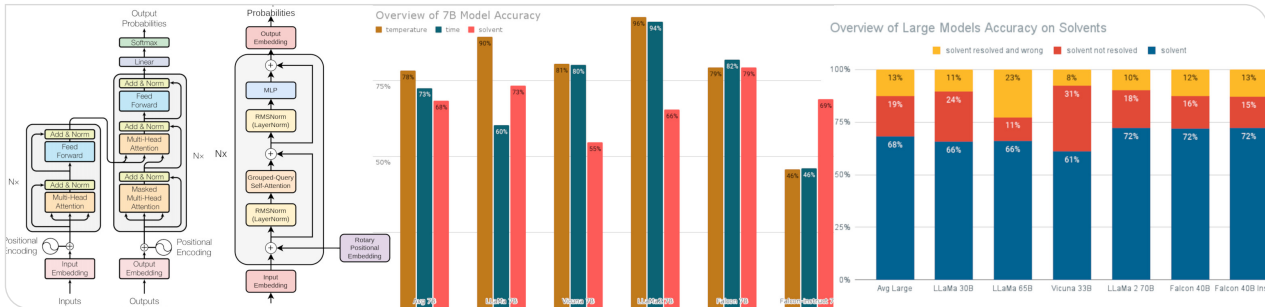


Benchmarking Large Language Models for Zero-Shot Automated Information Extraction from Scientific Literature

Felix Karg | 12. October 2023

Reviewer: T.T.-Prof. Dr. Pascal Friederich; Second Reviewer: Prof. Jan Niehues; Advisor: Tobias Schlöder



Motivation

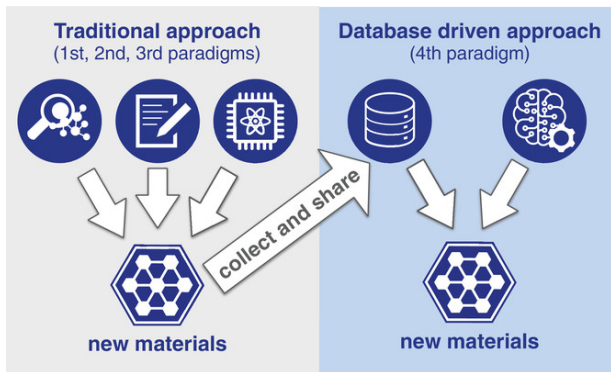


Image Source: [1]

Machine Learning (ML) models are increasingly used in screening steps for materials discovery and property prediction [2–4]. Yet, most previous research is not available in a machine-readable format.

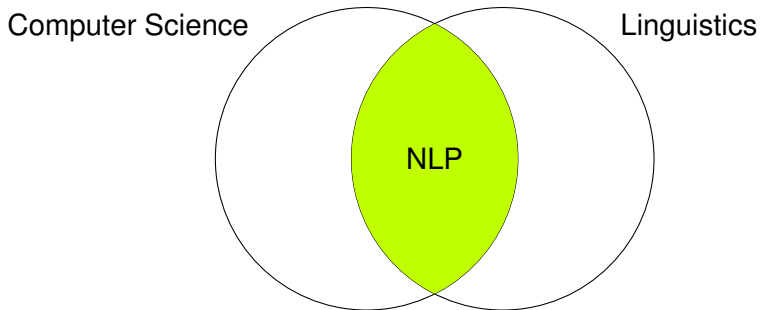
Scientific Questions

There are three main questions this work aims to answer:

- 1 Can I demonstrate high accuracy in zero-shot automated information extraction from scientific literature using open-access Large Language Models (LLMs)?
- 2 How do currently available open-access LLMs compare for this task?
- 3 How easy is it to fine-tune open-access LLMs for this task? How much does the accuracy increase from fine-tuning?

While we're at it, create an automated pipeline for information extraction from unstructured text.

Natural Language Processing



Goal: Make computers “understand” documents.

Information Extraction for Automated Experimentation

Information Extraction is the Natural Language Processing (NLP) task of extracting structured (machine-readable) information from unstructured text.

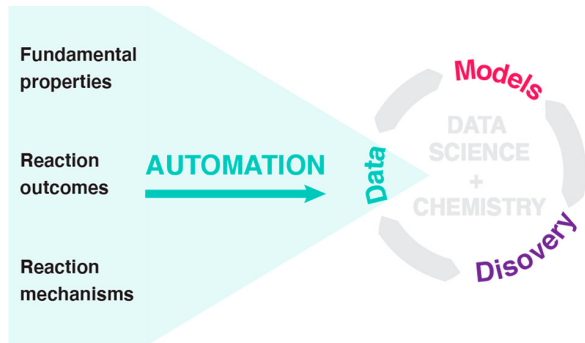


Image Source: [5]

Namend Entity Recognition

Named Entity Recognition (NER) is the NLP task of extracting structured (machine-readable) information from unstructured text.

