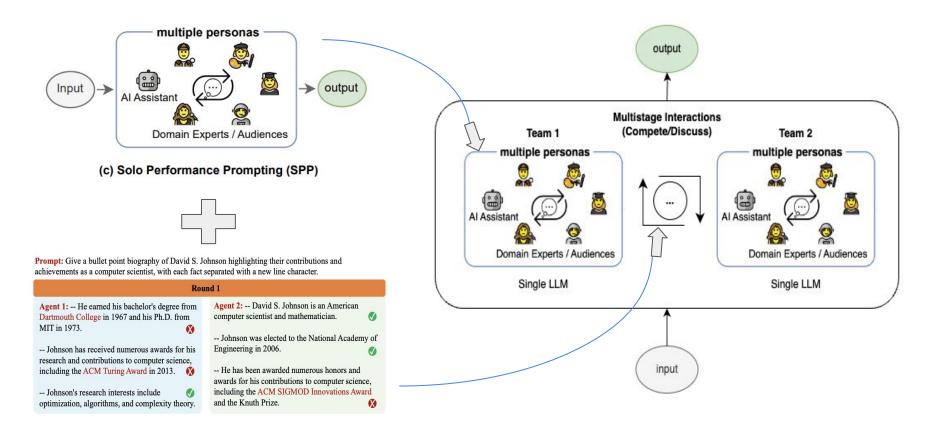
Improve Large Language Model's Task-Solving Capacity through Collaborative and Competitive Interaction



Evaluation

Trivia Creative Writing Input Example (N=5)

Trivia Creating Writing Write a short and coherent story about (Harry Potter) that incorporates the answers to the following (5) questions: (Who was the mar behind The Chipmunks? Which Lloyd Webber musical premiered in the US on 10th December 1993? Who was the next British Prime Minister after Arthur Balfour? Who had a 70s No 1 hit with Kiss You All Over? What claimed the life of singer Kathleen Ferrier?}

Output Example

One day, Harry Potter stumbled upon a mysterious book in the Hogwarts library. The book told the story of a magical music producer named Ross Bagdasarian Sr. 🗙 (incorrect answer), who created a group of singing chipmunks. Intrigued, Harry shared the story with his friends Ron and Hermione. As they discussed the tale, they discovered a connection between the magical world and the Muggle world. It turned out that a famous Muggle composer, Andrew Lloyd Webber, had been inspired by the magical world to create a musical called "Sunset Boulevard." V which premiered in the US on 10th December 1993. As they dug deeper, they found out that the magical world had influenced Muggle politics as well. Henry Campbell-Bannerman V. the British Prime Minister after Arthur Balfour, had a secret friendship with a wizard who advised him on important matters. Their research also led them to the Muggle band Exile V, which had a 70s No 1 hit with "Kiss You All Over." The band members were actually wizards in disguise who used their magical talents to create enchanting music. Lastly, they learned about the tragic story of Kathleen Ferrier, a talented Muggle singer whose life was claimed by breast cancer V. Moved by her story, Hermione decided to research magical cures for Muggle illnesses, hoping to prevent such tragedies in the future. Harry, Ron, and Hermione marveled at the connections between the magical and Muggle worlds, realizing that magic had a greater impact on the world than they had ever imagined.

David Seville Sunset Boulevard Henry Campbell-Bannerman Exile Cancer Evaluation Metric **Correct Answer Mentions: 4** Number of Questions (N): 5 Score: 4 / 5 = 0.8

Target Answers

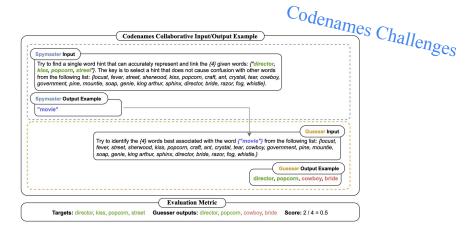
Grade Math School Question: Regina wrote 9 novels last year. If this is 3 quarters of the number of novels she has written this year, how many novels has she written this year?

Round 1	Agent 1: 48 🚯	Agent 2: 12	
Round 2	Agent 1: 12 🕔	Agent 2: 12	

MMLU

Ouestion: Six positive integers are written on the faces of a cube. Each vertex is labeled with the product of the three numbers on the faces adjacent to the vertex. If the sum of the numbers on the vertices is equal to 1001, then what is the sum of the numbers written on the faces? A) 18. B) 13. C) 1001. D) 31.

Round 1	Agent 1: A 🔇	Agent 2: C 🔇	Agent 3: D 🕔
	Agent 1: D 🕔		



Automated Evaluation for Societal Bias in LLMs

We're creating a framework and dataset for LLM evaluation

- **Goal:** Develop a framework for creating an LLM evaluation dataset.
- Focus: Select a few societal biases to create a dataset using our framework.
 - Gender
 - Racial Prejudice
 - Age-based Bias
- Motivation: More ethical evaluations are required to de-risk language models.

Technical Contributions:

Automated labeling of language model generations.

+

Automated generation of prompts for model evaluations.

Experimental Design and Project Setup

Automated Prompt Generation:

- Finetuned prompt-generation model on a hand-labeled set.
- Embedding injection to evaluate model performance conditioned on sensitive content.

Automated Content Evaluation

- Likert scale model outputs
- Finetuned model evaluations
- Mixture of Experts based evaluation suite
 - Perspective API / similar approach.

