LANGUAGE MODELS CAN (KIND OF) REASON: A SYSTEMATIC FORMAL ANALYSIS OF CHAIN-OF-THOUGHT

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ABSTRACT

Large language models (LLMs) have shown remarkable reasoning capabilities given chain-of-thought prompts (examples with intermediate reasoning steps). Existing benchmarks measure reasoning ability indirectly, by evaluating accuracy on downstream tasks such as mathematical reasoning. However, it is unclear *how* these models obtain the answers and whether they rely on simple heuristics rather than the generated chain-of-thought. To enable systematic exploration of the reasoning ability of LLMs, we present a new synthetic question-answering dataset called PRONTOQA, where each example is generated from a synthetic world model represented in first-order logic. This allows us to parse the generated chain-of-thought into symbolic proofs for formal analysis. Our analysis on INSTRUCTGPT and GPT-3 shows that LLMs are quite capable of making correct individual deduction steps, and so are generally capable of reasoning, even in fictional contexts. However, they have difficulty with *proof planning*: When multiple valid deduction steps are available, they are not able to systematically explore the different options.

1 INTRODUCTION

The ability to reason—drawing new conclusions from provided facts—is a hallmark of human intelligence. Recently, chain-of-thought (CoT) prompting has enabled large language models (LLMs) to perform logical reasoning tasks with impressive accuracy (Wei et al., 2022b; Chowdhery et al., 2022; Lewkowycz et al., 2022). In CoT prompting, each example consists of a *question* (e.g., "$\frac{6}{3} - 1$?"), a short description of the reasoning required to answer the question called the *"chain-of-thought"* (e.g., "$\frac{6}{3}$ is 2. $2 - 1$ is 1."), and a *label* (e.g., "1"). When prompted with a few CoT examples, the elicited reasoning allows LLMs to predict the label with much higher accuracy than standard question-answer prompting. However, it is unclear to what extent these models can reason due to several confounding factors. First, existing studies primarily rely on question-answering tasks from real-world settings such as math word problems (Cobbe et al., 2021; Han et al., 2022; Weston et al., 2016). It is likely that LLMs have already acquired the knowledge through pretraining and simply retrieve the answer rather than reason over it. Second, the reasoning task may contain spurious correlations that allow the model to obtain the correct answer through shortcuts (Zhang et al., 2022). In this work, we systematically investigate the reasoning capability of LLMs by directly evaluating their predicted chains-of-thought (the interpretable proof steps), rather than the predicted label.

To enable easy analysis of the CoT, we construct a new synthetic question-answering dataset called PRONTOQA, for **Pr**oof and **Onto**logy-Generated **Q**uestion-**A**nswering, where each example is generated from an ontology and has a unique proof (see figure 1 for an example). We convert the proofs into syntactically simple sentences using a simple grammar so that the inverse process is relatively easy: From the predicted CoT, we are able to semantically parse each sentence into a formal language and reconstruct the underlying proof steps. We then directly analyze the model's reasoning by inspecting each step in the reconstructed proof and comparing them against the groundtruth proof.[1]

We systematically evaluate INSTRUCTGPT (Ouyang et al., 2022) and the original GPT-3 (Brown et al., 2020) on PRONTOQA by controlling a number of variables that characterize the complexity of the reasoning task, such as the ontology type and the number of proof steps required. Our analysis shows that these models are quite good at producing valid *individual* proof steps, even on fictional and counterfactual ontologies. However, LLMs have difficulty with *proof planning*: when the models encounter a point in the proof where multiple valid proof steps are available, they sometimes select

[1] All code and data generation scripts are available at `[anonymized]`.

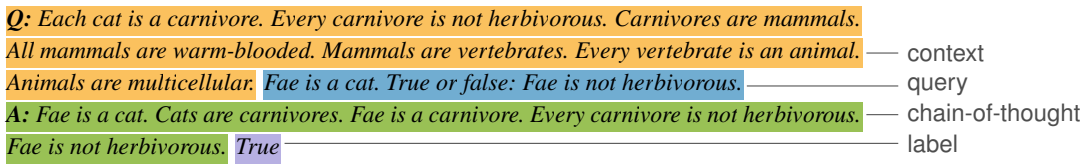


FIGURE 1: A question-answering example from PRONTOQA, with each component highlighted and labeled.

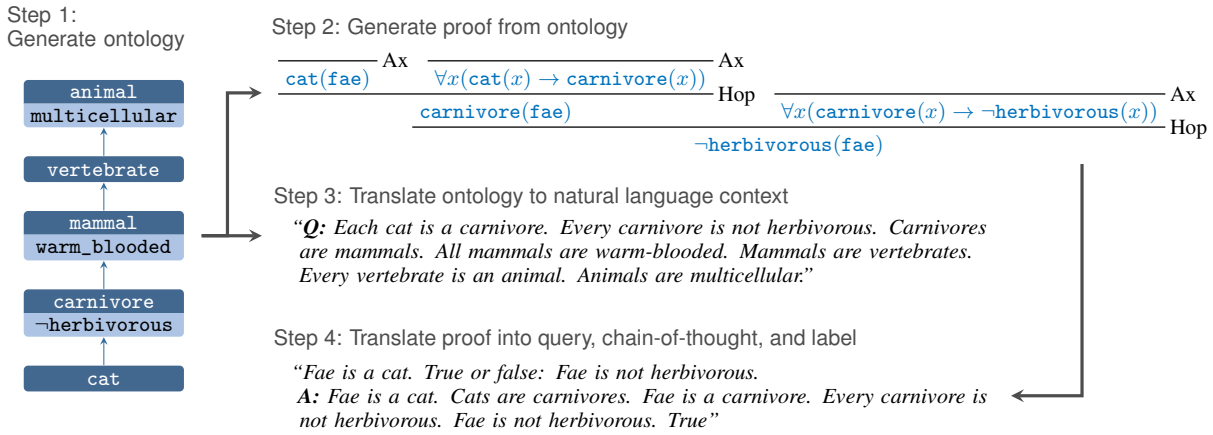


FIGURE 2: Schematic of the generative process for each example in PRONTOQA. **Step 1:** We generate an ontology from a prior distribution, shown here as a tree. Each node denotes a concept (e.g. `mammal`), each with an optional property (e.g. `warm_blooded`), and each blue edge denotes a "subtype of" relation. **Step 2:** Generate proof from the ontology. Each horizontal black line indicates a proof step, with its premises written above the line and the conclusion written below. **Step 3:** Convert the ontology into a natural language context. **Step 4:** Convert the proof into a natural language query, chain-of-thought, and answer label. There is a one-to-one correspondence between the conclusion of each proof step and the sentences in the chain-of-thought.

the wrong step, and this often leads to an incomplete proof and subsequently an incorrect answer. Interestingly, the models are much less likely to be misled with a true ontology, suggesting that the world knowledge acquired during pretraining plays an important role in LLM reasoning.

