### LLMs cannot *find* reasoning errors, but can *correct* them!

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#### **Abstract**

While self-correction has shown promise in improving LLM outputs in terms of style and quality (e.g. Chen et al., 2023; Madaan et al., 2023), recent attempts to self-correct logical or reasoning errors often cause correct answers to become incorrect, resulting in worse performances overall (Huang et al., 2023). In this paper, we break down the self-correction process into two core components: mistake finding and **output correction**. For mistake finding, we release BIG-Bench Mistake, a dataset of logical mistakes in Chain-of-Thought reasoning traces. We provide benchmark numbers for several state-of-the-art LLMs, and demonstrate that LLMs generally struggle with finding logical mistakes. For output correction, we propose a backtracking method which provides large improvements when given information on mistake location. We construe backtracking as a lightweight alternative to reinforcement learning methods, and show that it remains effective with a reward model at 60-70% accuracy.

### 1 Introduction

Large Language Models (LLMs) have dominated the field of NLP in recent years, achieving state-of-the-art performance in a large variety of applications. In particular, LLMs have demonstrated the ability to solve tasks with zero- or few-shot prompting, giving rise to prompting methods such as Chain-of-Thought (CoT) (Wei et al., 2022), Self-Consistency (SC) (Wang et al., 2023), ReAct (Yao et al., 2022), etc.

Recent literature on few- or zero-shot prompting has focused on the concept of *self-correction*, i.e. having an LLM correct its own outputs (Shinn et al., 2023; Miao et al., 2023; Madaan et al., 2023; Chen et al., 2023; Saunders et al., 2022). (See Pan et al. (2023) for a review of the literature.)

However, Huang et al. (2023) note that while self-correction may prove effective for improving model outputs in terms of style and quality, there is limited evidence that LLMs can identify and fix their own reasoning and logical errors without external feedback. For example, Reflexion (Shinn et al., 2023) and RCI (Kim et al., 2023) both use ground truth correctness as a signal to halt the self-correction loop. Initially observed by Madaan et al. (2023) on a math reasoning dataset, Huang et al. (2023) further demonstrate this shortcoming of self-correction in 2 additional datasets.

While previous work typically present self-correction as a single process, we divide it into **mistake finding** and **output correction**.

Mistake finding is a fundamental reasoning skill that has been studied and utilised extensively in philosophy, psychology, and mathematics, spawning concepts such as critical thinking, and logical and mathematical fallacies. One might expect that the ability to find mistakes should also be an important requirement for LLMs. However, our results show that state-of-the-art LLMs currently *cannot* find mistakes reliably.

Output correction involves partially or completely changing previously generated outputs. In the context of self-correction, this is typically done with outputs generated by the same model (see Pan et al. (2023) for an overview of different strategies). Despite LLMs' inability to find mistakes, our results show that they can *correct* outputs using our backtracking method, if given information about the mistakes, for example via a small, supervised reward model.

Our contributions for this paper are as follows:

 With Chain-of-Thought prompting, any task can be turned into a mistake-finding task. We collect and release<sup>1</sup> to the research community BIG-Bench Mistake, a dataset of CoT-style traces<sup>2</sup>

<sup>\*</sup>Work done during an internship at Google Research.

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<sup>&</sup>lt;sup>1</sup>https://github.com/WHGTyen/BIG-Bench-Mistake.

<sup>&</sup>lt;sup>2</sup>In this paper, we refer to a set of CoT reasoning steps as

generated using PaLM 2, and annotated according to where the first logical mistake is. To our knowledge, BIG-Bench Mistake is the first dataset of its kind that goes beyond problems in mathematics.

- 2. We produce benchmark results for our dataset to test the reasoning capabilities of state-of-the-art LLMs. We demonstrate that current state-of-the-art LLMs **struggle with mistake finding, even for objective, unambiguous cases**. We hypothesise that this is a main contributing factor to LLMs' inability to self-correct reasoning errors, and we call on the research community to pursue further improvements on the mistake finding task.
- 3. We propose **backtracking** as an output correction technique that makes use of mistake location information to improve performance on the original task. We demonstrate that this method corrects outputs that are originally incorrect, with minimal effect on outputs that are originally correct.
- 4. We construe backtracking as a form of "verbal reinforcement learning" (Shinn et al., 2023), allowing iterative improvement on CoT outputs without requiring any weight updates. We propose that backtracking can be used with a trained classifier as a reward model, and demonstrate the effectiveness of backtracking at various reward model accuracies.

#### 2 BIG-Bench Mistake

BIG-Bench Mistake consists of 2186 sets of CoTstyle traces. Each trace was generated by PaLM 2-L-Unicorn, and annotated with the location of the first logical error. An example trace is shown in Table 1, where the mistake location<sup>3</sup> is the 4<sup>th</sup> step.