Effects of the silica **MAT** content and temperature on the magnetic properties **PRO** of Fe₄NiO₈Zn **MAT** / O₂Si **MAT** nanocomposites **DSC** have been studied by electron paramagnetic resonance **CMT** (EPR **CMT**) technique.

MAT stands for Materials, **PRO** stands for Material Property, **DSC** is Descriptor and **CMT** is Characterization method. The goal of NER is to automatically detect entities that fall into these pre-defined semantic types.

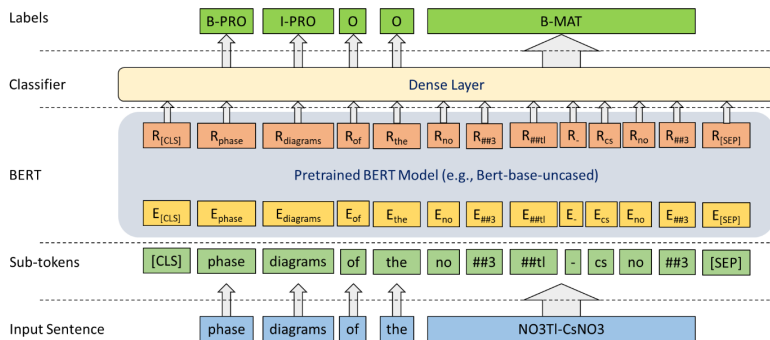
Example and partial description taken from [6] (supposedly taken from [7]), visualized using the spaCy python library [8].

Rule-Based Entity Recognition

Easy: Regular Expressions! ChemTagger [9], and others [10, 11] demonstrated that it works!
Except ...

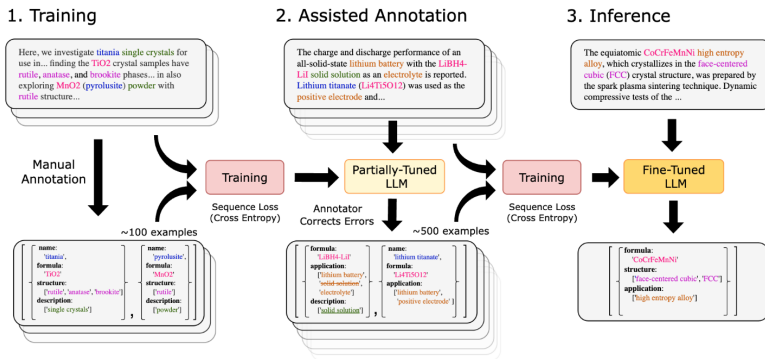
- “The mixture was filtered and the filtrate was kept at *room temperature* to obtained needle like colorless crystals of 1 after a month.” [12]
- “... distilled water, and dried at *ambient temperature* to give 39 mg of ...” [13]
- “... was added into 1 mL *boiling methanol solution* of btpe ...” [14]
- ...

Language Models for Information Extraction



NER modeled as a sequence-to-sequence labeling problem can achieve high accuracy using Bidirectional Encoder Representation from Transformers (BERT)-based Language Models (LMs). Image Source: [6]

Large Language Models for Structured Information Extraction

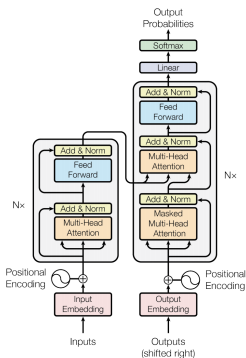


Other work focused on Entity Relation extraction, with mixed results for NER.
Image Source: [15]

Basic Terminology

- **Token:** String of arbitrary length, usually 3-4 characters
 - Refer to my previous talk about the transformer architecture for more details on internals
- **Context Length:** Amount of tokens a model can process concurrently as input
- **Single-shot / Multi-shot:** Evaluation setting in which a LLM is being provided with one or multiple examples of the task to fulfill
- **Zero-shot:** Evaluation setting in which no task examples are provided, or the model has been fine-tuned for

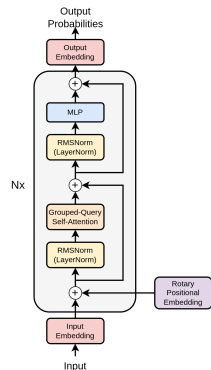
The Transformer Architecture



Original Transformer Architecture
Image Source: [16]

