CausalBench: A Comprehensive Benchmark for Evaluating Causal Reasoning Capabilities of Large Language Models

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Abstract

Causal reasoning, a core aspect of human cognition, is essential for advancing 1 large language models (LLMs) towards artificial general intelligence (AGI) and 2 reducing their propensity for generating hallucinations. However, existing datasets 3 for evaluating causal reasoning in LLMs are limited by narrow domain coverage 4 and a focus on cause-to-effect reasoning through textual problems, which does 5 not comprehensively assess whether LLMs truly grasp causal relationships or 6 merely guess correct answers. To address these shortcomings, we introduce a 7 novel benchmark that spans textual, mathematical, and coding problem domains. 8 Each problem is crafted to probe causal understanding from four perspectives: 9 cause-to-effect, effect-to-cause, cause-to-effect with intervention, and effect-to-10 cause with intervention. This multi-dimensional evaluation method ensures that 11 12 LLMs must exhibit a genuine understanding of causal structures by correctly answering questions across all four dimensions, mitigating the possibility of cor-13 rect responses by chance. Furthermore, our benchmark explores the relationship 14 15 between an LLM's causal reasoning performance and its tendency to produce hallucinations. We present evaluations of state-of-the-art LLMs using our bench-16 mark, providing valuable insights into their current causal reasoning capabili-17 ties across diverse domains. The dataset is publicly available for download at 18 https://huggingface.co/datasets/CCLV/CausalBench. 19

20 **1** Introduction

Causal reasoning, the ability to understand and infer causal relationships between variables, is a 21 fundamental aspect of human cognition and plays a crucial role in decision-making, problem-solving, 22 and learning [1]. For large language models (LLMs), causal reasoning refers to the ability to 23 accurately identify, represent, and reason about causal relationships described in text, mathematical 24 equations, or code snippets [1]. Developing strong causal reasoning abilities in LLMs is essential 25 for progress toward artificial general intelligence (AGI), as it enables models to understand not just 26 correlations but the underlying mechanisms driving outcomes [3]. This understanding is crucial for 27 making accurate predictions, generating insightful explanations, and adapting to new situations, as 28 core components of AGI. 29

However, existing causal reasoning benchmarks have several limitations that hinder their ability to 30 comprehensively evaluate the causal reasoning capabilities of LLMs. First, current benchmarks often 31 focus on a single perspective of causal reasoning, such as cause-to-effect, lacking a multifaceted 32 assessment that considers effect-to-cause reasoning and the impact of interventions. This narrow 33 focus allows models to correctly answer causal questions by chance without truly understanding the 34 underlying causal relationships [5]. Second, current benchmarks are primarily text-based, lacking 35 diversity in problem types, such as mathematical and coding problems that can encapsulate causal 36 dependencies. Incorporating these diverse problem formats would enable a more robust evaluation 37

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of LLMs' capacity to reason about causality across various modalities. Third, the limited scale of 38 existing benchmarks may not provide a sufficiently comprehensive assessment of LLMs' causal 39

reasoning abilities due to the limited scale of the benchmark dataset. 40

To address these limitations, we propose CausalBench, a comprehensive benchmark for evaluating the 41 causal reasoning capabilities of LLMs. CausalBench comprises four perspectives of causal reasoning 42 for each scenario: cause-to-effect, effect-to-cause, cause-to-effect with intervention, and effect-to-43 cause with intervention. This multi-perspective approach mitigates the potential for correct answers 44 by chance and provides a more accurate evaluation of LLMs' understanding of causal relationships. 45 Moreover, CausalBench includes a diverse set of problem types spanning textual, mathematical, and 46 coding domains, enabling a comprehensive assessment of causal reasoning abilities across different 47 modalities. The benchmark consists of more than 60,000 problems and employs six evaluation 48 metrics to measure LLMs' causal reasoning performance. 49 The major contributions of CausalBench are three-fold: (1) evaluating four causal reasoning perspec-50 tives per scenario to robustly assess causal understanding, (2) incorporating a diverse problem set

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spanning math, code, and natural language for cross-modal evaluation, and (3) implementing strict 52

quality control measures, including a causal inference engine check and human expert review, to 53 ensure the benchmark's validity and reliability. By addressing the limitations of existing benchmarks, 54

CausalBench aims to provide a more comprehensive and accurate evaluation of the causal reasoning 55

capabilities of LLMs, facilitating progress towards AGI. 56

Related Works 2 57

Existing datasets and benchmarks for evaluating causal reasoning primarily focus on commonsense 58 causality [9, 31, 32], which assesses the alignment between commonsense knowledge about causal 59 relationships in humans and language models. These datasets, such as WikiWhy [9], CausalWorld 60 [31], and UCLM [32], provide valuable insights into how well language models capture and reason 61 about everyday causal relationships. However, they do not explicitly evaluate the models' ability to 62 perform formal causal reasoning based on well-defined rules and principles from the field of causal 63 inference. Some recent works have started to explore more formal aspects of causal reasoning in 64 language models. For example, CRASS [28] focuses specifically on counterfactual reasoning, which 65 involves reasoning about alternative outcomes based on hypothetical changes to past events. While 66 counterfactual reasoning is an important aspect of causal inference, CRASS does not cover the full 67 spectrum of causal inference tasks, such as interventional and observational reasoning. Another 68 concurrent work by Kiciman et al. [16] evaluates language models on various causality-related tasks, 69 including causal sufficiency analysis, causal discovery, and counterfactual reasoning. However, their 70 evaluation primarily relies on the conceptual knowledge accrued from the training data rather than 71 formal causal inference, except for their causal sufficiency analysis. This means that the models' 72 performance may be influenced by spurious correlations or memorization from the training data 73 rather than a genuine understanding of causal principles. 74