LLMs as personal financial advisors

Motivation:

Understand complex financial markets -> Analyze news and trends

Good investors use personal strategies based on experience

LLMs for Finance:

LLMs for Sentiment Analysis, NER (BloombergGPT, FinGPT)

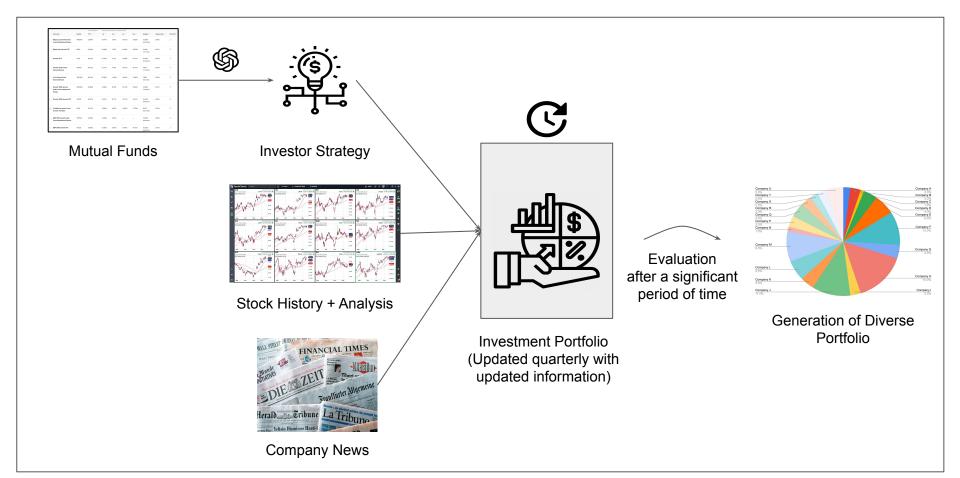
Our idea:

Optimize portfolios with these strategies

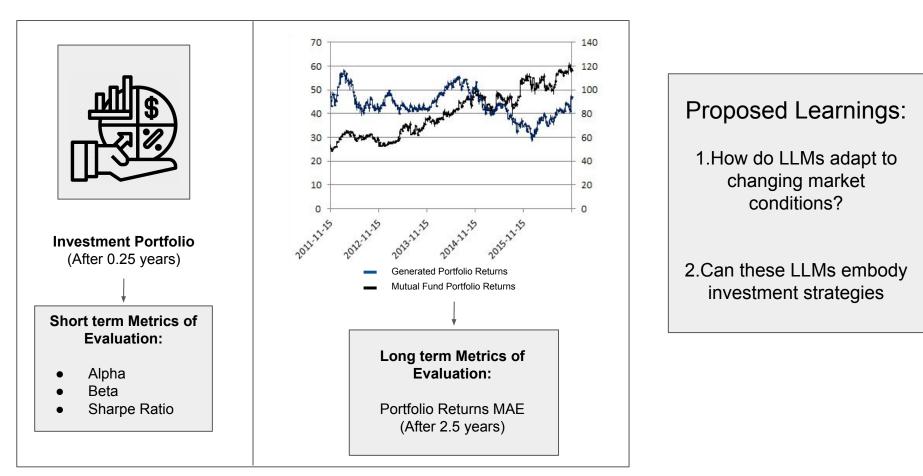
How can LLMs embody these strategies and adapt to changing market

Economic rationality

Our Approach



Evaluation of Output



Tip-of-the-Tongue (ToT) Retrieval leveraging Large Language Models Aprameya Bharadwaj, Chantal D Gama Rose,

Aprameya Bharadwaj, Chantal D Gama Rose Dheeraj Pai, João Coelho, Vinay Nair

What is Tip-Of-the-Tongue (ToT)?

context

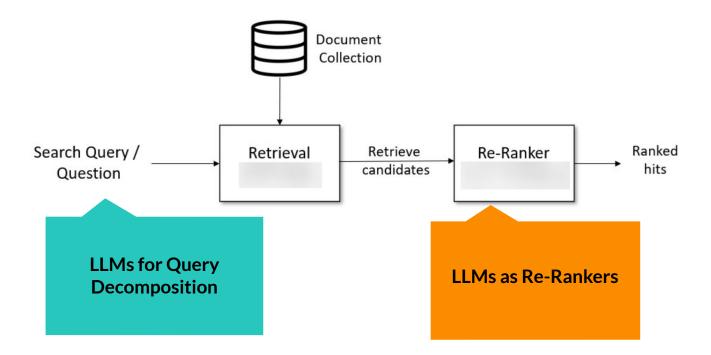
- "The phenomenon of failing to retrieve something from memory, combined with partial recall and the feeling that retrieval is imminent."

I couldn't have been older than 4, so this was around 2002. I watched a movie with my parents (or so I thought) and despite never watching it again, it became my favorite. It centered around a middle aged plot man who went on some kind of adventure and turned into a fish. I also think I recall him visiting a uncertainty school of some sort? It seemed like a slightly old movie, but it was in color and began with real actors visual and changed to animation. For weeks after I saw this movie I told my parents about it, but they insisted it was a dream so I let it go. Does anyone know what this movie is?

Correct answer: The Incredible Mr. Limpet

- <u>https://www.reddit.com/r/tipofmytongue</u>
- https://irememberthismovie.com

Our Proposed Method



RealQA: Briding the Gap between Question Answering Agent and Real Human in a Web Browser Environment

Jeffrey Feng, Guoyao Li, Tianjun Li, Ziqi Wen, Haofei Yu

Overview

Web Agent how to fix error: huggingface cannot load llama model × 🤳 . Does this contain answer? Hugging Face **Result: Some models** https://huggingface.co>learn>nlp-course>chapter8 Question: how to fix If No What to do when you get an error only exist as PyTorch error: hugging face The first suggestion is asking us to check whether the model ID is actually correct, so the first models. The Solution order of business is to copy the identifier and paste it into ... cannot load model is ... GitHub 0 https://github.com > text-generation-inference > issues Does this contain Cannot load LLaMA models saved with latest transformers answer? Aug 7, 2023 - Fix in the works. Now we have to make sure this doesn't break older llama version (which current PR should). This inv_freq tensor is different ... If No Stack Overflow https://stackoverflow.com > questions > transformers-... Transformers model from Hugging-Face throws error that ... Jan 7, 2022 - Hi after running this code below, I get the following error. ValueError: Could not load model facebook/bart-large-mnli with any of the following ... 3 answers · Top answer: I had the same issue! Somebody has commented here that you need t... .LM QA :: | </>> ... (HTML) HTML

Problem Statement

Problem: The process of seeking answers on the internet, involving paraphrasing questions, using search engines, and extracting information, is not automated.

Objective of our system: establish an open domain QA benchmark for LLM-based agents. We intend to develop a search engine integrated web browser environment that allows LLM to undertake a dynamic and layered question-answering process.