2 RELATED WORK

There are a number of research directions related to our work. There are efforts to tweak or extend CoT prompting to elicit more sophisticated reasoning behavior (Creswell et al., 2022; Anil et al., 2022; Dohan et al., 2022), and they have shown that these prompting extensions to CoT can improve the elicited reasoning behavior of LLMs, even with smaller models. Rather than presenting a new prompting approach, the goal of this work is to measure the reasoning ability elicited by CoT. There are other datasets that have been designed or used to measure the reasoning capabilities of transformer-based models and LLMs (Han et al., 2022; Tafjord et al., 2021; Weston et al., 2016). They show that LLMs are able to answer questions that require reasoning in the few-shot setting with reasonable accuracy. These datasets are largely consistent with the real-world, and so they may confound measuring reasoning ability with retrieval ability. In addition, they evaluate the predicted labels, which may not necessarily be a good measure of reasoning ability. As in our approach, Dasgupta et al. (2022) specifically looked at whether LLMs can reason in fictional or counterfactual settings and found that reasoning ability is indeed negatively affected in these settings. However they did not analyze individual steps of reasoning to better understand the cause of the errors. Since we are able to formally evaluate the LLM's predicted CoT step-by-step, we are able to perform a more fine-grained analysis of their reasoning ability. Zhang et al. (2022) showed that BERT is not able to learn to reason robustly, but they did not use CoT prompting and it is not obvious if their results generalize to LLMs, which we evaluate.

There are two broad research approaches for reasoning in NLP: (1) reasoning over a formal symbolic language, possibly with neuro-symbolic methods and/or semantic parsing (Saparov & Mitchell,

2022; Kapanipathi et al., 2021; Dong et al., 2019; Rocktäschel & Riedel, 2017), or (2) reasoning directly over natural language (Chen et al., 2021; Bostrom et al., 2022; 2021; Welleck et al., 2021; Bhagavatula et al., 2020). While PRONTOQA is generated from symbolic ontologies, the examples themselves are in natural language, and so provides value to both research approaches.

3 PRONTOQA: A SYNTHETIC DATASET FOR LOGICAL REASONING

We create a new dataset, called PRONTOQA for **Pr**oof and **Onto**logy-Generated **Q**uestion-**A**nswering, where each question is generated from a symbolic ontology and proof to facilitate formal analysis of the predicted CoT. To focus the scope of our exploration, and to limit the complexity of the generated questions to those within reach of current LLMs, we only consider questions that are answerable using repeated applications of the modus ponens deduction rule. More formally, *modus ponens* is a simple deduction rule where given the premises $\forall x(f(x) \rightarrow g(x))$ and $f(a)$, we conclude $g(a)$ (e.g., given "All cats are carnivores" and "Fae is a cat," we conclude "Fae is a carnivore;" see figure 6 in the Appendix).[2] This rule can easily be chained together to construct proofs with a controllable number of steps.

We generate CoT examples consisting of: the context, query, CoT, and label, where the *context* is a short paragraph containing information relevant to answer the *query* (see figure 1 for an example). Each example is translated from a proof and ontology such that the inverse process is simple: the sentences in an example can be easily and uniquely parsed into symbolic logical forms amenable to formal analysis. More specifically, as shown in figure 2, we: (1) first generate an ontology from a set of concepts, (2) generate a proof by traversing the ontology, (3) translate the ontology into the natural language context, and (4) translate the proof into the query, CoT, and label by mapping logical forms to natural language sentences. We describe each step in further detail below.

Ontology generation. The first step is to generate a small hierarchical *ontology*. The ontology is a collection of concepts (e.g., `mammal`, `cat`, `carnivore`, etc) and subtype relations between them (e.g., $\forall x(\texttt{cat}(x) \rightarrow \texttt{carnivore}(x))$). The ontology also describes properties of concepts (e.g., $\forall x(\texttt{mammal}(x) \rightarrow \neg\texttt{cold_blooded}(x))$). To generate questions that are not overly complex for LLMs, we restrict the ontologies to be *linear* (i.e. in the tree, every node has exactly 0 or 1 child nodes).

Proof generation. We generate proofs from the ontology by choosing a starting node uniformly at random, and generating the initial axiom indicating that an entity has a specific type (e.g., $\texttt{cat}(\texttt{fae})$). Then, we walk up the tree, with each step corresponding to an application of a deduction rule (i.e., a *proof step*). Each proof step consists of zero or more *premises* and one *conclusion*. We stop when we reach a node (e.g., $\texttt{carnivore}(\texttt{fae})$), or a node property (e.g., $\neg\texttt{herbivorous}(\texttt{fae})$), such that the number of generated proof steps matches the target number of steps.

Translation to natural language example. Given a generated ontology and proof, we now translate it into a natural language CoT example consisting of the question (context and query), CoT, and label. We describe how each component is generated below:

We use a simple grammar to convert the formal statements of the ontology into the natural language utterances that make up the context. Every edge in the ontology is converted into sentences such as "All cats are carnivores" or "Every cat is a carnivore." Properties of nodes are also converted into sentences of the form "All mammals are not cold-blooded," etc.

The query is generated by using the same grammar to convert the initial axiom in the proof into a natural language sentence (e.g., "Fae is a cat"). We then determine with probability 0.5 whether to ask if the conclusion of the proof is true or if its negation is false, and convert it into a natural language "true or false" query (e.g., "True or false: Fae is not herbivorous.") and label (e.g., "True").

We convert the ordered sequence of proof steps into the CoT by translating the conclusion of each proof step into a CoT sentence.

Avoiding shortcuts. We have to be careful to remove any shortcuts in the question that would allow the model to "guess" the answer without reasoning. In fact, we find that without any distractors, INSTRUCTGPT is able to predict the "true"/"false" label almost perfectly. INSTRUCTGPT can utilize

[2]Note that in natural deduction, this rule is actually a composition of two deduction steps: given $\forall x(f(x) \rightarrow g(x))$, we use universal elimination to conclude $f(a) \rightarrow g(a)$, and given $f(a)$, we use implication elimination to conclude $g(a)$.

