed across the corresponding inputs and outputs. Additionally we also evaluate the rate at which an LLM generates valid programs (follows all instructions mentioned in 4.2.1) which we term as the **Valid Rate**.

Table 1: **Benchmark performance:** We compute the pass@1 and edit similarity as the coarse and fine-grained evaluation, respectively, for each model. ■- indicates mixture-of-experts (or MoE) model and ★- indicates reasoning model.

Model	**First Code Block**			**Last Code Block**		
	Pass@1	**Edit Sim**	**Valid Rate**	**Pass@1**	**Edit Sim**	**Valid Rate**
Codestral-22B	0.1552	0.1758	0.8351	0.1552	0.1763	0.8354
Qwen2.5-32B-Instruct	0.2006	0.2277	0.8854	0.2016	0.2382	0.8818
Qwen2.5Coder-32B-Instruct	0.2087	0.2362	0.7947	0.2228	0.2536	0.8019
QwQ-32B ★	0.1865	0.0954	0.8455	0.253	0.1752	0.8552
Qwen3-32B	0.2147	0.2198	0.8748	0.25	0.2587	0.8767
Qwen3-30B-A3B ★■	0.2913	0.3	0.9093	0.2913	0.3	0.9093
DeepSeek-R1-Distill-Qwen-32B ★	0.122	0.1137	0.7778	0.126	0.1179	0.7851
DeepSeek-R1 ★■	0.3044	0.3513	**0.9469**	0.3065	0.3518	**0.9527**
o3-mini ★	0.0464	0.0533	0.7921	0.0474	0.0543	0.801
o4-mini ★	0.3871	0.4154	0.7387	0.3871	0.4154	0.7387
Gemini 2.5 Flash Preview 04-17 ★	0.4617	0.5215	0.8148	0.4617	0.5215	0.8148
Claude-3.5-Sonnet	0.2732	0.3416	0.9275	0.2732	0.3416	0.9275
Claude-3.7-Sonnet ★	**0.5111**	**0.5647**	0.8478	**0.5403**	**0.5918**	0.8574
Claude-3.7-Sonnet (Thinking Mode) ★	0.5050	0.5288	0.9135	0.5111	0.5393	0.9168

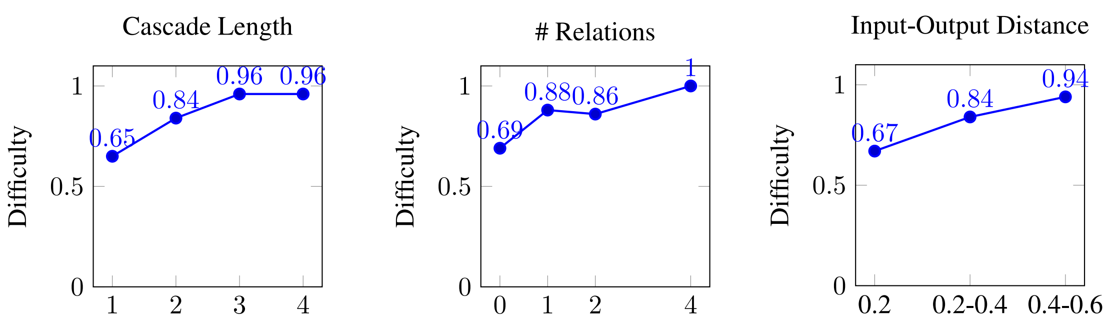

Figure 2: **Understanding Empirical Instance Difficulty:** We visualize the distribution of the inverted pass rate empirical difficulty or d_{pass} when varying complexity related features like: 1) Cascade Length, 2) No. of Relations and 3) Input-Output Distance.

5.4 Instance Complexity vs Empirical Instance Difficulty

We investigate how predictive the complexity of an $<\vec{i}, \vec{p}, \vec{o}>$ triple is about the empirical difficulty $d(\vec{i}, \vec{p}, \vec{o})$ of the instance. We use the notion of empirical/observed difficulty described in C.1 and measure instance complexity using features described in C.2. Based on these complexity features, we perform several analyses on the predictive power of the instance complexity on the empirical instance difficulty.