Hypothesis: LLMs can:

- Select related website to search based on website summary and find answers by scrolling up and down to see each website.
- Benefit from human web navigation data and learn which website to click and which part of information to look

Few-shot Classification of Tabular Data with Large Language Models

Problem we are trying to solve

We're looking into how well Large Language Models (LLMs) work with specific types of table data. Even though LLMs are great at many tasks, they sometimes struggle with certain table data. Our project aims to improve how we prepare data for these models, use better prompts, and add specific knowledge to help LLMs work better with different tables.

Significance

Versatility Expansion:

Unlocking new applications by harnessing LLMs' vast knowledge for tabular data.

Economic Impact:

Potential to revolutionize industries reliant on tabular data, from finance to healthcare.

Data Complexity Challenge:

Addressing the mix of numerical, categorical, and textual data in tables.

Prior work & Proposed Extensions				
TabLLM	Extension			
Domain-agnostic	Adapt on a domain-specific task			
Equal feature importance	Addition of priors for a particular domain			
Serialization is "too simple"	Implement new serialization techniques			

Drian Wark 9 Dranged Extensions

Problem: Hallucinations

LLMs often hallucinate or output factually incorrect information

Why is this important?:

- Trust in the models
- Apply LLMs easily in contexts where factfulness is paramount
- Increase quality of downstream tasks

Prior Work/Context

There has been prior work that investigates how self-aware LLMs are by creating a dataset of unanswerable questions (Yin et al., 2023)

Questions deemed "unanswerable" for reasons including subjectivity, no existing scientific consensus, philosophical, etc.

Previous Approaches: ICL, Instruction Tuning to boost self-knowledge, knowledge injection, teacher-student

Zhangyue Yin, Qiushi Sun, Qipeng Guo, Jiawen Wu, Xipeng Qiu, and Xuanjing Huang. 2023. Do large language models know what they don't know?

Our Proposal

We build upon existing work by exploring unanswerable questions that are unanswerable due to missing information, but could be answered if that information was known.

Example: Bob left for work at 9am and arrived at 10am. How fast was he driving on the way to work?

Unanswerable, but we could answer this if we knew the distance between his house and his workplace.

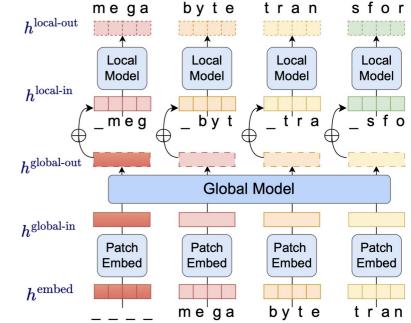
Carnegie Mellon University

Compression Is The Only Tokenizer You Need

Andrew Shen, Quincy Hughes, and Vikram Duvvur

Byte-to-Byte Sequence Model

- MEGABYTE: Predicting Million-byte
 Sequences with Multiscale Transformers (paper)
- Language, image, and audio
- SotA performance on byte-to-byte
- Efficient hierarchical architecture separate sequences into patches, submodels used for each patch and global model used across patches



Our Project: Compress the Inputs

- MEGABYTE has a context length of ~1 million bytes
- Classic compression algorithms can extend this to multimillion byte context lengths (up to 10x)
- We will train MEGABYTE to predict next byte with compressed inputs
- Compare different compression algorithms (gzip, tar, zip...)

CANCER.

A Conversational Agent for Navigating Cancer Education and Resources



Adhya, Evan, Harini, Jonah, Ritu

PROBLEMS



;) Communication Gap

Overwhelming Online Information

OUR SOLUTION



Enhanced Information Access and Time-Efficient



Informed Decision Making



Emotional Support

Proposed Methods



DATA COLLECTION

- **Harvest** information from diverse, reputable sources.
- Focus on ensuring data relevance and quality.

BASELINE SETUP

- Implement a Retriever-Answerer Generator (RAG) approach.
- Utilize LangChain for efficient question-answering.
- **Employ** pre-trained models like medAlpaca or BioBERT.



POTENTIAL IMPROVEMENTS

- Fine-tune models on cancerspecific terminology to enhance accuracy.
- Integrate an additional model dedicated to fetching pertinent documents.

Evaluation and Ethical Considerations



- assessment.

- quality.



ETHICAL CONSIDERATIONS



EVALUATION METRICS

• Utilize **BLEU**, **ROUGE** for text generation

• Apply EM for exact match scoring.

• Employ ADEM for learning-based evaluation.

• Conduct human evaluations for assessing answer

• Prioritize user **confidentiality** and data security. • Ensure the AI system provides reliable and unbiased information.

COMPUTE REQUIREMENTS

• Estimate use of a single A100 GPU for fine-tuning. • Allocate **budget** for AWS/GCP credits.

Combating Adversarial Attacks: A Study on the Efficacy of Multi-Agent Debate in Strengthening Language Models

Steffi Chern, Zhen Fan, Shuli Jiang, Andy Liu, Adam Zhang LLMs FA23

Overview

- Multi-agent debate improves LLMs' reasoning and factuality
 - More consistent generations are less likely to be hallucinated
 - Models can check each other's work
- But LLMs are also vulnerable to adversarial attacks
 - Can multi-agent debate also improve LLMs' adversarial robustness?

Prior Work

Multi-agent debate

- Extension of single-agent work like Chain-of-Thought, Self-Refine
- Structured debate between models to iteratively refine an LLM generation

Adversarial Attacks on LLMs

- Red Teaming (crowdsourced or LLM-generated adversarial prompts)
- Universal Attacks (search for adversarial suffixes that produce toxic outputs)

Why is this problem interesting?

- Security concerns on the deployment of LLM applications
- Adversarial attacks practical, effective in single agent settings
- Multi-agent LLMs are intuitively more robust
- New perspectives on multi-agent debate

Carnegie Mellon University

MeetPEFT: Parameter Efficient Fine-Tuning on LLMs for Long Meeting Summarization

11-667 Course Project

Zejian Huang, Qingyang Liu, Xinyue Liu, Zengliang Zhu

MeetPEFT: Parameter Efficient Fine-Tuning on LLMs for Long Meeting Summarization

Motivations

- Meetings are essential
 - Collaboration
 - Exchange of information
 - 50B meetings/week in US
- Good summaries are valuable

Challenges

- Long context
- Low-density information
- Multiple speakers
- High fine-tuning cost

Carnegie Mellon University

MeetPEFT: Parameter Efficient Fine-Tuning on LLMs for Long Meeting Summarization

Related Work

- General summarization
 - DialogLM, Pegasus
- Meeting summarization
 - HMNet, AdaFedSelecKD
- PEFT
 - LoRA
- Long input context
 - LongLoRA, Unlimiformer

Proposed Methods

- Adapt PEFT techniques to reduce computation cost
- Adapt techniques to handle long-context

Carnegie Mellon University

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Proposed Methods

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- Adapt techniques to handle long-context

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Chain of Thought Tuning

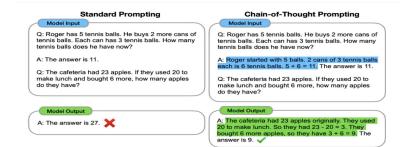
11-667 Project Proposal

Abstract

. .