Step type	**Example** (the conclusion of each step is highlighted green)
Strictly-valid atomic correct step, or *canonical step*	*"Fae is a cat. Cats are carnivores. Fae is a carnivore. Every carnivore is not herbivorous. Fae is not herbivorous. True"* **(this is the gold CoT for this example)**
Strictly-valid atomic misleading step	*"Fae is a cat. Cats are carnivores. Fae is a carnivore. Every carnivore is a mammal. Fae is a mammal..."*
Strictly-valid non-atomic correct step	*"Fae is a cat. Fae is a carnivore. Every carnivore is not herbivorous. Fae is not herbivorous. True"*
Strictly-valid non-atomic misleading step	*"Fae is a cat. Cats are carnivores. Fae is a carnivore. Fae is a mammal. Every mammal is a vertebrate..."*
Broadly-valid correct step	*"Fae is a cat. Every cat is not herbivorous. Fae is not herbivorous..."*
Broadly-valid misleading step	*"Fae is a cat. Every cat is a mammal. Fae is a mammal..."*
Invalid step	*"Fae is a cat. Cats are carnivores. Fae is a carnivore. Every carnivore is a cat. Fae is a cat..."*

TABLE 1: The types of proof steps (and examples thereof) into which we categorize each step in the predicted chain-of-thought from LLMs. Compare the given chain-of-thought examples with the gold example provided in the first row.

the heuristic that whether the queried property is mentioned in the context implies whether or not it is true. For instance, if the example is asking "Sally is a cat. True or false: Sally is a vertebrate," the model can simply look for a string "Every ___ is (not) a vertebrate," regardless of the content in the blank. Due to the generative process of these examples, this kind of sentence is guaranteed to appear exactly once in the context. Thus, to ensure that such a heuristic is not informative, we add a distractor sentence by generating a novel concept that is disconnected from the ontology tree, and we assign to this new concept the negation property that is queried by the question. So in the above example, if the ontology has the rule "Every mammal is a vertebrate," a possible distractor sentence is "Every insect is not a vertebrate." We insert this distractor sentence into a random position in the context.

A unique feature of PRONTOQA is that it is easily programmable, with a handful of tunable knobs which we use to generate examples with varying degrees of complexity and study different aspects of reasoning in LLMs. These variables are described in greater detail in section 5.1.

4 FORMAL ANALYSIS OF PREDICTED PROOFS

Instead of measuring the accuracy of the predicted answers (i.e. "true" or "false"), we would like to directly evaluate the predicted CoT to check if the model derives the right answer for the right reason. We endeavor to analyze whether the model is able to apply deduction rules correctly at each proof step (i.e., local correctness), but also whether the model can plan ahead and work toward proving the answer for the query (i.e., global correctness). To measure the local correctness of a given proof step, we compute whether the step follows from one or more applications of deduction rules, and whether it requires additional rules beyond those of the gold proofs. To measure the global correctness, we wish to identify proof steps that deviate from the gold proof.

To achieve this, we parse each sentence of the predicted CoT into logical form. We then compute whether that logical form is provable from previous logical forms via one or more applications of deduction rules. This logical form corresponds to the conclusion of a proof step. We then evaluate the correctness of each proof step by categorizing it according to three dimensions:

1. *Validity:* Is the current proof step provable from previous steps? If it is provable using only the deduction rules that appear in the gold proofs, we say the step is *strictly-valid*. If it is provable with a more powerful proof calculus, like natural deduction, we say the step is *broadly-valid*. Otherwise, we say the step is *invalid*.

   For example, given the premises, "Cats are carnivores" and "Carnivores are mammals," the step with conclusion "Cats are mammals" is broadly-valid since an additional deduction rule is required to prove it: given $\forall x(f(x) \rightarrow g(x))$ and $\forall x(g(x) \rightarrow h(x))$, conclude $\forall x(f(x) \rightarrow h(x))$.

2. *Atomicity:* Is the current proof step provable from previous steps with *exactly one* application of a deduction rule? If so, we say the proof step is *atomic*. Otherwise, it is *non-atomic*. Note that since all broadly-valid steps are non-atomic, this distinction is only useful for strictly-valid steps.

   For example, given the premises, "Fae is a cat," "Cats are carnivores," and "Carnivores are mammals," the step with conclusion "Fae is a mammal" is non-atomic since the step "Fae is a carnivore" was skipped.

3. *Misleading:* If the current proof step's premises are part of the gold proof, but its conclusion is not, then we say the proof step is *misleading*. Otherwise, it is *correct*.

   For example, given the premises "Fae is a carnivore," "All carnivores are not herbivorous," and "Carnivores are mammals," and the goal is to prove "Fae is not herbivorous," the step "Fae is a mammal" is misleading since even though the step is strictly-valid, it does not help in proving the goal.

The types of proof steps are listed in table 1 along with examples. For brevity, we refer to strictly-valid atomic correct steps as *canonical steps*. Psuedocode of the procedure to evaluate proofs is given in algorithm 1 in the Appendix.

Metrics. Given the above categorization of proof steps, we could define the correctness of a proof strictly by requiring the gold proof to be a subset of the predicted proof (so all corresponding proof steps must be canonical). But it is not obvious that this metric, which we call *strict proof accuracy*, would accurately measure the reasoning ability of the model. As such, we also consider more relaxed metrics: (a) we allow predicted proof steps to be strictly-valid non-atomic correct, which we call *"skip" proof accuracy*, (b) we allow predicted proof steps to be broadly-valid, which we call *broad proof accuracy*, or (c) we allow predicted proof steps to be strictly- or broadly-valid, which we call *valid proof accuracy*. The ordering of the sentences in the CoT is important: the conclusion of each proof step must come after the premises.

5 RESULTS

5.1 EXPERIMENTAL SETUP

In each experiment, we generate question-answering examples, perform CoT prompting on the LLMs, and analyze the predicted CoTs. We run the experiments on INSTRUCTGPT (model sizes 350M, 1.3B, 6.7B, 175B versions `001` and `002`) and the original GPT-3 (model size 175B), with greedy decoding (Ouyang et al., 2022; Brown et al., 2020). We use 8-shot in-context learning, so each input to the LLM consists of 8 fully-labeled questions followed by a single test question with missing CoT and label. The model's task is to predict the CoT and label for the test question. Note that all examples across all inputs are independently and identically generated from PRONTOQA.

There are a number of variables that we control when generating examples in PRONTOQA: (1) the number of hops, (2) the ordering of the sentences in the context, and (3) the type of the ontology. The number of hops directly controls the difficulty of the generated example, and we experiment with 1, 3, and 5 hops.

We control the ordering of the context sentences produced by the ontology: We either traverse the tree top-down (i.e. preorder) or bottom-up (i.e. postorder), generating a sentence for each traversed edge/node. The ordering also affects the difficulty of the generated example: if the context sentences are generated bottom-up, they will follow the same order as the steps in the gold proof. On the other hand, if they are generated top-down, the order is reversed, and the task may be more difficult.

To avoid any confounding effects from knowledge acquired during pretraining, PRONTOQA generates examples with fictional concept names (e.g. "wumpus" instead of "cat," etc). But we are also interested in measuring this confounding effect, and so in addition to fictional ontologies, we also generate "true" and "false" ontologies. True ontologies use real concept names and are consistent with the real-world (we randomly sample from a list of three hand-coded real ontologies). False ontologies use real concept names but the trees are generated using the random process described above, and so it is very likely to generate a false statement, such as "All mammals are cats."

For each combination of variables, we run the model on 400 examples, for a total of 48 experiments. We compute 95% confidence intervals for each experiment since the number of correct proofs is distributed according to a binomial with a latent parameter that represents the model's accuracy (Wilson, 1927).