6 Results

6.1 Benchmark Performance

Table 1 presents the pass@1, edit_sim, and valid rate for all models described in Section 5.2 for both the first and last code block. For most models, the last code block yields the best results, so we extract only those for further analysis. Surprisingly, o3-mini performs the worst, despite being a strong reasoning model, while Claude-3.7-Sonnet (without reasoning) achieves the best results. Interestingly, we also notice that Claude-3.7-Sonnet with reasoning (thinking mode) performs slightly worse, but in general, reasoning models, especially closed-source ones, perform the best. Some models might generate fewer valid programs overall, but a higher proportion of those may be functionally correct. For instance, o4-mini has a pass rate of 0.3871 with only 0.7387 valid rate, whereas DeepSeek-R1 achieves a higher valid rate of 0.9527 but a lower pass rate of 0.3065.

Table 2: **Model-wise instance difficulty breakdown:** Logistic Regression analysis of complexity features with instance difficulty (d_{pass}), for each model. Larger coefficients mean a feature is more predictive of difficulty, and the standard error reflects the reliability of the estimate. Cells are colored according to the rank order of the coefficients for the model from smallest to largest: 1st, 2nd, 3rd, 4th, 5th

Model Name	Feeding		Counter-Feeding		Counter-Bleeding		Cascade Length		Input-Output Dist	
	coef	std err	coef	std err	coef	std err	coef	std err	coef	std err
o3-mini ★	-0.046	0.2	4.7	4.1e+03	3	4e+03	0.047	0.24	0.12	0.2
DeepSeek-R1-Distill-Qwen-32B ★	-0.07	0.22	0.033	0.24	2.9	2.2e+03	0.43	0.29	1.5	0.22
Codestral-22B	0.065	0.18	0.14	0.24	-0.06	0.12	0.29	0.22	1.3	0.19
QwQ-32B ★	-0.053	0.15	-0.032	0.15	3	2.3e+03	0.41	0.19	0.91	0.15
Qwen2.5-32B-Instruct	-0.13	0.16	-0.026	0.18	-0.067	0.12	0.8	0.23	0.81	0.14
Qwen2.5Coder-32B-Instruct	0.08	0.15	0.28	0.23	-0.072	0.1	0.34	0.17	0.75	0.13
Qwen3-32B	-0.015	0.13	0.18	0.17	0.00016	0.11	0.51	0.15	0.21	0.1
Claude-3.5-Sonnet	0.094	0.13	0.1	0.15	0.078	0.11	0.18	0.15	1.2	0.14
Qwen3-30B-A3B ★■	-0.12	0.12	-0.0035	0.13	0.057	0.11	0.59	0.16	0.85	0.12
DeepSeek-R1 ★■	-0.03	0.11	-0.0087	0.11	0.12	0.11	0.23	0.14	1	0.12
o4-mini ★	0.17	0.093	0.013	0.084	-0.028	0.077	0.37	0.1	-0.027	0.081
Gemini 2.5 Flash Preview 04-17 ★	-0.036	0.087	0.03	0.087	0.17	0.11	0.55	0.11	0.21	0.082
Claude-3.7-Sonnet ★	0.02	0.083	0.16	0.089	0.12	0.092	0.61	0.1	-0.19	0.082

Varying thinking tokens for strong open- and closed-source models (Figure 6) shows marginal impact, confirming the benchmark's difficulty.

6.2 Understanding Empirical Instance Difficulty:

To investigate whether the <$\vec{i}$, $\vec{p}$, $\vec{o}$> triple instance complexity predicts empirical instance difficulty (as described in Section 5.4), we first visualize the distribution of inverse pass rate difficulty, d_{pass}, across different cascade lengths, relation counts, and input-output distances in Figure 2. We observe a nearly monotonic trend between each complexity feature and empirical difficulty. We also analyze the correlations between these features and both d_{pass} and inverse edit_sim difficulty d_{edit} in Table 5. While most features show statistically significant positive correlations with difficulty, the majority are only weakly or very weakly correlated. Cascade length and input-output distance exhibit the strongest correlations. We believe this reflects the multi-faceted nature of difficulty, where factors like relations, cascade length, and input-output distance each contribute, but none alone serves as a strong predictor. Additionally, the count of bleeding relations shows no statistically significant correlation. An analysis of relation counts in program sequences after removing the "degenerate programs" revealed that only 2 out of 992 instances contained one or more bleeding relations. This highlights a limitation of our current rejection sampling approach.

