

LLM Agents

Slido: https://app.sli.do/event/rzAMNVhnNM58rKG74nFaZd

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Overview of Course Contents

- Week 1: Logistics & Overview
- Week 2: N-gram Language Models
- Week 3: Word Senses, Semantics & Classic Word Representations
- Week 4: Word Embeddings
- Week 5: Sequence Modeling & Recurrent Neural Networks (RNNs)
- Week 6: Language Modeling with Transformers
- Week 8: Transformer and Pretraining
- Week 9: Large Language Models (LLMs) & In-context Learning
- Week 10: Knowledge in LLMs and Retrieval-Augmented Generation (RAG)
- Week 11: LLM Reasoning
- Week 12: Reinforcement Learning for Post-Training LLMs
- Week 13: LLM Alignment & Agents
- Week 15 (after Thanksgiving): Project Presentations



(Recap) The Evolution of GPT Models: ChatGPT

- GPT-1: decoder-only Transformer pretraining
- GPT-2: language model pretraining is multi-task learning
- GPT-3: scaling up & in-context learning
- ChatGPT: language model alignment

			ChatGPT	
GPT-1	GPT-2	GPT-3	(GPT-3.5)	
2018	2019	2020	2022	



(Recap) Overview: Language Model Alignment

- Ensure language models behaviors are aligned with human values and intent for general tasks/applications
- "HHH" criteria (Askell et al. 2021):
 - Helpful: Efficiently perform the task requested by the user
 - Honest: Give accurate information & express uncertainty
 - Harmless: Avoid offensive/discriminatory/biased outputs







Paper: https://arxiv.org/pdf/2112.00861

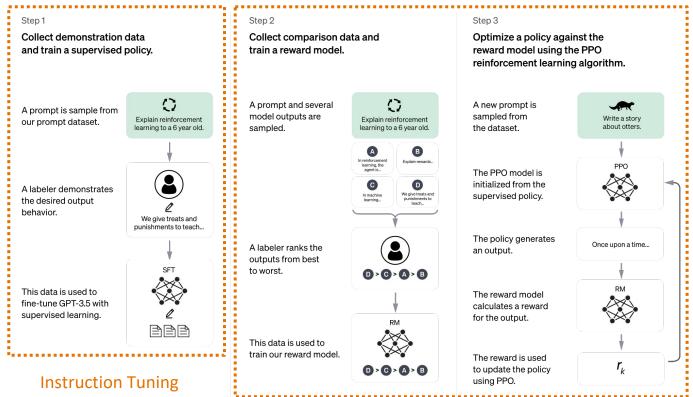
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(Recap) Language Model Alignment: Post-training

- Pretrained language models are **not** aligned
- Objective mismatch
 - Pretraining is to predict the next word in a sentence
 - Does not involve understanding human intent/values
- Training data bias
 - Text from the internet can contain biased, harmful, or misleading information
 - LMs don't distinguish between good and bad behavior in training data
- (Over-)generalization issues
 - LMs' generalization can lead to outputs that are inappropriate in specific contexts
 - Might not align with intended ethics/honesty standard



(Recap) Language Model Alignment Techniques

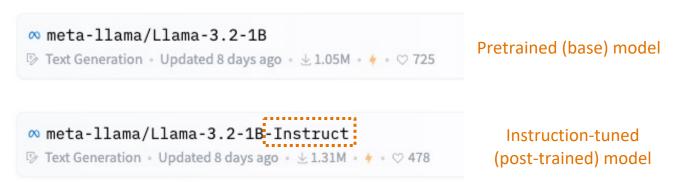


Reinforcement Learning from Human Feedback (RLHF)



(Recap) Overview: Instruction Tuning

- Train an LM using a diverse set of tasks
 - Each task is framed as an instruction followed by an example of the desired output
 - The goal is to teach the model to follow specific instructions (human intent) effectively
- The resulting model can perform a variety of tasks **zero-shot** (w/o requiring in-context demonstrations)
- The instructions can also be in chat format tuning an LM into a chatbot





(Recap) Instruction Tuning: Introduction

- **Setting**: fine-tune LLMs with task-specific instructions on diverse tasks
- Goal: enable LLM to better understand user prompts and generalize to a wide range of (unseen) tasks zero-shot

