To whom it may concern,

What follows is my MSc Thesis done for the MSc in Artificial Intelligence at City, University of London, in the 2023/2024 term.

The thesis has already been examined and approved with a grade over the distinction level. This grade will be added to the transcript and finalised in the coming months.

Regards,

-Martin



City, University of London MSc in Artificial Intelligence Project Report Year 2023/2024

Knowledge Grounding in Language Models: An Empirical Study

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Project Repository: https://github.com/mfixman/rag-thesis

October 2 2024

Declaration

By submitting this work, I declare that this work is entirely my own except those parts duly identified and referenced in my submission. It complies with any specified word limits and the requirements and regulations detailed in the assessment instructions and any other relevant programme and module documentation.

In submitting this work I acknowledge that I have read and understood the regulations and code regarding academic misconduct, including that relating to plagiarism, as specified in the Programme Handbook. I also acknowledge that this work will be subject to a variety of checks for academic misconduct.

Signed: Martin Fixman

Acknowledgements

I wanted to express my gratitude to my supervisor, Dr. Tillman Weyde (with apologies for getting his first name wrong for months), to Dr. Chenxi Whitehouse, the original author of the preprint, and to Dr. Pranava Madhyastha for helping me take this great step in my academic career. This was not an easy thesis to research and write, but the guidance and advice I received from each of the three collaborators helped me fully understand the context I was working on and in conducting meaningful research.

My most important takeaway from the thesis, which I learned thanks to the work from my collaborators, is my deeper understanding of how to conduct a rigorous academic project. I plan to pursue a doctorate degree in the near future, and I am sure that the knowledge I gained in this project will make my future projects more thorough and efficient, and greatly improve my future academic work.

I also wanted to acknowledge the work done by the entire MSc in Artificial Intelligence in City St. Georges, University of London, for making a fantastic course. I learned a lot in many subjects and areas, even in ones which I barely had an idea were so broad. I also made a lot of contacts and good friends, who will definitely continue being a presence in my life after this MSc. Most important of all, I had fun, and any doubts I had on returning to academia after many years in the industry were completely unfounded.

In particular, I wanted to acknowledge Dr. Esther Mondragón for being an outstanding professor and administrator, and for taking a very strong stance in ensuring that the standards for this Master's degree remain high. My experience in this program was fantastic, and I hope the same continues being true for future students.

Abstract

In recent years large language models have exploded in quality and prevalence, and they have become crucial for work in a wide range of areas. However, their tendency to produce hallucinations presents a critical challenge in contexts where precision and correctness are crucial.

Retrieval-Augmented Generation (RAG), which leverages external information to provide more accurate and contextually appropriate responses, has been proposed as a solution to this problem. However, this solution is far from perfect as it's unclear when a large language model will choose to generate answers using the context provided by RAG over the knowledge in its parametric memory.

This thesis explores the *Knowledge Grounding* of various large language models. In particular, it attempts to answer a research question: **How does a large language** model respond to questions when context information contradicts or supports its inherent parametric knowledge?

To investigate this, we develop a diverse dataset comprising questions on various topics and using diverse data. We use this dataset to construct queries with counterparametric context, i.e. the context information contradicts the answer given by the model without context, and parametric context. We test models of different architectures and sizes to find out which type of answer they choose. We also analyse the *perplexity* of these answers to give us an indication on certainty of the model in its answer, and observe differences in the perplexity between answers that agree or disagree with the context information.

Our findings suggest that smaller models and models that encode the entire input sequence into an internal representation before outputting an answer might produce more answers sourced from the RAG-provided context, therefore avoiding hallucinations. In particular, the smaller models Meta-Llama-3.1-8B and Flan-T5-XL tend to have better knowledge grounding and fewer hallucinations than their larger versions, while encoder-decoder Seq2Seq models tend to outperform Decoder-only models. As an additional analysis we investigate methods for determining whether a given response originates from the RAG context or the model's internal memory from the query's resulting perplexity. This might be used to develop methods to prevent hallucinations in large language models that use RAG indexing.

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1 Introduction and Objectives

1.1 Problem Background

In recent years, Large Language Models (LLMs) have become ubiquitous in solving general problems across a wide range of tasks, from text generation to question answering and logic problems. However, recent research suggests that answering questions using solely the parametric knowledge of these models, i.e. what is encoded in the parameters after training, might not be the most effective way to obtain desired behaviour (Yao et al. 2023).

One potential approach to improving the performance of LLMs on knowledge problems is Retrieval-Augmented Generation (RAG) (Lewis et al. 2020). RAG involves retrieving relevant text related to a query and incorporating it into the model's input, enhancing the model's ability to generate accurate and contextually appropriate responses.

As RAG-enhanced systems become more widespread, studies on the performance of different retrieval systems and their interaction with LLMs have become crucial. Many explore the performance on downstream tasks depending on both the retriever and the generator (Ghader et al. 2023, Brown et al. 2020), examining whether the knowledge is grounded in the context. Retrieval-Augmented models, such as ATLAS (Izacard et al. 2022) and RETRO (Borgeaud et al. 2022), use this approach to fine-tune a model on both a large body of knowledge and on a retriever for a given index.

Well-grounded models with RAG-generated data that is anchored in verifiable and accurate sources can improve the performance of large language models. In the context of queries enhanced with RAG, we prefer knowledge sourced from context which came from the index, since they are much less likely to be "hallucinations" or mistakes from the model.

This project aims to understand the performance of various large language models when queries with added context by measuring their knowledge grounding on a dataset consisting of a large variety of questions across a wide range of topics. We follow the approach by Yu et al. of running queries with counter-parametric context to understand whether a particular answer originates from the model's inherent knowledge (i.e., its training data) or from the provided context (i.e., the context retrieved by RAG).

This thesis builds on this knowledge to improve our understanding of how different LLMs interact with the given context in the problem of question answering. Specifically, we research whether these interactions vary depending on the type of question being answered for models of different architectures and sizes, contributing to a more nuanced understanding of LLM performance in diverse knowledge domains.

1.2 Research Question

This thesis attempts to answer the following question:

How does a large language model respond to questions when given context information that contradicts or agrees with its inherent parametric knowledge?

The rest of this section gives an overview of the steps we take to answer this question.

1.3 Research Objectives and Beneficiaries

This thesis is structured around three different sub-objectives to deepen our understanding knowledge grounding in large language models.

1. Creating a representative dataset of questions.

This is necessary as existing Q&A datasets are not suitable for our objectives.