6.3 Model-wise Instance Difficulty Breakdown

Finally, to understand which complexity features of an <$\vec{i}$, $\vec{p}$, $\vec{o}$> triple each model struggles with, we perform logistic regression analysis on the inverse pass rate difficulty, d_{pass}. Specifically, we treat the complexity features like the counts of the F, CB, CF relations, cascade length, and input-output distance as the independent variables and d_{pass} as the dependent variable. We exclude bleeding here due to its infrequency as seen in section 6.2. Table 2 depicts the regression coefficients for each complexity feature per model. We observe that cascade length and input-output distance affect the log probability of sample difficulty the most, while the relation counts individually have a lower impact. However, there is a noticeable difference between the transparent relation (feeding) and the opaque relations (counter-feeding and counter-bleeding). As predicted, weaker models struggle more with opaque relations compared to better-performing models. For both feeding and counter-feeding features, reasoning models generally yield coefficients with smaller magnitudes compared to non-reasoning models. This trend supports the hypothesis that reasoning models are better suited for PBE tasks and are more robust to the presence of complex relational structures within programs.

7 Discussion

While reasoning models have been successful at math and coding tasks, this paper addresses a question posed by earlier researchers Naik et al. [2024, 2025]: **Are reasoning models useful for practical and scientifically important problems like historical linguistics?** While Naik et al. [2025] showed that LLMs can succeed at very simple forward reconstruction tasks, especially when trained on carefully designed synthetic data, we evaluate the latest advancement in modeling, reasoning models, on more realistic and complex forward reconstruction problems. These problems feature cascades with multiple programs (and with multiple relations between programs). This was enabled by three technical innovations: (1) algorithms for classifying pairs of arbitrary string rewrite programs as feeding, bleeding, or neutral, (2) a proof of the algorithms' correctness, and (3) a rejection sampling method that facilitated the generation of large numbers of problems at scale. This pipeline yielded a set of nearly 1k instances that even state-of-the-art reasoning LLMs struggle with. Claude-3.7-Sonnet, the best-performing model, achieves only a 54% pass rate and while it can solve some (33%) complex problems, it fails to solve nearly 40% of the simple problems.

The benchmark reveals two things: (1) Reasoning models have great potential to solve more realistic forward reconstruction problems (2) They still struggle with several complexity features (e.g. cascade length and complex relations between programs) and as consequence are not reliable enough to be employed in practice for forward reconstruction. Given the kind of benchmark we have developed (limited though it is by "degenerate programs" and skews in the program distribution), it is now possible to evaluate how well reasoning models perform on tasks that involve abstract inductive reasoning and planning. Work like this will blaze the trail towards reasoning models able to induce programs from pairs of examples without relying on heuristic crutches or domain knowledge.

8 Conclusion & Future Work

Most state-of-the-art LLMs, including the latest reasoning models, struggle with the kind of inductive reasoning needed in historical linguistics. Our results highlight the need to investigate the cause and explore better training methods, like verifier-based reinforcement learning, to better align models with historical linguists' needs. We also plan to improve our benchmark generation pipeline in terms of sampling efficiency and improving the rejection sampling constraints to avoid degenerate programs to generate even more challenging problems.

9 Limitations

Although the benchmark generation process proposed by our study is successful at finding challenging problems, it does suffer from some key limitations that need to be improved to generate more diverse and challenging data. Firstly, sampling efficiency is a concern since the rejection sampling process discards too many data points (roughly 94% of the generated data is discarded), which makes it harder to apply additional constraints. Additionally, it also produces a lot of "degenerate programs" especially for bleeding relations which makes the data distribution less challenging and diverse. Other limitations include the fact that our regression analysis sometimes fails to obtain good estimates for coefficients (high std. error) and the complexity features like cascade length and input-output distance are also highly correlated (since a longer cascade with naturally lead to more changes between the input and output) which means the complexity features aren't truly independent.

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A Benchmark Details

A.1 Licensing

We create a new benchmark for a completely logical version of the task of forward reconstruction that requires inductive reasoning and multi-step planning. Our benchmark contains 992 instances and is released under the CC BY-SA 4.0 license. Additionally, we produce code that allows you to sample more data, which we also release under the MIT license.

A.2 Benchmark Statistics

Figure 3 shows the distribution of all complexity features in our dataset.