FINETUNED LANGUAGE MODELS ARE ZERO-SHOT LEARNERS

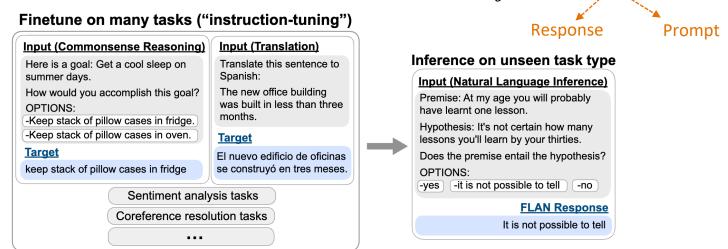
Jason Wei*, Maarten Bosma*, Vincent Y. Zhao*, Kelvin Guu*, Adams Wei Yu, Brian Lester, Nan Du, Andrew M. Dai, and Quoc V. Le Google Research

Paper: https://arxiv.org/pdf/2109.01652



(Recap) Instruction Tuning: Method

- Input: task description
- Output: expected response or solution to the task
- Train LLMs to generate response tokens given prompts $\min_{m{ heta}} \log p_{m{ heta}}(m{y}|m{x})$



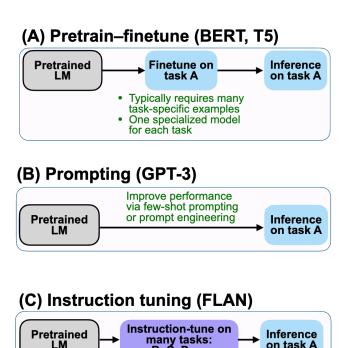
Paper: https://arxiv.org/pdf/2109.01652



(Recap) Instruction Tuning vs. Other Paradigms

- Task-specific fine-tuning does not enable generalization across multiple tasks
- In-context learning requires few-shot demonstrations

Instruction tuning enables zero-shot cross task generalization



B, Ć, D, ...

Model learns to perform

many tasks via natural

language instructions

Inference on

unseen task

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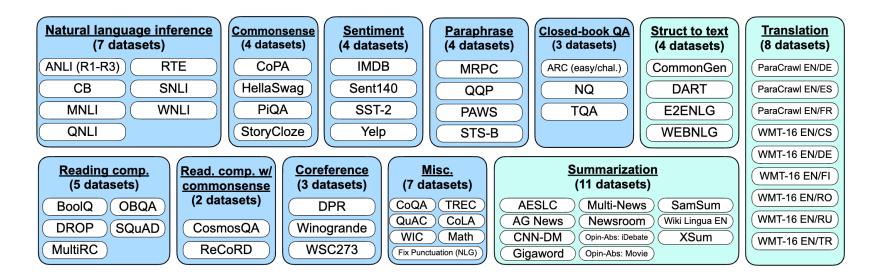
(Recap) Instruction Tuning vs. Pretraining

- Both instruction tuning and pretraining are multi-task learning paradigms
- Supervision
 - Pretraining: self-supervised learning (raw data w/o human annotation)
 - Instruction tuning: supervised learning (human annotated responses)
- Task format
 - Pretraining: tasks are implicit (predicting next tokens)
 - Instruction tuning: tasks are explicit (defined using natural language instructions)
- Goal
 - Pretraining: teach LMs a wide range of linguistic patterns & general knowledge
 - Instruction tuning: teach LMs to follow specific instructions and perform a variety of tasks



(Recap) FLAN: Collection of Instruction Tuning Datasets

62 datasets (12 task clusters) covering a wide range of understanding + generation tasks