In contrast, our proposed dataset, CausalBench, is grounded in the principles of causal inference 75 76 [11, 25, 26]. CausalBench provides a comprehensive and principled framework for assessing the causal reasoning capabilities of language models, ensuring that the models are evaluated on their 77 ability to perform formal causal inference rather than relying on spurious correlations or memorization 78 from training data. By encompassing a diverse set of causal scenarios (text, code, and math), 79 four causal perspectives (cause to effect, effect to cause, cause to effect with intervention, and 80 effect to cause with intervention), and explanations associated with ground truth for each test case, 81 CausalBench offers a rigorous and systematic approach to benchmarking causal reasoning in LLMs. 82 It is designed to test the models' ability to reason about causal relationships in a variety of domains, 83 including natural language, programming code, and mathematical equations. In summary, while 84 existing datasets and benchmarks have made contributions to the study of causal reasoning in language 85 models, CausalBench offers a more comprehensive, principled, and rigorous approach to evaluating 86 formal causal inference capabilities across multiple domains. By grounding the evaluation in the 87 principles of causal inference and providing a diverse set of test cases with associated explanations, 88 CausalBench aims to set a new standard for benchmarking causal reasoning in LLMs. 89

90 3 Dataset Construction Process and Method

The construction of CausalBench involves three key steps: manual generation of initial test cases, 91 scaling up using LLM such as GPT-4 Turbo, and quality control through causal inference engines 92 together with human verification. Initially, we manually create a set of test cases covering four aspects 93 of causal inference: (a) cause to effect, (b) effect to cause, (c) cause to effect with intervention, and (d) 94 effect to cause with intervention to ensure a comprehensive evaluation of causal reasoning capabilities 95 from different perspective. To expand the dataset, we then use GPT-4 Turbo with few-shot prompting, 96 97 leveraging the model's ability to generate additional test cases that adhere to the desired format and 98 cover the four causal inference aspects. The few-shot prompts are designed to guide GPT-4 Turbo 99 in producing a diverse and extensive set of problems that maintain consistency with the manually 100 generated cases. Afterward, we implement a quality control process involving validation through causal inference engines and review by human experts. The causal inference engines verify the 101 logical consistency and correctness of the generated test cases, while human experts review and refine 102 the dataset to maintain high standards of quality and relevance. 103



104 3.1 Workflow Overview

Figure 1: Workflow overview of the CausalBench dataset construction process.

105 3.2 Manual Analysis and Generation

For the text problems of our Benchmark, we randomly selected 100 questions from the CLADDER 106 dataset [10] and manually analyzed them to determine their category within (1) inference from 107 cause to effect, (2) effect to cause, (3) cause to effect with intervention, or (4) effect to cause with 108 intervention. These perspectives represent different dimensions of causal reasoning; (1) Cause to the 109 effect: Given the cause, what is the likelihood of the effect? (2) Effect to cause: Given the effect, 110 what is the likelihood of the cause? (3) Cause to effect with intervention: If an intervention is added 111 to the causal relationship, given the cause, what is the likelihood of the effect? and (4) Effect to cause 112 with intervention: If an intervention is added to the causal relationship, given the effect, what is the 113 likelihood of the cause? 114

After categorizing the selected cases from the CLADDER dataset, we expanded them by creating additional questions for the other three perspectives. For example, if a case was classified as "cause to effect", we generated corresponding questions for "effect to cause", "cause to effect with intervention", and "effect to cause with intervention" manually.

To correctly expand other perspective questions and their ground truths, we visualized the relationships
 between variables using causal diagrams and analyzed these relationships by calculating conditional
 probabilities. Causal diagrams represent variables as nodes and causal relationships as directed edges.
 For example, consider the following hypothetical scenario:

Imagine a self-contained, hypothetical world with only the following conditions, and without any unmentioned factors or causal relationships: Parents' intelligence has a direct positive effect on parents' social status and child's intelligence. Other unobserved factors has a positive direct effect on parents' social status and child's intelligence. If a child is intelligent, would it be more likely that this child had intelligent parents?



Figure 2: Causal Graph Example

In this scenario, the causal diagram would have four nodes: Parents' intelligence, Parents' social
status, Child's intelligence, and Other unobserved factors. There would be directed edges from
Parents' intelligence to Parents' social status and Child's intelligence, from Other unobserved factors
to Parents' social status and Child's intelligence, and from Parents' social status to Child's intelligence.
Conditional probabilities can be estimated based on the causal graph.