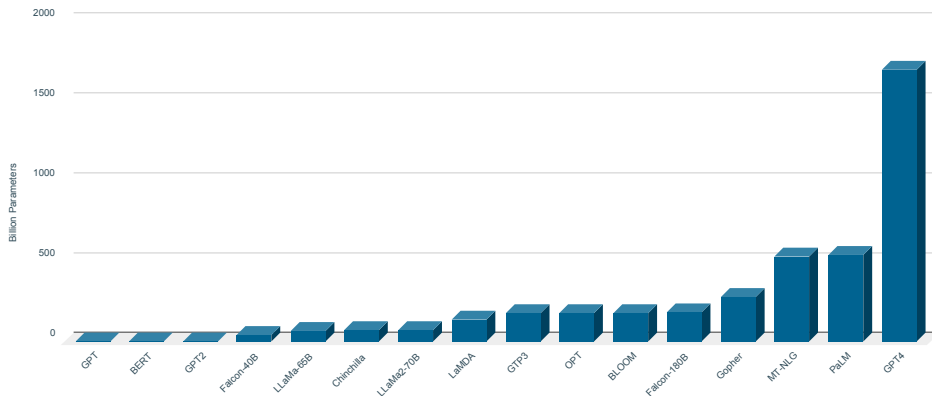
Most Prominent Changes:

- Activation Function: Swish Gated Linear Unit (SwiGLU) [17] instead of Rectified Linier Unit (ReLU)
- Positional Encoding: Rotary Positional Encoding (RoPE) [18], and *on each layer*
- Normalization with RMSNorm [19] *before* instead of after each layer
- Attention: Often a variant of Sparse Attention [20] or FlashAttention [21]
- Most Recently: The usage of Grouped Query Attention (GQA) [22]



Modern Transformer Architecture

Large Language Model Parameter Count



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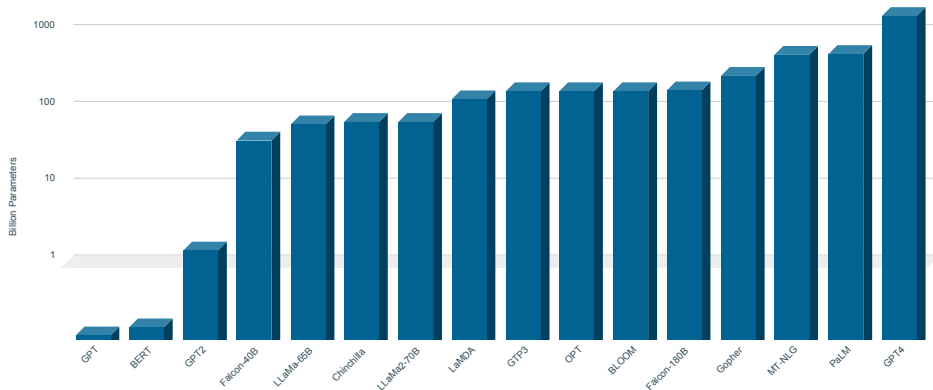
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Large Language Model Parameter Count (logscale)



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Training Large Language Models

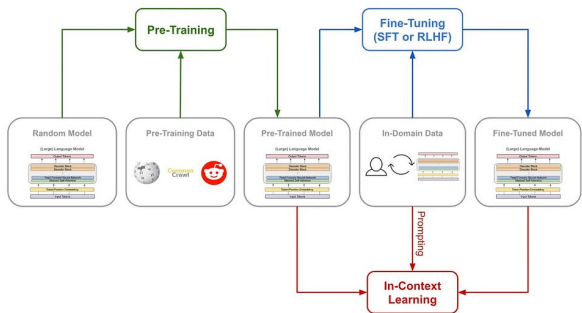


Image Source: [23]

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Criteria for Models

TODO: fix color scheme

- 1 It is possible to get the full model weights.
- 2 The selected models ought to be decently capable causal language models.
- 3 Ceteris paribus, a smaller model is better.