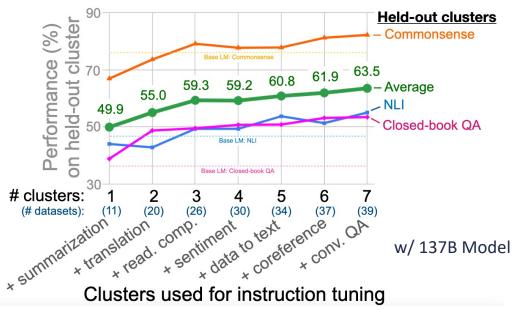


Paper: https://arxiv.org/pdf/2109.01652



(Recap) Generalization Improves with More Clusters

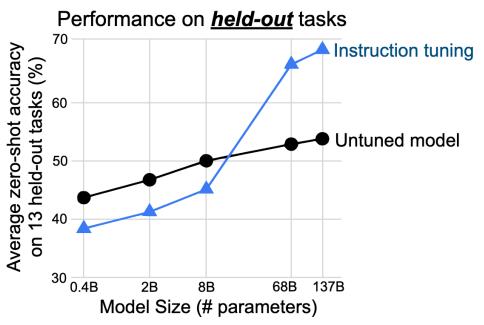
- Held out three clusters from instruction tuning: Commonsense, NLI, Closed-book QA
- More clusters and tasks used in instruction tuning => better generalization to unseen clusters





(Recap) Instruction Tuning with Different Model Sizes

- Instruction tuning can hurt small model (< 8B) generalization
- Instruction tuning substantially improves generalization for large models



(Recap) Chat-style Instruction Tuning

- Instruction tuning can also be used to build chatbots for multi-turn dialogue
- Instructions may not correspond strictly to one NLP task, but mimic a human-like dialogue
- Multi-turn instruction tuning training data example:

```
{"role": "user", "content": "What's the weather like today?"},
{"role": "assistant", "content": "It's sunny with a high of 75 degrees."},
{"role": "user", "content": "Great! What about tomorrow?"},
{"role": "assistant", "content": "Tomorrow will be partly cloudy with a high of 72 degrees."}
```

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(Recap) Limitations of Instruction Tuning & Why RLHF

Costly human annotations

- Instruction tuning requires human annotators to write down the entire expected responses
- RLHF only relies on preference labels (which response is better?)

Open-ended generation

- Open-ended creative generation (e.g., story writing) inherently has no single "right" answer
- RLHF uses human feedback to determine which response is more creative/appealing

Token-level learning

- Instruction tuning applies the language modeling loss -> penalizes all token mistakes equally regardless of their impact on the overall quality of the output (e.g., a grammatical error might be less critical than a factual inaccuracy)
- RLHF uses human feedback to prioritize the error types that are more important to correct

Suboptimal human answers

- Instruction tuning may learn the suboptimal patterns written by humans
- Identifying a better answer from a few options is usually easier than writing an optimal answer entirely



(Recap) Overview: RLHF

- Human feedback collection
 - Generate multiple responses using the model given the same prompt
 - Human evaluators rank responses of the model based on helpfulness/honesty/safety...
- Reward model training
 - A reward model is trained on human feedback data to predict the quality of responses
 - Higher reward = more preferred by human evaluators
- Policy optimization
 - Use reinforcement learning algorithms to further train the LM to maximize the reward predicted by the reward model
 - Encourage the model to produce outputs that align better with human preferences

Training language models to follow instructions with human feedback

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(Recap) RLHF Illustration

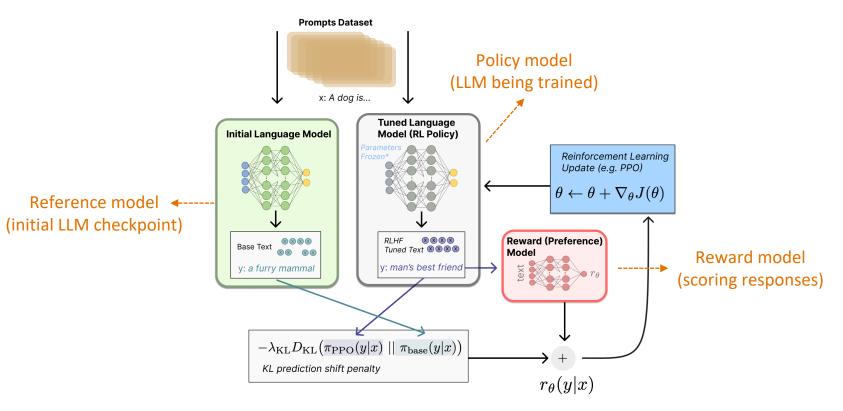


Figure source: https://huggingface.co/blog/rlhf



(Recap) Preference Data Construction

- Goal of reward model: score the quality of LLM's output based on human feedback
- Can we directly ask human annotators to assign a scalar score (e.g., 1-10) to a single

response?