Top left: The B, F, CB, and CF counts reveal that most instances have no relations; 10.6% have one, and only 2.4% have two or more. This suggests unexpectedly low complexity, likely due to degenerate programs in the ground truth cascades $\vec{p}$. Despite this, even strong models like Claude-3.7-Sonnet struggle with the data.

Top middle: Feeding is the most common relation type, present in 85 instances. In contrast, counter-feeding and counter-bleeding are rare, and bleeding occurs in only two cases. This skew likely results from the removal of degenerate programs, many of which were involved in bleeding relations.

Top right: Cascade lengths are mostly short, with 70.6% of instances having a single-program ground truth. Still, 25% have two programs, and 5% have more than two, indicating some structural complexity.

Bottom left: Normalized Levenshtein distance between inputs and outputs is low in most cases: 74.5% are below 0.2, 23.5% fall between 0.2 and 0.4, and only 2% exceed 0.4. No instance exceeds a distance of 0.6.

Bottom right: Word-level differences show that 46% of examples differ by one word, 31% by two, 17% by three, 5% by four, and 1% by all five, reflecting a range of surface-level complexity.

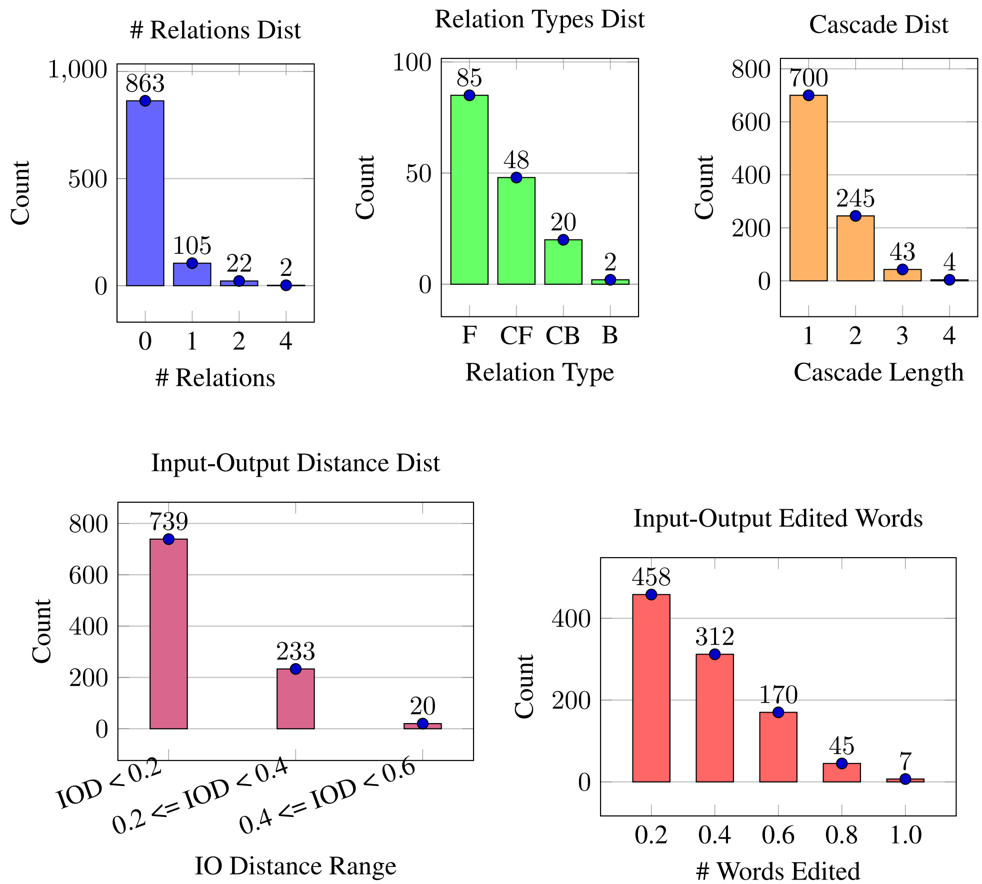

Figure 3: Distribution plots for complexity features in our benchmark.

B Method Details

B.1 Program Extraction

Since we evaluate all kinds of LLMs, including reasoning models that may first produce intermediate outputs and then iteratively refine or improve them by reflection, we account for this by evaluating both the first and last code block produced by each model.