Using the causal graph and conditional probabilities, we can categorized the original questions as effect-to-cause. The probability of the child being intelligent given that the parents are intelligent is higher than the probability of the child being intelligent given that the parents are unintelligent, so the ground truth is yes. Then extend the questions to cover four perspectives by adjusting the questioning logic and incorporating interventions into the causal path diagram, and calculate ground truth for each questions.(examples are provided in the Appendix)

Finally, we obtained 100 causal scenarios, with 400 causal questions. They serve as the foundation for our few-shot prompting approach, providing examples for GPT-4 Turbo on how to identify the type of the initial question and generate additional questions for the remaining perspectives. By using these examples in a few-shot prompting setting, we guide the model to generate additional perspective questions with answers for all other causal scenarios in the CLADDER dataset.

For coding and mathematical problems, we manually created 100 code scenarios and 100 math scenarios, each containing causal relationships, and designed four perspective questions for each scenario. These questions addressed causal issues based on the relationships described in the scenarios (examples are provided in the Appendix). We then used causal graphs and conditional probabilities to manually generate the ground truths and employed few-shot prompts with GPT-4 Turbo to generate additional code, math scenarios and questions with corresponding answers.

In summary, the manual analysis and generation process involved visualizing causal relationships 150 using causal diagrams and calculating conditional probabilities for each scenario. We modified the 151 152 questioning approach and added interventions to expand each problem into four forms, covering cause-153 to-effect, effect-to-cause, cause-to-effect with intervention, and effect-to-cause with intervention, and generated ground truths for each question. By the end of this section, we had created 100 sets of 400 154 text-based questions with ground truths, 100 sets of 400 coding questions with ground truths, and 155 100 sets of 400 math questions with ground truths. These manually generated samples serve as the 156 foundation for our few-shot prompting approach, which utilizes GPT-4 Turbo to generate additional 157 test cases. 158

159 3.3 Scaling Up with LLMs

After manually generating and verifying an initial set of questions, we employed GPT-4 Turbo to scale up the dataset. The scale-up process was divided into three parts: text problems, coding problems, and mathematical problems.

For the text problems, we provided GPT-4 Turbo with original CLADDER dataset[10] questions with manually expanded questions along with their ground truths. By learning from these samples, GPT-4 ¹⁶⁵ Turbo was tasked with reading the remaining CLADDER scenarios (around 10,000 problems) and ¹⁶⁶ their corresponding questions, determining the question perspective, expanding the scenario into the ¹⁶⁷ other three perspectives, and generating the associated ground truths. This process ensures every text

causal scenario has four dimension questions and corresponding ground truths.

In the case of coding problems, we supplied GPT-4 Turbo with the 100 manually created code examples containing causal relationships. Using these examples as a foundation, GPT-4 Turbo generated an additional 2,000 code snippets, each incorporating causal relationships. For each newly generated code snippet, GPT-4 Turbo created four perspectives of questions and provided the corresponding ground truths, ensuring a comprehensive evaluation of causal reasoning in the context of programming.

Similarly, for mathematical problems, GPT-4 Turbo was employed to generate 2,000 new mathematical scenarios across various domains, such as probability theory, mathematical statistics, differential equations, and complex analysis. For each mathematical scenario, GPT-4 Turbo generated four types of questions and their associated ground truths, assessing the model's ability to reason about causal relationships in mathematical contexts.

By leveraging the capabilities of GPT-4 Turbo, we were able to create a dataset across all three problem categories. The text problems were augmented by automatically generating additional question perspectives and ground truths based on the existing CLADDER scenarios. The coding and mathematical problems were scaled up by having GPT-4 Turbo create new scenarios containing causal relationships and generate the corresponding questions and ground truths. This scale-up process resulted in a more comprehensive and diverse dataset, enabling a thorough evaluation of causal reasoning abilities in large language models across various domains.

187 3.4 Quality Control

188 3.4.1 Causal Inference Engine Design

To ensure the accuracy and consistency of the generated questions and answers, we developed a causal inference engine. This engine utilizes causal diagrams and conditional probabilities associated with each question to compute the answers for all questions. The causal inference engine serves as a verification layer, comparing the answers generated by the language model. If the answer generated by the language model differs from the answer generated by the causal inference engine, the case will be manually inspected, and the ground truth will be generated by human experts. Here are the Causal Inference Engine design details:

196 Input

- A causal scenario described in natural language, code, or mathematical equations, including
 causal relationships among variables, known conditions, etc.
- A causal query, which is a question based on causal scenario

200 Steps

1. Causal Graph Extraction:

(a) For natural language scenarios, we identify variables and causal relationships, and 202 construct causal graphs (G := (V, E)) by implementing a pipeline consisting of semantic 203 parsing and coreference resolution modules. The semantic parsing module first uses 204 the Stanford Parser [12] to perform syntactic parsing and obtain the sentence structure. 205 Then, it applies Compositional Semantics [13] to recursively map the syntactic parse 206 tree to a logical form, based on the principle of compositionality. The coreference 207 resolution module uses techniques such as the mention-pair model [14] to determine 208 which mentions refer to the same entity, and merges the variables corresponding 209 to coreferent mentions. From the outputs of the semantic parsing and coreference 210 resolution modules, the pipeline automatically extracts variables from nouns and 211 noun phrases, and identifies causal relationships indicated by verbs and conjunctions 212 expressing causality [15]. Finally, the causal graph construction module takes the 213 extracted variables as nodes (V) and causal relationships as directed edges (E) to 214 automatically build the causal graph [1]. 215