Our traces span across a set of 5 tasks<sup>4</sup> from the BIG-bench dataset (Srivastava et al., 2023): word sorting, tracking shuffled objects, logical deduction, multi-step arithmetic, and Dyck languages. CoT

## Sort the following words alphabetically: List: hypochlorite ponderosa phone credulity

Thought 1:	I should start by looking at the first letter of the words in the list. The first letter: "hypochlorite": "h" (8). "ponderosa": "p" (16). "phone": "p" (16). "credulity": "c" (3).
Thought 2:	We now have: (3) "credulity" < (8) "hypochlorite" < (16) ["ponderosa" ? "phone"].
Thought 3:	Now let's sort this subpart ["ponderosa"? "phone"] by looking at their second letters. The second letter: "ponderosa": "o" (15). "phone": "h" (8).
Thought 4:	We now have: (8) "phone" < (15) "ponderosa" for the subpart. Hence, we have "credulity" < "phone" < "ponderosa". (MISTAKE)

Thought 5: I have now sorted all the words. The answer is credulity hypochlorite phone ponderosa

Table 1: Example of a CoT trace for the word sorting task. In this example, there is a mistake in Thought 4 because the ordering "credulity" < "phone" < "ponderosa" is missing the word *hypochlorite*.

prompting is used to prompt PaLM 2 to answer questions from each task. As we wanted to separate our CoT traces into distinct steps, we follow the method used by Yao et al. (2022) and generate each step separately, using the newline as a stop token.

In this dataset, all traces are generated with temperature = 0. The correctness of answers are determined by exact match. Prompts can be found at https://github.com/WHGTyen/BIG-Bench-Mistake.

#### 2.1 Annotation

Each generated trace is annotated with the first logical error. We ignore any subsequent errors as they may be dependent on the original error.

Note that traces can contain a logical mistake yet arrive at the correct answer. To disambiguate the two types of correctness, we will use the terms **correct**<sub>ans</sub> and **incorrect**<sub>ans</sub> to refer to whether the final **ans**wer of the trace is correct. **Accuracy**<sub>ans</sub> would therefore refer to the overall accuracy for the task, based on how many final answers are correct. To refer to whether the trace contains a logical **mis**take (rather than the correctness of the final answer), we will use **correct**<sub>mis</sub> and **incorrect**<sub>mis</sub>.

### 2.1.1 Human annotation

For 4 of the 5 tasks, we recruit human annotators to go through each trace and identify any errors.

a trace.

 $<sup>^{3}</sup>$ As some traces may not contain mistakes, we use the term *mistake location* as a multi-class label that can refer to either the integer N where the  $N^{th}$  step contains the first mistake, or that there are no mistakes.

<sup>&</sup>lt;sup>4</sup>These 5 tasks were selected because 1) Anil et al. (2023) demonstrate that PaLM 2 performs poorly on these tasks, so it is likely to generate mistakes in CoT traces; 2) any mistakes that may occur are likely to be unambiguous, therefore minimising subjectivity during annotation; and 3) identifying mistakes for these tasks does not require expertise knowledge of a specific domain.

Annotators have no domain expertise but are given guidelines<sup>5</sup> to complete the task.

Before annotation, we sample a set of 300 traces for each task, where 255 (85%) are incorrect<sub>ans</sub>, and 45 (15%) are correct<sub>ans</sub>. Since human annotation is a limited and expensive resource, we chose this distribution to maximise the number of steps containing mistakes and to prevent over-saturation of correct steps. We also include some correct<sub>ans</sub> traces because some may contain logical errors despite the correct answer, and to ensure that the dataset included examples of correct steps that are near the end of the trace. This also prevents annotators from feeling forced to find a mistake in all traces. To account for this skewed distribution, results in section 4 are split according to whether the original trace is  $correct_{ans}$  or  $incorrect_{ans}$ .

Following Lightman et al. (2023), annotators are instructed to go through each step in the trace and indicate whether the step is correct or not (binary choice). Annotators only submit their answers until all steps have been annotated, or there is one incorrect step. If an incorrect step is identified, the remaining steps are skipped. This is done to avoid ambiguities where a logically correct deduction is dependent on a previous mistake. We make our annotation guidelines available at https://github.com/WHGTyen/BIG-Bench-Mistake, and we include a screenshot of the user interface in Figure 3.

Each trace has been annotated by at least 3 annotators. If there are any disagreements, we take the majority label. We calculate Krippendorff's alpha (Hayes and Krippendorff, 2007) to measure inter-rater reliability (see Table 2).

Task	Krippendorff's $\alpha$
Word sorting	0.979
Tracking shuffled objects	0.998
Logical deduction	0.996
Multistep arithmetic	0.984

Table 2: Inter-rater reliability for the human-annotated tasks, measured by Krippendorff's alpha.

#### 2.1.2 Automatic annotation

For Dyck languages, we opt for mostly automatic annotation instead of human annotation as the traces show limited variation in phrasing and solution paths.

For each trace, we generate a set of standard

steps based on the format used in the prompt examples. Using pattern matching, we can identify whether each model-generated step also conforms to the same format. If so, we compare the two and assume that the trace is incorrect if the symbols do not match. Additionally, we also account for edge cases such as where the final two steps are merged into one, or variations in presentation where some symbols are placed in quotes and some are not. We release the code at https://github.com/WHGTyen/BIG-Bench-Mistake along with our dataset.

#### 3 Benchmark results

Table 4 shows the accuracy of GPT-4-Turbo, GPT-4, and GPT-3.5-Turbo on our mistake-finding dataset. For each question, the possible answers are either that there are no mistakes, or, if there is a mistake, the number N indicating the step in which the first mistake occurs. A model's output is only considered correct if the location matches exactly, or the output correctly indicates that there are no mistakes.