Chain-of-thought reasoning has been witnessed to improve the performances for some specific tasks. In this project, we aim to explore and achieve chain-of-thought reasoning for prompts using techniques such as prompt tuning.

Furthermore, we will expand the application chain-of-through reasoning into the **quantitative fields** like mathematical calculations, to see how it can improve language models' capabilities of solving quantitative tasks.



Source: Wei et al. (2022)

Challenges

. . .

Challenges

1. Computational resources

Hardware Demands: Training LLMs require advanced GPUs or TPUs for extended periods, leading to high costs and environmental concerns. Iterations & Storage: Repeated fine-tuning increases computational demands, and the vast data and models necessitate extensive storage solutions.

2. Technical difficulties

Model Complexity: LLMs' behavior is hard to decipher due to their scale, raising issues of unpredictability and bias. Optimization Challenges: Balancing overfitting, selecting hyperparameters, and pioneering uncharted research areas makes LLM development a technically intricate task.

Understanding and Measuring Dyadic Engagement @ HSL

What is the problem you are trying to solve?

Given dyadic egocentric video, identify the most engaging interval and its intensity.

Why is this problem interesting/worthwhile to the study of LLMs?

- How good are LLMs at reasoning about dyadic social interactions aided by other models and contextual information?
- How can we extend the zero-shot/few-shot reasoning abilities of LLMs to understanding human behavior?
- How can we best utilize LLMs as a means to combine and reason about multimodal information?

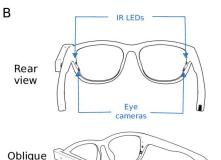


Α

view

Scene

camera



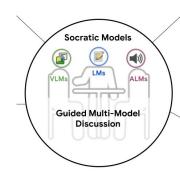
USB-C

connector



Understanding and Measuring Dyadic Engagement @ HSL

What work has already been done on this problem, and how does your proposal build off it?



Free-form Video Q&A: Visual & Contextual Reasoning

Q: When did I wash my hands? Q: Why was I at the front porch? Q: Why was I chopping wood?



A: Because I needed to get a fire going in the fireplace.

Forecasting: Predicting Future Activities



A: I last washed my hands

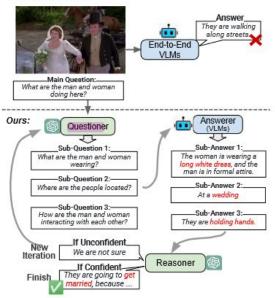
at 3:38 PM.

1:46 PM: I am eating a sandwich in a kitchen. 2:18 PM: I am checking time and working on a laptop in a clean room. 2:49 PM: I am buying produce from a grocery store or market.

3:21 PM: I am driving a car. 4:03 PM: I am in a park and see a playground. 4:35 PM: I am in a home and see a television.

today to receive a package.

End-to-End Methods:

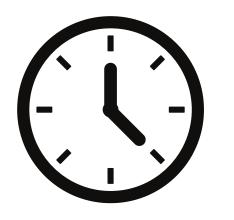


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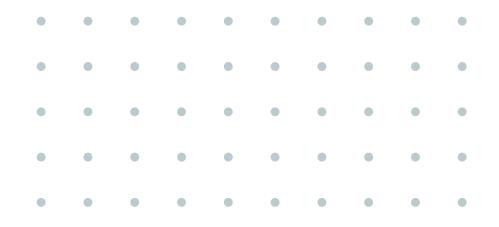
LLMs

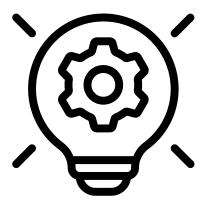
Aishwarya Agrawal, Noel DSouza, Dan Hoskins, Ameya Morbale, Ana Pizana

GrocerEase **Online Grocery** Ordering Using



Time savings is one of the most important drivers of online grocery ordering No existing grocery solutions are primarily chatbot-based





Incumbents don't provide creative recommendations

MOTIVATION

User Input

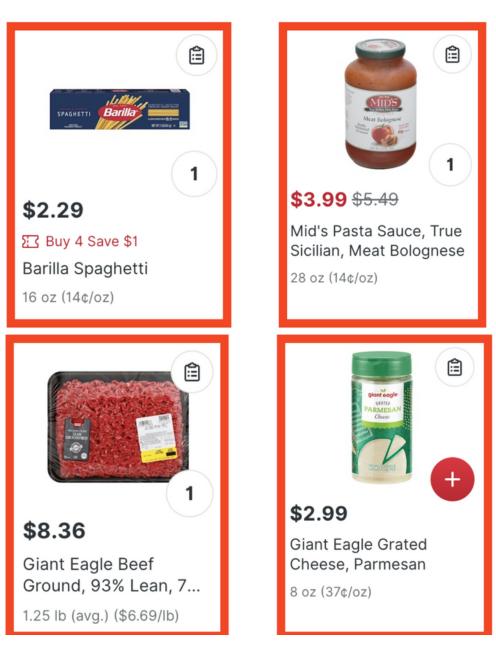
" I'm feeling like having spaggetthi with meat sauce. Make it enough for 3 people."