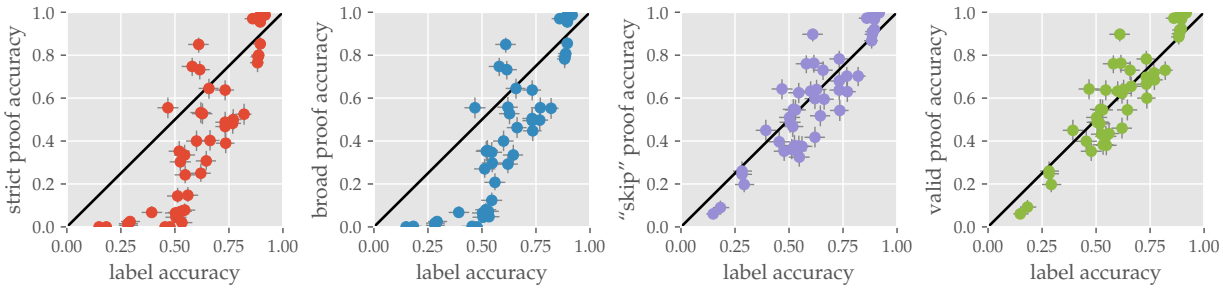


FIGURE 3: Scatter plots of label accuracy vs proof accuracy of all GPT-3 experiments in this paper. The black line indicates perfect agreement between label accuracy and proof accuracy. Label accuracy is not well-correlated with strict or broad proof accuracy, and is better correlated with "skip" and valid proof accuracy, suggesting that label accuracy is a good measure of reasoning ability.

5.2 DO CORRECT ANSWERS IMPLY CORRECT REASONING?

Label accuracy may not necessarily measure whether the model is performing reasoning correctly, since the model may find ways to guess the label via heuristics or spurious correlations. To gauge whether label accuracy is a good metric and which proof accuracy metric is best to measure reasoning ability, we investigate how label accuracy is related to the various proof accuracy metrics. We plot the proof accuracy vs label accuracy (i.e., simply checking whether the predicted label "True" or "False" is correct) of every experiment that we conducted in figure 3. Each point in the scatter plot corresponds to one of our 48 experiments described above. We observe that the label accuracy is poorly correlated with strict proof accuracy, and that strict proof accuracy may underestimate the model's reasoning performance. Rather, the most permissive accuracy metric has the highest correlation with label accuracy, suggesting that GPT-3 is indeed performing the reasoning to answer the question, rather than relying on heuristics. It also suggests that the most permissive proof accuracy metric is most appropriate for measuring the reasoning ability of the model.

5.3 PROOF ANALYSIS RESULTS

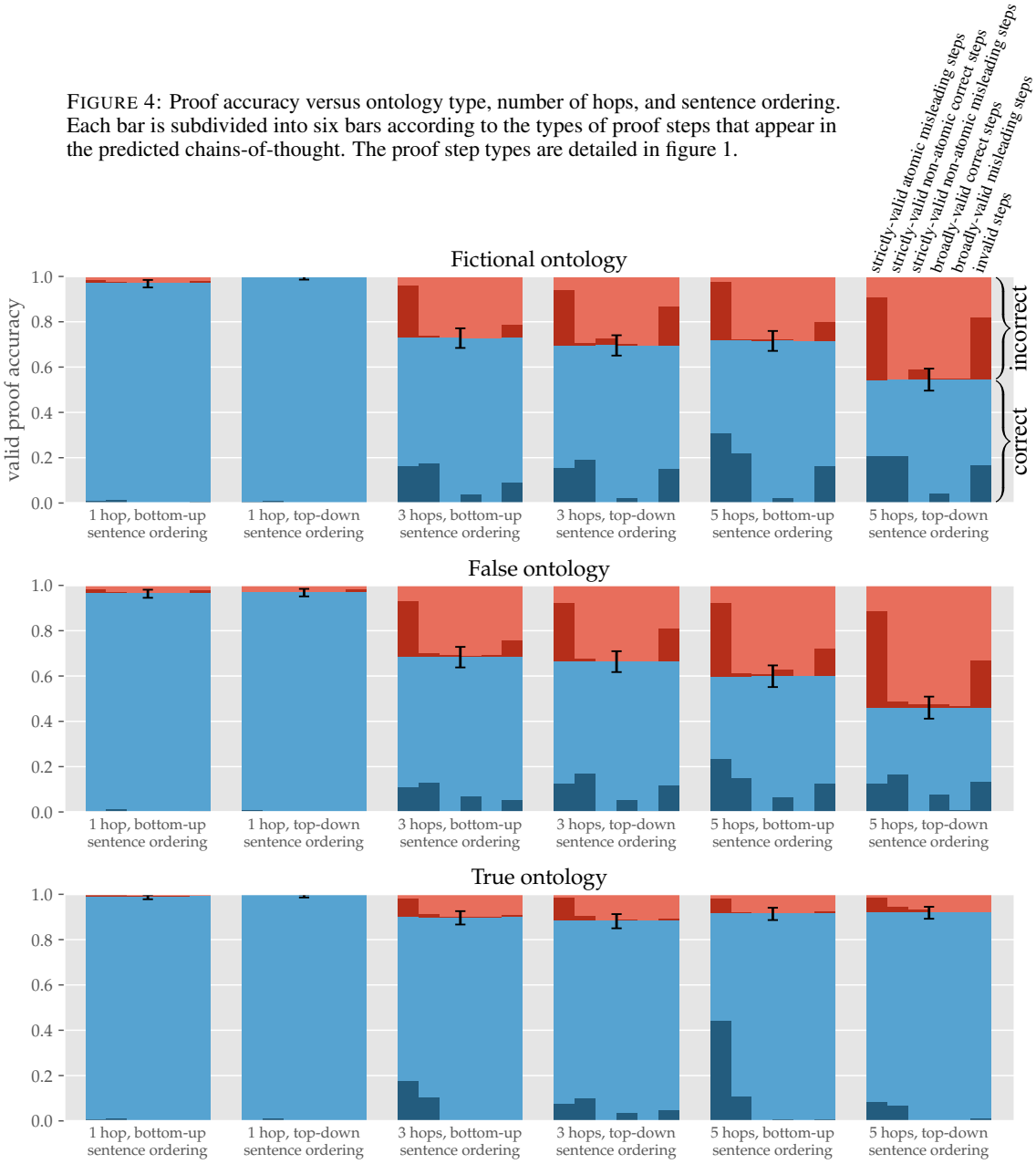
Reasoning is an emergent ability. We investigated how reasoning ability is affected by model size. In figure 7 in the Appendix, proof accuracy increases considerably when increasing the model size from 350M to 1.3B and 6.7B. However, only version `002` of the 175B INSTRUCTGPT model is able to perform better than chance, suggesting that the reasoning ability tested by our experiments could be an emergent ability (Wei et al., 2022a). We were not able to conclusively discern the cause of the significant difference in performance between version `001` and `002`. One possible factor is the maximum token limit of version `002` is roughly twice that of version `001`. In fact, the original GPT-3 seems to perform as well as, if not slightly better than, version `001` of INSTRUCTGPT. In addition, we notice that the frequency of invalid steps decreases as the model size increases, and so larger models seem to be better at making valid steps, whether or not those steps are actually useful.