All models are given the same 3-shot prompts<sup>6</sup>. We use three different prompting methods:

- **Direct trace-level prompting** involves using the whole trace as input to the model and directly prompting for the mistake location. The model must output either the number representing the step, or "No".
- Direct step-level prompting prompts for a binary Yes/No output for every step, indicating whether or not the step is correct. In each generation call, the input contains the partial trace up to (and including) the target step, but does not contain results for previous steps. The final answer is inferred from where the first "No" output occurs (subsequent steps are ignored).
- CoT step-level prompting is an extension of direct, step-level prompting. Instead of a binary Yes/No response, we prompt the model to check the (partial) trace through a series of reasoning steps. This method is the most resource intensive of all three methods as it involves generating a whole CoT sequence for every step. Due to cost and usage limits, we are unable to provide results from GPT-4-Turbo here. As with direct step-level prompting, the final answer is

<sup>&</sup>lt;sup>5</sup>See https://github.com/WHGTyen/BIG-Bench-Mistake for further details.

 $<sup>^6\</sup>mathrm{Prompts}$  can be found at https://github.com/WHGTyen/BIG-Bench-Mistake.

Task	Num. of correct <sub>ans</sub> traces	Num. of incorrect <sub>ans</sub>	Num. of incorrect <sub>mis</sub> traces	Total
Word sorting	45	255	266	300
Tracking shuffled objects	45	255	260	300
Logical deduction	45	255	294	300
Multistep arithmetic	45	255	238	300
Dyck languages	482	504	650	986
Dyck languages (sampled)	88	504	545	592

Table 3: Breakdown of correctness and mistake distribution in our dataset. Correctness<sub>ans</sub> is based on exact matching. Dyck languages (sampled) refers to the set of traces which have been sampled so that the tratio of  $correct_{ans}$  to  $incorrect_{ans}$  traces matches the other tasks.

inferred from where the first "No" output occurs (subsequent steps are ignored).

#### 3.1 Discussion

All three models appear to struggle with our mistake finding dataset. GPT-4 attains the best results but only reaches an overall accuracy of 52.87 with direct step-level prompting.

Our findings are in line with and builds upon results from Huang et al. (2023), who show that existing self-correction strategies are ineffective on reasoning errors. In our experiments, we specifically target the models' *mistake finding* ability and provide results for additional tasks. We show that state-of-the-art LLMs clearly struggle with mistake finding, even in the most simple and unambiguous cases. (For comparison, humans can identify mistakes without specific expertise, and have a high degree of agreement, as shown in Table 2.)

We hypothesise that LLMs' inability to find mistakes is a main contributing factor to why LLMs are unable to self-correct reasoning errors. If LLMs are unable to *identify* mistakes, it should be no surprise that they are unable to self-correct either.

Note that the mistakes in our dataset are generated using PaLM 2 L (Unicorn), and traces were sampled according to whether the final answer was correct or not. Therefore, we expect that using PaLM 2 itself to do mistake finding will produce different and likely biased results. Further work is needed to elucidate the difference between crossmodel evaluation and self-evaluation.

#### 3.2 Comparison of prompting methods

As we compare results across the three methods, we find that the accuracy on traces with no mistakes goes down<sup>7</sup> considerably from direct, trace-level

prompting to CoT, step-level prompting. Figure 1 demonstrates this trade-off.

We hypothesise that this is due to the number of outputs generated by the model. Our three methods involve generating increasingly complex outputs, starting with direct, trace-level prompting requiring a single token, then direct, step-level prompting requiring one token per step, and finally CoT step-level prompting requiring several sentences per step. If each generation call has some probability of identifying a mistake, then the more calls made on each trace, the more likely the model will identify at least one mistake.

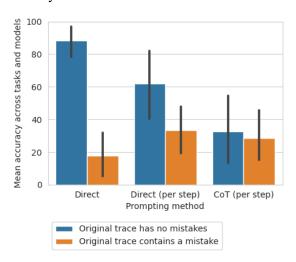


Figure 1: Graph of mistake location accuracies for each prompting method (excluding GPT-4-Turbo which we do not have CoT step-level results for). Blue bars show accuracies on traces with no mistakes, so the model must predict that the trace has no mistake to be considered correct; orange bars show accuracies on traces with a mistake, so the model must predict the precise location of the mistake to be considered correct.

# 3.3 Few-shot prompting for mistake location as a proxy for correctness

In this section, we investigate whether our prompting methods can reliably determine the correctness $_{ans}$  of a trace rather than the mistake location. Our motivation was that even humans

<sup>&</sup>lt;sup>7</sup>Note that the traces in BIG-Bench Mistake are sampled to contain more incorrect<sub>ans</sub> traces than correct<sub>ans</sub> traces (and therefore more incorrect<sub>mis</sub> traces than correct<sub>mis</sub> traces), so the overall mistake location accuracy appears higher for per-step prompting in Table 4, despite the poor accuracy for correct<sub>mis</sub> traces. For a full set of split by correctness<sub>mis</sub>, see

Model	Direct	Direct	CoT (step)				
Model	(trace)	(step)	Cor (sucp)				
W	Word sorting (11.7)						
GPT-4-Turbo	36.33	33.00	_				
GPT-4	35.00	44.33	34.00				
GPT-3.5-Turbo	11.33	15.00	15.67				
Trackir	ng shuffle	ed objects (	5.4)				
GPT-4-Turbo	39.33	61.67	_				
GPT-4	62.29	65.33	90.67				
GPT-3.5-Turbo	10.10	1.67	19.00				
Log	ical dedu	iction (8.3)					
GPT-4-Turbo	21.33	75.00	_				
GPT-4	40.67	67.67	10.33				
GPT-3.5-Turbo	2.00	25.33	9.67				
Multistep arithmetic (5.0)							
GPT-4-Turbo	38.33	43.33	_				
GPT-4	44.00	42.67	41.00				
GPT-3.5-Turbo	20.00	26.00	25.33				
Dyc	k langua	ges† (24.5)					
GPT-4-Turbo	15.33*	28.67*	_				
GPT-4	17.06	44.33*	41.00*				
GPT-3.5-Turbo	8.78	5.91	1.86				
	Over	all					
GPT-4-Turbo	30.13	48.33	_				
GPT-4	39.80	52.87	43.40				
GPT-3.5-Turbo	10.44	14.78	14.31				