What are the steps for making a simple cake?

- 1. Warm up the oven.
- Grease a cake pan.
- 3. Blend dry ingredients in a bowl.
- 4. Incorporate butter, milk, and vanilla.
- Mix in the eggs.
- 6. Pour into the prepared pan.
- 7. Bake until golden brown.
- 8. Add frosting if desired.

Different human evaluators can be very inconsistent in assigning absolute scores!



(Recap) Preference Data with Pairwise Comparisons

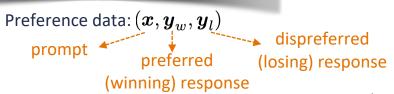
Humans are better at relative judgments than absolute ones

What are the steps for making a simple cake?

- 1. Preheat oven to 350°F (175°C).
- 2. Grease and flour a cake pan.
- In a bowl, combine 2 cups flour, 1.5 cups sugar, 3.5 tsp baking powder, and a pinch of salt.
- Add 1/2 cup butter, 1 cup milk, and 2 tsp vanilla; mix well.
- Beat in 3 eggs, one at a time.
- 6. Pour batter into the pan.
- Bake for 30-35 minutes or until a toothpick comes out clean.
- Let cool, then frost or serve as desired.

What are the steps for making a simple cake?

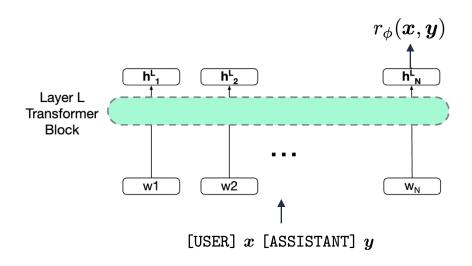
- 1. Warm up the oven.
- 2. Grease a cake pan.
- 3. Blend dry ingredients in a bowl.
- 4. Incorporate butter, milk, and vanilla.
- Mix in the eggs.
- 5. Pour into the prepared pan.
- 7. Bake until golden brown.
- Add frosting if desired.





Reward Model Setup

Goal: train a reward model to assign a higher reward to y_w than y_l

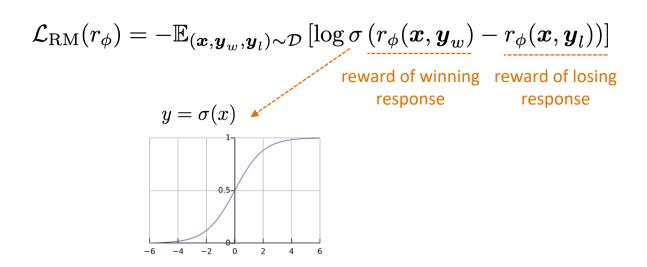


Apply a linear layer at the last token representation to learn a scalar output



Reward Model Training

Bradley-Terry pairwise comparison objective



Optimizing LLMs with the Reward Model

- The trained reward model serve as a proxy for human judgment (higher reward = more preferred by humans)
- Maximize the reward of generated responses from the LLM (policy model)

$$\max_{ heta} \mathbb{E}_{m{y} \sim p_{ heta}(\cdot | m{x})} \left[r_{\phi}(m{x}, m{y})
ight]$$
LLM output reward of LLM probability generated response

What if our reward model is imperfect?



Issues with Naïve Optimization of Rewards

- Reward models are still only approximations of true human preferences
 - Can be noisy or incomplete (e.g., not well-generalized out-of-domain)
- Solely maximizing the reward leads to several issues
 - Exploiting reward model flaws: The LLM might learn to "hack" the reward model, finding
 ways to achieve high reward without actually possessing the desired behavior
 - Mode collapse: The LLM might converge to a narrow distribution of outputs that achieve high reward, but lack diversity and fail to generalize to different situations
 - Loss of pretrained knowledge: Over-optimization for the reward model can cause the LLM to unlearn desirable properties in the initial pretrained model (e.g., grammar, factuality)