For the remainder of the paper, our results focus on the 175B INSTRUCTGPT model (version `002`). Our main results are in figure 4 where we show the proof accuracy and distribution of proof step types for all experiments.

Real-world knowledge helps reasoning. We investigate the extent to which reasoning ability is affected by whether the ontology is fictional, "true," or "false." Evidently from figure 4, the LLM seems to perform comparably in the fictional and "false" ontology settings (accuracy is slightly worse with a "false" ontology). However, when using the "true" ontology, the model performs considerably better, and its performance does not deteriorate when increasing the number of hops from 3 to 5. The language model is able to utilize its background knowledge from pretraining to "skip" hops, and is therefore not as negatively affected by the increased number of hops. This is consistent with the findings of Dasgupta et al. (2022).

Evidently, the model's reasoning is heavily reliant on real-world knowledge, and this may be a problem for generalizability: such as when applying LLMs to novel scenarios or to scenarios that are not well-represented in the training data.

FIGURE 4: Proof accuracy versus ontology type, number of hops, and sentence ordering. Each bar is subdivided into six bars according to the types of proof steps that appear in the predicted chains-of-thought. The proof step types are detailed in figure 1.

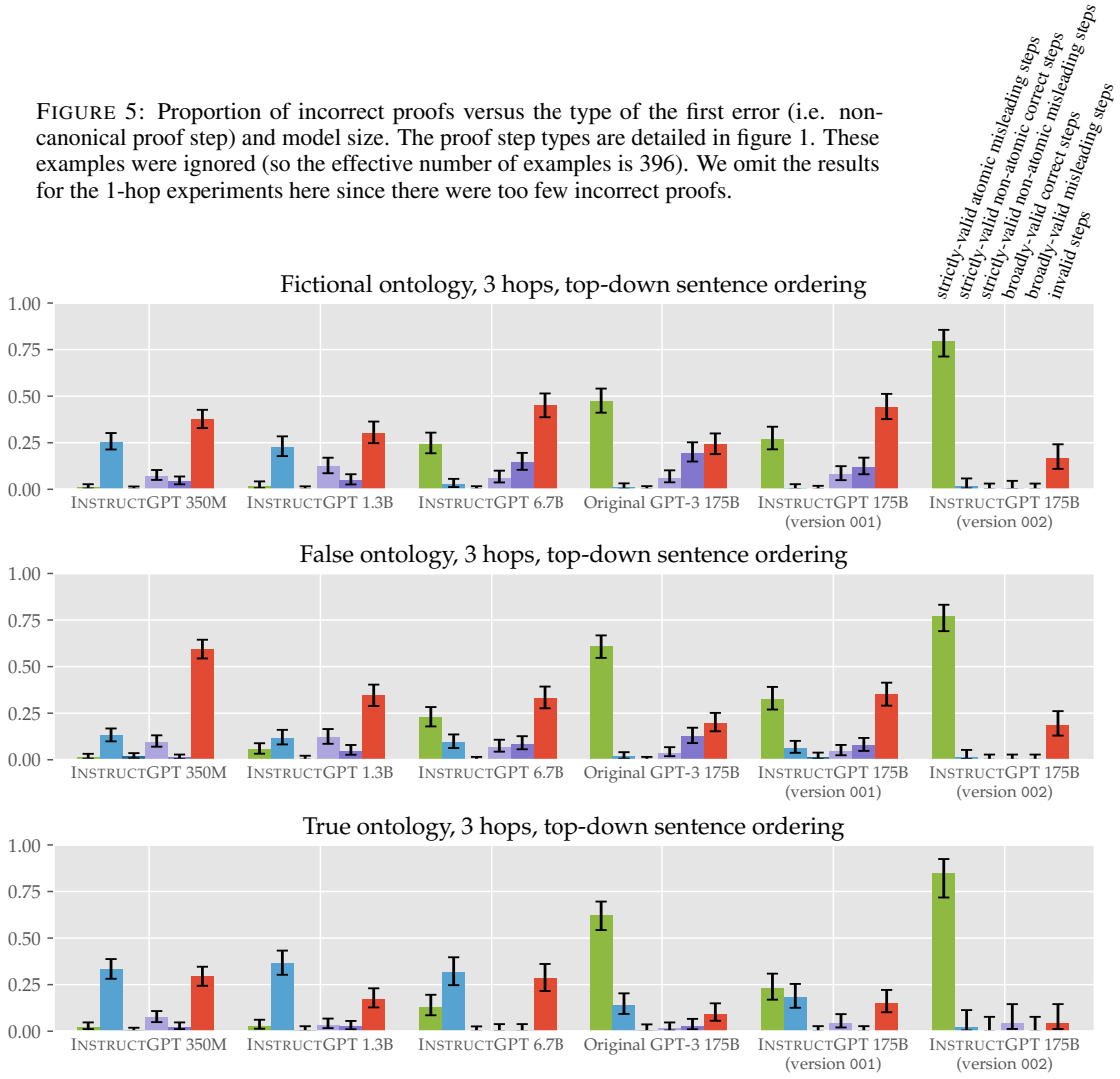


Longer proofs are still challenging. We investigate the extent to which reasoning ability is affected by the number of hops in the proof. We also see from figure 4 that the model handles 1- and 3-hop examples quite accurately but struggles with 5-hop top-down examples, with accuracy falling to chance. So while it is able to perform reasoning to an extent, its ability becomes more limited as the number of hops increases.

Sentence ordering affects reasoning. We also tested how reasoning ability is affected by the ordering of the context sentences. We notice in figure 4 that as the number of hops increases, the model becomes sensitive to the ordering of the sentences (top-down vs bottom-up traversal of the ontology). This may be due to the fact that the order of the gold proof steps mirrors the bottom-up traversal, and is the reverse of the top-down traversal. Thus, the task may be made more difficult for language models if the context sentences are ordered top-down.

How do LLMs reason step-by-step? We explore how often certain types of proof steps appear in correct vs incorrect proofs, and whether proof accuracy is correlated with the presence of specific types of proof steps. Figure 4 breaks down the bars further (in darker red and blue) to indicate the fraction of examples that contain proof steps other than canonical steps. We make the following observations:

FIGURE 5: Proportion of incorrect proofs versus the type of the first error (i.e. non-canonical proof step) and model size. The proof step types are detailed in figure 1. These examples were ignored (so the effective number of examples is 396). We omit the results for the 1-hop experiments here since there were too few incorrect proofs.