B.2 Prompt Template

We show the prompt template used for the PBE forward reconstructions task below. This prompt includes the exact instructions and examples given to all the LLMs for performing this task.

PBE Forward Reconstruction Prompt

Follow the instructions below to solve the code completion task:
We will provide the input corpus and corresponding output corpus. Each element in the corpus is a string, and the output is transformed from the corresponding input using an ordered sequence of "replace" programs. You need to find the correctly constructed and ordered sequence of "replace" programs to transform the entire input corpus into the output corpus. Note that the programs can interact with each other in a way that reduces or increases the number of times they are applied on a given input based on where they are ordered in the sequence. This makes it very important to apply them in the correct order.
The programs should be written using only the Python `replace` function. For example, for a program that replaces all occurrences of "ab" with "bc" it should be written as: `replace('ab', 'bc')`
Here is an example of the full task:

```
### Inputs
["abc", "ebc", "aba"]

### Outputs
["edc", "edc", "aba"]

### Program Sequence
```python
["replace('bc','dc')", "replace('ad','ed')"]
```

While generating the program sequence, you need to abide by the following restrictions:

1. Each program must transform exactly {program_length} characters. For example if program_length = 2 it only allows programs like `replace('bc','dc')` since 'bc' and 'dc' both have 2 characters but programs such as `replace('abc','dc')` or `replace('bc','adc')` are not allowed since input length 'abc' and the output length 'adc' of the respective programs are greater than 2.
2. The maximum number of programs is {program_num}
3. You should only consider the Python "replace" function for specifying programs (each program is a Python replace function). You cannot use any other Python modules or functions.
4. Strictly follow the markdown style convention while presenting your final program sequence, and make sure to enclose it in the ` ```python ` markdown style code block.

Now, please generate the sequence of programs corresponding to the following input corpus and output corpus:

```
Inputs
{inputs_list}

Outputs
{outputs_list}

Program Sequence
```

B.3 Licenses for Evaluated Models

We list the licenses used for each evaluated open and closed source models in Table 3.

C Experimental Details

C.1 Empirical Difficulty

We define the empirical difficulty as the observed difficulty of an <$\vec{i}, \vec{p}, \vec{o}$> triple based on the ability of the set of evaluated models $\mathcal{M}$ to come up with a functionally correct solution. Specifically we
```

Table 3: Licenses for open and closed source models.

Model	License
Qwen2.5-32B-Instruct	Apache 2.0
Qwen3-32B-Instruct	Apache 2.0
Claude-3.5-Sonnet	API (Anthropic EULA)
Codestral-22B	Mistral Non-Production License (MNPL)
Qwen2.5Coder-32B-Instruct	Apache 2.0
QwQ-32B	Apache 2.0
DeepSeek-R1-Distill-Qwen-32B	MIT
o3-mini	API (OpenAI EULA)
o4-mini	API (OpenAI EULA)
Gemini 2.5 Flash Preview 04-17	API (Google EULA)
Claude-3.7-Sonnet	API (Anthropic EULA)
Qwen3-30B-A3B	Apache 2.0
DeepSeek-R1	MIT

operationalize it by averaging the inverted pass@1 (d_{pass}) or edit_sim (d_{edit}) for a given <$\vec{i}, \vec{p}, \vec{o}$> triple across all models $M \in \mathcal{M}$ as follows (where $\hat{\vec{p}} = M(\vec{i}, \vec{o})$):

$$d_{pass}(\vec{i}, \vec{p}, \vec{o}) = \frac{1}{|\mathcal{M}|} \sum_{M \in \mathcal{M}} 1_{\hat{\vec{p}}(\vec{i}) \neq \vec{o}}$$

$$d_{edit}(\vec{i}, \vec{p}, \vec{o}) = \frac{1}{|\mathcal{M}|} \sum_{\hat{\vec{p}} \in \mathcal{M}(\vec{i}, \vec{o})} \frac{\mathrm{dist}(\hat{\vec{p}}(\vec{i}), \vec{o})}{\mathrm{dist}(\vec{i}, \vec{o})}$$

C.2 Instance Complexity

For the instance complexity, we utilize three kinds of features: 1) counts of B, F, CB, CF relations, 2) number of programs in the ground truth program sequence $\vec{p}$, and 3) the normalized Levenshtein edit distance between the inputs ($\vec{i}$) and outputs ($\vec{o}$) or $\mathrm{dist}(\vec{i}, \vec{o})$. Additionally, we discard the degenerate programs described in 5.1 before extracting the complexity features.