2. Building an experimental framework to understand the source of the answer to a query given by a large language model.

This will give us information about which models chooses to answer questions using its learned parametric knowledge or the given context, and whether it depends on the question asked.

3. Enhancing the framework to understand the reasoning behind each answer

We use the perplexity of a model's response on both answers to understand why a certain answer was chosen, and we attempt to predict the source of the answer with this number alone. This could help RAG-enhanced systems prevent hallucinations by repeating the index search in answers which might contradict the given context.

This project will contribute to the body of knowledge on the study of large language models, knowledge grounding, and how to improve retrieval-augmented generation models.

It will benefit researchers in this areas, along with developers attempting to create new large language models that are less sensitive to hallucinations along with the users of those new models.

1.4 Overview of Methods

1.4.1 Creating a representative dataset of questions

We require a dataset of questions that's useful for answering our research question. This dataset should allow us to understand whether each response came from the model's parametric memory or from the RAG-provided context, and should be reasonably representative of the world to prevent biases.

In particular, the questions should allow us to easily create counterparametric answers to later add as context to our queries. We follow the example of Yu et al. on creating questions that can be easily answered with short responses, and later using these answers to create counterparametric context.

We enhance the work by Yu et al. by adding a much larger and broader set of questions from a large variety of topics.

The criterion for solving this objective is to generate such a dataset that can be used in the experiments for this thesis.

1.4.2 Building an experimental framework to understand the source of an LLM's answer

Little is currently understood about the factors that control the source of knowledge of an answer in a large language model, and whether the generated text comes from the query's context or from memorised parametric information.

Previous research found out that, when the context of a query contradicts the ground knowledge of a model, the final answer is affected by the size and architecture of the model used (Yu et al. 2023).

This thesis extends this research by testing the representative set of questions and counterfactuals described in the previous section with both Seq2Seq and Decoder-only models of various sizes. We also research the cases when the answer doesn't correspond to either the parametric or contextual knowledge, and why the model chooses a third type of answer when adding counterfactual context.

The criterion for solving this objective is calculating data about the source of the answering from querying the models with the queries generated on Section 1.4.1, including the amount of answers sourced by the query's context and from the parametric knowledge of the model, and analysing and understanding these numbers.

1.4.3 Enhancing the framework to understand the reasoning behind each answer

Yu et al. showed that there is a correlation between the probability of a large language model choosing a parametric answer over a counterfactual contextual answer and the amount of times this answer appears in the ground truth data of the model. This gives us clues on whether the result of a query came from parametric or contextual knowledge for morels with access to its ground truth, as is the case in models like Pythia (Biderman et al. 2023).

Unfortunately, most open-source large language models provide only the model weights and do not give us access to the source data being used to train it and therefore do not allow this kind of analysis.

The **perplexity** score of answer gives a measure of how "certain" a large language model is of its answer (Jiang et al. 2021). We hypothesise that we can use this metric to serve as a reliable indicator of whether a particular answer came from a large language model's memory or whether it was derived from the provided context.

The criterion for solving this objective is calculating the perplexity data that's behind the source of the decision for a model to get data from the query's context or from parametric data, along with reflections on the reason why each model has these numbers.

Additionally, we should establish whether it's possible to create an estimator that can predict the source of an answer from the perplexity alone.

2 Context

This research is the latest on a long line of academic articles on retrieval-augmented generation, comparing and contrasting parametric knowledge with contextual information, and how to enhance knowledge on large language models.

This section summarizes key articles that informed this research.

2.1 Foundational Papers on Large Language Models

Large language models have exploded in popularity since the development of transformer architecture (Vaswani et al. 2017). This architecture relies entirely on self-attention mechanisms rather than recurrent layers, which allow the model to weigh the importance of different words in a sequence relative to each other, irrespective of their position. This mechanism enables the model to capture complex dependencies and relationships across long sequences more effectively than traditional models.

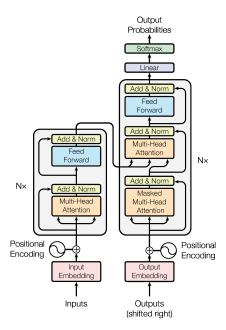


Figure 1: Transformer Architecture, from "Attention is all you need" (Vaswani et al. 2017).

GPT models (Radford & Narasimhan 2018) improve upon this architecture by running a supervised task-specific fine-tuning round after the unsupervised pre-training on large amount of test data. Later models, starting from GPT-2, use zero-shot transfer learning to improve their performance (Radford et al. 2019). Zero-shot learning (Norouzi et al. 2014) trains a model to perform a task without having been explicitly trained on examples of that task; instead, it leverages knowledge gained from pre-training to infer and generalise to new tasks with the context on the prompt.

By adding only a few examples of the task at hand, a model can improve generalisation

to new tasks with a limited amount of labelled data. GPT-3 uses this to understand the structure and nature of a task with a few examples (Brown et al. 2020).

Despite these improvements in sequential models, the models still present many faults in question-and-answer tasks (Jiang et al. 2021). Hallucinations are not uncommon, even for queries that ask questions that can be answered with short answers.

2.2 Architectures of Large Language Models

In this subsection we present two different large language model architectures that are used widely for this research. This thesis uses and compares four models using the Flan-T5 and Llama architectures.

2.2.1 Seq2Seq Models: T5 and Flan-T5

The T5 model (Raffel et al. 2020), developed by Google Brain in 2020, is an encoder-decoder Seq2Seq model that treats every processing problem as a text-to-text task. This way it uses transfer learning to learn many different kinds of tasks from a single source of training data.

The model is trained using only masked language modelling and treating every problem as a supervised text-to-text task where both the input and output are in text form. The data is later fine-tuned to make it able to solve other tasks.

Flan-T5 uses the same architecture as T5, but fine-tuned on tasks to follow explicit instructions (Chung et al. 2022). This scales well on larger tasks and larger model sizes, and it's particularly effective on problems requiring a chain-of-thought.

These models have strong performance while adding little or not existing context, and are capable capable to understand explicit instructions which can generalise to new task types, improving the downstream task performance (Longpre et al. 2023).

2.2.2 Decoder-only Models: GPT and Llama

GPT models use a transformer-based decoder-only architecture trained to solve the problem of causal language modelling, or predicting the next token in a sequence (Radford & Narasimhan 2018, Radford et al. 2019, Brown et al. 2020). These models generate text by predicting tokens one-by-one rather than encoding internal information of a query, such as Seq2Seq models.

GPT models are good at solving a variety of tasks they they not trained in with little or no context. Its autoregressive nature specialised it at generating human-like text, so it's widely used for chatbots and content creation.