Table 4: Mistake finding accuracy across 5 tasks. The average number of steps in the CoT reasoning traces in each task is indicated in brackets. Unless otherwise indicated, the number of traces in each task is shown in Table 3. We also provide scores split by correctness $_{ans}$  of the original trace in Figure B.

- $\dagger$  indicates that traces were sampled to contain 15% correct<sub>ans</sub> and 85% incorrect<sub>ans</sub> traces (see Table 3).
- \* indicates that traces were sampled to contain 45 correct<sub>ans</sub> and 255 incorrect<sub>ans</sub> traces to reduce costs.

use mistake finding as a strategy for determining whether an answer is correct or not, such as when going through mathematical proofs, or working through argumentation. Additionally, one might think that directly predicting the correctness $_{ans}$  of a trace may be easier than having to pinpoint the precise location of an error.

We calculate averaged F1 scores based on whether the model predicts that there is a mistake in the trace. If there is a mistake, we assume the model prediction is that the trace is incorrect $_{ans}$ . Otherwise, we assume the model prediction is that the trace is correct $_{ans}$ .

In Table 5, we average the F1s using  $correct_{ans}$  and  $incorrect_{ans}$  as the positive label, weighted according to the number of times each label occurs.

M- 1-1	Direct Direct (trace) (step)		CoT (step)	
Model				
	Word so	orting		
GPT-4-Turbo	87.73	86.68	_	
GPT-4	81.50	85.12	81.19	
GPT-3.5-Turbo	6.58	35.07	77.79	
Trac	king shuf	fled object	ts	
GPT-4-Turbo	52.23	74.31	_	
GPT-4	76.38	75.69	95.03	
GPT-3.5-Turbo	32.04	77.61	78.11	
I	ogical de	duction		
GPT-4-Turbo	86.46	81.79	_	
GPT-4	84.54	83.38	23.96	
GPT-3.5-Turbo	10.34	67.62	61.31	
Mı	ultistep a	rithmetic		
GPT-4-Turbo	71.17	86.24	_	
GPT-4	72.97	78.67	79.67	
GPT-3.5-Turbo	3.76	53.18	64.08	
	Dyck lan	guages		
GPT-4-Turbo	51.96	85.87	_	
GPT-4	62.33	85.73	79.60	
GPT-3.5-Turbo	46.57	79.31	77.79	

Table 5: Weighted average F1 scores for predicted correctness<sub>ans</sub> of traces across 5 tasks. Baseline is 78 if we only select the incorrect<sub>ans</sub> label. As in Table 4, traces for the Dyck languages task has been sampled to match the ratio of  $correct_{ans}$  to  $incorrect_{ans}$  traces of the other tasks. See Table 3 for a full breakdown.

Note that the baseline of predicting all traces as incorrect achieves a weighted F1 average of 78.

The weighted F1 scores show that prompting for mistakes is a poor strategy for determining the correctness of the final answer. This is in line with our previous finding that LLMs struggle to identify mistake locations, and also builds upon results from Huang et al. (2023), who demonstrate that improvements from Reflexion (Shinn et al., 2023) and RCI (Kim et al., 2023) are only from using oracle correctness<sub>ans</sub> information.

#### 4 Backtracking

Madaan et al. (2023) and Huang et al. (2023) both demonstrate that self-correction is only effective with external feedback – for example, both Shinn et al. (2023) and Kim et al. (2023) rely on oracle labels for improvements – but there is often no external feedback available in many real-world applications.

As an alternative, we explore the possibility of replacing external feedback with a lightweight classifier trained on a small amount of data. Analogous to reward models in conventional reinforcement learning, this classifier detects any logical errors in a CoT trace, which is then fed back to the generator model to improve on the output. This can be done over multiple iterations to maximise improvements.

We propose a simple backtracking method to improve model outputs based on the location of logical errors:

- 1. First, the model generates an initial CoT trace. In our experiments, we use temperature = 0.
- 2. We then determine the mistake location in this trace using a reward model.
- 3. If there are no mistakes, we move onto the next trace. If there is a mistake (e.g. at Thought 4 in the example trace in Table 1), we prompt the model again for the same step but at temperature = 1, generating 8 outputs. We use same prompt and the partial trace containing all steps up to but not including the mistake step (e.g. up to Thought 3, prompting for Thought 4).
- 4. From the 8 outputs, we filter out any options that match what was previously identified as a mistake. From the remaining outputs, we select one with the highest log-probability.
- 5. Finally, with the new, regenerated step in place of the previous one, we generate the remaining steps of the trace again at temperature = 0.