216	(b)	For code scenarios, we identify variables and their dependencies, and construct causal
217		graphs by implementing a pipeline that analyzes the code structure, control flow, and
218		data flow. The pipeline first uses a code parser, such as the ast module [17] in Python, to
219		generate an abstract syntax tree (AST). It then performs control flow analysis using tech-
220		niques like control flow graphs (CFGs) [18] and program dependence graphs (PDGs)
221		[21], and data flow analysis using def-use chains [19] and static single assignment
222		(SSA) form [20], to identify execution paths, dependencies between statements, and
223		variable dependencies. These analyses help automatically extract variables and their
224		relationships from the code structure. Finally, the causal graph construction module
225		takes the extracted variables as nodes (V) and their dependencies as edges (E) to build
226		the causal graph based on the code semantics [1], capturing the causal relationships
227		between variables and enabling further reasoning and analysis.

- (c) For math scenarios, we identify variables and their functional relationships, and con-228 struct causal graphs by implementing a pipeline that parses and analyzes the mathe-229 matical equations. The pipeline first uses a math expression parser, such as the SymPy 230 library [22] in Python, to convert the equations into an abstract syntax tree (AST) 231 representation. It then traverses the AST to identify variables and their functional 232 relationships, such as dependencies and algebraic operations, using techniques like 233 symbolic differentiation [23] and expression simplification [24]. These analyses help 234 automatically extract variables and their relationships from the equation structure. 235 Finally, the causal graph construction module takes the extracted variables as nodes (V) 236 and their functional relationships as directed edges (E) to build the causal graph based 237 on the equation semantics, similar to the approach in [1]. The resulting causal graph 238 captures the causal relationships between variables in the mathematical equations, 239 enabling further reasoning and analysis. 240
- 241 2. **Query Classification:** Classify the causal query into one of the three levels of the Ladder 242 of Causation (Association, Intervention, Counterfactuals). Formalize the query into the 243 corresponding causal language, as discussed in [4].

3. Estimand Derivation:

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- (a) For text and math scenarios, we construct a module that uses causal inference algorithms (e.g., do-calculus [25], counterfactual inference formulas [26]) to derive the estimand based on the causal graph and query type.
- (b) For code scenarios, we use program analysis techniques (e.g., symbolic execution, data dependency analysis, control flow analysis) to derive the estimand based on the code structure and query type. This involve simulating interventions on code variables and analyzing the resulting program behavior.
- 4. Data Matching: Match the terms in the estimand with the available data or constraints in the scenario to obtain a computable estimand expression. Check the completeness and consistency of the data. Raise warnings or errors if critical data is missing. For code scenarios, this involve executing the code with specific inputs and observing the outputs. This step is similar to the data matching phase in [4].

5. Causal Effect Estimation:

- (a) Calculate the causal effect value based on the estimand expression and the available data, yielding the answer to the query.
- (b) For scenarios with unobserved confounders, use instrumental variable estimation [27]
 or front-door adjustment [25].
- (c) For code scenarios, this involve comparing program behaviors under different interven tions.
- This step is inspired by causal effect estimation phase in [4].

265 Output

• Answer to the causal query, including the estimated causal effect, confidence interval, and key assumptions.

In a summary, our Causal Inference Engine extends the original design presented in [4] by incorporating domain-specific graph extraction and estimand derivation techniques to handle causal inference problems in text, code, and math scenarios. The overall pipeline remains consistent with the one described in [4], but the internal methods are adapted to the specific structures and semantics of each domain.

273 3.4.2 Quality Control Process

After expansion with GPT4-Turbo, we obtained around 10000 x 4 text-based questions, 2000 x 4 math questions, and 2000 x 4 coding questions, along with their GPT-4 Turbo generated answers. To ensure the accuracy of the ground truth of each questions, we employed a strict quality control process as showing below:

We used the causal inference engine introduced above to independently solve the problems and generate its own set of answers. We compared the answers generated by GPT-4 Turbo and the causal inference engine. If two answers were the same, we updated the answer as ground truth. If any of the answers were inconsistent, we conducted a manual analysis of the question and answers to determine the correct answer and update ground truth accordingly.

This multi-step quality control process, involving the use of causal inference engine and human expert check, ensures that the final dataset contains accurate and reliable questions and answers. The manual review of inconsistent answers further enhances the quality of the dataset by addressing any discrepancies or edge cases that the models may encounter.