Llama models improve several limitations of GPT by training smaller models on more data (Touvron et al. 2023), which generally achieves better performance (Hoffmann et al. 2022), and various improvements to the transformer architecture.

These models outperform GPT models on most benchmarks, despite being considerably smaller, by prioritising training efficiency and parameter optimisation. Further improvements to later versions of this model include fine-tuning in a post-training round using reinforcement learning from human feedback and training with longer contexts (Martin et al. 2023), and adding multilingual data to the training data (Dubey et al. 2024).

Llama 3 includes a set of Instruct models, which like Flan-T5 are fine-tuned to following instructions.

One of the inherent limitations of Decoder-only architectures is the challenge of maintaining coherence over long contexts. Additionally, they struggle with using accurate data from the query when it contradicts its parametric knowledge.

2.3 Retrieval-Augmented Generation

Large pre-trained language models store factual knowledge in their parameters. Their ability to access factual information from their source data without the risk of hallucinating incorrect information is limited, which affects their performance on knowledge-intensive tasks such as question-and-answer problems.

Retrieval-Augmented Generation (RAG) attempts to solve this problem by adding extra non-parametric data in a context gathered from an index with a separately-trained retriever (Lewis et al. 2020). This retrieved context is fed back to the original query as a combined representation containing this extra data. A diagram with an overview of this method is presented in Figure 2.

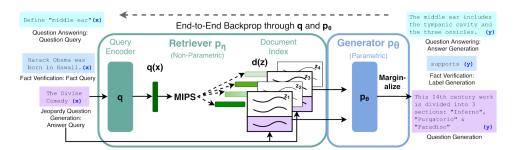


Figure 2: An overview of the RAG approach, combining a pre-trained retriever with a pre-trained model. From "Retrieval-Augmented Generation for Knowledge-Intensive NLP tasks" (Lewis et al. 2020)

RAG can be effective in preventing hallucinations by incorporating relevant external information into the generation process, ensuring that responses are more grounded in factual data from a knowledge base. However, this method is not perfect even after adding contextual data to the query the model could generate a response using its learned parametric memory while ignoring the data retriever by the RAG model.

2.4 Knowledge Grounding on Queries with Added Context

Knowledge grounding is the process by which a large language model incorporates external knowledge into its output generation. In the context of queries with context provided by RAG, a well-grounded model would ensue that answers are consistent with the knowledge in the index rather than in the model's inherent knowledge if they are contradictory.

Various attempts have been made at understanding how good the knowledge grounding of a RAG system is, and on what is the optimal configuration of RAG.

In "RAGGED: Towards Informed Design of Retrieval Augmented Systems" (Hsia et al. 2024), the authors create a framework to evaluate these systems and find that different models suit substantially varied RAG setups. In particular, the performance of the models decreases strongly in Decoder-only models such as Llama when the context passages provides more context, while Seq2Seq models such as Flan-T5 have better performance.

"Characterizing Mechanisms for Factual Recall in Language Models" (Yu et al. 2023), which is one of the main sources for this thesis, finds that when there is disagreement between the model's knowledge and the provided context then the architecture and size of the large language model will affect the probability of the model choosing to use the context (which is much less prone to hallucinating) as an answer rather than its parametric knowledge.

This paper also introduces a novel way to test this hypothesis by creating a dataset with questions and counterfactual context, an example of which is shown in Listing 1. By adding counterparametric information to the context, this method allows us to understand whether an answer came is parametric (that is, came from the memory of the model) or contextual (that is, came from the provided context).

```
The capital of {country} is {in context city}
Q: What is the capital of {country}?
A:
```

Listing 1: Example of queries used in (Yu et al. 2023). These queries form the basis and inspiration for the dataset creation done in this thesis

3 Methods

How does a large language model respond when given context that contradicts its parametric, learned knowledge? Why does it choose this answer?

To understand this, we build a new framework for testing a large language model's answers when presented with contradictory information. We test this framework with models of various architectures and sizes to get insights about our responses.

Following the example set in Section 1.3, we split this work into three sub-objectives.

3.1 Creating a representative dataset of questions

As argued in Section 1.4.1, the research of this thesis requires a large dataset of questions from a variety of categories to test large language models.

3.1.1 Dataset Description

The dataset we aim to create for this research is designed to be a comprehensive and versatile tool for evaluating large language models. By selecting a wide variety of questions questions we ensure that the dataset will provide meaningful insights of the grounding of LLMs across a wide spectrum of domains.

Our dataset should have the following properties.

1. Questions should have short, unambiguous answers.

Our goal is to compare these answers both for equality, on the LLM's perplexity at generating this result. Longer answers make this objective harder to interpret since two long answers might have a higher chance of being both correct. Ensuring our answers are short reduces the space of different but equivalent answers.

2. Questions must cover a large and diverse set of topics.

Parametric answers are sourced from the training data of a large language model, which might be biased towards certain topics or groups of people. For example, it is known that Wikipedia contains a significant geographical bias on biographies (Beytía 2020), and that this affects the probability of choosing to answer from parametric or contextual knowledge(Yu et al. 2023). We require a large and diverse and set of topics to counteract potential biases.

3. Questions must allow for the creation of counterparametric answers.

In order to test a model's knowledge grounding, this thesis requires understanding whether an answer came from contextual versus inherent knowledge. A simple way to do this is to repeat and enhance the approach used by Yu et al. of adding counterparametric answers to a query context. This allows us to to easily disambiguate whether an answer came from the model's inherent parametric memory or from the given context. This approach is only possible if the set of answers allows us to create a set of alternative answers that are plausibly correct and have the same format as the parametric answer, but are still counterparametric.

The existing literature uses various existing question-and-answer datasets. We believe that none of these datasets are a good fit for this research due to not following some of the three desired properties. However, understanding them can be useful when designing the final dataset.

Natural Questions Dataset Created by Google Research (Kwiatkowski et al. 2019), and commonly used in research related to understanding the answers of LLMs in question-and-answer problems (Hsia et al. 2024, Mallen et al. 2023, Ghader et al. 2023). While the dataset provides an excellent range of questions and existing literature to compare these results to, the lack of question categorisation is an obstacle in our objective to generate counterparametric answers.

Human-Augmented Dataset Sometimes used in research related to quality control of large language models (Kaushik et al. 2020). However, the high cost associated in generating this dataset would limit the size of our questions.

