

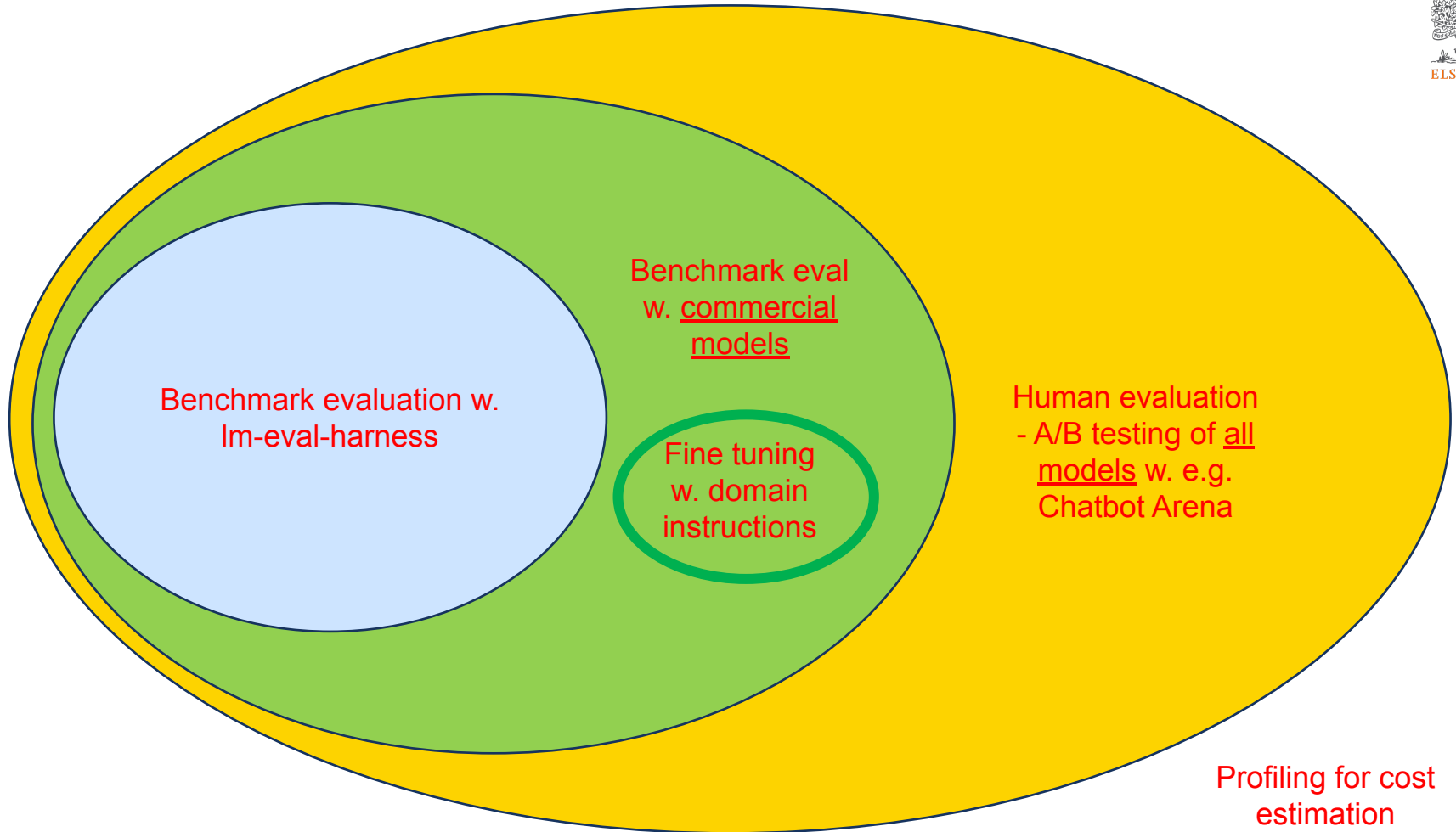
# NLP4Chemistry

Exploring the Fringe

Camilo Thorne, Saber Akhondi

May 2024 - COLING/LREC '24



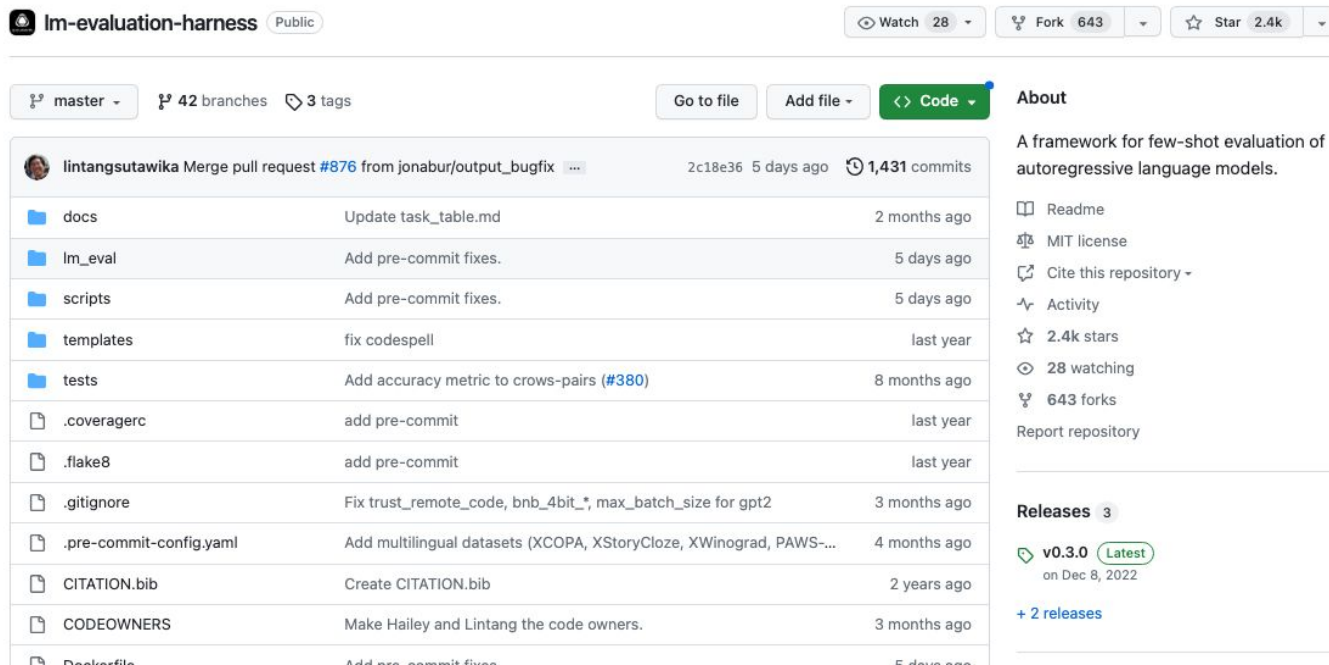


# Benchmark Evaluation



# Benchmark evaluation w. lm-eval-harness [2022]

<https://github.com/EleutherAI/lm-evaluation-harness>



The screenshot shows the GitHub repository page for **lm-evaluation-harness** by EleutherAI. The repository is public and has 28 watches, 643 forks, and 2.4k stars. It is currently on the **master** branch, with 42 other branches and 3 tags. The repository description states it is a framework for few-shot evaluation of autoregressive language models. The file list includes folders for docs, lm\_eval, scripts, templates, and tests, as well as various configuration and documentation files. The right sidebar shows the 'About' section with links to the README, MIT license, and repository activity, and the 'Releases' section showing the latest release, **v0.3.0**, dated December 8, 2022.

**lm-evaluation-harness** Public

Watch 28 Fork 643 Star 2.4k

master 42 branches 3 tags

Go to file Add file Code

**lintangsutawika** Merge pull request #876 from jonabur/output\_bugfix 2c18e36 5 days ago 1,431 commits

File/Folder	Description	Time
docs	Update task_table.md	2 months ago
lm_eval	Add pre-commit fixes.	5 days ago
scripts	Add pre-commit fixes.	5 days ago
templates	fix codespell	last year
tests	Add accuracy metric to crows-pairs (#380)	8 months ago
.coveragerc	add pre-commit	last year
.flake8	add pre-commit	last year
.gitignore	Fix trust_remote_code, bnb_4bit_*, max_batch_size for gpt2	3 months ago
.pre-commit-config.yaml	Add multilingual datasets (XCOPA, XStoryCloze, XWinograd, PAWS-...)	4 months ago
CITATION.bib	Create CITATION.bib	2 years ago
CODEOWNERS	Make Hailey and Lintang the code owners.	3 months ago
... (truncated)	...	...