Regularized Reward Optimization

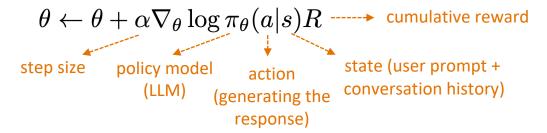
Add a penalty for drifting too far from the initial SFT checkpoint

$$\max_{\theta} \mathbb{E}_{\boldsymbol{y} \sim p_{\theta}(\cdot | \boldsymbol{x})} \left[r_{\phi}(\boldsymbol{x}, \boldsymbol{y}) - \beta \log \left(\frac{p_{\theta}(\boldsymbol{y} | \boldsymbol{x})}{p_{\text{SFT}}(\boldsymbol{y} | \boldsymbol{x})} \right) \right]$$
Maximize reward
Prevent deviation from the initial (SFT) model hyperparameter

- Penalize cases where $p_{ heta}(m{y}|m{x}) > p_{ ext{SFT}}(m{y}|m{x})$
- In expectation, it is known as the Kullback-Leibler (KL) divergence $ext{KL}(p_{ heta}(m{y}|m{x})\|p_{ ext{SFT}}(m{y}|m{x}))$

Optimization with Reinforcement Learning (RL)

- Why reinforcement learning:
 - No supervised data available (only a reward model)
 - Encourage the model to explore new possibilities (generations) guided by the reward model
- Optimization: policy gradient methods
 - Optimize the policy (LLM) by adjusting the parameters in the direction that increases expected rewards
- REINFORCE (simplest policy gradient method):





Overview: Direct Preference Optimization (DPO)

- Overall, the RLHF framework is very complicated
 - Need to first train a reward model
 - Need to do online sampling
 - Performance is very sensitive to many hyperparameters
- Direct Preference Optimization (DPO): optimize LM parameters directly on preference data by solving a binary classification problem (without an explicit reward model)

Direct Preference Optimization: Your Language Model is Secretly a Reward Model

Rafael Rafailov*† Archit Sharma*† Eric Mitchell*†

Stefano Ermon^{†‡} Christopher D. Manning[†] Chelsea Finn[†]

†Stanford University ‡CZ Biohub {rafailov,architsh,eric.mitchell}@cs.stanford.edu

Paper: https://arxiv.org/pdf/2305.18290

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Further Reading on RLHF

- RAFT: Reward rAnked FineTuning for Generative Foundation Model Alignment [Dong et al., 2023]
- <u>Iterative Preference Learning from Human Feedback: Bridging Theory and Practice for RLHF under KL-Constraint</u> [Xiong et al., 2023]
- SLiC-HF: Sequence Likelihood Calibration with Human Feedback [Zhao et al., 2023]
- <u>SimPO: Simple Preference Optimization with a Reference-Free Reward</u> [Meng et al., 2024]

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Agenda

- LLM Agent Overview
- Multimodal LLMs
- Tool Usages
- Code Assistant

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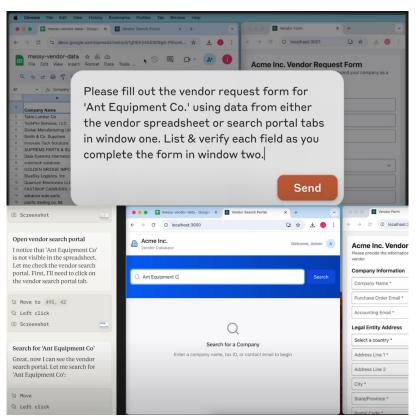
Overview: Language Agents

- Language agents: systems that interact with users using natural language as an interface to execute real-world tasks
- LLMs serve as the foundation for language agents
 - Natural language understanding: comprehend and interpret user input in text
 - Natural language generation: generate coherent & appropriate responses/actions
 - Reasoning: enable multi-step reasoning or problem-solving/decision-making
- Examples:
 - **Virtual assistants**: understand user commands and carry out tasks (e.g., setting reminders, playing music, controlling smart home devices)
 - Code agents: assist developers by generating code snippets, suggesting improvements, and explaining how certain pieces of code work
 - Business operations: break down high-level goals (e.g., "create a marketing campaign"), search and synthesize information, and execute steps autonomously (e.g., interacting with external API/tools)



Claude 3.5: Computer Use







WebShop: Language Agents for Online Shopping

Instruction: i am looking for x-large, red color women faux fur lined winter warm jacket coat, and price lower than 70.00 dollars

Current Query: women fur jacket coat

Results

Page 1 (1-10) of 50 total results

Back to Search

Next >







Current Action: click[Back to Search]