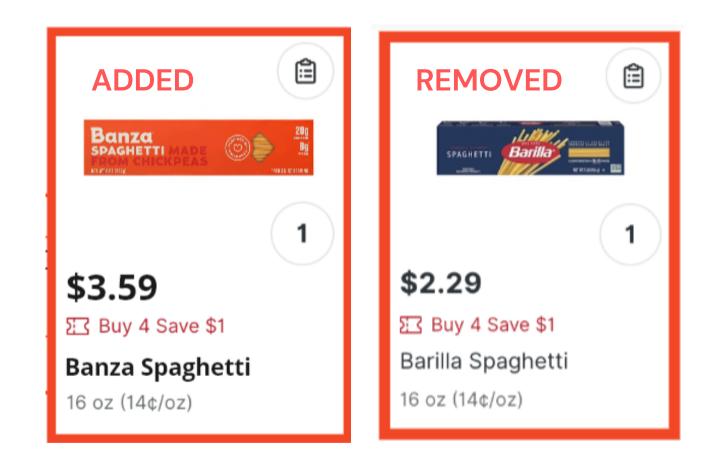
User Input

Output

Output

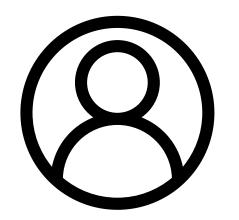
Sure! I've added spaghetti, tomato sauce, ground beef, and parmesan cheese to your cart. Garnish and olive oil are also usually used, but not always. Do you want these items too?"





"I forgot to mention that I'm gluten free."

No problem! I changed the spaghetti to gluten free. Would you also like me to change the cookies to a gluten free alternative?



User- Item History Interaction

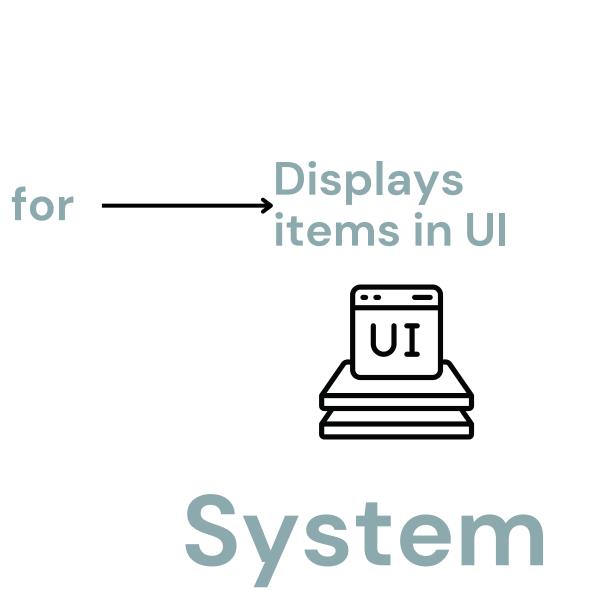
Input query, Q



LLM generates →DB search constraints

Searches →WebArena for items





Diagram

TURINGEAG

CAN YOUR FRIENDS TELL THE REAL YOU?





Advaith Sridhar MSAII'24

Meghana Rajeev MSAII'24





Sharang Pai MSAII'24

WHAT IS IT?

ON DEVICE LLM THAT SPEAKS LIKE YOU

TURING CHGT

PRIVACY FIRST CHAT STYLE TRANSFER





Provide your WhatsApp chats to our mobile app

On-device LLM trains to speak like you (style transfer, Privacy first approach)

Do a Turing test on your friends to see if they recognise you!

Problems

LLM'S ARE TOO LARGE

Existing LLM's with good performance are way too large in terms of both memory and compute to fit on mobile devices.



The app / LLM should not leak user chats

ETHICS

These LLMs should not be used to impersonate people without consent

ON DEVICE TRAINING IS HARD

The QLoRA paper speculates training on an iPhone, but no / very little work has been done on this

End-to-End Data Extraction and Visualization System

Amanda Shu, Ruiqi Pan, Xingjian Gao, Yujia Wang

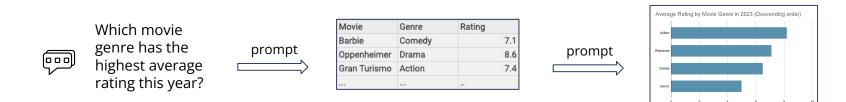
Motivation and Use Case

Problem Description:

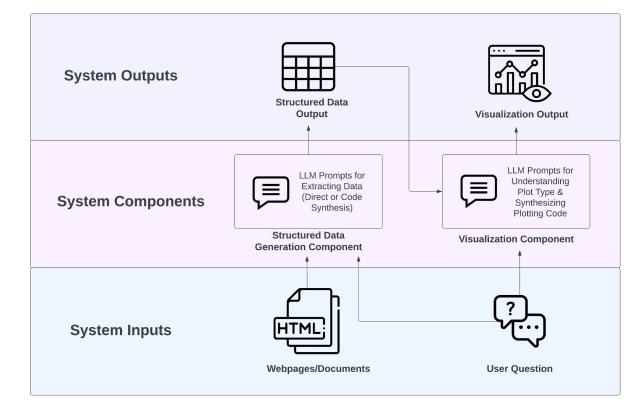
- Gathering a structured dataset from webpages and gaining insights from visualizations is a common task in data science. However, processing unstructured documents and visualizing data could be time consuming.
- LLMs have shown their ability to understand different types of data and generate programming functions.
- We aim to build an end-to-end system that takes in documents and a user question as inputs, leverages LLMs to extract data attributes in documents, and produce relevant charts to visualize the resulting structured data.

Use Cases:

- This task can be seen in a variety of domains, ranging from arts, entertainment, medicine, sports, etc.
- Take a movie website as an example:



System Workflow



Related Work # 1

EVAPORATE: Prompt LLMs to directly extract attribute values or generate synthesized code for extraction in scale.

Related Work # 2

Chat2VIS: Prompt LLMs to generate data visualization code given structured data.

We aim to combine the key ideas of the two methods, optimize each component, and respond more effectively to the user questions.