**About**

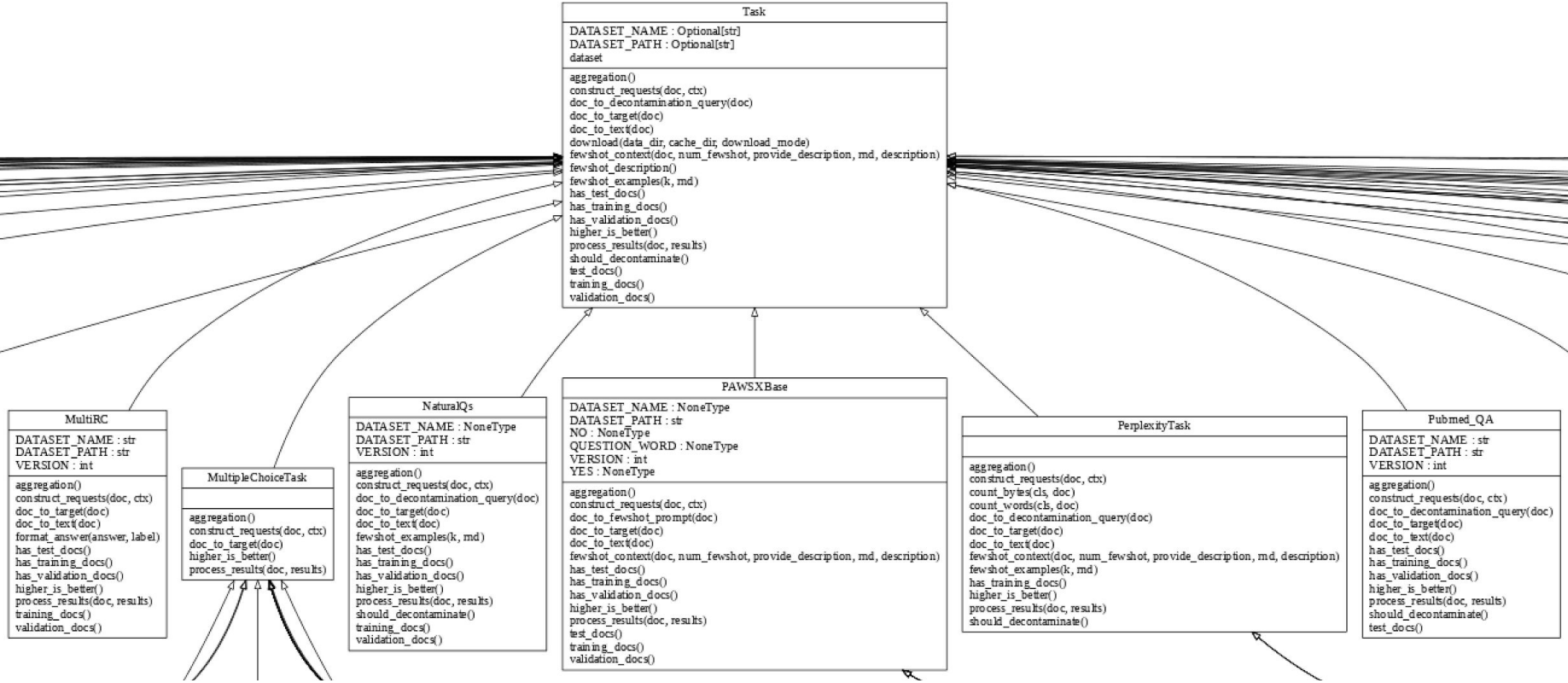
A framework for few-shot evaluation of autoregressive language models.

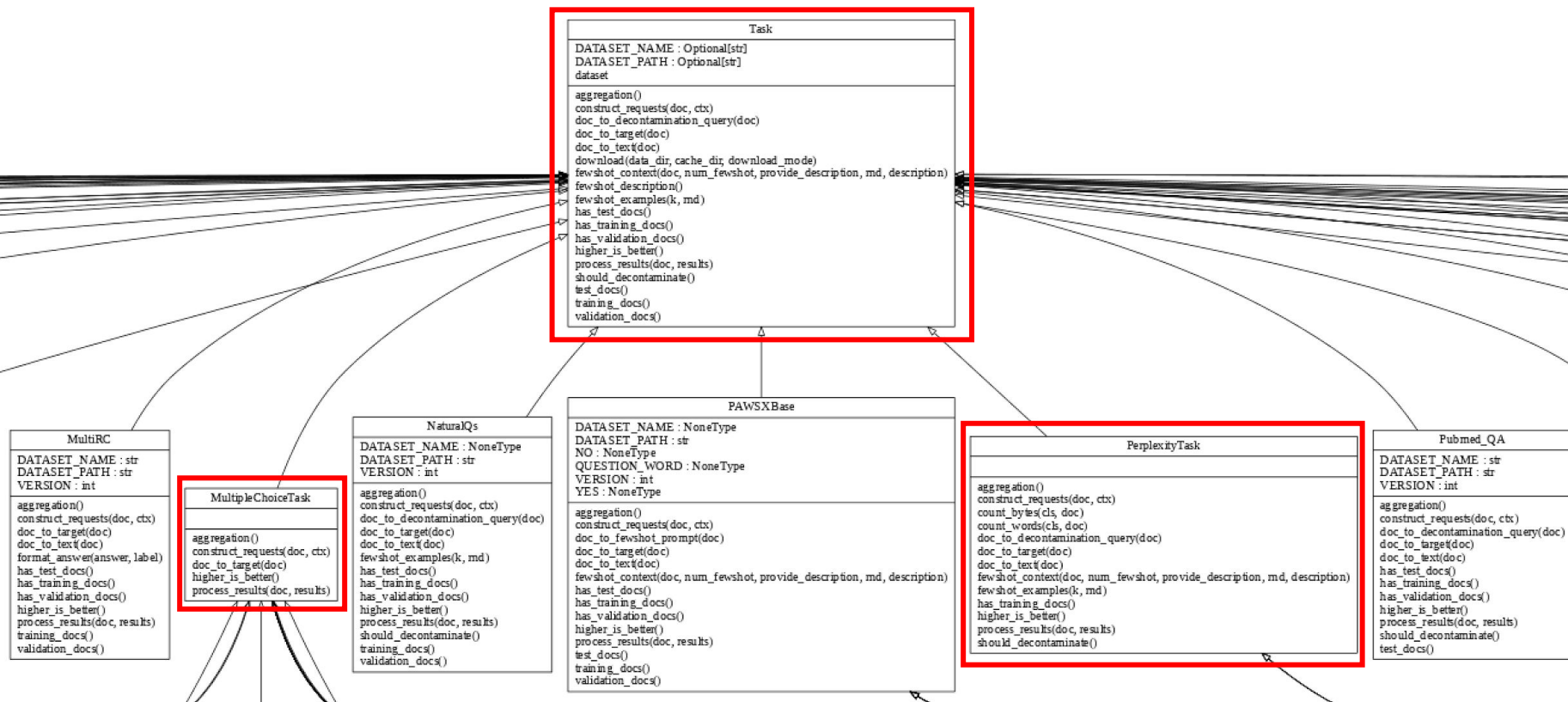
- Readme
- MIT license
- Cite this repository
- Activity
- 2.4k stars
- 28 watching
- 643 forks
- Report repository