Our backtracking method provides several benefits over existing self-correction methods:

- Unlike Shinn et al. (2023), Kim et al. (2023), etc., our approach does not depend on oracle knowledge of the answer. Instead, it relies on information (for example from trained a reward model) about logical errors, which can be determined on a step-by-step basis using a reward model. Logical errors can occur in correct<sub>ans</sub> traces, or not occur in incorrect<sub>ans</sub> traces<sup>8</sup>.
- Unlike Shinn et al. (2023), Miao et al. (2023), and many others, backtracking does not rely on any specific prompt text or phrasing, thereby reducing associated idiosyncrasies.
- Compared to approaches that require regenerating the entire trace, backtracking reduces computational cost by reusing previous steps that are known to be logically sound.

• Backtracking improves on the quality of the intermediate steps directly, which can be useful in scenarios that require correct steps (e.g. generating solutions to math questions), and also generally improves interpretability.

Backtracking with mistake location information from a reward model can be construed as a lightweight RL method. However, unlike conventional deep reinforcement learning:

- Backtracking with a reward model does not does not require any training of the original generator model. Once the reward model is trained, it can be used for backtracking with any LLM as the generator, and can also be updated independently of the generator LM. This can be especially helpful when LLMs are frequently updated to new checkpoints.
- Backtracking only requires training of a small reward model. Compared to methods that require training of the generator model, backtracking is far more efficient in terms of computing resources and available data.
- The process of backtracking is more interpretable than updating the weights of the generator model directly, as is required for many deep RL methods. It clearly pinpoints the location at which an error occurs, which can help the debugging process and allow faster development and iterations of models.

#### 4.1 Backtracking with gold mistake location

As an initial experiment, we use labels from BIG-Bench Mistake to test if an LLM is able to correct logical errors using backtracking, independent of its inherent ability to identify these errors or any other reward model.

For example, if the mistake location is in step 4, we use backtracking to regenerate that step and continue the rest of the chain. If the mistake location is that there are no logical mistakes, we do not backtrack and use the original result.

#### 4.1.1 Results

The results are shown in Table 6. To show that performance increases are not due to randomly resampling outputs, we compare our results to a random baseline, where a mistake location<sup>9</sup> is randomly se-

 $<sup>^{8}</sup>$ Having no logical errors in incorrect $_{ans}$  traces is much rarer but does exist, for example when the answer is correct but is not captured by exact match, or if the original question is faulty and has multiple possible answers.

<sup>&</sup>lt;sup>9</sup>As described above, the mistake location can be either the number representing the step, or that there are no mistakes. If there are no mistakes, we do not use backtracking and simply use the original trace.

	With <b>mistal</b>	ke location	With <b>rando</b>	Avg. num.	
Task	<b>∆</b> accuracy ✓	∆accuracy <sub>x</sub>	∆ accuracy ✓	$\Delta$ accuracy <sub>x</sub>	of steps
Word sorting	-11.11	+23.53	-15.56	+11.76	11.7
Tracking shuffled objects	-6.67	+43.92	-6.67	+20.39	5.4
Logical deduction	-11.43	+36.86	-13.33	+21.57	8.3
Multistep arithmetic	-0.00	+18.04	-8.89	+10.59	5.0
Dyck languages	-6.82	+18.06	-15.91	+5.16	24.5

Table 6: Absolute differences in accuracy ans before and after backtracking. "With mistake location" indicates that backtracking was done using oracle mistake locations from the dataset; "With random location" indicates that backtracking was done based on randomly selected locations.  $\Delta accuracy_{\checkmark}$  refers to differences in accuracy ans on the set of traces whose original answer was correct ans;  $\Delta accuracy_{\checkmark}$  for traces whose original answer was incorrect ans. The average number of steps in a trace is shown to demonstrate the likelihood of randomly selecting the correct mistake location in the random baseline condition.

lected for each trace and we perform backtracking based on the random location.

Note that Table 6 separates results into numbers for the correct set and the incorrect set, referring to whether the *original* trace was correct<sub>ans</sub> or not. This gives a clearer picture than the overall accuracy<sub>ans</sub>, which would be skewed by the proportion of traces that were originally correct<sub>ans</sub> (15%) and incorrect<sub>ans</sub> (85%).

Scores represent the absolute differences in accuracy<sub>ans</sub>. We perform backtracking on both correct<sub>ans</sub> and incorrect<sub>ans</sub> traces, as long as there is a mistake in one of the steps.

 $\Delta$ accuracy, refers to differences in accuracy<sub>ans</sub> on the set of traces whose *original* answer was correct<sub>ans</sub>. Note that we take losses here because, despite the correct answer, there is a logical mistake in one of the steps. Therefore, the answer may change to an incorrect one when we backtrack.

 $\Delta \mathbf{accuracy}_{\mathbf{X}}$  is the same but for incorrect<sub>ans</sub> traces, so the answers may have been corrected, hence increasing accuracy<sub>ans</sub>.

For example, for the word sorting task, 11.11% of traces that were originally correct<sub>ans</sub> became incorrect<sub>ans</sub>, while 23.53% of traces that were originally incorrect<sub>ans</sub> became correct<sub>ans</sub>.

#### 4.1.2 Discussion

The scores show that the gains from correcting incorrect $_{ans}$  traces are larger than losses from changing originally correct answers. Additionally, while the random baseline also obtained improvements, they are considerably smaller than if the true mistake location was used. Note that tasks involving fewer steps are more likely to improve performance in the random baseline, as the true mistake location is more likely to be identified.