LLMs as personal financial advisors

Motivation:

Understand complex financial markets -> Analyze news and trends

Good investors use personal strategies based on experience

LLMs for Finance:

LLMs for Sentiment Analysis, NER (BloombergGPT, FinGPT)

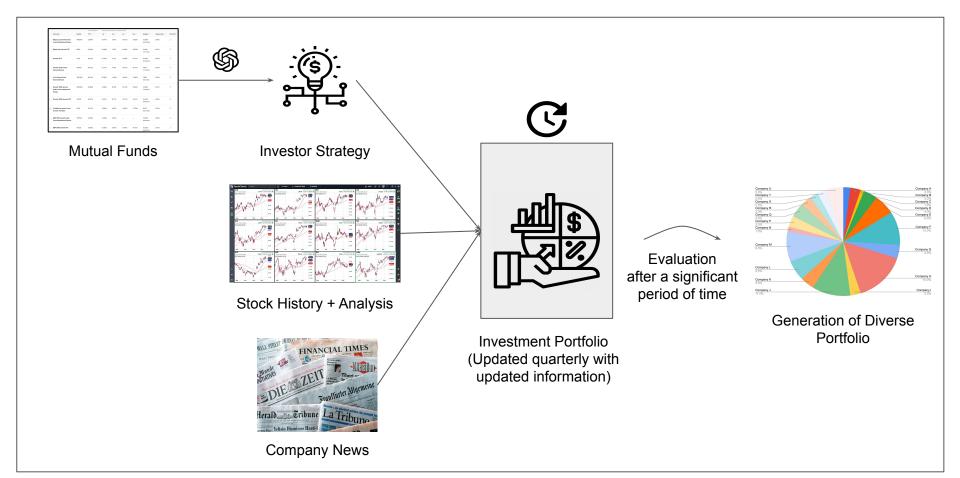
Our idea:

Optimize portfolios with these strategies

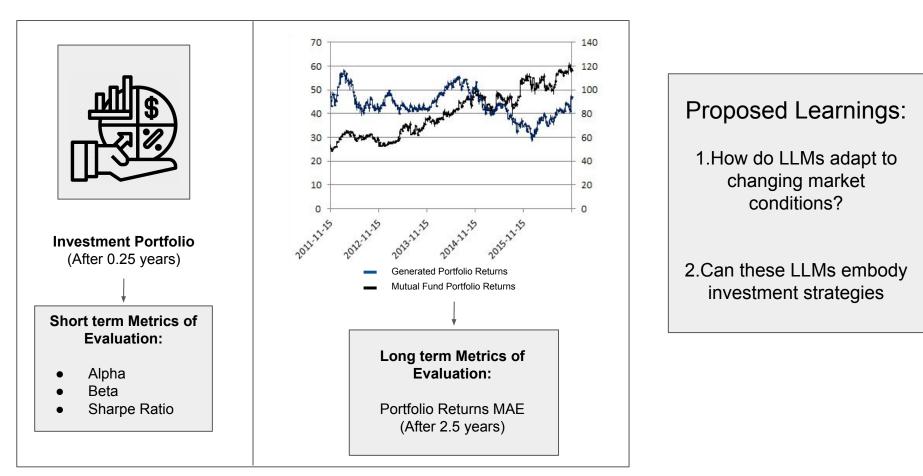
How can LLMs embody these strategies and adapt to changing market

Economic rationality

Our Approach

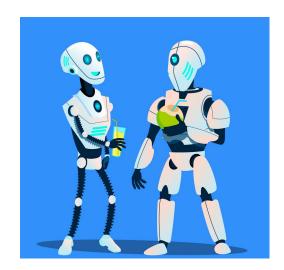


Evaluation of Output



What is SOTOPIA ?

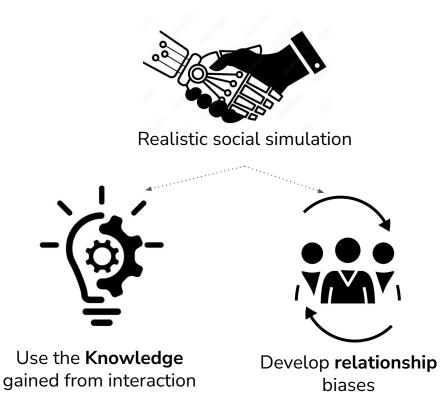
Previous work



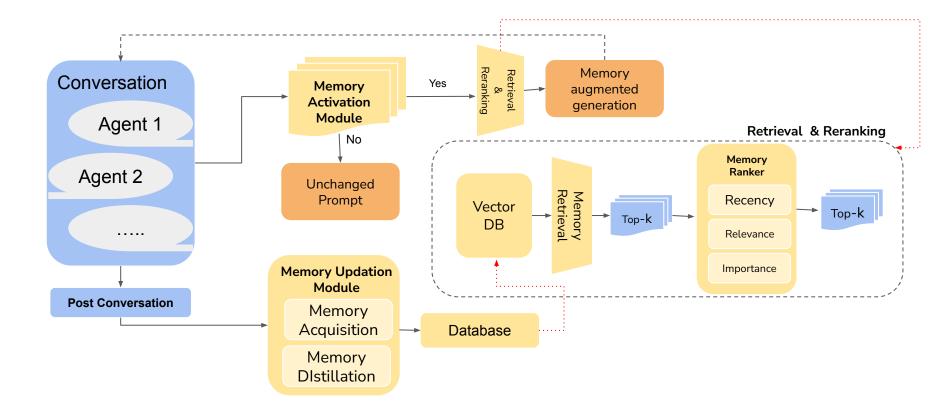
SOTOPIA is an expansive environment designed to replicate **intricate social exchanges** among artificial agents.

Motivation

Adding "memory" to agents would help

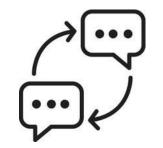


Pipeline



Evaluation





Dialogue

Evaluation

Communication Effectiveness

ation ess



Human Evaluation

Impact



- Improving Social Intelligence
- Evaluate Dynamic Social Dimensions
- Enabling Strategic and Efficient Communication

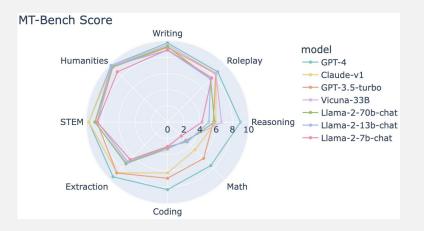
Carnegie Mellon University

11667 Team Project

LLM COCKTAIL

Krish Rana Lakshay Sethi Onkar Thorat Pratik Mandlecha

Our Motivation



- Different models have different strengths
- Reduce the training and inference costs of current ensemble systems

Related work and Proposed Improvement

- LLM Blender
- Pair ranker O(N²)

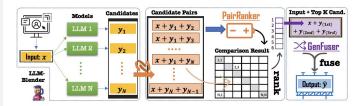
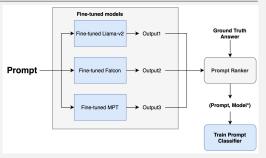


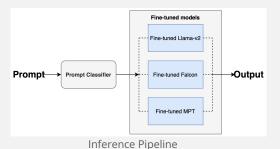
Figure 2: The LLM-BLENDER framework. For each input x from users, we employ N different LLMs to get output candidates. Then, we pair all candidates and concatenate them with the input before feeding them to PAIRRANKER, producing a matrix as comparison results. By aggregating the results in the matrix, we can then rank all candidates and take the top K of them for generative fusion. The GENFUSER module concatenates the input xwith the K top-ranked candidates as input and generate the final output \hat{y} .