Language Models

- LLaMa 7B, 13B, 30B, 65B
- Vicuna 7B, 13B, 33B
- LLaMa 2 7B, 13B, 70B
- Falcon 7B, 40B
- Falcon-instruct 7B, 40B

Schema

The schema provided for the model to follow. Model output termination would happen after generation of a token for `"` for strings or `,` for numbers, or a number of other dedicated 'end of generation' tokens, e.g. `<EOS>`.

```
1 schema = {  
2     "type": "object",  
3     "properties": {  
4         "additive": {"type": "string"},  
5         "solvent": {"type": "string"},  
6         "temperature": {"type": "number"},  
7         "temperature_unit": {"type": "string"},  
8         "time": {"type": "number"},  
9         "time_unit": {"type": "string"},  
10    },  
11 }
```

Prompt

Prompt used to generate output. "{output}" delineates where the model provides an answer.

```
prompt = "{paragraph}\nOutput result in the following JSON schema format:\n{schema}\nResult: {output}"
```

Output

Exemplary output based on the prompt and schema shown before.

```
1 output = {  
2   "additive": "acid",  
3   "solvent": "water",  
4   "temperature": 80,  
5   "temperature_unit": "C",  
6   "time": 24,  
7   "time_unit": "h",  
8 }
```

Data Source

- SynMOF_M [3]
 - Publicly Accessible
 - Manually Extracted
 - 778 Labels
 - Temperature Information is in °C
 - Timeframe (Durations) in h.
 - Chemical Compounds via cid
- Corresponding Synthesis Paragraphs

Unit Equality

Time and Temperature
Compounds **TODO: this**

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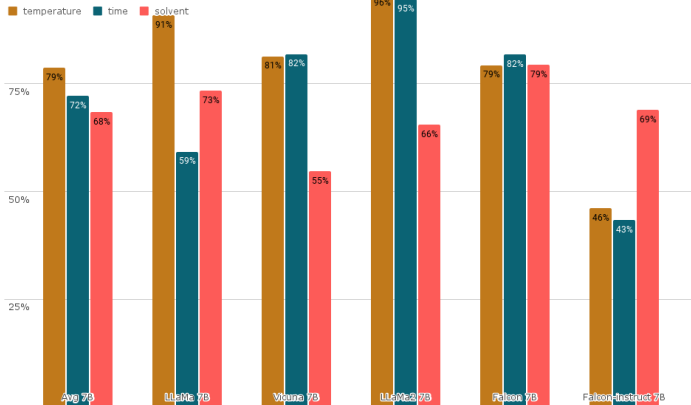
Compound Equality: cid

Foreshadowing:

- 'water'
- cid 962
- 'Synonyms': 319
- Includes 'distilled water' and 'H2O'
- But not 'distilled H2O'
- Even though this occurs verbatim in eight synthesis paragraphs

Accuracy Overview I

Overview of 7B Model Accuracy



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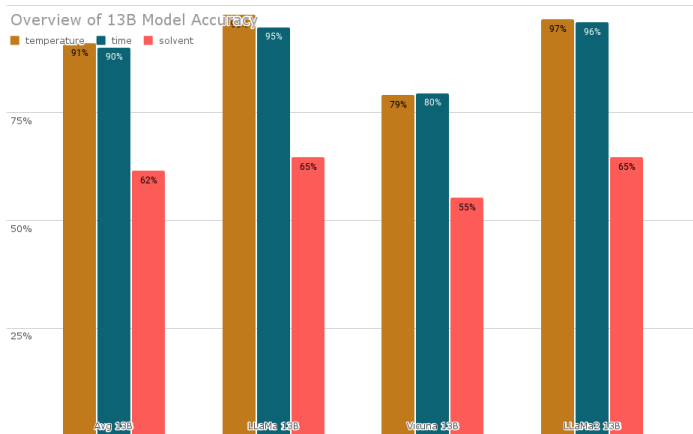
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Accuracy Overview II



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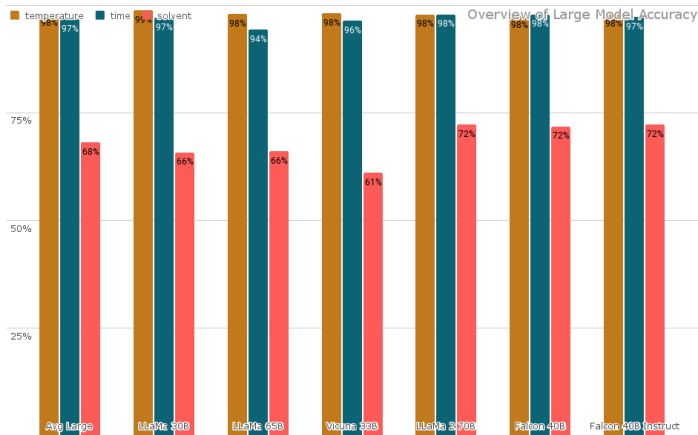
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Accuracy Overview III