Countries' Capitals Question Dataset Used in "Characterizing Mechanisms for Factual Recall in Language Models" (Yu et al. 2023), this dataset contains a single question about the capital city of certain countries which can be easily transformed to a counterparametric question. This format is ideal for the research done in this thesis, but having a single type of question will not allow a deep dive into the source of each answer in a general question.

3.1.2 Dataset Creation

Instead of using an existing dataset, this research takes inspiration from countries' capital queries used in the paper by Yu et al., and creates a similar but larger and more varied dataset of questions and answers from a wide range of topics, assuring questions can be grouped by question pattern so that the formats of their answer are similar. This way, we can emulate the approach used in that paper of reusing the answer from a certain question as the counterfactual context of another.

This dataset will be used for the experiments of this thesis. Since it might be useful for future research, it will also be presented as its own result.

Since this thesis requires a set of questions that covers a large set of topics, we first generate by hand a list of various categories of questions. Each one of these categories refers to the subject of the question, rather than the answer.

For each category we create a set of base questions and another set of objects. We ensure that for all the objects, and specially in the case of people, the resulting list of objects represents a wide variety of objects from across the world

For each category, we generate a set of questions by matching every one of its base questions with every one of its objects. An example of this approach is shown in Table 1.

This list of questions will enable the research on whether the answers given by large language models depend on the category and the format of the questions.

Category	Base Questions	Object	Queries
Person	Q: What is the date of birth of {person}? A: The date of birth of {person} is Q: In what city was {person} born? A: {person} was born in	Che Guevara Confucius	Q: What is the date of birth of Che Guevara? A: The date of birth of Che Guevara is Q: What is the date of birth of Confucius? A: The date of birth of Confucius is Q: In what city was Che Guevara born? A: Che Guevara was born in Q: In what city was Confucius born? A: Confucius was born in
City	Q: What country is $\{city\}$ in? A: $\{city\}$ is in	Cairo Mumbai Buenos Aires London	Q: What country is Cairo in? A: Cairo is in Q: What country is Mumbai in? A: Mumbai is in Q: What country is Buenos Aires in? A: Buenos Aires is in Q: What country is London in? A: London is in

Table 1: Some examples of the base-question and object generation that are fed to the models for finding parametric answers. For each category, we match every base question to every object to create a longer set of questions. In this example, the *Person* category contains 2 base questions and 2 objects, resulting in 4 questions; the *City* category contains 1 base question and 4 objects, also resulting in 4 questions.

3.2 Building an experimental framework to understand the source of an LLM's answer

3.2.1 Model Selection

In order to understand the knowledge grounding of a wide variety of large language models, the queries generated in Section 3.1 are tested with four models of different architectures and sizes. These models are listed in Table 2.

	Seq2Seq Model	Decoder-Only Model
Smaller	Flan-T5-XL	Meta-Llama-3.1-8B-Instruct
Larger	Flan-T5-XXL	Meta-Llama-3.1-70B-Instruct

Table 2: The four large language models chosen for this research.

All of the models used in this research leverage autoregressive attention using the transformer architecture (Vaswani et al. 2017), where each token attends to its preceding tokens, maintaining the temporal order of the sequence. This approach allows them to generate coherent and contextually relevant text by sampling from this learned distribution, while also capturing long-range dependencies and complex patterns in language.

Both Sequence-to-Sequence models are based on T5 models (Raffel et al. 2020), which employ an encoder-decoder architecture: while an encoder processed the input sequence

into a context vector, and an decoder generates an input sequence from this vector. The Flan-T5 models are fine-tuned to follow instructions, and have improved zero-shot performance compared to the original T5 models (Chung et al. 2022).

Flan-T5-XL contains approximately 3 billion parameters. This is considerably bigger than the base Flan-T5 model (Chung et al. 2022), which will provide better accuracy of its parametric answers.

Flan-T5-XXL contains 11 billion parameters, has higher accuracy on the parametric answers as the XL model (Chung et al. 2022). However, how the higher amount of parameters will affect its knowledge grounding when running our experiment is still unknown.

Decoder-only models generate answers one token at a time from the input query. Given a sequence of tokens, they generate text one token at a time by attempting to solve the problem of predicting the following token (Radford & Narasimhan 2018).

This thesis uses the -Instruct versions of the latest Llama models (Dubey et al. 2024), which use this architecture and fine-tune it to tasks of instruction-following. These models are specially adept at complex prompts. Of the models used in this thesis, Meta-Llama-3.1-8B-Instruct has 8 billion parameters, while Meta-Llama-3.1-70B-Instruct has 70 billion.

The properties of the models are summarised in Table 3.

Model	Architecture	Trained On	Parameters
Flan-T5-XL	Seq2Seq	Public NLP Datasets	3 Billion
Flan-T5-XXL	Seq2Seq	Public NLP Datasets	11 Billion
	· ·	Web text, code, instruction datasets Web text, code, instruction datasets	

Table 3: Model cards of the large language models used in this research.

3.2.2 Understanding the source of the answer in each model

The first step to understanding the knowledge grounding of large language models is to create queries that contain data that contradicts its parametric knowledge as part of the context. By comparing the result to the existing answers it becomes trivial to understand whether an answer came from the model's memory, the queries' context, or neither of these.

Following the approach done by Yu et al., for every query we randomly sample from the set of answers of the same base question for answers that are different to the parametric answer which is given by the original query. An example of this random sampling can be found in Table 4.

We later add this *counterparametric answer* to the context, to form a new query and query

Base Question	Object	Parametric Answer	Counterparametric Answer	Question with Counterparametric Context
	Che Guevara	June 14, 1928	965 AD	Context: [the date of birth of Che Guevara is 965 AD]. Q: What is the date of birth of Che Guevara? A: The date of birth of Che Guevara is
Q: What is the date of birth of {person}? A: The date of birth of {person} is	Ibn al-Haytham	965 AD	June 14, 1928	Context: [the date of birth of Ibn al-Haytham is June 14, 1928]. Q: What is the date of birth of Ibn al-Haytham? A: The date of birth of Ibn al-Haytham is
	Boyan Slat	27 January 1994	February 23, 1868	Context: [the date of birth of Boyan Slat is February 23, 1868]. Q: What is the date of birth of Boyan Slat? A: The date of birth of Boyan Slat is
	W.E.B Du Bois F	February 23, 186	8 June 14, 1928	Context: [the date of birth of W.E.B Du Bois is June 14, 1928]. Q: What is the date of birth of W.E.B Du Bois? A: The date of birth of W.E.B Du Bois is
Q: What country	Cairo	Egypt	India	Context: [Cairo is in India] Q: What country is Cairo in? A: Cairo is in
is {city} in? A: {city} is in	Mumbai	India	Egypt	Context: [Mumbai is in Egypt]. Q: What country is Mumbai in? A: Mumbai is in

Table 4: Using the same question format allows us to repurpose previous parametric answers as counterparametric ones. In this example, we randomly sample answers from the same base question but referring to a different object to find counterparametric answers, which we later add to the context of the query.

the same model again with the added counterparametric context. This is exemplified in Table 5.