1. Most predicted proof steps are strictly-valid, in both correct and incorrect proofs.
2. LLMs tend to skip steps by producing non-atomic steps, just as humans do when they verbalize their reasoning.
3. Most incorrect proofs contain misleading steps and invalid steps. This suggests that the source of the incorrect reasoning is either a due to a misleading step or an invalid step that causes the model to produce steps that do not belong to the gold proof.

Intriguingly, some correct proofs also contain misleading steps and invalid steps, which implies that the model is sometimes able to recover from these "mistakes" and return to the gold proof. We analyze this behavior in greater detail in section 5.4.

5.4 WHAT LEADS TO A MISTAKE?

We investigate whether specific types of proof steps are causing the the largest INSTRUCTGPT model to produce reasoning errors. To do so, we identify the first step in each incorrect proof that is not a canonical step. We observe in figure 5, among incorrect proofs, strictly-valid atomic misleading steps appear in the proof first far more often than other non-canonical step types, including invalid steps. This indicates that for the best-performing models, the main source of reasoning error is from misleading steps, since most predicted steps are strictly-valid and atomic. That is, imagining the space of proof steps as a graph where each edge represents a single valid step, INSTRUCTGPT almost always performs a walk in this graph. Once INSTRUCTGPT encounters a branch where one path at the fork follows the correct proof and the other paths do not, INSTRUCTGPT will select the incorrect direction with some frequency and is then not able to return to the correct path. Therefore, it seems

that while LLMs are able to produce valid proof steps with high probability, they have difficulty with proof planning/strategizing.

We were also curious to see if this relationship held in smaller models. We see in the bottom three rows of figure 5 that smaller models are more prone to making invalid steps or non-atomic steps as their first non-canonical step. But as model size increases, the frequency of these types of steps decreases, and is instead superseded by misleading steps.

Looking again at figure 4, we note that many correct proofs also contain misleading steps, and so it must be the case that INSTRUCTGPT sometimes returns to the correct proof path at some point after making a misleading step. To investigate this behavior more closely, we count the number of steps that the model takes *after* making a misleading step until it produces a step in the gold proof and plot the histogram in figure 9 in the Appendix. We observe that, in general, the more time the model spends outside the correct proof path, the less likely it becomes to return to the correct proof.

6 CONCLUSION AND FUTURE WORK

In this work, we introduced a synthetic fictional question-answering dataset called PRONTOQA designed to evaluate the reasoning ability of LLMs. We evaluated INSTRUCTGPT and GPT-3 on PRONTOQA and found that while the largest model was generally able to perform reasoning, even with fictional and counterfactual inputs, it had difficulty with proof planning and selecting the correct proof step when there are multiple available.

PRONTOQA, and our high-level approach more broadly, could be used to compare LLM reasoning with that of humans, and to explore which aspects of human reasoning were acquired by LLMs from their pretraining. As our work has shown that LLMs are able to reason to a degree, it is yet unclear where the model acquired this ability. Are there portions of the pretraining data that teach the model to reason? Our work shows that relying on CoT prompting is not sufficient for more complex reasoning, such as in mathematical domains. Rather, our results suggest that reasoning systems stand to benefit from more sophisticated proof planning/search strategies, such as neurosymbolic approaches where part of the reasoning can be done over interpretable symbolic structures. PRONTOQA can be used to train new reasoning systems, or to pretrain/fine-tune LLMs to hopefully improve their reasoning capability.

The inability of LLMs to plan ahead in their reasoning might be related to recent work illuminating the theoretical computational limitations of such models (Merrill et al., 2022).

Since our analysis was limited to modus ponens, proof lengths of at most 5, and semantically simple sentences, it remains to be seen whether LLMs are able to produce longer proofs, or reason with other deduction rules, or over more semantically complex sentences/logical forms.

Our analysis also revealed a possible way forward to rectify this shortcoming: Even after making a misleading step, INSTRUCTGPT sometimes "returned" to the correct proof. We could relax the constraint that the chains-of-thought always reflect the shortest correct proof of the answer. It is reasonable for humans to explore a space of possible solutions before arriving at the correct answer, and we could mimic this in LLMs by allowing the CoT to explore alternative paths in the space of proof steps, even if those paths are not ultimately part of the underlying shortest proof. This kind of search strategy is analogous to depth-first search (DFS) in graphs. We could provide in-context examples of chains-of-thought that follow a DFS, with the hope that the model is able to learn to perform DFS when given a new test example, thereby improving the likelihood that it finds the correct answer.

Our results suggest that the model's greedily-predicted CoT may not necessarily maximize the likelihood globally, according to the LLM. As such, we can extend the CoT paradigm where after every predicted step in the CoT, we perform beam search decoding to find the top-k most likely values for the next step. We can then perform beam search over the proof steps (i.e., sentences) rather than over the tokens, in order to hopefully find more globally optimal predicted proofs that lead to the correct answer.

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A DEDUCTION RULES

Figure 6 outlines the two deduction rules that we utilize in PRONTOQA.

Deduction rules in general form

$$\frac{f(a) \quad \forall x(f(x) \to g(x))}{g(a)}\ \text{Hop}$$

$$\frac{}{A}\ \text{Ax}$$

Examples

$$\frac{\texttt{cat}(\texttt{fae}) \quad \forall x(\texttt{cat}(x) \to \texttt{carnivore}(x))}{\texttt{carnivore}(\texttt{fae})}\ \text{Hop}$$

i.e. Given that "Fae is a cat" and "All cats are carnivores," we conclude that "Fae is a carnivore."

$$\frac{}{\texttt{cat}(\texttt{fae})}\ \text{Ax}$$

i.e. Assume that "Fae is a cat" is an axiom.

FIGURE 6: The two deduction rules that constitute the restricted proof calculus in our experiments. All proofs in PRONTOQA are composed of instances of only these two rules. Here, A is any expression, and $f(a)$ is any expression where the variable x in f is substituted with any term a (and similarly for $g(a)$).