C.3 Inference/Sampling Parameters

We show the sampling parameters used for all the models in Table 4. The max tokens are the total output tokens the model can generate (including thinking tokens), while the thinking budget(s) captures only the chain-of-thought or reasoning related tokens. The top-p is the cumulative probability cutoff used for nucleus sampling, while the temperature is for controlling the degree of randomness in the sampling. We report the max tokens and thinking tokens wherever possible based on the providers (for some models you can only control the total tokens, while for some you can only control thinking tokens). For some models like Gemini 2.5 Flash Preview, the model has a mode where it first reasons about how much thinking is required based on how complex it determines the problem to be. We use this setting for the experiments in Table 1. However, we also do experiments comparing the effect of varying token budgets (2048, 4096, 8192) for QwQ and Gemini 2.5 Flash Preview, hence we highlight the default setting used for Table 1 for these models in bold.

D Additional Results

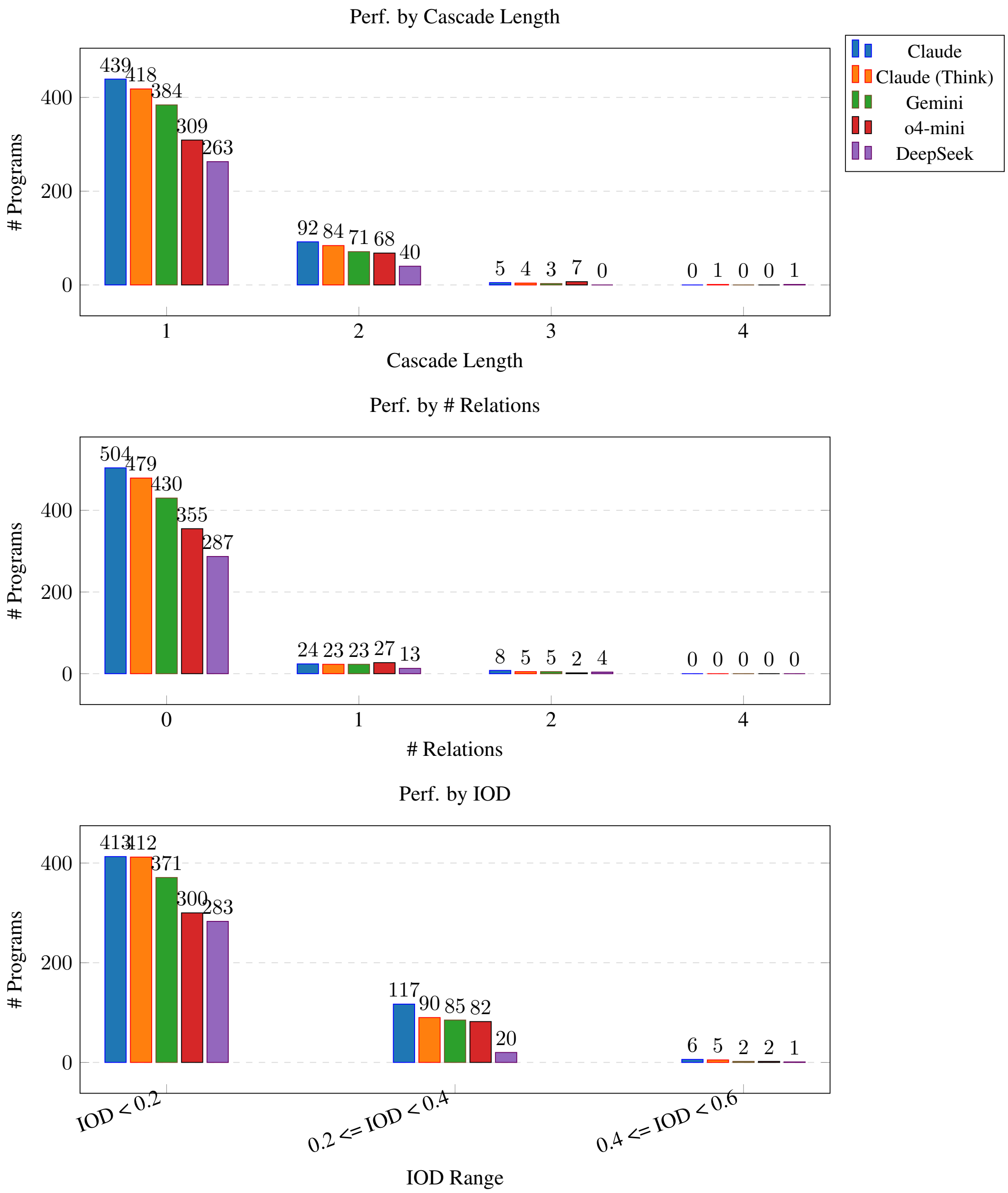

Figure 4: Model performance breakdown across different structural features.

Table 4: Sampling parameters used for inference across all models. “Max tokens” refers to the total number of tokens (output + thinking tokens) for models that support it. "Top-p" controls nucleus sampling. "Temperature" sets the randomness of token selection. "Thinking budget" is the number of thinking tokens, applicable only to models that support this feature.