To ensure that the results are simple to interpret and minimise the effect of randomness, once we select the queries we follow the example of Hsia et al. and use Greedy Decoding to generate the answer. While beam search with tends to produce more accurate results for long answers (Sutskever et al. 2014, Wu et al. 2016) and there are many other sampling methods that tend to produce better results (Holtzman et al. 2020), this is likely to not have an effect on experiments shorter answers (Raffel et al. 2020).

We compare the generated answer with the context to the previously generated parametric answer, and we categorise the answer:

Parametric answers are equal to the answer given by the model when queried without context. This answer would come from the parametric memory of the model, and could potentially indicate an hallucination not present in the context.

Contextual answers are equal to the context given in the query. In a RAG context, this would be the answer retrieved from the index.

Other answers are neither of these, and this answer comes from a mis-interpretation of the input by the model or from some other source.

To minimise the amount of problems caused by large language models generating extra information, we define two strings to be equal by truncate the text until the first period or <EOS> token, removing punctuation and stop words, and finding whether one of the answers is a subsequence of another.

We later found out that this approach to compare strings could be improved, and understanding whether two generated answers are identical is an ongoing problem. This is later explained in the Future Work section in Section 6.3.1.

Question with counterparametric context	Model Answer	Category
Context: [the nearest major body of water to Windhoek is the Rio de la Plata] Q: What is the nearest major body of water to Windhoek? A: The nearest major body of water to Windhoek is	the Atlantic Ocean	Parametric
Context: [the date of birth of Che Guevara is 965 AD]. Q: What is the date of birth of Che Guevara? A: The date of birth of Che Guevara is	965 AD	Contextual
Context: [Rome is in Georgia] Q: What country is Rome in? A: Rome is in	the United States	Other

Table 5: Example for results for three questions. We enhance each question with a context containing data that is different to the answer given by the model for this question. We later categorise the source of the answer as **Parametric** if it came from the model's inherent memory, **Contextual** if it came from the context, or **Other** if it's neither of these. Note that, in the third query, the model is interpreting the question as asking about Rome in the US State of Georgia, rather than the country of Georgia.

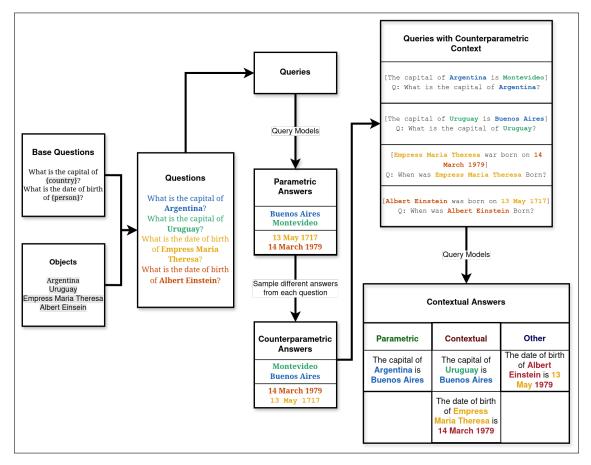


Figure 3: Example diagram of steps taken to calculate the sets of Parametric, Contextual, and Other answers. The terms in this diagram are explained in the Glossary. The following steps are shown:

- 1. Generate questions by combining every base question with every object of the same category.
- 2. Query each model, and get a set of parametric answers.
- 3. Shuffle these parametric answers along the same base question to get counterparametric answers.
- $4. \ \, {\rm Query \ the \ model \ again, \ using \ the \ counterparametric \ answers \ as \ context.}$
- 5. Group the answers according to their source.

3.2.3 Understanding the result by finding the mean attention of the context and question areas

When comparing different architectures, it's useful to understand how much attention they give to the context compared to the rest of the query.

Given that all our model architectures employ attention mechanisms (Chung et al. 2022, Dubey et al. 2024), we can estimate the relative importance of the tokens in each section of the query by calculating the average self-attention each token receives within its respective section. Specifically, we compute the mean self-attention weights, which serve as a proxy for the emphasis the model places on different parts of the input.

This approach is formalized in Equation (1), where we define the mean self-attention for tokens in the context and query sections.

$$A: \mathbb{R}^{\text{batch} \times |\text{layer}| \times |\text{attn_head}| \times Q \times K}$$

$$m_{b,q,k} = \frac{1}{|\text{layer}| \times |\text{attn_head}|} \sum_{\substack{i=0\\j=0}}^{\text{layer}} A_{b,i,j,q,k}$$

$$d_{b,q} = m_{b,q,q}$$

$$s_{b,i} = (d_{b,i} - \min(d_b)) / (\max(d_b) - \min(d_b))$$

$$\text{attn}_{\text{ctx}} = \frac{1}{|\text{ctx}|} \sum_{i \in \text{ctx}} s_{b,i} \quad \text{attn}_{\text{rest}} = \frac{1}{|\text{rest}|} \sum_{i \in \text{rest}} s_{b,i}$$

$$(1)$$

In this equation, A is the 5-tensor representing the attention weights. $m_{b,q,k}$ represents the mean attention all layers and heads, while d_b represents the diagonal of these attentions which correspond to the self-attentions.

We normalise the values for the tokens in each query to s_i in order to being able to compare them between different query, and average then among the context tokens and the rest of the query. This results in two results that can be compared between different queries.

3.3 Enhancing the framework to understand the reasoning behind each answer

3.3.1 Perplexity Score

The Perplexity score of an answer is normally used to measure the inverse of the certainty that the model has of a particular answer (Brown et al. 2020, Borgeaud et al. 2022). In a sense, it's the "surprise" of a model that a certain answer is correct.

We can define the probability of a model choosing a token x_n with context x_1, \ldots, x_{n-1} from a query Q by calculating the softmax value of all the logits for the possible words for this token.

The probabilities of of the answer generated from a query can be accumulated to calculate the negative log-likelihood NLL, which is used to calculate the perplexity PPL using the formulas from Equations (2) and (3).