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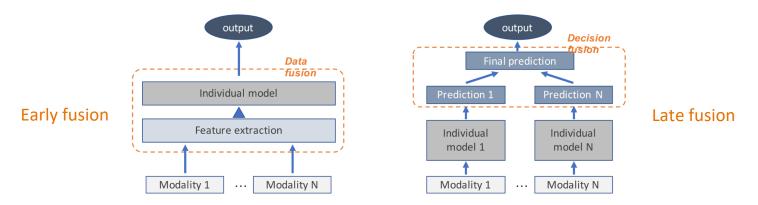
Overview: Multimodal LLMs

- Process and understand multiple types of data (e.g., text, images, audio, and video)
- More comprehensive and contextually rich understanding & generation
- Multimodal input processing (common):
 - Accept and process different types of input data
 - Examples: understanding the content of an image, transcribing and interpreting speech, analyzing video content, or integrating information from sensor data
- Multimodal output generation (less common):
 - Generate output in various modalities
 - Examples: creating realistic images from text descriptions, translating speech to text, or generating music according to user descriptions



Overview: Multimodal Architecture

- Architecture:
 - Require modality-specific architectures (e.g., vision/audio/video encoders)
 - Usually LLMs serve as the strong base
- Multimodal fusion: fuse information from different modalities
 - Early fusion: Combine raw input data from different modalities before processing
 - Late fusion: Process each modality separately and then combine the representations later





Overview: Multimodal Datasets

Training datasets need to contain paired examples of different modalities => teach the model the relationships between different types of data



Source: https://www.barnorama.com/wp-content/uploads/2016/12/03-Confusing-Pictures.jpg

What is unusual about this image?

The unusual aspect of this image is a man ironing clothes on the back of a minivan or van. This is not a typical place to perform this activity, as one would usually iron clothes in a more stationary and safe location, such as a home, using a regular ironing board.

Figure source: https://arxiv.org/pdf/2304.08485



Visual Instruction Tuning

- Goal: fine-tune a multimodal LLM to learn to follow instructions for tasks that involve both visual and textual information
- **LLaVA** (Large Language and Vision Assistant): combine a pretrained vision encoder (e.g., CLIP) with a large language model (e.g., Llama) for visual instruction tuning

Visual Instruction Tuning

Haotian Liu^{1*}, Chunyuan Li^{2*}, Qingyang Wu³, Yong Jae Lee¹

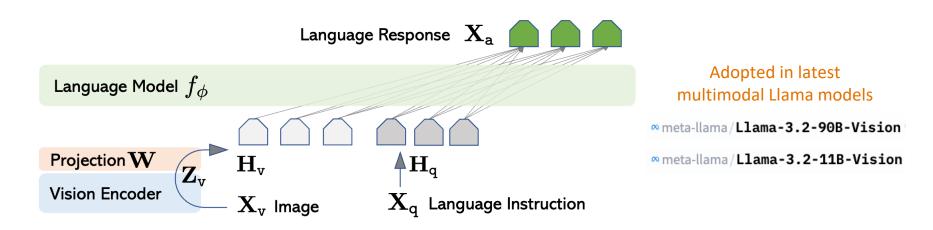
¹University of Wisconsin–Madison ²Microsoft Research ³Columbia University https://llava-vl.github.io

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LLaVA: Architecture

- Learn a projection matrix (W) to convert imagine representations (Z_v) to text embeddings (H_v)
- Concatenate visual tokens (H_v) with text tokens (H_q) as input to the model



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LLaVA: Results

Sometimes I just look at pictures of the earth from space and I marvel at how beautiful it all is.



User LLaVA Can you explain this meme in detail?