287 4 Benchmark Results

288 4.1 Baseline of Mainstream LLMs

We tested several state-of-the-art large language models, including GPT-4, Claude-3, LLAMA-3, and 289 others, on our CausalBench. The evaluation metrics included: Four-Type Questions Group Correction 290 Rate, Overall Correction Rate (Ignore Question Type), From Cause to Effect without Intervention 291 Correction Rate, From Effect to Cause without Intervention Correction Rate, From Cause to Effect 292 with Intervention Correction Rate, and From Effect to Cause with Intervention Correction Rate. For 293 each causal scenario, there are four questions: cause-to-effect without intervention, effect-to-cause 294 without intervention, cause-to-effect with intervention, and effect-to-cause with intervention. The 295 Four-Type Questions Group Correction Rate represents the proportion of scenario cases where all 296 four types of questions of one scenario are all answered correctly by the large language models. 297 If any of the four questions of a scenario is answered incorrectly, the scenario is considered to be 298 answered incorrectly by the LLM. The Overall Correction Rate (Ignore Question Type) is calculated 299 300 by dividing the total number of correctly answered questions by the total number of questions, without 301 categorizing the questions by type and scenario. The From Cause to Effect without Intervention 302 Correction Rate is calculated by dividing the number of correctly answered "From Cause to Effect without Intervention" type questions by the total number of this type of questions. Similarly, the 303 From Effect to Cause without Intervention Correction Rate is calculated by dividing the number of 304 correctly answered "From Effect to Cause without Intervention" type questions by the total number of 305 this type of questions. The remaining two metrics, From Cause to Effect with Intervention Correction 306 Rate and From Effect to Cause with Intervention Correction Rate, follow the same calculation method 307 as the previous two metrics, focusing on their respective question types. 308

Here are the tables showing LLMs' performance on text, math, and code problems.

Model Four-Type Questions Group Correction Rate (%)		Overall Correction Rate (Ignore Question Type) (%)	From Cause to Effect without Intervention Correction Rate (%)	From Effect to Cause without Intervention Correction Rate (%)	From Cause to Effect with Intervention Correction Rate (%)	From Effect to Cause with Intervention Correction Rate (%)
GPT-4 Turbo	36.9	73.3	74.4	71.2	73.8	73.7
Claude3-Opus	36.8	72.6	74.1	70.9	73.2	72.2
Mistral-7B	25.5	63.6	58.7	66.5	64.2	65.0
Llama3-70B	21.8	61.5	62.6	59.6	63.8	60.1
Llama2-7B	20.7	62.1	62.8	64.0	56.4	65.4
GPT-3.5	16.7	57.8	57.6	58.5	56.2	58.7
Gemma-7b-it	12.8	50.7	50.0	46.9	53.6	52.1
Bloomz	4.2	41.7	41.0	40.7	41.7	43.6
AquilaChat	1.9	31.1	28.7	32.4	33.1	30.4

Table 1: LLM Performance on Text Problems

Model	Four-Type Questions Group Correction Rate (%)	Overall Correction Rate (Ignore Question Type) (%)	From Cause to Effect without Intervention Correction Rate (%)	From Effect to Cause without Intervention Correction Rate (%)	From Cause to Effect with Intervention Correction Rate (%)	From Effect to Cause with Intervention Correction Rate (%)
Mistral-7B	62.0	87.2	78.9	85.6	85.3	98.9
GPT-4 Turbo	61.4	88.7	78.6	88.3	91.7	96.0
Claude3-Opus	54.6	85.9	74.7	87.1	86.5	95.4
Llama3-70B	40.8	80.7	56.8	86.8	82.0	97.1
Gemma-7b-it	38.3	79.2	50.4	82.8	91.1	92.0
AquilaChat	25.3	68.1	57.0	67.8	69.2	78.3
Bloomz	23.9	69.2	53.3	76.8	67.3	79.7
GPT-3.5	15.9	63.3	47.1	71.5	48.6	86.1
Llama2-7B	2.8	42.3	45.3	54.2	17.5	52.4

Table 2: LLM Performance on Math Problems

Model	Four-Type Questions Group Correction Rate (%)	Overall Correction Rate (Ignore Question Type) (%)	From Cause to Effect without Intervention Correction Rate (%)	From Effect to Cause without Intervention Correction Rate (%)	From Cause to Effect with Intervention Correction Rate (%)	From Effect to Cause with Intervention Correction Rate (%)
Llama3-70B	43.8	77.0	82.0	75.7	73.9	76.0
Claude3-Opus	39.6	71.3	78.6	71.3	68.7	66.5
GPT-4 Turbo	37.2	71.0	80.6	67.5	73.2	62.5
Gemma-7b-it	32.3	68.4	74.1	67.7	66.0	65.4
Mistral-7B	31.4	66.8	67.5	68.3	61.3	70.2
GPT-3.5	25.0	64.5	71.9	65.4	59.8	60.6
Llama2-7B	22.6	61.9	79.0	45.5	76.3	46.8
Bloomz	17.5	52.4	49.6	56.8	46.4	56.8
AquilaChat	14.7	47.3	36.8	56.4	38.9	57.2

 Table 3: LLM Performance on Code Problems

310 4.2 Test Result Summary

The evaluation results of state-of-the-art large language models on CausalBench provide valuable insights into their causal reasoning capabilities across textual, mathematical, and coding problem domains:

Overall, the models achieved higher correction rates on mathematical problems compared to textual and coding problems. For instance, GPT-4 achieved an 88.7% overall correction rate on math problems, while scoring 73.3% and 71.0% on text and code problems, respectively. This suggests that causal reasoning in mathematical contexts is relatively easier for LLMs compared to natural language and programming domains.