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Note on Interesting Outliers

7B

- LLaMa-7B accuracy on temperature and time vary substantially across models, but are mostly similar within one model
- solvent accuracy of Vicuna bad somehow
- Bad temperature and time accuracy of Falcon-instruct
- Decent performance from LLaMa 2 overall

13B

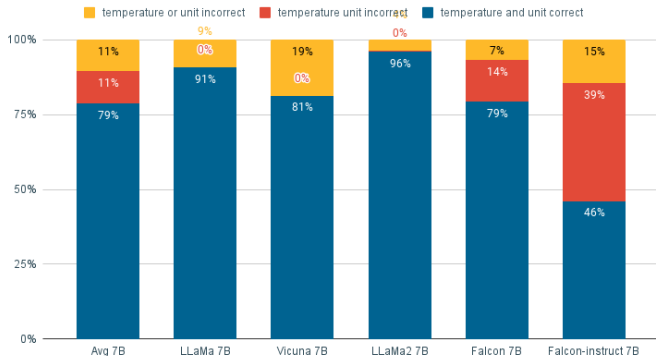
- Vicuna still lagging behind, though while Falcon does not have a 13B variant, it should still be worse
- Accuracy on solvent seems to have gotten worse, on average and for individual models

30B+

- Average Accuracy very high
- solvent accuracy only 72% though, that was higher in 7B models!

Unit Confusion I

Overview of 7B Models Accuracy on Temperature



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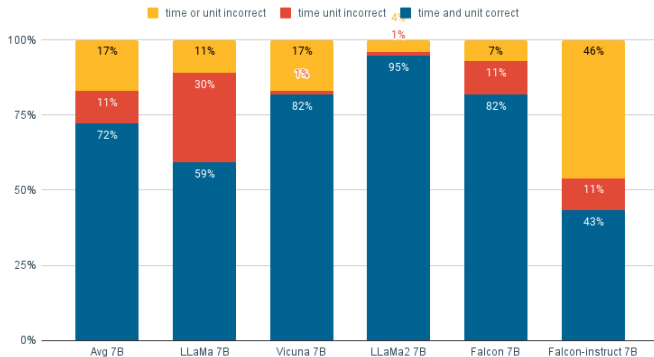
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Unit Confusion II

Overview of 7B Models Accuracy on Time



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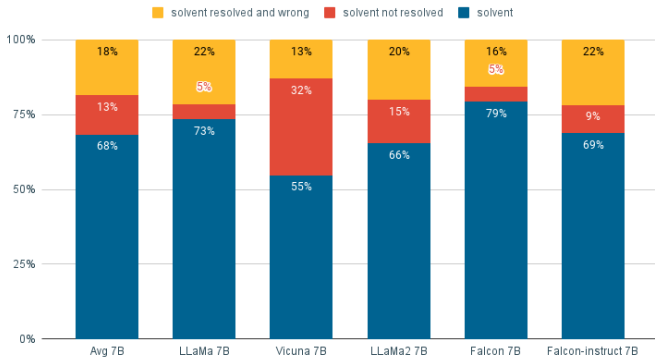
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Note on Unit Confusion

- Does happen fewer than 0.5% (0-4 cases) for models sized 13B or more

Solvent Resolution I

Overview of 7B Models Accuracy on Solvents



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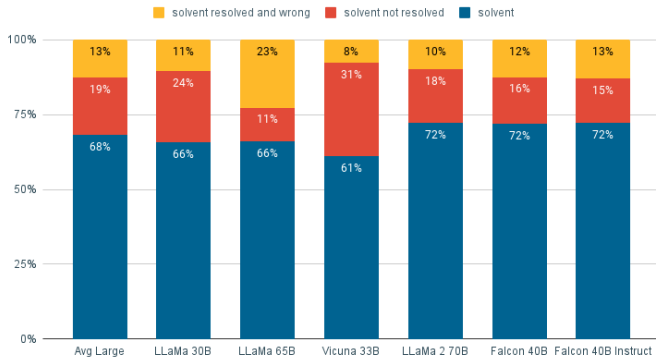
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Solvent Resolution II

Overview of Large Models Accuracy on Solvents



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Solvent Resolution?

One hypothesis: Models *are* getting more accurate, but there is a failure in resolving the compounds.

Remember ‘distilled H2O’?

This may be true in particular for the solvent N,N-DIMETHYLACETAMIDE (cid 31374), where the synthesis paragraphs contain none of its 125 synonyms in 34 cases (or about 4.37% of the dataset).