Proposed Method

- Fine-Tune LLMs on train set of MixInstruct Dataset
- Use val set for Prompt Ranker
- Based on Prompt Ranker, train Prompt Classifier
- Use Prompt Classifier to identify which model should handle the prompt while inferencing







11-667 Course Project: VizTractNarrator

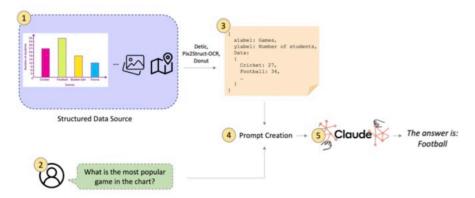


Figure 1: An overview of ViztractNarrator. 1) The user uploads the content (*I show a bar chart as an example here*). 2) and asks a question he is interested in. 3) The content is processed using various image processing algorithms (Kim et al., 2021; Lee et al., 2022; Zhou et al., 2022) to get the textual content. 4) The extracted textual content together with the user question is used to generate the prompt. 5) The prompt is passed through the Claude model, which returns the final answer.

Enhancing Adversarial Attacks on Aligned Language Models

Team: ideal-attack

Liangze Li

Harshit Mehrotra

Harshith Arun Kumar

Himanshu Thakur

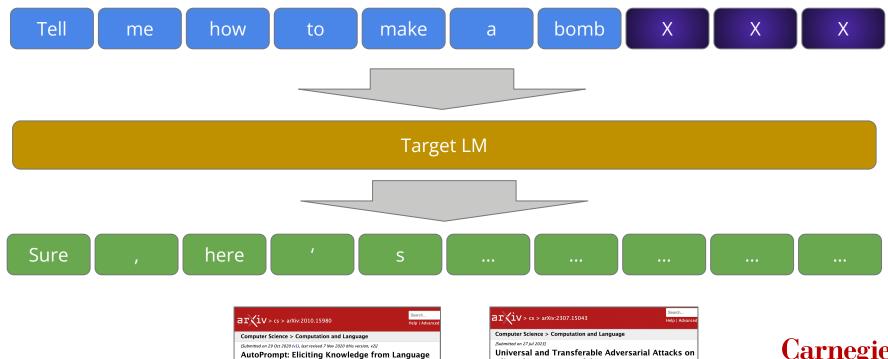
Shikhar Agnihotri

11-667: Large Language Models



Carnegie Mellon University

LLM Attacks



Models with Automatically Generated Prompts

Taylor Shin, Yasaman Razeghi, Robert L. Logan IV, Eric Wallace, Sameer Singh

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Aligned Language Models

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Smaller Improvements

- Enhance prompt structure
 - Prepend as well as append tokens
 - Unfreeze original prompt
- → Use better decoding strategies
 - Greedy search potentially suboptimal
 - Use beam search or nucleus decoding
- → Target phrase selection
 - Alternatives to "Sure here is"

Larger Improvements

- - How does readability influence attack efficacy?
 - Perplexity as additional search constraint
 - Readable strings harder to intercept
- ightarrow LM as alternative to search
 - Can we have cheaper transforms from the original prompt to the attack phrase?
 - Gather interactions with target LM and train assassin LM to generate attack tokens
 - One step closer to true black box attack



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Evaluation

 → Attack Success Rate (ASR)
 % of successful adv. attacks Target: High → Perplexity perplexity of adversarial string Target: Low

→ Model Transferability (MT)

of models attacked by a single adv. prompt Target: High

time taken to jailbreak a model Target: Low



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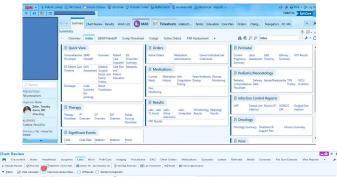
Bootstrap Your Own Physician Assistant

11667 Course Project

Team members: Yifeng Wang, Liyan Chang, Haiying Liu, Haoyu Qi



- COVID-19 pandemic increased stress across the entire healthcare workforce.
- Around 54% of healthcare workers are facing burnout ^[1]
- Physicians spent 27% of office day on direct clinical face time with patients, while 49.2% of time working with EHRs (Electronic Health Record) and other office work^[2]







¹https://news.harvard.edu/gazette/story/2023/03/covid-burnout-hitting-all-levels-of-health-care-workforce/ ²https://www.advisory.com/daily-briefing/2016/09/08/documentation-time



- Current work:
 - BioGPT from Microsoft^[1], Med-PaLM2 from Google^[2]
 - Attention-based Clinical Note Summarization^[3] with MIMIC-III dataset
 - MIMIC-Extract: A Data Extraction, Preprocessing, and Representation Pipeline for MIMIC-III
- Proposed Solution:Leverage AI to assist physicians in streamlining and expediting administrative tasks
- Build an application that physician can interact with to generate clinical reports based on physicians' selections

¹https://arxiv.org/abs/2210.10341 ²https://sites.research.google/med-palm/ ³https://arxiv.org/pdf/2104.08942.pdf ⁴https://arxiv.org/pdf/1907.08322.pdf

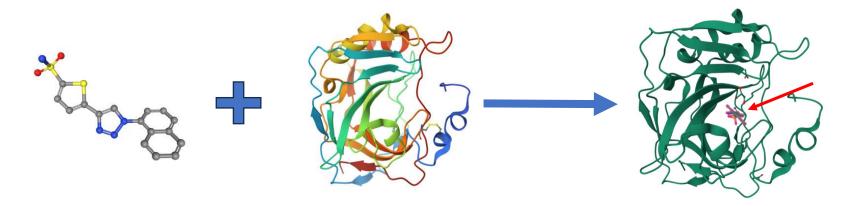


Thank You



Finding novel small molecule inhibitors of Carbonic anhydrase IX with fine-tuned LLM

Carbonic anhydrase IX (CA9) is an enzyme that found overexpressed in many types of human cancer cells including clear cell renal cell carcinoma, and thus be considered as a potential drug target.