While our numbers do show that our gains are

higher than our losses, it should be noted that changes in the overall accuracy depends on the original accuracy achieved on the task. For example, if the original accuracy on the tracking shuffled objects task was 50%, the new accuracy would be 68.6%. On the other hand, if the accuracy was 99%, the new accuracy would drop to 92.8%. As our dataset is highly skewed and only contains 45 correct<sub>ans</sub> traces per task, we leave to future work to assess the effectiveness of backtracking in a more comprehensive way.

# 4.2 Backtracking with a simulated reward model

We show in subsection 4.1 that backtracking can be used to correct CoT traces using gold mistake location labels. To explore what level of accuracy reward model is needed when gold labels are not available, we use backtracking with *simulated* reward models, designed to produce labels at different levels of accuracy. We use accuracy $_{RM}$  to refer to the accuracy of the simulated reward model at identifying mistake locations.

For a given reward model at X% accuracy  $_{RM}$ , we use the mistake location from BIG-Bench Mistake X% of the time. For the remaining (100-X)%, we sample a mistake location randomly. To mimic the behaviour of a typical classifier, mistake locations are sampled to match the distribution found in the dataset. We also ensure that the sampled location does not match the correct location.

#### 4.2.1 Results

Results are shown in Figure 2. We can see that the losses in  $\Delta \operatorname{accuracy}_{\checkmark}$  begins to plateau at 65%. In fact, for most tasks,  $\Delta \operatorname{accuracy}_{\checkmark}$  is already larger than  $\Delta \operatorname{accuracy}_{\checkmark}$  at around 60-70% accuracy<sub>RM</sub>. This demonstrates that while higher accuracies produce better results, backtracking is still effective

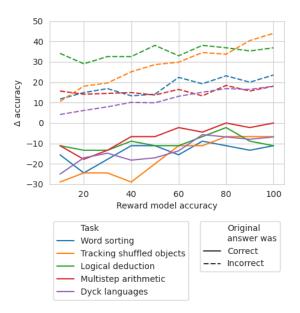


Figure 2:  $\triangle$ accuracy, and  $\triangle$ accuracy, on each dataset as accuracy, increases.

even without gold standard mistake location labels.

#### 4.3 Reward Modeling

We perform a preliminary investigation of if mistake-finding can benefit from a dedicated reward model and if learning to find mistakes in a set of tasks can transfer to finding mistakes in out-of-distribution tasks. We fine-tuned a PaLM 2-XS-Otter model based on our available data for 20k steps and choose the checkpoint with the best validation results. We hold out one task for evaluation while training the reward model on the other 4 tasks.

Held-out task	Difference
Word sorting	+11.66
Tracking shuffled objects	+19.67
Logical deduction	-0.67
Multi-step arithmetic	+4.00
Dyck languages	+22.59

Table 7: Absolute difference in mistake finding accuracy between PaLM 2-L-Unicorn and a small, trained reward model.

Note the reward model we train is significantly smaller than our inference model. We show the relative improvements and losses in Table 7 vs. a zero-shot baseline on PaLM 2-L-Unicorn. We see gains for 4 out of 5 of the tasks. This provides initial indication that it maybe possible to train separate reward model classifiers to assist in backtracking and that these reward models do not have to be large. Further, a reward model can work on mistakes that are out-of-distribution. However, we

believe more data may be necessary to improve results across the board on all tasks. We leave the collection of this larger dataset and a more rigorous investigation of the trade-offs of model size vs. performance of the reward model to future work.

We also leave for future work the effect of backtracking iteratively with a reward model: for example, the generator model may make another mistake after backtracking for the first time, which can then be identified and corrected again.

#### 5 Related work

**Datasets** To our knowledge, the only publicly available dataset containing mistake annotations in LLM outputs is PRM800K (Lightman et al., 2023), which is a dataset of solutions to Olympiad-level math questions. Our dataset BIG-Bench Mistake covers a wider range of tasks to explore the reasoning capabilities of LLMs more thoroughly. Additionally, the generator LLM used in PRM800K has been fine-tuned on 1.5B math tokens as well as a dataset of step-by-step math solutions. For this paper, we wanted to explore few-shot in-context learning methods, which is typically used in real-world applications with API-based LLMs.

**Self-correction** Pan et al. (2023) present a plethora of self-correction methods in recent literature. While their list includes training-time correction strategies such as RLHF (Ouyang et al., 2022) and self-improve (Huang et al., 2022), our backtracking method falls into the category of post-hoc correction, where the correction process is applied to outputs that have already been generated.

Our paper focuses on correction of logical and reasoning errors, rather than stylistic or qualitative improvements. Previous post-hoc correction methods that are applied to reasoning errors include Reflexion (Shinn et al., 2023) and RCI (Kim et al., 2023), both of which cause performance deterioration when the oracle label is not used (Huang et al., 2023). Other methods such as Self-Refine (Madaan et al., 2023) and iterative refinement (Chen et al., 2023) focus on qualitative or stylistic improvements rather than correcting logical errors.

#### 6 Conclusion

In this paper, we describe and release our dataset BIG-Bench Mistake for mistake finding, and propose a backtracking method to correct logical errors in CoT style traces. We show that LLMs generally struggle with finding logical errors without external feedback, but argue that this feedback can come from a reward model instead. Finally, we demonstrate the effectiveness of backtracking, both with gold standard labels as well as with simulated reward models at lower levels of accuracy.

#### Limitations

One main limitation of our dataset is that it features tasks that are artificial and unrealistic for real-world applications. We made this choice to minimise ambiguity and subjectivity during the mistake finding process, but further work needs to be done to determine the effectiveness of backtracking in a more realistic setting.