Model	Max Tokens	Top P	Temperature	Thinking Budget(s)
Codestral-22B	2048	0.95	0.7	-
Qwen2.5-32B-Instruct	512	0.95	0.7	-
Qwen2.5Coder-32B-Instruct	512	0.95	0.7	-
QwQ-32B	-	0.95	0.6	2048, 4096, **8192**
Qwen3-32B	2048	0.95	0.7	-
Qwen3-30B-A3B	2048	0.95	0.7	-
DeepSeek-R1-Distill-Qwen-32B	2048	0.95	0.7	2048
DeepSeek-R1	32768	0.95	0.7	dynamic
o3-mini	-	0.95	0.7	4096
o4-mini	-	0.95	0.7	4096
Gemini 2.5 Flash Preview 04-17	dynamic	0.95	0.7	**dynamic**, 2048, 4096, 8192
Claude-3.5-Sonnet	2048	0.9	0.5	-
Claude-3.7-Sonnet	2048	0.9	0.5	-
Claude-3.7-Sonnet (Thinking Mode)	12000	-	1	2048

Table 5: **Understanding empirical instance difficulty:** Spearman Rank (ρ) and Kendall Tau (τ) correlation between the instance difficulty (d_{pass}) and (d_{edit}) and all the complexity features.

Instance Difficulty	Bleeding		Feeding		Counter-Bleeding		Counter-Feeding		Cascade Length		Input-Output Dist	
	r	p value	r	p value	r	p value	r	p value	r	p value	r	p value
d_{pass} (ρ)	0.06	p >0.05	0.2	p <0.0001	0.09	p <0.005	0.17	p <0.0001	0.39	p <0.0001	0.33	p <0.0001
d_{pass} (τ)	0.05	p >0.05	0.18	p <0.0001	0.08	p <0.005	0.15	p <0.0001	0.33	p <0.0001	0.24	p <0.0001
d_{edit} (ρ)	0.02	p >0.05	0.13	p <0.0001	0.11	p <0.0005	0.1	p <0.005	0.14	p <0.0001	0.17	p <0.0001
d_{edit} (τ)	0.02	p >0.05	0.11	p <0.0001	0.09	p <0.0005	0.08	p <0.005	0.12	p <0.0001	0.12	p <0.0001

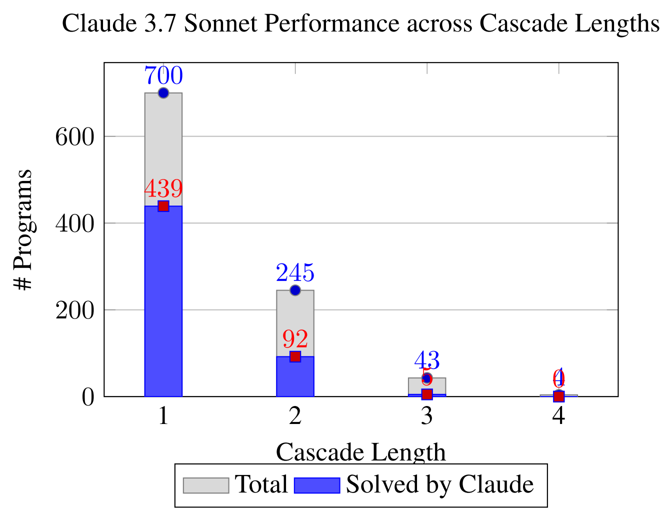

Figure 5: Superimposed performance bars for Claude 3.7 Sonnet.