The meme in the image is a creative and humorous take on food, with a focus on chicken nuggets, as the center of the universe. The meme begins with the phrase "Sometimes I just look at pictures of the Earth from space and I marvel at how beautiful it all is..." The main image features a tray of cooked chicken nuggets, with the chicken pieces positioned to resemble the continents and islands on a world map. The meme playfully suggests that the chicken nuggets represent the Earth, and the various locations depicted in the photo are

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Tool Usages with LLMs

- Motivation: many task execution requires accessing & using external tools (e.g., calculator, calendar, search engines)
- Toolformer: train LMs to use various tools and automatically decide when and how to use which tool

Toolformer: Language Models Can Teach Themselves to Use Tools

Timo Schick Jane Dwivedi-Yu Roberto Dessì† Roberta Raileanu Maria Lomeli Luke Zettlemoyer Nicola Cancedda Thomas Scialom

Meta AI Research †Universitat Pompeu Fabra



Types of Tools Considered

Automatically decide when & which tool to use during text generation

Question answering syst	em
-------------------------	----

The New England Journal of Medicine is a registered trademark of [QA("Who is the publisher of The New England Journal of Medicine?") → Massachusetts Medical Society] the MMS.

Calculator

Out of 1400 participants, 400 (or [Calculator(400 / 1400) $\rightarrow 0.29$] 29%) passed the test.

Machine translation

The name derives from "la tortuga", the Spanish word for $[MT("tortuga") \rightarrow turtle]$ turtle.

Wikipedia search

The Brown Act is California's law [WikiSearch("Brown Act") → The Ralph M. Brown Act is an act of the California State Legislature that guarantees the public's right to attend and participate in meetings of local legislative bodies.] that requires legislative bodies, like city councils, to hold their meetings open to the public.



Tool Learning via In-context Learning

- Provide example API calls in context
- LLMs learn to generate API calls for new data

In-context examples

Your task is to add calls to a Question Answering API to a piece of text. The questions should help you get information required to complete the text. You can call the API by writing "[QA(question)]" where "question" is the question you want to ask. Here are some examples of API calls:

Input: Joe Biden was born in Scranton, Pennsylvania.

Output: Joe Biden was born in [QA("Where was Joe Biden born?")] Scranton, [QA("In which state is Scranton?")] Pennsylvania.

Input: Coca-Cola, or Coke, is a carbonated soft drink manufactured by the Coca-Cola Company.

Output: Coca-Cola, or [QA("What other name is Coca-Cola known by?")] Coke, is a carbonated soft drink manufactured by [QA("Who manufactures Coca-Cola?")] the Coca-Cola Company.

Input: x

Output:

Generate API calls for new data

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Filtering API Calls

- Some API calls are beneficial for the LLM to execute the task, while others are not
- Helpful API calls typically reduce the loss for generating future tokens



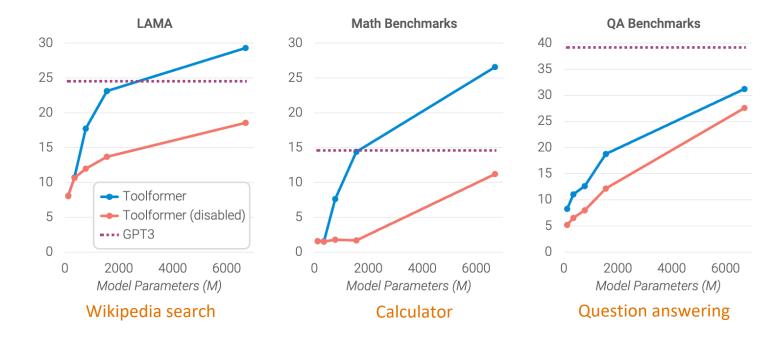
Filter out API calls which do not reduce the loss

$$c_i^2$$
 = Which country is Pittsburgh in? r_i^2 = United States $L_i(c_i^2 o United States)$ > $\min(L_i(c_i^2 o \varepsilon), L_i(\varepsilon))$ API call does not help reduce the loss



Tool Usage Ability vs. Model Scale

Larger models more effectively learn how to appropriately use tools



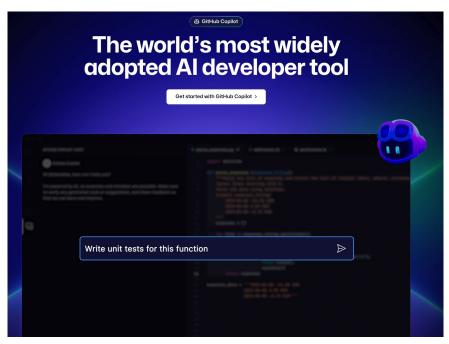
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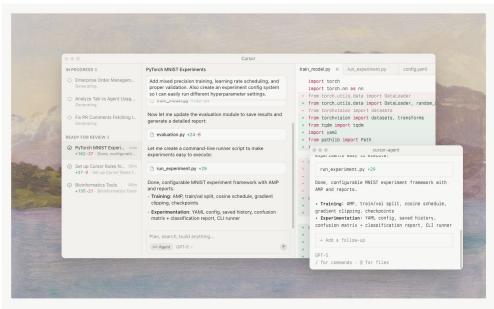
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LLMs as Code Assistants