Another limitation is that our paper does not evaluate backtracking on the original datasets on BIG-Bench, only showing results on the limited set that we sampled in a skewed manner, in order to maximise the value of the human annotators' time. We leave the full evaluation to future work.

#### References

- Rohan Anil, Andrew M Dai, Orhan Firat, Melvin Johnson, Dmitry Lepikhin, Alexandre Passos, Siamak Shakeri, Emanuel Taropa, Paige Bailey, Zhifeng Chen, et al. 2023. Palm 2 technical report. *arXiv* preprint arXiv:2305.10403.
- Pinzhen Chen, Zhicheng Guo, Barry Haddow, and Kenneth Heafield. 2023. Iterative translation refinement with large language models. *arXiv preprint* arXiv:2306.03856.
- Andrew F Hayes and Klaus Krippendorff. 2007. Answering the call for a standard reliability measure for coding data. *Communication methods and measures*, 1(1):77–89.
- Jiaxin Huang, Shixiang Shane Gu, Le Hou, Yuexin Wu, Xuezhi Wang, Hongkun Yu, and Jiawei Han. 2022. Large language models can self-improve. *arXiv* preprint arXiv:2210.11610.
- Jie Huang, Xinyun Chen, Swaroop Mishra, Huaixiu Steven Zheng, Adams Wei Yu, Xinying Song, and Denny Zhou. 2023. Large language models cannot self-correct reasoning yet. *arXiv* preprint arXiv:2310.01798.
- Geunwoo Kim, Pierre Baldi, and Stephen McAleer. 2023. Language models can solve computer tasks. *arXiv preprint arXiv:2303.17491*.
- Hunter Lightman, Vineet Kosaraju, Yura Burda, Harri Edwards, Bowen Baker, Teddy Lee, Jan Leike, John Schulman, Ilya Sutskever, and Karl Cobbe. 2023. Let's verify step by step. *arXiv preprint arXiv:2305.20050*.

- Aman Madaan, Niket Tandon, Prakhar Gupta, Skyler Hallinan, Luyu Gao, Sarah Wiegreffe, Uri Alon, Nouha Dziri, Shrimai Prabhumoye, Yiming Yang, et al. 2023. Self-refine: Iterative refinement with self-feedback. *arXiv preprint arXiv:2303.17651*.
- Ning Miao, Yee Whye Teh, and Tom Rainforth. 2023. Selfcheck: Using Ilms to zero-shot check their own step-by-step reasoning. arXiv preprint arXiv:2308.00436.
- Long Ouyang, Jeffrey Wu, Xu Jiang, Diogo Almeida, Carroll Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, et al. 2022. Training language models to follow instructions with human feedback. *Advances in Neural Information Processing Systems*, 35:27730–27744.
- Liangming Pan, Michael Saxon, Wenda Xu, Deepak Nathani, Xinyi Wang, and William Yang Wang. 2023. Automatically correcting large language models: Surveying the landscape of diverse self-correction strategies. *arXiv preprint arXiv:2308.03188*.
- William Saunders, Catherine Yeh, Jeff Wu, Steven Bills, Long Ouyang, Jonathan Ward, and Jan Leike. 2022. Self-critiquing models for assisting human evaluators. *arXiv preprint arXiv:2206.05802*.
- Noah Shinn, Federico Cassano, Edward Berman, Ashwin Gopinath, Karthik Narasimhan, and Shunyu Yao. 2023. Reflexion: Language agents with verbal reinforcement learning.
- Aarohi Srivastava, Abhinav Rastogi, Abhishek Rao, Abu Awal Md Shoeb, Abubakar Abid, Adam Fisch, Adam R Brown, Adam Santoro, Aditya Gupta, Adrià Garriga-Alonso, et al. 2022. Beyond the imitation game: Quantifying and extrapolating the capabilities of language models. *arXiv preprint arXiv:2206.04615*.
- Aarohi Srivastava, Abhinav Rastogi, Abhishek Rao, Abu Awal Md Shoeb, Abubakar Abid, Adam Fisch, Adam R Brown, Adam Santoro, Aditya Gupta, Adrià Garriga-Alonso, et al. 2023. Beyond the imitation game: Quantifying and extrapolating the capabilities of language models. *Transactions on Machine Learning Research*.
- Mirac Suzgun, Nathan Scales, Nathanael Schärli, Sebastian Gehrmann, Yi Tay, Hyung Won Chung, Aakanksha Chowdhery, Quoc V Le, Ed H Chi, Denny Zhou, et al. 2022. Big-bench-hard/cotprompts. https://github.com/suzgunmirac/BIG-Bench-Hard/tree/main/cot-prompts. Accessed: 2023-10-31.
- Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc V. Le, Ed H. Chi, Sharan Narang, Aakanksha Chowdhery, and Denny Zhou. 2023. Self-consistency improves chain of thought reasoning in language models. In *ICLR* 2023.

Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, brian ichter, Fei Xia, Ed Chi, Quoc V Le, and Denny Zhou. 2022. Chain-of-thought prompting elicits reasoning in large language models. In *Advances in Neural Information Processing Systems*, volume 35, pages 24824–24837. Curran Associates, Inc.

Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik Narasimhan, and Yuan Cao. 2022. React: Synergizing reasoning and acting in language models. *arXiv preprint arXiv:2210.03629*.