The Four-Type Questions Group Correction Rate, which measures the proportion of scenarios where all four reasoning perspectives are correctly answered, was consistently lower than the Overall Correction Rate (Ignore Question Type) across all problem types. For example, GPT-4 achieved a 61.4% Four-Type Questions Group Correction Rate on math problems, compared to an 88.7% Overall Correction Rate. This indicates that LLMs often struggle to maintain a comprehensive understanding of causal relationships when questioned from multiple perspectives.

The introduction of interventions in the causal scenarios led to mixed results in correction rates across models and problem types. In the text domain, the correction rates slightly decreased for most models when interventions were introduced. However, in the math domain, the correction rates generally improved with interventions. For instance, GPT-4's performance increased from 78.6% to 91.7% on cause-to-effect questions with intervention in math problems. In the coding domain, the impact of interventions varied across models, with some showing improvements and others exhibiting a decline in performance.

Among the tested models, GPT-4 and Claude-3 consistently outperformed other large language models
 (LLMs) across most problem types and reasoning dimensions, achieving the highest correction rates.
 Mistral demonstrated strong performance in mathematical problems but exhibited shortcomings in
 code-related tasks. Conversely, LLAMA-3 showed robust performance in code-related problems but
 faced challenges with text and mathematical tasks.

337 5 Correlation with Hallucination

To analyze the correlation between LLMs' causal reasoning ability and their hallucination rate, we referred to the LLMs' performance on hallucination datasets. The hallucination evaluation results were obtained from the Hallucination Leaderboard, developed by Vectara [30]. This leaderboard provides a comparison of LLM performance in maintaining a low hallucination rate and ensuring factual consistency when summarizing a set of facts.

Model	Hallucination Rate	Factual Consistency Rate	Answer Rate	Average Summary Length (Words)
GPT 4 Turbo	2.5 %	97.5 %	100.0 %	86.2
Llama3-70B	4.5 %	95.5 %	99.2 %	68.5
Mistral 7B Instruct-v0.2	4.5 %	95.5 %	100.0 %	106.1
Llama2-7B	5.6 %	94.4 %	99.6 %	119.9
Claude3-Opus	7.4 %	92.6 %	95.5 %	92.1
Google Gemma-7b-it	7.5 %	92.5 %	100.0 %	113.0

Table 4: Performance of LLMs on the Hallucination Dataset

The hallucination evaluation process involves measuring the hallucination rate, factual consistency rate, answer rate, and average summary length. These metrics provide a comprehensive understanding of each model's tendency to hallucinate and its ability to maintain factual accuracy [30].

After comparing the LLMs' performance on CausalBench with their performance on the Hallucination evaluation leaderboard provided by Vectara on Huggingface [30], we found that models with stronger causal reasoning abilities tend to exhibit lower hallucination rates. For instance, GPT-4 Turbo, LLAMA-3-70B, and Mistral-7B, which demonstrated superior performance on causal reasoning tasks, also had low hallucination rates. In contrast, models like Google Gemma-7b-it and LLAMA-2-7B, which showed weaker performance on our CausalBench, had higher hallucination rates of 7.5% and 5.6%, respectively.

This trend indicates a potential link between a model's ability to understand and reason about causal relationships and its likelihood of not producing hallucinations. Further research is required to explore this correlation in more depth and to understand the underlying mechanisms driving this relationship.

356 6 Impact and Limitations

357 6.1 Impact

For the first time, we innovatively propose four types of questioning approaches for the same causal 358 scenario: cause-to-effect, effect-to-cause, cause-to-effect with intervention, and effect-to-cause with 359 intervention. We also calculate the proportion of cases where large language models correctly answer 360 all four types of questions for a given causal scenario. This effectively avoids the situation where 361 large language models coincidentally answer causal questions correctly without understanding the 362 causal relationships embedded in the causal scenario, thereby improving the accuracy of the dataset's 363 test results. By providing causal reasoning problems spanning multiple domains(text, code, math), it 364 addresses the limitations of existing causal datasets and offers a more comprehensive and robust tool 365 for assessing the causal reasoning abilities of language models. The findings in this paper suggest that 366 models with stronger causal reasoning capabilities tend to exhibit lower hallucination rates, providing 367 a new perspective on exploring the relationship between causal reasoning and reducing hallucinations. 368 369 CausalBench has the potential to become a benchmark for driving progress in causal reasoning in artificial intelligence. 370

371 6.2 Limitations

CausalBench has several limitations that need to be addressed in future work. These include the need for further expanding the domain coverage, increasing the scale of the dataset, incorporating causal discovery tasks and exploring the intrinsic mechanisms between causal reasoning and hallucinations through more empirical studies.

376 7 Conclusion

In this paper, we present CausalBench, a comprehensive benchmark dataset for evaluating the causal reasoning capabilities of large language models. CausalBench innovatively proposes four types of questioning approaches for each causal scenario: cause-to-effect, effect-to-cause, cause-to-effect with intervention, and effect-to-cause with intervention. By calculating the proportion of cases where models correctly answer all four question types, CausalBench effectively assesses whether LLMs truly understand the underlying causal relationships, mitigating the impact of models coincidentally providing correct answers without causal comprehension.