**Releases** 3

**v0.3.0** Latest on Dec 8, 2022

+ 2 releases





```
import datasets

from lm_eval.base import PerplexityTask
from lm_eval.utils import escaped_split

class ICSRPerplexity(PerplexityTask):
    """
    We re-use here the ICSR data, but we throw away the labels.
    We ask the model to generate the abstracts, and measure LM perplexity.
    """
    VERSION = "0.1.0"
    DATASET_PATH = "icsr"
    DATASET_NAME = "icsr-perplexity"

    def __init__(self, data_dir=None, cache_dir=None, download_mode=None):
        self.data_dir = data_dir
        self.dataset = datasets.load_dataset(
            path=self.DATASET_PATH,
            name=self.DATASET_NAME,
            data_dir=data_dir,
            cache_dir=cache_dir,
            download_mode=download_mode,
            field="data",
        )
        self._training_docs = None
        self._fewshot_docs = None

    def download(self, data_dir=None, cache_dir=None, download_mode=None):
        raise TypeError("cannot download an arbitrary JSON dataset")

    def has_validation_docs(self):
        return False

    def has_training_docs(self):
        return False

    def has_test_docs(self):
        return True

    def test_docs(self):
        return map(self._process_doc, self.dataset["test"])

    def _process_doc(self, doc):
        return doc['Abstract']
```

- Extend task (sub) class
- Implement custom constructor
- Implement or override super-class methods

```
MODEL_REGISTRY = {  
    "hf": gpt2.HFLM,  
    "hf-causal": gpt2.HFLM,  
    "hf-causal-experimental": huggingface.AutoCausalLM,  
    "hf-seq2seq": huggingface.AutoSeq2SeqLM,  
    "gpt2": gpt2.GPT2LM,  
    "gpt3": gpt3.GPT3LM,  
    "anthropic": anthropic_llms.AnthropicLM,  
    "textsynth": textsynth.TextSynthLM,  
    "dummy": dummy.DummyLM,  
}
```

## Library supports:

- HF-supported **decoder-only** models + architectures
- HF-supported **encoder-decoder** models + architectures
- OpenAI legacy models (GPT3, GPT4)
- Anthropic Claude v1

Datasets need to be formatted into HF **Dataset** JSON format

Models and datasets by default fetched from HF remote servers

But they can also be deployed locally, provided HF formats are satisfied





# lm-eval-harness leaderboard [2022-]

[https://huggingface.co/spaces/HuggingFaceH4/open\\_llm\\_leaderboard](https://huggingface.co/spaces/HuggingFaceH4/open_llm_leaderboard)

## 🤖 Open LLM Leaderboard

LLM Benchmark
Metrics through time
About
FAQ
Submit

Search models or licenses (e.g., 'model\_name; license: MIT') and press ENTER...

Select columns to show

☒ Average
☒ ARC
☒ HellaSwag
☒ MMLU
☒ TruthfulQA
☒ Winogrande
☒ GSM8K
☐ Type

☐ Architecture
☐ Precision
☐ Merged
☐ Hub License
☐ #Params (B)
☐ Hub
☐ Model sha

Hide models

☒ Private or deleted
☒ Contains a merge/mcmerge
☒ Flagged
☐ MoE

Model types

☒ pretrained
☒ continuously pretrained
☒ fine-tuned on domain-specific datasets
☒ chat models [RLHF, DPO, IFT, ...]

☒ base merges and moerges
☐ ?

Precision

☒ float16
☒ bfloat16
☐ 8bit
☐ 4bit
☐ GPTQ
☐ ?

Model sizes (in billions of parameters)

☐ ?
☐ ~1.5
☐ ~3
☒ ~7
☒ ~13
☐ ~35
☐ ~60
☐ 70+

T	Model	Average	ARC	HellaSwag	MMLU	TruthfulQA	Winogrande	GSM8K
🔖	<a href="#">zhengr/MixIAO-78x2-MoE-v8.1</a>	77.5	73.81	89.22	64.92	78.57	87.37	71.11
💬	<a href="#">yunconglang/Truthful_DPO_TenGao_FusionNet_78x2_MoE_13B</a>	77.44	74.91	89.3	64.67	78.02	88.24	69.52
🔖	<a href="#">yunconglang/DARE_TIES_13B</a>	77.1	74.32	89.5	64.47	78.66	88.08	67.55
🔖	<a href="#">yunconglang/13B_MATIL_DPO</a>	77.08	74.66	89.51	64.53	78.63	88.08	67.1
🔖	<a href="#">yunconglang/MoE_13B_DPO</a>	77.05	74.32	89.39	64.48	78.47	88	67.63
🔖	<a href="#">yan-poleg/Experiment26-7B</a>	76.74	73.38	89.15	64.32	78.24	84.93	70.43
🔖	<a href="#">MISAIR/multi_verse_model</a>	76.74	72.87	89.2	64.4	77.92	84.77	71.27
🔖	<a href="#">chihoonlee10/T3Q-Mistral-Orca-Math-DPO</a>	76.7	72.95	89.23	64.42	78.41	84.93	70.28
🔖	<a href="#">yan-poleg/Experiment26-7B</a>	76.67	73.12	89.12	64.3	78.04	85	70.43
🔖	<a href="#">xwttz/experiment26-truthy-itex-0</a>	76.65	73.29	89.11	64.35	77.86	84.93	70.36
🔖	<a href="#">nbeerbower/bophades-mistral-truthy-DPO-7B</a>	76.63	73.38	89.28	64.73	77.88	85.16	69.37
🔖	<a href="#">yan-poleg/Experiment30-7B</a>	76.62	73.38	89.13	64.28	77.98	84.93	70.65