Fine-Tuning: Excerpt 1

Excerpt of what could be found in a custom dataloader. text describes any string the model may be provided as input. The tokenizer converts any string to a list of tokens and an attention mask, among other things. Similar code can be found in tutorials and official sources, e.g. Microsoft [24]

```
1  text_encodings = tokenizer(text, ...)
2
3  return {
4      "input_ids": text_encodings["input_ids"],
5      "attention_mask": text_encodings["attention_mask"],
6      "label": text_encodings["input_ids"],
7  }
```

Fine-Tuning: Failure 1

A model fine-tuned like this returns the following. The " where actually inserted during conversion to json from jsonformer.

```
1 output = {  
2     "additive": "",  
3     "solvent": "",  
4     "temperature": "",  
5     "temperature_unit": "",  
6     "time": "",  
7     "time_unit": "",  
8 }
```

Fundamentally, no idea what is going on. It works for others, and it could still be one of many different things that actually happened.

Fine-Tuning: Excerpt 2

- Using the HuggingFace `trl` (Transformer Reinforcement Learning) library
- `DataCollator` are used for batch-processing inputs
- `DataCollatorForLanguageModeling` abstracting away tokenization, uses `"text"`-key for training in other examples
- Specifically, the example uses `DataCollatorForCompletionOnlyLM`, deriving from it

Fine-Tuning: Failure 2

Error when providing DataCollatorForCompletionOnlyLM with a dataloader similar to those in examples. Counterintuitively, this is not a **KeyError**.

```
1 |----- Traceback (most recent call last) -----|
2 |           ...                                     |
3 |    372 |    model.train() # put the model in training mode |
4 |    > 373 |    trainer.train()                         |
5 |    ...
6 | ValueError: You should supply an encoding or a list of encodings
7 | to this method that includes "input_ids", but you provided []
```

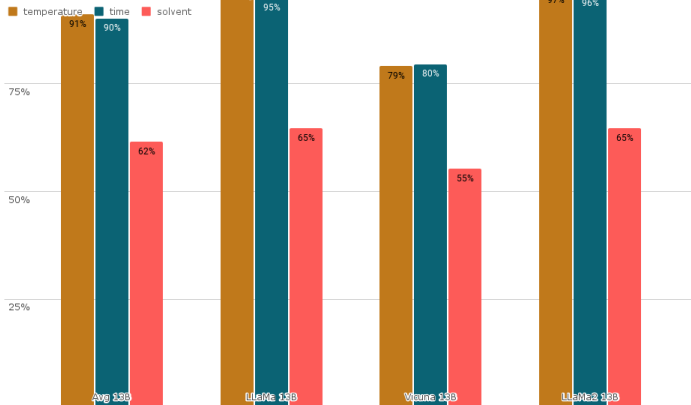
It also fails when manually tokenizing before the DataCollator (providing tokenized "input_ids" etc. as key, using this or a different DataCollator).

Conclusion

- Zero-shot automated information extraction from scientific literature was successfully demonstrated.
- Capabilities of different open-access LLMs were measured and compared. Furthermore, frequent mistakes were analyzed and provided insight in failure modes.
- Fine-Tuning was substantially harder than initially assumed, and eventually abandoned for this work.

Surprises

Overview of 13B Model Accuracy



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Surprises: Implications

GPU requirements for 4-bit quantized LLaMA models

LLaMA Model	Minimum VRAM Requirement	Recommended GPU Examples
LLaMA-7B	6GB	RTX 3060, GTX 1660, 2060, AMD 5700 XT, RTX 3050
LLaMA-13B	10GB	AMD 6900 XT, RTX 2060 12GB, 3060 12GB, 3080, A2000

Image Source: [25]

Modern consumer hardware can achieve throughputs of 30 to 40 tokens per second, depending on the specific GPU used [25].

Outlook

A number of questions where answered, this newfound knowledge provides the opportunity to ask better questions.

- How many of the unresolved solvent cases where actually correct?
- What is the accuracy of a correctly modeled additive?
- How can the prompt be improved?
- How does zero-shot accuracy compare with fine-tuned models?
- How do these models compare with next-gen models such as GPT4 or Falcon-180B?
- How do LLMs compare to established masked language models for NER?

What are your Questions?

All code and artifacts can be found at

<https://github.com/fkarg/mthesis>.

A tagged commit marks the state of submission.