NLL
$$(x_1, ..., x_n \mid Q) = -\frac{1}{n} \sum_{i=1}^n \log_2 P(x_i \mid Q, x_1, ..., x_{i-1})$$
 (2)

$$PPL(x_1, ..., x_n \mid Q) = 2^{NLL(x_1, ..., x_n \mid Q)}$$
(3)

3.3.2 Perplexity of the parametric answer with counterparametric context and vice-versa

Note that, in these experiments, the token x_n does not necessarily have to be the most likely result generated by the model when applying the query x_1, \ldots, x_{n-1} .

Therefore it becomes necessary to use teacher-forcing (Lamb et al. 2016) to feed some answer to the model regardless of what's the most likely answer for each successive token. This allows us to calculate the perplexity scores of the parametric answers for both the contextless query and the one with counterparametric context, and the perplexity scores of the contextual answers for these two queries.

For a given parametric answer p_1, \ldots, p_n and different counterparametric answer q_1, \ldots, q_m , a query without context Q, and a query with this counterparametric context Q' we can calculate four different perplexity scores P_0, P_1, P_2, P_3 as shown in Table 6.

Since the parametric answer is by definition the response of the model to the regular query, $P_0 \leq P_1$ and the perplexity of the parametric value is lower than the perplexity of any other answer on query Q.

Figure 4 contains an example of the calculation of the perplexity values for a particular query in a case where the contextual answer is considerably less surprising than the parametric answer.

		Tokens			
		Parametric p	Counterparametric q		
Context	Base Query	$P_0 = \operatorname{PPL}\left(p_1, \dots, p_n \mid Q\right)$	$P_1 = \operatorname{PPL}\left(q_1, \dots, q_m \mid Q\right)$		
	Counterparametric Context	$P_2 = \operatorname{PPL}(p_1, \dots, p_n \mid Q')$	$P_3 = \operatorname{PPL}(q_1, \dots, q_m \mid Q')$		

Table 6: We calculate four different perplexity values: one for each set of tokens, and one for each query context. We care about P_2 and P_3 , which are the perplexities at getting the parametric and counterfactual answers in a query with counterfactual context.

Similar to the work done earlier in this section, we say that the perplexity of an answer is **Parametric** if the probability of getting the parametric answer is greater than the probability of getting the contextual answer; that is, $P_2 < P_3$. Contrary to this, we consider an answer **Contextual** if $P_2 > P_3$.

For simplicity and to the myriad of possible token and probability combinations, in this experiment we do not analyse the case when an answer is preferred to either of these two.

3.3.3 Predicting whether an answer came from memory or from context

One question remains: if the response of the query with counterparametric context Q' is a certain answer x_1, \ldots, x_n , can we predict whether this answer is came from the model's memory p or from the given context q without requiring an extra query?

We propose investigating the value of the perplexity $PPL(x_1, ..., x_n \mid Q')$ and comparing it to the distribution of perplexities on queries with added counterparametric context P_2 and P_3 . The probability of this value being on one distribution or another might give us a good idea of the source the model used for generating the answer.

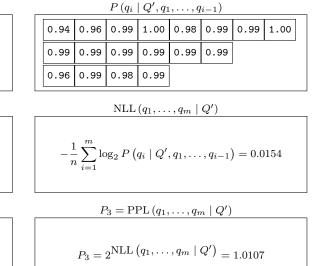
Base Query QQ: Where is The Son of Man primarily housed? A: The Son of Man is currently in Parametric Answer Tokens p_1, \ldots, p_n collection National Gallery of Canada Ottawa Ontario Canada $P(p_i \mid Q', p_1, \ldots, p_{i-1})$ 4e-05 | 0.87 | 0.93 | 0.06 0.94 0.26 0.04 0.61 0.98 0.72 0.49 0.59 0.90

 $\mathrm{NLL}\left(p_1,\ldots,p_n\mid Q'\right)$

 $-\frac{1}{n}\sum_{i=1}^{n}\log_2 P\left(p_i \mid Q', p_1, \dots, p_{i-1}\right) = 2.0566$

 $P_2 = \operatorname{PPL}(p_1, \dots, p_n \mid Q')$

 $P_2 = 2^{\text{NLL}} (q_1, \dots, q_m \mid Q') = 4.1599$



Query with Counterparametric Context Q'[Context: The Son of Man is housed in in the refectory of the Convent of Santa Maria delle

Q: Where is The Son of Man primarily housed?

Counterparametric Answer Tokens q_1, \ldots, q_m

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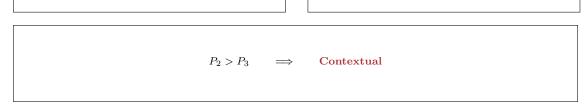


Figure 4: Example of perplexity calculation for the parametric and counterparametric answers in a query with the counterparametric context. For each large language model, we calculate the probability of getting each parametric token p_1, \ldots, p_n and each counterparametric token $q_1 \ldots q_m$ in the query with added context Q', and we accumulate that into two perplexity values. Note that, due to teacher forcing, the calculation finds the probability of the next token p_i given the previous tokens of the searched answer p_1, \ldots, p_{i-1} rather than given the most likely tokens. For example, once we feed the string "National Gallery of Canada in", the probability of the next token being "Ottawa" is very high. In the same way, despite the perplexity of the token "collection" following the initial token "the" is very high, the perplexity of the following tokens in the parametric answer is considerably lower.

4 Results

We followed the methods explained in Section 3 to create a new dataset and run the models listed Section 3.2.1 in order to measure their knowledge grounding of each one of these models when adding counterparametric context.

This section presents the results from these runs.

4.1 Creating a representative dataset of questions

As described in Section 1.4.1 and explained in Section 3.1, we require a new and diverse dataset in order to run this data and answer the research question.

We manually create a set of 4760 questions using the method explained in Section 3.1.

In order to be able to reuse objects for different questions, we separated the questions and objects in 9 different categories.

- 1. **Person** Historical people living from early antiquity to the present day from all around the globe. The questions have short, unambiguous answers, such as date of birth or most famous invention.
- 2. City Cities from all over the globe. Questions may include population, founding date, notable landmarks, or geographical features.
- 3. **Principle** Scientific principles, discovered from the 16th century forward. Questions about their discovery, use, and others.
- 4. **Element** Elements from the periodic table. Questions may cover discovery, atomic number, chemical properties, or common uses.
- 5. **Book** Literary works from various genres, time periods, and cultures. Questions may involve authors, publication dates, plot summaries, or literary significance.
- 6. **Painting** Famous artworks from different art movements and periods. Questions may cover artists, creation dates, styles, or current locations.
- 7. **Historical Event** Significant occurrences that shaped world history, from ancient times to the modern era. Questions may involve dates, key figures, causes, or their historical consequences.
- 8. **Building** Notable structures from around the world, including ancient monuments, modern skyscrapers, and architectural wonders. Questions may cover location, architect, construction date, or architectural style.
- 9. **Composition** Musical works from various genres and time periods. Questions may involve composers, premiere dates, musical style, or cultural significance.