# ChemLLM [2023]

- Open release of chemistry LLM evaluation benchmarks
- "Promptified" version of known benchmarks
  - USPTO-50k
  - PubChem
  - ...

Ability	Task	Task Type	Dataset	#ICL candidates	#test	Evaluation Metrics
Understanding	Name Prediction	Generation	PubChem	500	100	Accuracy
	Property Prediction	Classification	BBBP, HIV, BACE, Tox21, ClinTox	2053, 41127, 1514, 8014, 1484	100	Accuracy, F1 score
Reasoning	Yield Prediction	Classification	Butchward-Hartwig, Suzuki-Miyaura	3957, 5650	100	Accuracy
	Reaction Prediction	Generation	USPTO-Mixed	409035	100	Accuracy, Validity
	Reagents Selection	Ranking	Suzuki-Miyaura	5760	100	Accuracy
	Retrosynthesis	Generation	USPTO-50k	40029	100	Accuracy, Validity
	Text-Based Molecule Design	Generation	ChEBI-20	26407	100	BLEU, Exact Match, etc
Explaining	Molecule Captioning	Generation	ChEBI-20	26407	100	BLEU, Chemists, etc

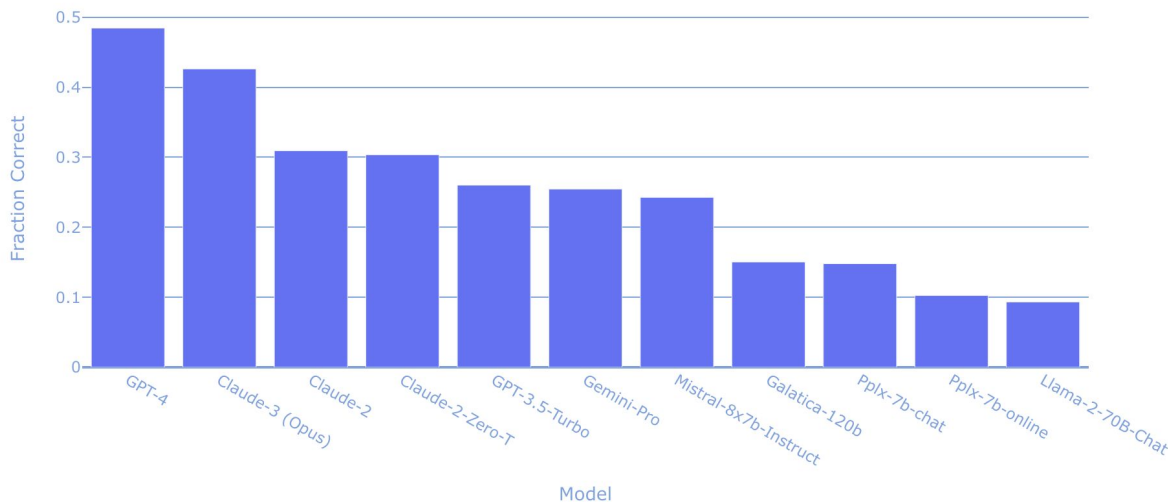
<https://github.com/ChemFoundationModels/ChemLLMBench>

# ChemBench [2024]

- Similar to ChemLLM, but focused on pharmaceutical domain
- Evaluation of open source models + leaderboard

<https://lamalab-org.github.io/chem-bench/leaderboard/>

Relies on  
completion  
"accuracy" for  
benchmarking!



# Challenges of metrics

Benchmark metrics focus too much on lexical match, **at the expense of topical relevancy!**

**doc\_id:** 3

**prompt\_0:** "Question: Pyridine synthesis via hetero-Diels-Alder reaction of 1,2,4-triazines and dienophiles (e.g. enamine) followed by extrusion of N<sub>2</sub> What is the name of the reaction? Answer: Boger Thermal Cycloaddition Question: How to synthesis L-valeric acid? Answer: The Marckwald Asymmetric Synthesis is a well-known reaction to synthesise L-valeric acid.It's a Chiral synthesis of L-valeric acid by pyrolysis of brucine salt of racemic  $\alpha$ -methyl- $\alpha$ -ethylmalonic acid Question: What is a Clauson-Kaas Synthesis? Answer: Synthesis of pyrrole derivative by the condensation between a primary aliphatic or aromatic amine and 2,5-dialkoxy-tetrahydrofuran in the presence of an acid catalyst Question: Which reaction type is able to convert trialkyl phosphite and alkyl halide to phosphonate? Answer: until"