The dataset encompasses a diverse set of problems spanning textual, mathematical, and coding domains, addressing the limitations of existing causal reasoning benchmarks. Evaluated on Causal-Bench, state-of-the-art LLMs demonstrate stronger performance on mathematical problems compared to textual and coding tasks. Notably, models with superior causal reasoning abilities tend to exhibit lower hallucination rates, suggesting a potential link between the two capabilities.

Despite its contributions, CausalBench has several limitations, including the need for expanded domain coverage and deeper exploration of the intrinsic mechanisms connecting causal reasoning and hallucination reduction. Future work will focus on addressing these limitations, further refining the evaluation metrics, and providing insights to advance the development of causal reasoning abilities in large language models. CausalBench serves as a robust tool and an important step towards achieving artificial general intelligence.

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505 Checklist

506	1.	For all authors
507 508		(a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
509		(b) Did you describe the limitations of your work? [Yes]
510		(c) Did you discuss any potential negative societal impacts of your work? [Yes]
511 512		(d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
513	2.	If you are including theoretical results
514		(a) Did you state the full set of assumptions of all theoretical results? [N/A]
515		(b) Did you include complete proofs of all theoretical results? [N/A]
516	3.	If you ran experiments (e.g. for benchmarks)
517 518		(a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
519 520		(b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
521 522		(c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [N/A]
523 524		(d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes]
525	4.	If you are using existing assets (e.g., code, data, models) or curating/releasing new assets
526		(a) If your work uses existing assets, did you cite the creators? [Yes]
527		(b) Did you mention the license of the assets? [Yes]
528		(c) Did you include any new assets either in the supplemental material or as a URL? [Yes]
529 530		(d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes]
531		(e) Did you discuss whether the data you are using/curating contains personally identifiable
532		information or offensive content? [Yes]
533	5.	If you used crowdsourcing or conducted research with human subjects
534 535		(a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
536 537		(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
538 539		(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

540 8 Appendix A: CausalBench Dataset Link

541 https://huggingface.co/datasets/CCLV/CausalBench

542 9 Appendix B: Text Question Example

543 Causal Scenario:

Imagine a self-contained, hypothetical world with only the following conditions, and without any unmentioned factors or causal relationships: Parents' intelligence has a direct positive effect on parents' social status and child's intelligence. Other unobserved factors has a positive direct effect on parents' social status and child's intelligence.

548 Question 1:

⁵⁴⁹ If a child is intelligent, would it be more likely that this child had intelligent parents?

550 Question Type:

⁵⁵¹ Inference from Effect to Cause without Intervention

552 Ground Truth:

- 553 Yes
- **Explanation:** The probability of the child being intelligent given that the parents are intelligent is higher than the probability of the child being intelligent given that the parents are unintelligent, so
- 556 the ground truth is yes.

557 Question 2:

⁵⁵⁸ If the parents are intelligent, is the child more likely to be intelligent?

559 Question Type:

560 Inference from Cause to Effect without Intervention

561 Ground Truth:

- 562 Yes
- **Explanation:** The probability of the child being intelligent given that the parents are intelligent is
- ⁵⁶⁴ higher than the probability of the child not being intelligent given that the parents are intelligent,
- since parent's intelligence has positive effect on child's intelligence.

566 Question 3:

- ⁵⁶⁷ If we intervene to make the parents intelligent (e.g., through education or training), is the child more
- 568 likely to be intelligent?

569 Question Type:

570 Inference from Cause to Effect with Intervention

571 Ground Truth:

- 572 Yes
- **Explanation:** By intervening to increase the parents' intelligence, the child's intelligence is more likely to increase due to the causal chain. Although other unobserved factors also affect the child's
- ⁵⁷⁵ intelligence, the direct positive effect of parents' intelligence still exists.
- 576 Question 4:
- ⁵⁷⁷ If we observe a child is intelligent, and then intervene to make the child unintelligent (e.g., through ⁵⁷⁸ some kind of impairment), does this make it less likely that the child's parents are intelligent?
- 579 **Question Type:**
- 580 Inference from Effect to Cause with Intervention
- 581 Ground Truth:

582 No

583 Explanation:

The child's intelligence is the result of the combined effects of parents' intelligence and other factors. Even if we intervene to decrease the child's intelligence, it does not change the parents' level of intelligence. Therefore, in this case, the change in the child's intelligence does not affect our judgment of whether the parents are intelligent or not.