### A Implementational details

# A.1 3-shot CoT prompting to generate traces for BIG-Bench Mistake

We use PaLM 2 L (Unicorn) to generate the traces used in BIG-Bench Mistake. All traces are generated at temperature = 0.

Our prompts and examples can be found at https://github.com/WHGTyen/BIG-Bench-Mistake. Our prompts are based on chain-of-thought prompts in the BIG-Bench Hard dataset (Suzgun et al., 2022), with four main changes:

- 1. Example CoT traces in the prompt is broken up into smaller steps (typically one sentence per step). This is done so that mistake location information is more precise.
- 2. Following Yao et al. (2022), each step in the prompt is signposted with "Thought 1", "Thought 2:", etc. This allows us to refer to the number of the step when prompting for mistake location.
- 3. For the logical deduction task, we find that the notation used in the original prompt with question marks is often inconsistent. It becomes difficult for annotators to determine whether a question mark is a mistake or not, because the correctness of the question mark is dependent on its interpretation. To minimise such ambiguity, the question mark notation is rewritten into text.
- 4. For the multistep arithmetic task, one of the prompt examples is altered to increase the length of the equation. This is because the BIG-Bench Hard dataset (where the prompts are taken from) only used equations of a specific length, but our dataset contains equations of averaged a variety of lengths, in accordance with the original BIG-Bench dataset (Srivastava et al., 2022).

Following Yao et al. (2022), we use the newline as the stop token, which generates one step with every generation call. We algorithmically append "Thought N:" before each step. This allows us to split up steps in a clear and systematic way. We stop generating once an answer is reached, which is detected using the following regex:

(?<=[Tt]he answer is).\*\$

# A.2 3-shot prompting to identify mistakes in BIG-Bench Mistake

As described in section 3, we explore three different methods of prompting for mistake location: direct trace-level prompting, direct step-level prompting, and CoT step-level prompting. We use 3-shot prompting for all methods, and our prompts and examples can be found at https://github.com/WHGTyen/BIG-Bench-Mistake.

Our prompts follow OpenAI's chat completion format. All results were obtained with temperature =0 and no stop tokens.

#### **B** Annotation

We release our annotation guidelines at https://github.com/WHGTyen/BIG-Bench-Mistake.

During annotation of the multistep arithmetic task, we found that the first CoT step given in the original BIG-Bench Hard prompt examples (Suzgun et al., 2022) was incorrect. Since all generated traces contained the same first step, we removed that step before showing traces to the annotators.

Figure 3 contains an example screenshot of the user interface. For every trace, we provide the input question as well as the target answer, with a note to be aware of errors that may occur in  $correct_{ans}$  traces.

Annotators can click on words to highlight the same word across the trace and the question text, which we found was particularly helpful for some tasks such as word sorting and tracking shuffled objects. Buttons on the right automatically become inactive if a previous step has been labelled as negative.

#### C Benchmark scores

Model	Direct	Direct	CoT (step)	Model Direct Direct	CoT (s
Model	(trace)	(step)	COT (Step)	(trace) (step)	COI (S
	Word so	rting		Word sorting	
GPT-4-Turbo	67.74	38.24	_	GPT-4-Turbo 32.71 32.33	_
GPT-4	88.24	82.35	58.82	GPT-4 28.20 39.47	30.83
GPT-3.5-Turbo	100.00	97.06	20.59	GPT-3.5-Turbo 0.00 4.51	15.04
Track	king shuf	fled objec	ets	Tracking shuffled objects	S
GPT-4-Turbo	90.00	77.50	_	GPT-4-Turbo 31.54 59.23	_
GPT-4	82.50	82.50	80.00	GPT-4 59.14 62.69	92.31
GPT-3.5-Turbo	67.50	0.00	0.00	GPT-3.5-Turbo 1.17 1.92	21.92
Lo	ogical de	duction		Logical deduction	
GPT-4-Turbo	100.00	83.33	_	GPT-4-Turbo 20.81 74.83	_
GPT-4	100.00	100.00	0.00	GPT-4 39.46 67.01	10.54
GPT-3.5-Turbo	100.00	50.00	100.00	GPT-3.5-Turbo 0.00 24.83	7.82
Mu	ltistep ar	ithmetic		Multistep arithmetic	
GPT-4-Turbo	57.69	40.32	_	GPT-4-Turbo 34.27 44.12	_
GPT-4	53.23	46.77	27.42	GPT-4 41.60 41.60	44.54
GPT-3.5-Turbo	96.77	79.03	58.06	GPT-3.5-Turbo 0.00 12.18	16.81
I	Dyck lang	guages		Dyck languages	
GPT-4-Turbo	96.42	30.00	_	GPT-4-Turbo 6.99 28.46	_
GPT-4	98.41	78.57	13.79	GPT-4 7.37 40.81	43.91
GPT-3.5-Turbo	95.74	4.76	0.00	GPT-3.5-Turbo 1.28 6.05	2.08

<sup>(</sup>a) Mistake finding accuracy for traces that do not contain mistakes (correct  $_{mis}$ ).

Table 8: Mistake finding accuracy across 5 tasks for  $\mathsf{correct}_{mis}$  and  $\mathsf{incorrect}_{mis}$  traces. The combined scores of Table 8a and Table 8b make up Table 4.

<sup>(</sup>b) Mistake finding accuracy for traces that contain mistakes (incorrect  $_{mis}$ ).



Figure 3: Screenshot of the user interface for a question from the tracking shuffled objects task.