**logit\_0:** "The reaction type that is able to convert trialkyl phosphite and alkyl halide to phosphonate is a Wacker reaction"

**truth:** " The Arbuzov Reaction is a well-known reaction to synthesise phosphonate.It's a Formation of a phosphonate from a trialkyl phosphite and an alkyl halide"

**Completion1:** "The reaction type that is able to convert trialkyl phosphite and alkyl halide to phosphonate is a Wacker reaction"

**Completion2:** "**The Arbuzov Reaction**" [closer as it captures the subject!]

**Truth:** "The Arbuzov Reaction is a well-known reaction to synthesise phosphonate. It's a Formation of a phosphonate from a trialkyl phosphite and an alkyl halide"

Completion	BLEURT	BLEU	ROUGE-1	ROUGE-2
Completion 1	0.166	0.137	0.533	0.186
Completion 2	-0.644	0.001	0.207	0.148

# Human Evaluation



# Human evaluation [2023]

- Benchmark evaluation cannot cover all the quality dimensions of LLMs
- Human evaluations rely on A/B testing:
  - Pits two generations of two (blinded) models for same input
  - Humans express a preference (A is better, B is better, tie)

## Two broad methods:

1. ELO scores
2. Votes w. IRR

The ELO score is a ranking score derived from chess. It is typically measured and updated after every single match. In the context of LLM “gamified” A/B testing it quantifies and aggregates user preferences towards a given model.

In what follows,  $E_A \in [0, 1]$  is the expected likelihood of  $A$  winning, whereas  $S_A$  is the “observed” likelihood with  $S_A = 1$  if  $A$  wins,  $S_A = 0$ , if  $A$  loses and  $S_A = 0.5$ . Let  $\text{ELO}_A$  be the initial ELO score of  $A$ . After playing a game the new ELO score of  $A$  is

$$\text{ELO}'_A = \text{ELO}_A + k \cdot (S_A - E_A)$$

where  $k$  denotes a scaling factor that determines how much influence each particular match can have on the overall ELO rating of the player.

# Chatbot arena leaderboard [2023-]



[Arena \(battle\)](#) [Arena \(side-by-side\)](#) [Direct Chat](#) [Vision Direct Chat](#) **Leaderboard** [About Us](#)

## LMSYS Chatbot Arena Leaderboard

[Vote](#) | [Blog](#) | [GitHub](#) | [Paper](#) | [Dataset](#) | [Twitter](#) | [Discord](#)

LMSYS Chatbot Arena is a crowdsourced open platform for LLM evals. We've collected over 500,000 human pairwise comparisons to rank LLMs with the [Bradley-Terry model](#) and display the model ratings in Elo-scale. You can find more details in our [paper](#).

[Arena](#) [Full Leaderboard](#)

Total #models: 89. Total #votes: 722,009. Last updated: April 13, 2024.

NEW! View leaderboard for different categories (e.g., coding, long user query)!

Code to recreate leaderboard tables and plots in this [notebook](#). You can contribute your vote at [chat.lmsys.org](#)!

Category  
Overall


Overall Questions  
#models: 89 (100%) #votes: 722,009 (100%)

Rank	Model	Arena Elo	95% CI	Votes	Organization	License	Knowledge Cutoff
1	<a href="#">GPT-4-Turbo-2024-04-09</a>	1259	+5/-5	21448	OpenAI	Proprietary	2023/12
1	<a href="#">GPT-4-1106-preview</a>	1254	+4/-4	66858	OpenAI	Proprietary	2023/4
1	<a href="#">Claude-3-Opus</a>	1253	+3/-3	66357	Anthropic	Proprietary	2023/8
2	<a href="#">GPT-4-0125-preview</a>	1249	+3/-4	54002	OpenAI	Proprietary	2023/12
5	<a href="#">Bard (Gemini Pro)</a>	1209	+6/-6	12435	Google	Proprietary	Online
5	<a href="#">Claude-3-Sonnet</a>	1202	+3/-3	69817	Anthropic	Proprietary	2023/8
5	<a href="#">Llama-3-70b-Instruct</a>	1198	+9/-11	2754	Meta	Llama 3 Community	2023/12
7	<a href="#">Command R+</a>	1193	+3/-3	37752	Cohere	CC-BY-NC-4.0	2024/3
7	<a href="#">GPT-4-0314</a>	1189	+4/-4	45288	OpenAI	Proprietary	2021/9
10	<a href="#">Claude-3-Haiku</a>	1181	+3/-3	61623	Anthropic	Proprietary	2023/8
11	<a href="#">GPT-4-0613</a>	1165	+3/-3	63963	OpenAI	Proprietary	2021/9
12	<a href="#">Mistral-Large-2402</a>	1158	+3/-4	40831	Mistral	Proprietary	Unknown
12	<a href="#">Qwen1.5-72B-Chat</a>	1153	+3/-4	30800	Alibaba	Qianwen LICENSE	2024/2
12	<a href="#">Claude-1</a>	1150	+5/-4	21824	Anthropic	Proprietary	Unknown
12	<a href="#">Mixtral-8x22b-Instruct-v0.1</a>	1147	+9/-11	2945	Mistral	Apache 2.0	2024/4

<https://chat.lmsys.org/?leaderboard>

# Human evaluation – A/B testing

[https://github.com/allenai/open-instruct/tree/main/human\\_eval](https://github.com/allenai/open-instruct/tree/main/human_eval)

**Human Evaluation**  
You are logged in as **admin**. [\[Log out\]](#)

<

Instance 1

>

Do you find the instance interesting, invalid, or too hard to complete? Please let us know by giving feedback here! (Optional)

☐ This example is interesting.