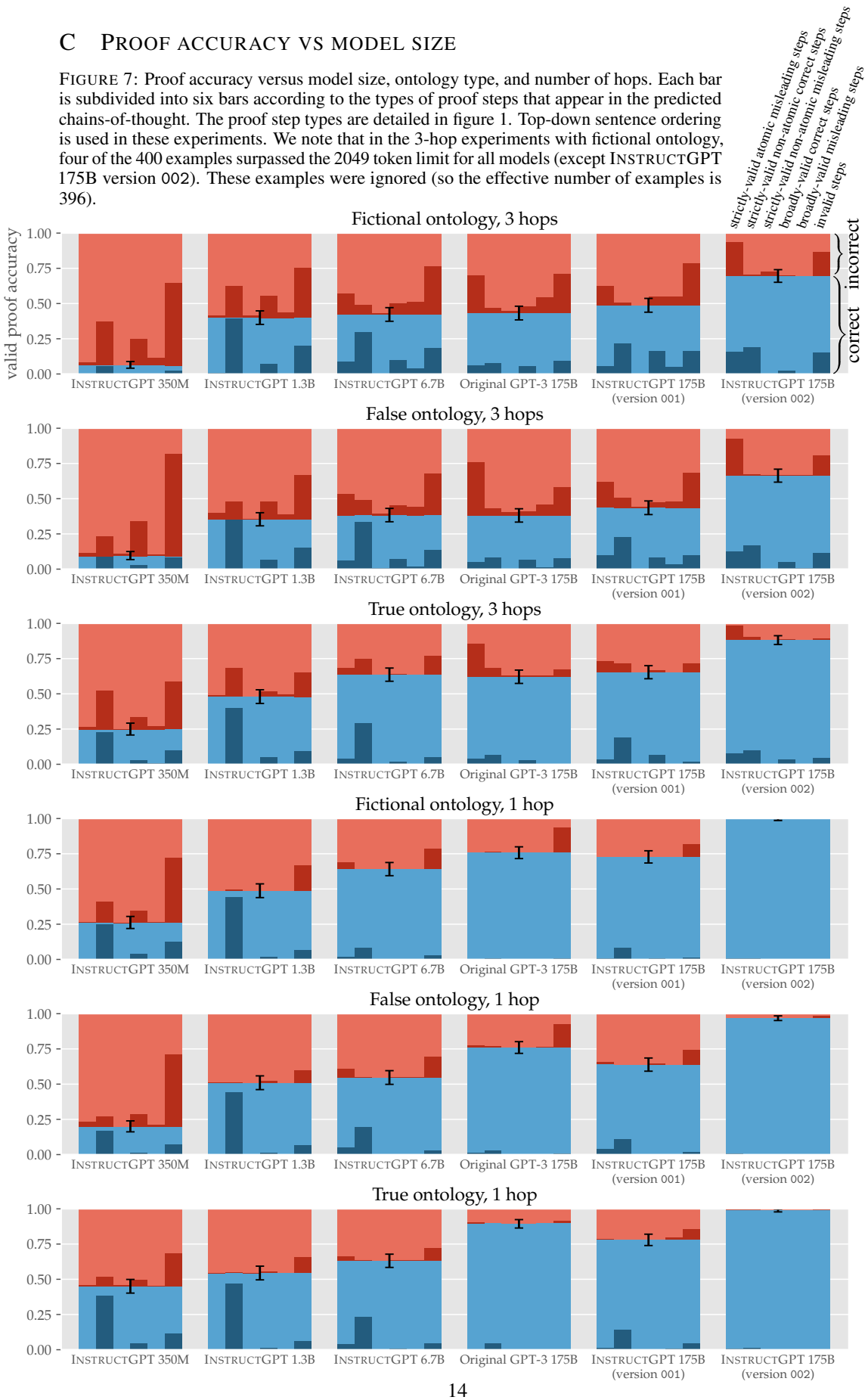
B HOW WE EVALUATE THE CHAIN-OF-THOUGHT

Algorithm 1: Our algorithm for reconstructing and evaluating the proof from the predicted chain-of-thought, and for computing whether each proof step is valid vs invalid, atomic vs non-atomic, misleading vs correct. Here, we use the notation $\varphi[x \mapsto c]$ to denote the substitution of all occurrences of the symbol x with c in the logical form φ. We use the helper function `is_provable` to compute whether a given logical form φ is provable from a set of axioms with one or more deduction rules. The function returns a tuple (P, k) where if $k \geq 0$, φ is provable in k steps using the premises P. Otherwise, φ is not provable.

```
function evaluate_cot(context sentences Q_1, ..., Q_m,
                      predicted chain-of-thought sentences C_1, ..., C_n,
                      gold chain-of-thought sentences T_1, ..., T_r)
    for i ∈ 1, ..., m do                                   /* parse the context */
        L_i^Q = semantic_parse(Q_i)
    for i ∈ 1, ..., r do                                   /* parse the gold chain-of-thought */
        L_i^T = semantic_parse(T_i)
    initialize S as an empty set
    for i ∈ 1, ..., n do                                   /* parse and evaluate the predicted chain-of-thought */
        L_i^C = semantic_parse(C_i)
        (P, k) = is_provable(L_i^C, {L_1^Q, ..., L_m^Q}, S)
        if k ≥ 0
            /* if we wish to use a stricter metric for proof accuracy, we can add
               conditions here (e.g., requiring atomicity by checking k = 1) */
            add L_i^C to S
        if P ⊆ {L_1^T, ..., L_r^T} and L_i^C ∉ {L_1^T, ..., L_r^T}
            /* the premises are in the gold proof but the conclusion is not */
            mark L_i^C as a misleading step
    return L_r^T ∈ S        /* the proof is correct if the final conclusion is provable */
function is_provable(logical form φ, set of axioms A, previous conclusions S)
    if φ ∈ A
        return ({φ}, 1)                                    /* provable by Ax step (strictly-valid) */
    else if φ ∈ S
        return ({φ}, 0)                                    /* already proved by previous step */
    else if φ has form g(c) or ¬g(c) for any constants g and c
        for a ∈ A ∪ S do
            if a has form ∀x(ψ → γ) where γ[x ↦ c] = φ
                (P, k) = is_provable(ψ[x ↦ c], A, S)
                if k ≥ 0
                    return (P ∪ {a}, k + 1{a ∈ A})         /* provable by Hop step (strictly-valid) */
    else if φ has form ∀x(ψ → γ)
        /* note:  we precompute this graph */
        let G be the graph where for any axiom in A with form ∀x(α → β), α and β are vertices and there is a
          directed edge from α to β
        if there is a path in G from ψ to γ
            /* provable with additional deduction rules (broadly-valid) */
            return ( axioms corresponding to path edges , length of path )
    return (∅, −1)                                         /* this step is not provable (i.e., invalid) */
```

C PROOF ACCURACY VS MODEL SIZE

FIGURE 7: Proof accuracy versus model size, ontology type, and number of hops. Each bar is subdivided into six bars according to the types of proof steps that appear in the predicted chains-of-thought. The proof step types are detailed in figure 1. Top-down sentence ordering is used in these experiments. We note that in the 3-hop experiments with fictional ontology, four of the 400 examples surpassed the 2049 token limit for all models (except INSTRUCTGPT 175B version 002). These examples were ignored (so the effective number of examples is 396).