10 Appendix C: Code Question Example

```
589 Causal Scenario:
```

```
class SalesData {
590
        int totalSales, newSubscriptions;
591
        double pricePerSubscription;
592
593
        public SalesData(int newSubscribers, double price) {
594
             this.newSubscriptions = newSubscribers;
595
596
             this.pricePerSubscription = price;
597
             updateSales();
        }
598
599
        public void updatePrice(double newPrice) {
600
             this.pricePerSubscription = newPrice;
601
             updateSales();
602
        }
603
604
        public void addSubscriptions(int additionalSubs) {
605
             this.newSubscriptions += additionalSubs;
606
607
             updateSales();
        ł
608
609
        private void updateSales() {
610
             totalSales = (int) (newSubscriptions * pricePerSubscription);
611
612
613
        public int getTotalSales() {
614
             return totalSales;
615
616
    }
617
618
   SalesData monthlyReport = new SalesData (100, 10.0);
619
   monthlyReport.addSubscriptions (50);
620
   monthlyReport.updatePrice(15.0);
621
```

622 **Question 1:**

⁶²³ If the number of new subscriptions increases, will total sales also increase, assuming no other ⁶²⁴ changes?

```
625 Question Type:
```

626 From cause to effect without intervention

```
627 Ground Truth:
```

628 Yes

```
629 Explanation:
```

The method 'addSubscriptions' adds new subscriptions and then immediately calls 'updateSales',

which recalculates total sales based on the new number of subscriptions and the current price per

- subscription. Therefore, with no other changes, increasing the number of new subscriptions directly
- leads to an increase in total sales.

634 Question 2:

⁶³⁵ Does an increase in total sales imply an increase in the price per subscription?

636 Question Type:

⁶³⁷ From effect to cause without intervention

638 Ground Truth:

639 No

640 **Explanation**:

An increase in total sales can occur either from an increase in the price per subscription or from an increase in the number of new subscriptions due to the calculation in 'updateSales'. Hence, an increase in total sales does not necessarily imply that the price per subscription has increased; it could also be due to an increase in the number of subscriptions.

645 Question 3:

⁶⁴⁶ If we manually increase the price per subscription, will this result in an increase in total sales?

647 Question Type:

648 From cause to effect with intervention

649 Ground Truth:

650 Yes

651 Explanation:

Increasing the price per subscription using 'updatePrice' method causes 'updateSales' to be called, calculating the new total sales using the increased price. Assuming the number of subscriptions

remains constant, this intervention in price directly causes an increase in total sales.

655 Question 4:

⁶⁵⁶ If total sales decrease after an intervention, does this mean we decreased the number of new subscrip-⁶⁵⁷ tions?

658 Question Type:

⁶⁵⁹ From effect to cause with intervention

660 Ground Truth:

661 No

662 Explanation:

A decrease in total sales after an intervention could be due to either a decrease in the number of new subscriptions or a decrease in the price per subscription. As these two factors multiply to compute total sales, the decrease could be attributed to either factor independently or both. Thus, a decrease in total sales does not definitively determine that the intervention was a decrease in the number of new subscriptions.

668 11 Appendix D: Math Question Example

669 Causal Scenario:

Investigate the influence of a linear operator transformation z = L(x) on a vector field x governed by

 $\frac{d}{dt}x = Mx$, where M is a constant matrix. The transformation L represents another linear operator with a constant matrix.

673 Question 1:

- If the transformation z = L(x) is applied immediately at t = 0 to a vector x_0 , followed by evolution
- under $\frac{d}{dt}x = Mx$ without further intervention, does the state z(t) at t = T exactly replicate the result
- of evolving x_0 directly under $\frac{d}{dt}x = Mx$ until t = T?
- 677 Question Type:
- 678 From cause to effect without intervention
- 679 Ground Truth:
- 680 No
- 681 Explanation:

Applying the transformation z = L(x) modifies the initial conditions. The trajectory of z(t) and x(t)would differ unless L commutes with the exponential of M, which generally is not the case. Hence, the state transformations under L can produce a distinct evolutionary path in comparison to the direct

evolution of x_0 .

686 Question 2:

⁶⁸⁷ Can the original vector x_0 be reliably determined at t = 0 after observing the vector z(t) at t = T, ⁶⁸⁸ without knowing if the transformation L was applied?

- 689 **Question Type:**
- 690 From effect to cause without intervention
- 691 Ground Truth:

692 No

693 Explanation:

⁶⁹⁴ Without information on the application of L, reconstructing the exact initial state x_0 from z(t) is ⁶⁹⁵ not straightforward. The application of L can alter the vector in ways that are not easily reversible,

- $_{696}$ especially if L and M are not designed to reveal their effects straightforwardly.
- 697 Question 3:

If an additional linear transformation H is applied at time t_1 as an intervention, will the final state z(T) at $T > t_1$ be independent of the initial transformation L and solely determined by M and H?

700 **Question Type:**

- 701 From cause to effect with intervention
- 702 Ground Truth:

703 No

704 Explanation:

The final state z(T) will depend on L, M, and H. The transformations imposed by L initially, and H later, both play critical roles. These factors, combined with the dynamics driven by M, contribute

to a state at T that relies on all three matrices, affected by their interaction and properties.

708 Question 4:

Based on knowing only the vector z(T) at time T, is it feasible to precisely identify the transformations (L, H, or both) that were previously applied?

- 711 Question Type:
- 712 From effect to cause with intervention
- 713 Ground Truth:

714 No

- 715 **Explanation:**
- ⁷¹⁶ Determining which transformations were applied based on the final vector z(T) alone is challenging
- $_{17}$ due to the overlapping effects matrices may have in transforming the state space. The interactions of L

- and H with the matrix exponential of M can result in equivalent states from different transformation sequences.