☐ This example is invalid.

☐ This example is too hard for me.

Comment:

Provide feedback

Design a skill assessment questioner for R (Programming Language).

Here are responses from two AI models.

A

Sure, here is a sample skill assessment questionnaire for R programming language:

1. What is the difference between a vector and a matrix in R?
2. How do you create a function in R?
3. What is the purpose of the "apply" family of functions in R?
4. How do you handle missing data in R?
5. What is the difference between a data frame and a tibble in R?
6. How do you create a scatterplot in R?
7. What is the purpose of the "dplyr" package in R?
8. How do you handle factors in R?
9. What is the difference between a "for" loop and a "while" loop in R?
10. How do you create a linear regression model in R?

B

1. What is R used for?
  - a. Data analysis and statistical computing
  - b. Web development
  - c. Mobile app development
  - d. Game development
2. What is the syntax for creating a vector in R?
  - a. `vector_name <- c(element1, element2, element3)`
  - b. `vector_name = c(element1, element2, element3)`
  - c. `vector_name = [element1, element2, element3]`
  - d. `vector_name <- [element1, element2, element3]`
3. What is the function used to read a CSV file in R?
  - a. `read.csv()`

Now please evaluate the two outputs based on your knowledge, preference, and any external tools (e.g., Google Search or Translate).

Q1: Is output A an acceptable response? An acceptable response should ① answer the user requests ② have no significant errors ③ have no meaningless text (e.g., repetition).

☐ Yes ☐ No

Q2: Is output B an acceptable response? An acceptable response should ① answer the user requests ② have no significant errors ③ have no meaningless text (e.g., repetition).

☐ Yes ☐ No

Q3: Please choose the response that you prefer (based on helpfulness).

A is clearly better

A is slightly better

Tie

B is slightly better

B is clearly better

Submit



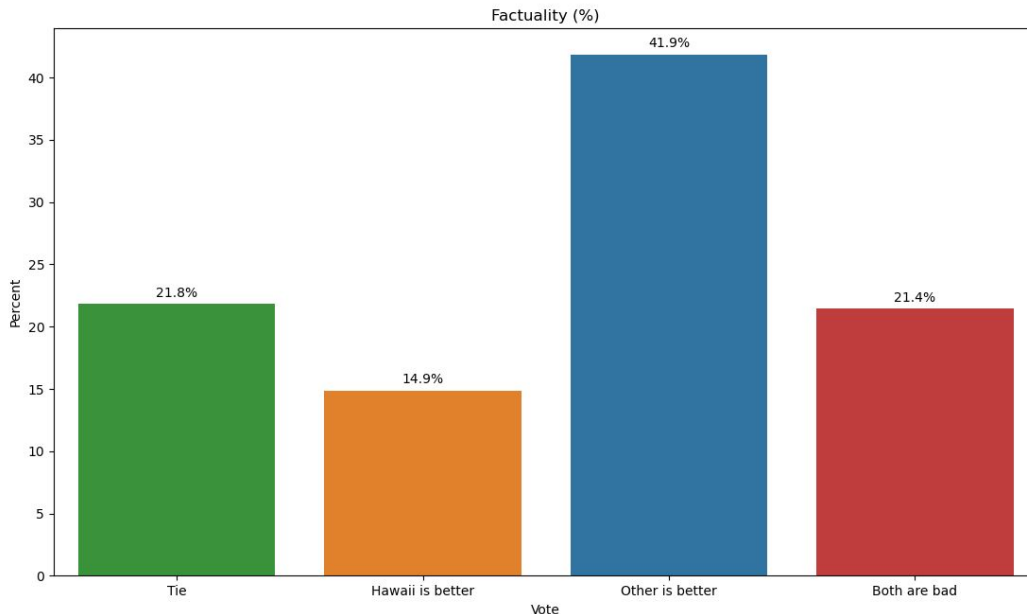
# Human evaluation – factuality [2024]

- ✓ Elsevier analysed the factuality of LLMs on custom LLS input prompts (NER, RE, open and closed book QA)
- ✓ >500 prompts judged by >40 content experts
- ✓ Alpha score / IRR > 0.6