D ADDITIONAL ERROR ANALYSIS

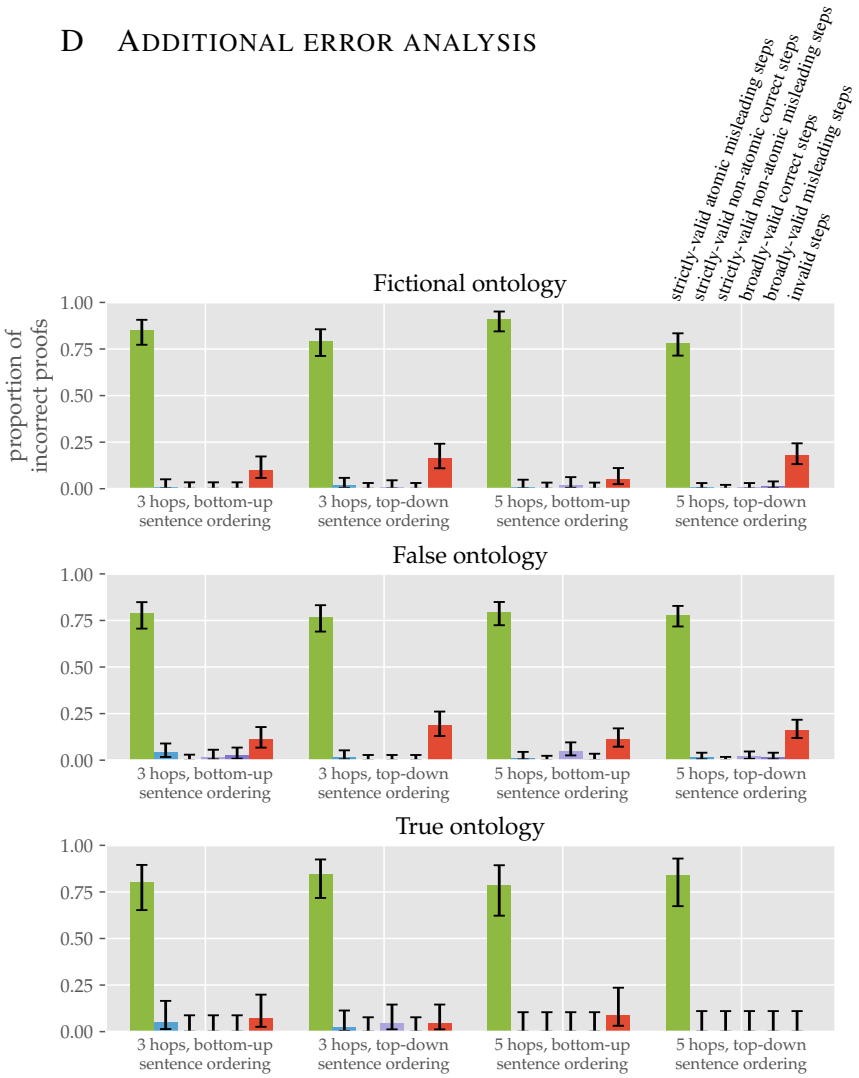


FIGURE 8: Proportion of incorrect proofs versus the type of the first error (i.e. non-canonical proof step), number of hops, and sentence ordering. The proof step types are detailed in figure 1. We note that in the 3-hop experiments with fictional ontology, four of the 400 examples surpassed the 2049 token limit for all models (except INSTRUCTGPT 175B version 002). These examples were ignored (so the effective number of examples is 396). We omit the results for the 1-hop experiments here since there were too few incorrect proofs.

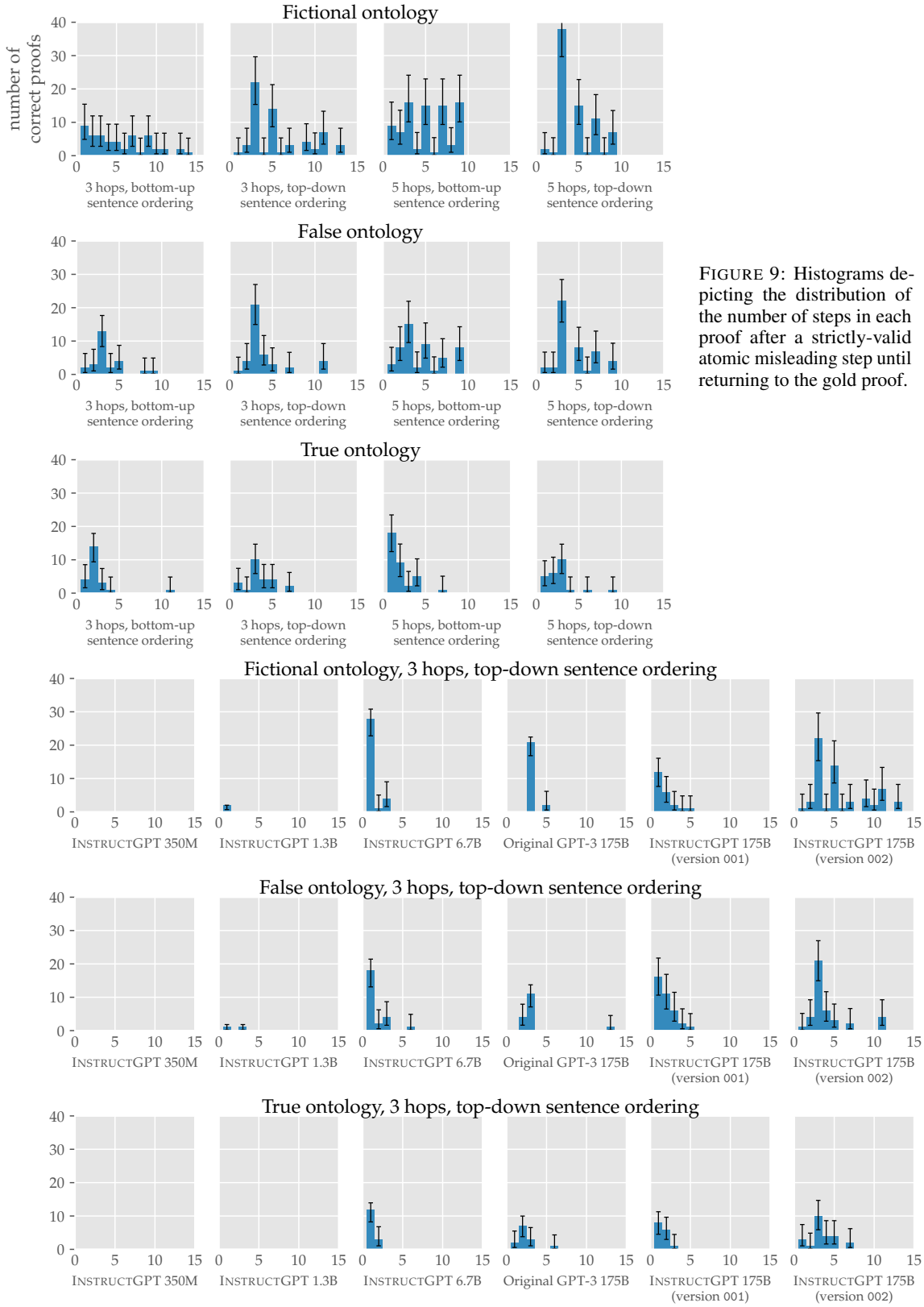


FIGURE 9: Histograms depicting the distribution of the number of steps in each proof after a strictly-valid atomic misleading step until returning to the gold proof.