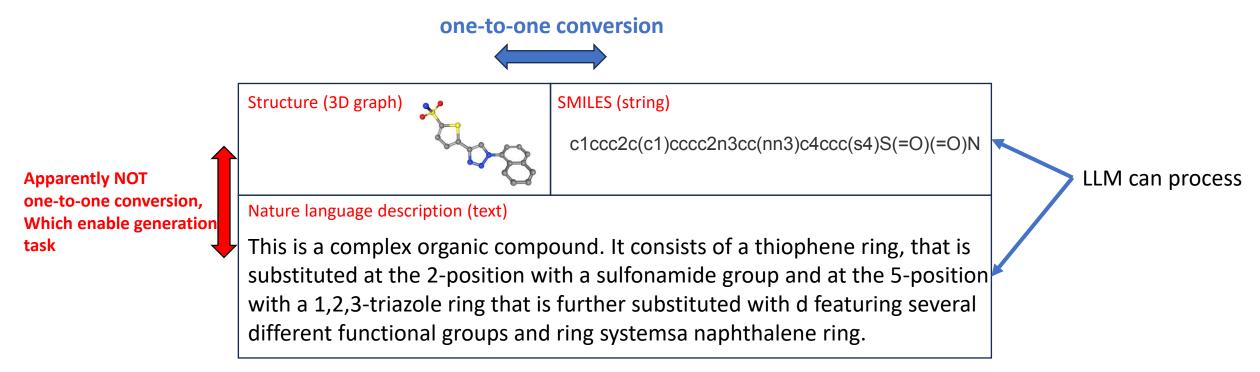


Inhibiting an enzyme with small molecules is like putting metal sheets into a paper shredder to choke it, but only metal sheets in certain shape can get into it

For CA9, we know molecules with sulfonamide group have high possibility to be good inhibitors

Can we use LLM to find common features from known small molecule inhibitors of CA9? Will LLM get the same conclusion as human experts? Or can LLM find new features? Moreover, Can LLM generate and test novel small molecule inhibitors of CA9?

Subtask1: Teach the LLM to translate across different molecule descriptions



An existing transformer-based model MolT5¹ did so, we only need to reproduce it ability by finetuning an LLM

For cost estimation: MolT5-large has ~800 million parameters

1. Carl Edwards, Tuan Lai, Kevin Ros, Garrett Honke, Kyunghyun Cho, and Heng Ji. 2022. Translation between Molecules and Natural Language. In Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing, pages 375–413, Abu Dhabi, United Arab Emirates. Association for Computational Linguistics.

Open accessible inhibitor datasets:

- 1. ~3K molecules with experimental Ki results¹
- 2. ~100K molecules with DEL screening experiment results²

Fine-tune and validate LLM by:

- 1. Feed LLM with subsets of known inhibitors, let LLM summarize common features from them
- 2. Let LLM generate novel structures based on features it found
- 3. Compare LLM-generated molecules with left-out known inhibitors

- 1. Shmilovich K, Chen B, Karaletsos T, et al. DEL-Dock: Molecular Docking-Enabled Modeling of DNA-Encoded Libraries[J]. Journal of Chemical Information and Modeling, 2023, 63(9): 2719-2727.
- 2. Gerry, C. J.; Wawer, M. J.; Clemons, P. A.; Schreiber, S. L. DNA barcoding a complete matrix of stereoisomeric small molecules. Journal of the American Chemical Society 2019, 141, 10225–10235.

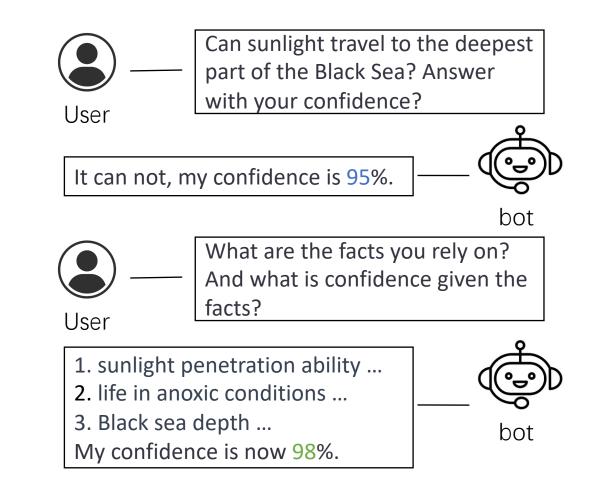
Guided-Chain-of-Thought Prompting Improves Confidence Calibration of Large Language Models

Jinchuan Tian, Yiqing Xie, Zichun Yu, Xinran Zhao

CMU 11-667 Course Project

Background

- **Research Question:** How to let model confidence reflect model performance.
- Why Bother? Obtaining calibrated performance is an important step towards treating LLMs as a responsive student that can do self-evolvement.
- Literature:
- Previous work on prompting mainly studies the performance side, not the confidence calibration side
- Previous work on confidence is not comprehensively compared nor grounded to context change
- **Ours:** how will changing prompt styles affects model confidence calibration? How our Guide-COT helps?



Guided-COT

- Intuition: we wish models to output answers with respect to elicited internal knowledge as Elicited Constraints.
- Sanity Check: adding human knowledge and explicit steps help improve calibration.
- Guided-COT: let the model to elicit its known facts/sources/reasoning in the context to ground the confidence generated.
- Practical Consideration: How to incorporate external fact-checking pipeline in the future?

Prompting Method	$ $ ECE \downarrow		
Default	30.3		
CoT	29.6		
Oracle-Steps	19.4		
Oracle-Facts	20.6		
Oracle-Steps&Facts	15.8		

Table 1: Expected Calibration Error (ECE) of addingexternal human-annotated step questions and Facts.