## Models

**A) Hawaii:** LSS-specific model (8b)

**B) Other:** LSS-fine tuned llama2 (7b), llama-2-chat (7b), GPT-3.5-turbo (175b)

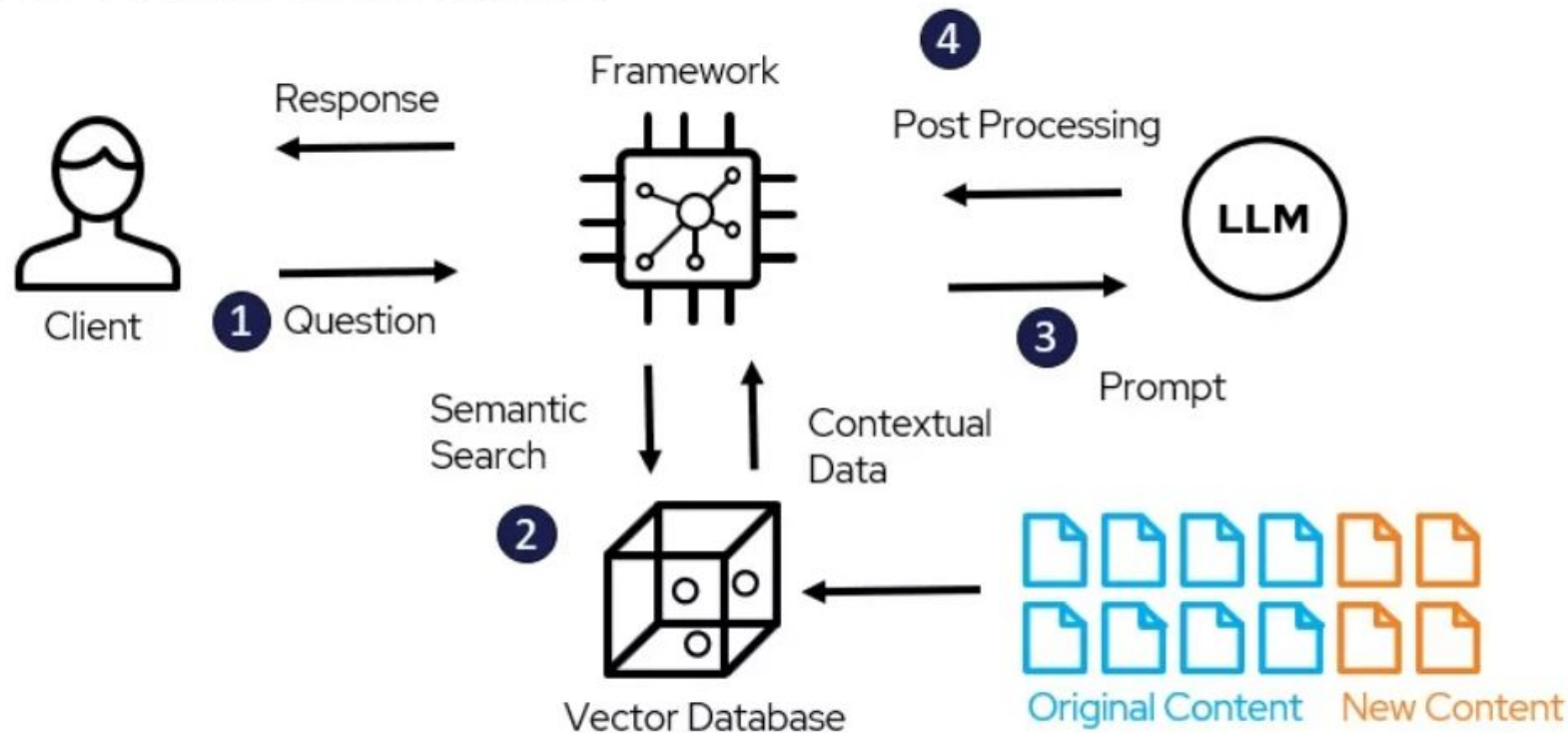


# RAG Systems



# Retrieval augmented generation [2022-]

## RAG Architecture Model

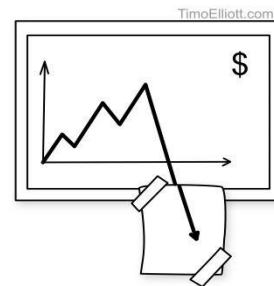
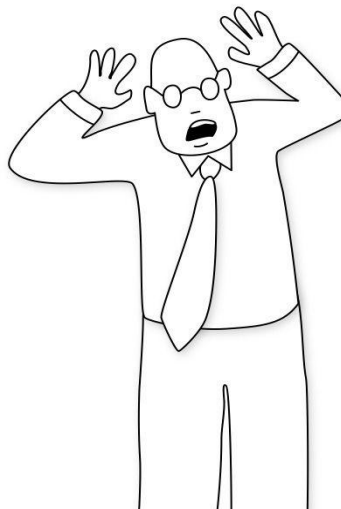
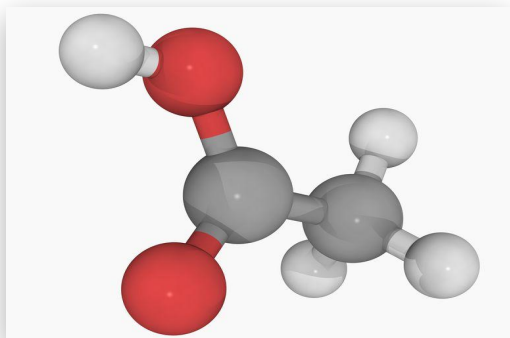


# References



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- § 2024 - Are large language models superhuman chemists?  
- <https://arxiv.org/abs/2404.01475>
- § 2024 - Retrieval-Augmented Generation for Large Language Models: A Survey  
- <https://arxiv.org/abs/2312.10997>

**Thank you!**



*"Quick! Somebody  
find me a  
data scientist!"*