https://github.com/features/copilot



Code Infilling

- Motivation: code is seldom written in a single left-to-right pass and is instead repeatedly edited and refined
- Need train an LLM to perform both left-to-right code generation and editing (masking and infilling)

INCODER: A GENERATIVE MODEL FOR CODE INFILLING AND SYNTHESIS

```
Daniel Fried*<sup>♥†♦</sup> Armen Aghajanyan*<sup>♥</sup> Jessy Lin<sup>♠</sup>
Sida Wang<sup>♥</sup> Eric Wallace<sup>♠</sup> Freda Shi<sup>△</sup> Ruiqi Zhong<sup>♠</sup>
Wen-tau Yih<sup>♥</sup> Luke Zettlemoyer<sup>♥†</sup> Mike Lewis<sup>♥</sup>

Facebook AI Research<sup>♥</sup> University of Washington<sup>†</sup>
UC Berkeley<sup>♠</sup> TTI-Chicago<sup>△</sup> Carnegie Mellon University<sup>♠</sup>

dfried@cs.cmu.edu, {armenag,mikelewis}@fb.com
```

Paper: https://arxiv.org/pdf/2204.05999

InCoder Training: Causal Masking

- Sample several spans of code in training documents
- Move these spans to the end of the document, with their original location denoted by special mask tokens
- LLM is trained to produce these entire masked documents => learn to generate insertion text conditioned on bidirectional context

Original Document

Masked Document

InCoder Inference: Code Editing

Various types of code editing: insert mask tokens at desired locations and use the model to generate content to be inserted

Type Inference

Variable Name Prediction

Docstring Generation

Multi-Region Infilling

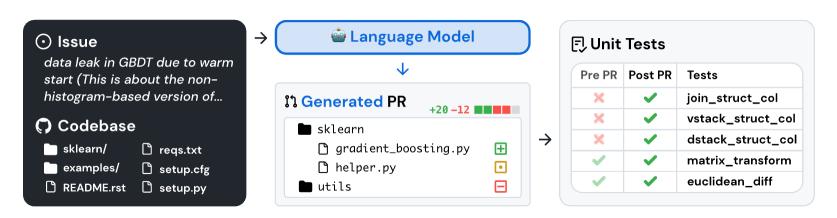
```
from collections import Counter

def word_count(file_name):
    """Count the number of occurrences of each word in the file."""
    words = []
    with open(file_name) as file:
        for line in file:
            words.append(line.strip())
    return Counter(words)
```



Code Agent Evaluation: SWE-Bench

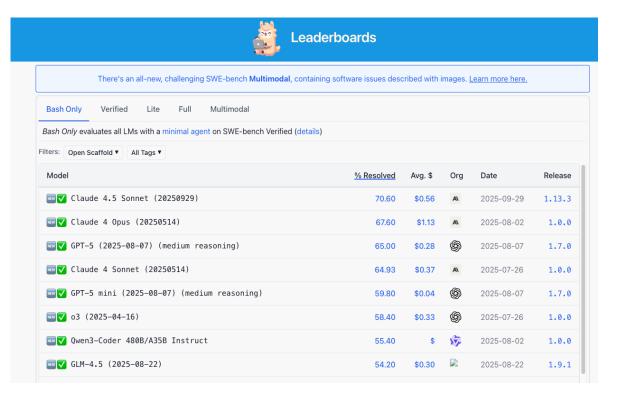
- Collect task instances from real-world Python repositories by connecting GitHub issues to merged pull request solutions that resolve related test
- Provided with the issue text and a codebase snapshot, LLMs generate a patch that is evaluated against real tests



Paper: https://arxiv.org/pdf/2310.06770



Latest Progress (As of 11/19/25) on SWE-Bench



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Thank You!

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