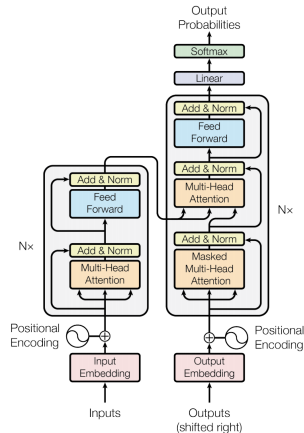


Image Source: [16]

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Glossary I

causal language model A causal language model predicts the likelihood of the next token based on a sequence of tokens (input). By sampling one of the predicted tokens and appending it to the input, output can be generated autoregressively. This in contrast to e.g. a masked language model. 15, 52

Falcon One of the LLMs used. Created by the Technology Innovation Institute (TII). 16, 26, 40

GPT2 The second generation **Generative Pretrained Transformer** LM from OpenAI [26]. 53

GPT3 The third generation **Generative Pretrained Transformer** LM from OpenAI [27]. 53

GPT4 The fourth generation **Generative Pretrained Transformer** LM from OpenAI [28]. Currently their most capable model. 40, 53

Glossary II

HuggingFace American deep learning ecosystem startup, having created the well established transformers framework which provides useful abstractions of most existing open-access Machine Learning models. 35

LLaMa A LLM from Meta. 16, 26, 52, 53

LLaMa 2 One of the LLMs used. It is the successor of LLaMa, also created by Meta. 16, 26

masked language model A masked language model predicts all masked (often missing) tokens in a sequence based on the context provided by the surrounding tokens. This in contrast to e.g. a causal language model. 40, 51

Meta Previously known as Facebook, Meta is a deep learning powerhouse and regularly open-sources new state-of-the-art machine learning models. 52

Glossary III

Microsoft Tech Giant, well-known for its operating system. Microsoft recently started intensive cooperation with OpenAI through a \$10 Billion USD investment, and started integrating GPT4 and other models throughout their services. 33

OpenAI American AI company, trailblazer at the frontier of scaling deep learning architectures and corresponding algorithmic breakthroughs. Their currently most well-known models are the Generative Pretrained Transformer (GPT) family of models, particularly GPT2, GPT3 and GPT4. 51, 53

Technology Innovation Institute Abu Dhabi-based machine learning research institute. 51

Vicuna One of the LLMs used. Based on LLaMa. 16, 26

Acronyms I

BERT Bidirectional Encoder Representation from Transformers 8

GPT Generative Pretrained Transformer 53

GQA Grouped Query Attention 11

LLM Large Language Model 3, 10, 37, 40, 51–53, 56

LM Language Model 8, 51

ML Machine Learning 2

MLP Multi-Layer Perceptron 56

NER Named Entity Recognition 6, 8, 9, 40

NLP Natural Language Processing 5, 6

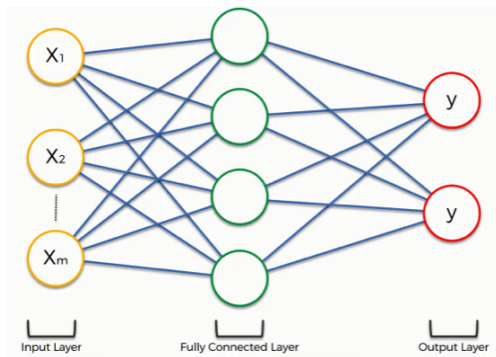
Acronyms II

ReLU Rectified Linier Unit 11, 56

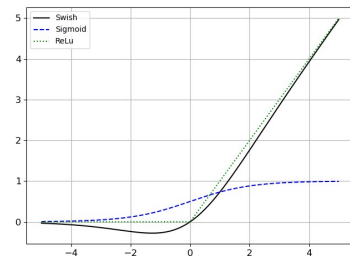
RoPE Rotary Positional Encoding 11

SwiGLU Swish Gated Linear Unit 11, 56

Multi-Layer Perceptron



Multi-Layer Perceptron (MLP) with one fully connected layer. Alternative names include 'dense', 'fully connected' and 'mlp' layer. Figure from [29].



Common activation function: ReLU, or recently for LLMs: SwiGLU.

InstructGPT: Following Instructions

“In human evaluations on our prompt distribution, outputs from the 1.3B parameter InstructGPT model are preferred to outputs from the 175B GPT-3, despite having 100x fewer parameters. Moreover, InstructGPT models show improvements in truthfulness and reductions in toxic output generation while having minimal performance regressions on public NLP datasets.”