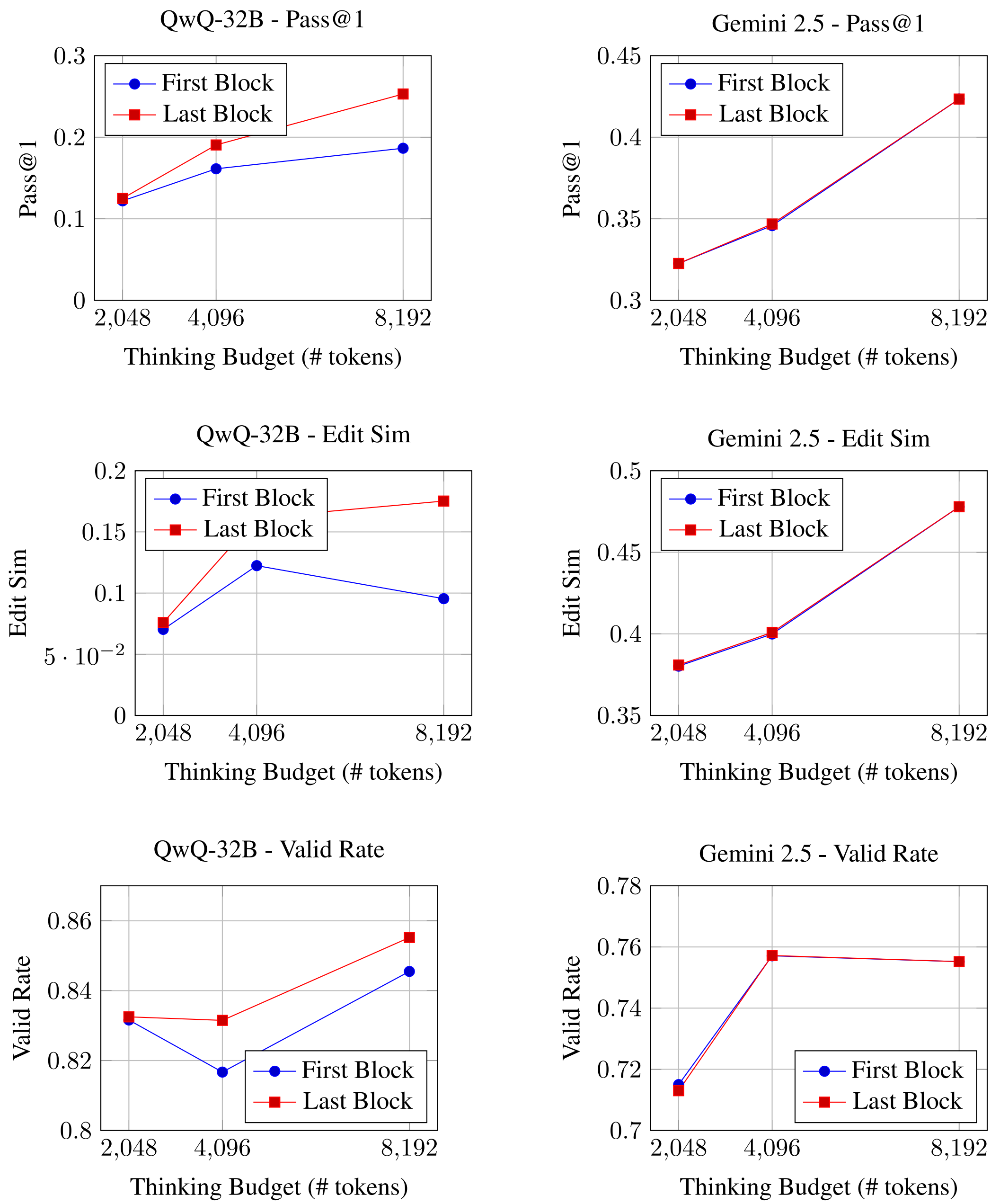

Figure 6: Evaluation Metrics comparison between **QwQ-32B** and **Gemini 2.5 Flash Preview 04-17** across variable thinking budgets (number of tokens)