Each one of these categories has a number of questions that are assigned one of the objects, following and enhancing the question-building approach used by Yu et al..

The final list of base questions and objects for all categories can be found in Appendix A. The total amount of these and composition of the 4760 questions can be found in Table 7.

Category	Base Questions	Objects	Total Questions
Person	17	57	969
City	17	70	1190
Principle	5	37	185
Element	15	43	645
Book	11	49	539
Painting	12	44	528
Historical Event	4	64	256
Building	9	22	198
Composition	10	25	250
Total	100	411	4760

Table 7: The amount of base questions, objects, and the total amount of questions in each category on the final dataset after merging the base questions with the objects of each respective category.

4.2 Building an experimental framework to understand the source of an LLM's answer

4.2.1 Building and running the framework

The code used for running this framework is present in Appendix C. This code roughly follows the diagram on Figure 3 to run the following steps.

- 1. Generate questions from base questions and objects: combine_questions.
- 2. Gather the parametric answers for each model: QuestionAnswerer.answerChunk.
- 3. Shuffle them to create counterfactual answers: sample_counterfactual_flips
- 4. Build new queries with these counterfactual answers as context: Question.format
- 5. Run the models again, and gather the corresponding answer type for each answer from the results: QuestionAnswerer.answerCounterfactuals.

The models were run on a server with 48 Intel(R) Xeon(R) CPU 3GHz CPUs, 376GB of RAM, and 2 NVIDIA A100 GPUs with 80GB of VRAM each that was kindly provided to Artificial Intelligence MSc students in City, University of London.

We estimate that it's possible to run this framework for all but the largest model, Meta-Llama-3.1-70B, using a single A100 GPU.

Appendix B explains the many options that can be run on knowledge_grounder.py to re-run this experiment or run similar ones.

4.2.2 Framework Results

The results of running the queries created in Section 3.1 with added counterparametric context on each of the four models the four models can be found in Table 8 and Figure 5.

Model	Parametric	Contextual	Other
flan-t5-xl	248	4284	228
flan-t5-xxl	242	4304	214
Meta-Llama-3.1-8B-Instruct	745	3662	353
Meta-Llama-3.1-70B-Instruct	1070	3303	387

Table 8: Amount of answers of each category when running our dataset on each of the four models. Seq2Seq models tend to generate using the parametric context more often than Decoder-only models, while for the latter the size of the model makes a large difference.

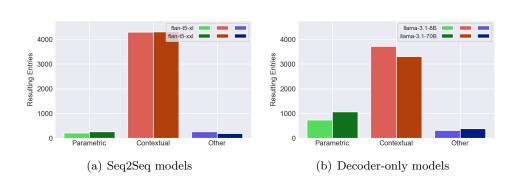


Figure 5: Results by type depending on which model; these are the same results as Table 8.

As hypothesised in Section 1.4.2, there are vast differences on how the models of different types and sizes act when presented with a context that contradicts their knowledge. This section contains an overview of the differences, which investigated further in Section 5.

A similar pattern emerges in most (but not all) of the categories, which can be seen in Tables 10 and 11 and Figures 6 and 7.

4.2.3 Calculating the attention of the context and question of each query

Using the method described in Section 3.2.3, we can find the attention each model gives, on average, to the tokens in the context part of the query, and how much to the rest.

Query Part	flan-t5-x1	flan-t5-xxl	Meta-Llama-3.1 -8B-Instruct	Meta-Llama-3.1 -70B-Instruct
Context	0.18	$0.22 \\ 0.05$	0.08	0.06
Rest	0.03		0.03	0.01

Table 9: Average normalised attention of the query on the tokens corresponding to the context of the query and o the rest. All models pay more attention to the context section of the query than to the rest, but Seq2Seq models tend to have a much higher ratio than decoder-only models.

	f	flan-t5-x1			flan-t5-xxl		
	Parametric	Contextual	Other	Parametric	Contextual	Other	
Person	32	900	37	23	890	56	
City	120	1030	40	78	1093	19	
Principle	13	164	8	9	168	8	
Element	6	637	2	102	515	28	
Book	26	488	25	18	457	64	
Painting	26	446	56	4	498	26	
Historical Event	11	217	28	1	254	1	
Building	14	174	10	0	189	9	
Composition	0	228	22	7	240	3	

Table 10: Results for running each one of the 10 categories separately on the Seq2Seq models. There is not a significant difference between categories.

	Meta-Llama-3.1-8B-Instruct			Meta-Llama-3.1-70B-Instruct		
	Parametric	Contextual	Other	Parametric	Contextual	Other
Person	40	833	96	209	614	146
City	117	1007	66	166	966	58
Principle	44	118	23	44	117	24
Element	218	385	42	275	347	23
Book	135	344	60	154	318	67
Painting	47	458	23	49	445	34
Historical Event	81	154	21	117	118	21
Building	27	163	8	31	159	8
Composition	36	200	14	25	219	6

Table 11: Results for running each one of the 10 categories separately on the Decoder-only models, there are a few differences in the results for different categories, which is likely caused by the average answer size.

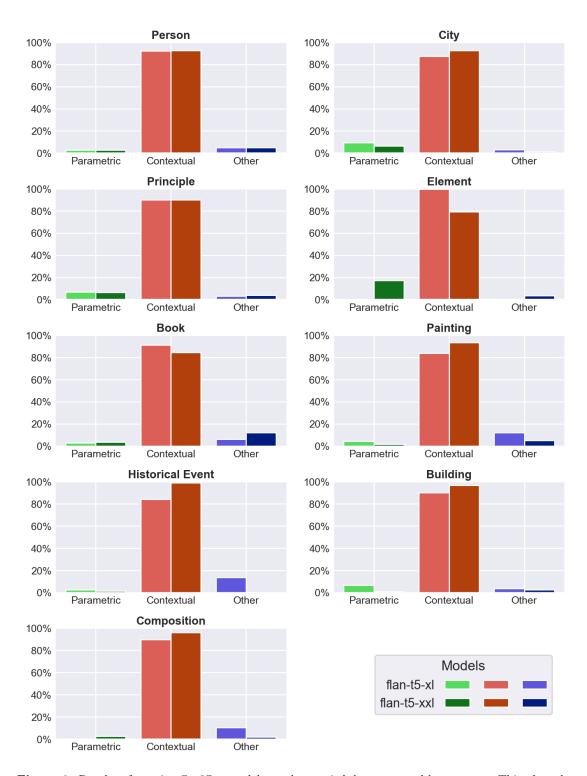


Figure 6: Results of running Seq2Seq models on the queried data, grouped by category. This plots the information shown in Table 10, and we can confirm that there isn't a significant difference in the source of the knowledge used to generate the answer depending on category.