Ouyang et. al. 2022 [30]

Reinforcement Learning from Human Feedback

Step 1

**Collect demonstration data,
and train a supervised policy.**

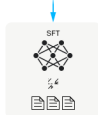
A prompt is
sampled from our
prompt dataset.



A labeler
demonstrates the
desired output
behavior.



This data is used
to fine-tune GPT-3
with supervised
learning.



Step 2

**Collect comparison data,
and train a reward model.**

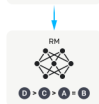
A prompt and
several model
outputs are
sampled.



A labeler ranks
the outputs from
best to worst.



This data is used
to train our
reward model.



Step 3

**Optimize a policy against
the reward model using
reinforcement learning.**

A new prompt
is sampled from
the dataset.



The policy
generates
an output.



The reward model
calculates a
reward for
the output.



The reward is
used to update
the policy
using PPO.



Image Source: [30]

RLHF originated from [31]

References

Glossary

Acronyms

MLP
○

Training LLMs
○●○○○○

ChatGPT

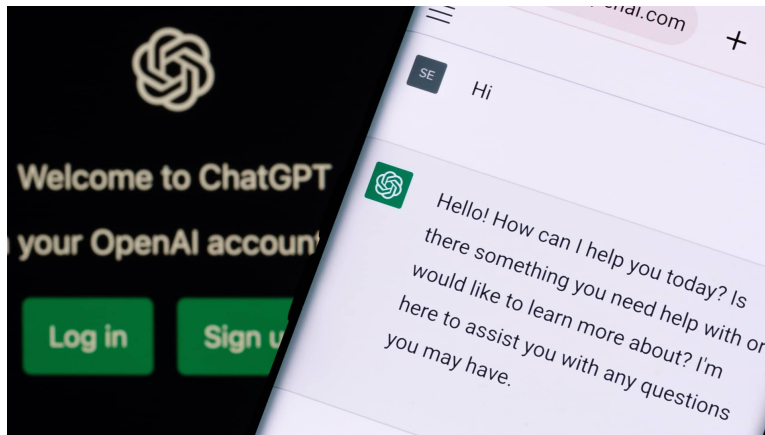


Image Source: [32]

ChatGPT Training Steps

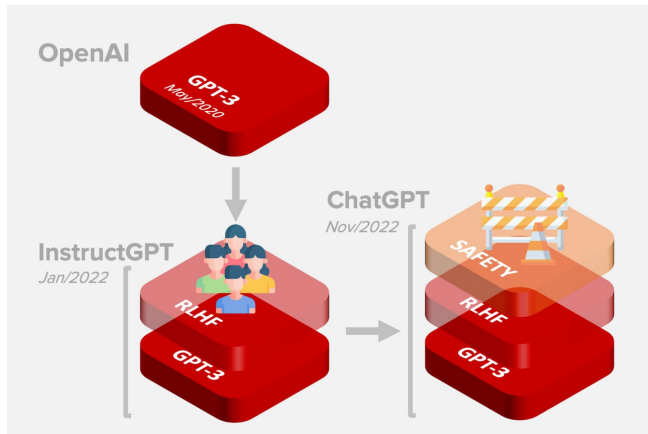


Image Source: [33]

References

Glossary

Acronyms

MLP
○

Training LLMs
○○○●○○

Constitutional AI

- 1 Prompt LLM with questions illiciting ethically questionable responses
- 2 Ask it to "rewrite this to be more ethical"
- 3 Fine-Tune to prefer rewritten response
- 4 Repeat a few times

Constitutional Results

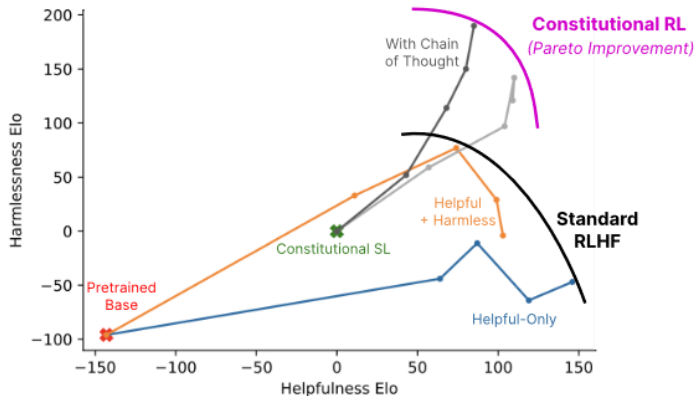


Image Source: [34]

References

Glossary

Acronyms

MLP
○

Training LLMs
○○○○○●