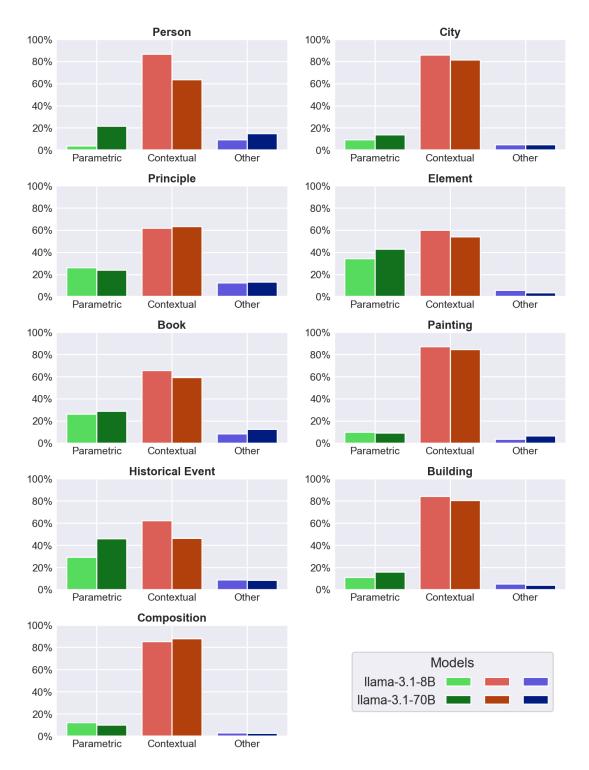


Figure 7: Results of running decoder-only models on the queried data, grouped by category. This plots the information shown in Table 11. Contrasting this to the previous plot, we can see that there is a significant difference in contexts that tend to have questions resulting in shorter answers, such as books and historical events, compared to sections that tend to have longer answers, such as persons.

4.3 Enhancing the framework to understand the reasoning behind each answer

We calculate the resulting perplexity of each query as explained in Section 3.3. These are accumulated in three distributions, depending on answer type, which are summarised in Tables 12 and 13 and Figure 8, and grouped by different categories in Figures 9 and 10, and later grouped by category in Figures 9 and 10.

	flan-	t5-xl	flan-t5-xxl		
	Parametric	Contextual	Parametric	Contextual	
count	588	4172	491	4269	
mean	7.02	1.55	12.01	1.24	
$\operatorname{\mathbf{std}}$	11.25	0.56	18.91	0.68	
10%	2.60	1.08	1.47	1.00	
25%	3.21	1.18	2.54	1.02	
50%	4.71	1.37	4.00	1.08	
75%	7.40	1.69	8.37	1.22	
90%	10.72	2.32	44.25	1.54	

Table 12: Distribution of perplexity values for Seq2Seq models. The perplexity of **Parametric** answers is consistently higher than the one of **Contextual** answers.

	Meta-Llama-3.	1-8B-Instruct	Meta-Llama-3.1-70B-Instruct		
	Parametric	Contextual	Parametric	Contextual	
count	289	4471	383	4377	
mean	1.64	1.20	1.56	1.22	
$\operatorname{\mathbf{std}}$	0.87	0.30	0.46	0.31	
10%	1.18	1.03	1.20	1.03	
25%	1.28	1.05	1.28	1.06	
50 %	1.45	1.11	1.43	1.12	
75%	1.72	1.23	1.68	1.25	
90%	2.22	1.43	2.04	1.49	

Table 13: Distribution of perplexity values for Decoder-only models. The same differences in Table 12 appear here, but to a lesser degree.

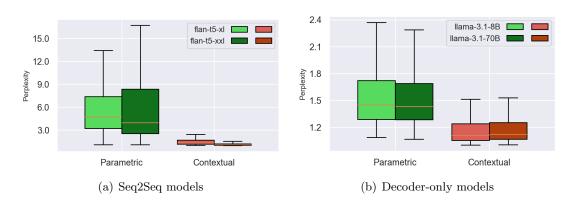


Figure 8: Perplexity distribution according to model architecture and size. These represent the same distributions as Tables 12 and 13.

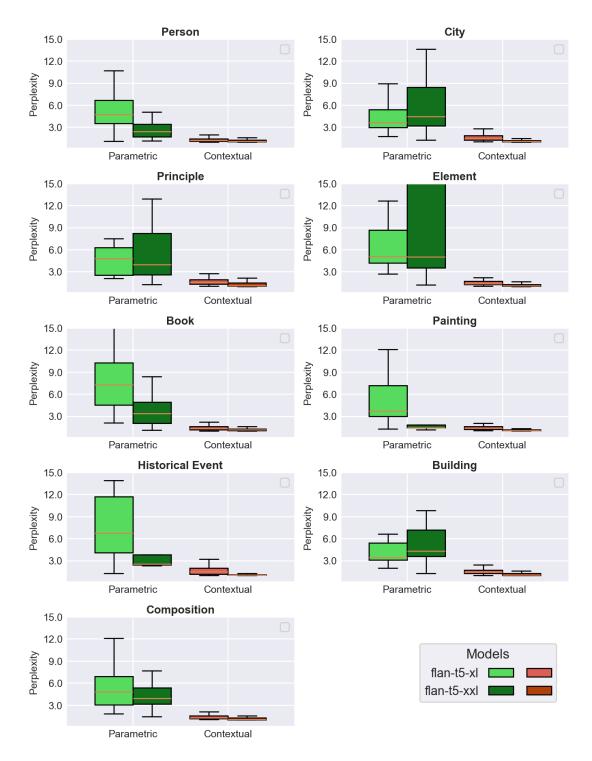


Figure 9: Box plots representing the distribution of the perplexities when running both Flan-T5 models, grouped by category. There are considerable differences in the distribution of perplexity values for **Parametric** answers, but not so much for **Contextual** answers. Still, the differences between this two are consistently large.

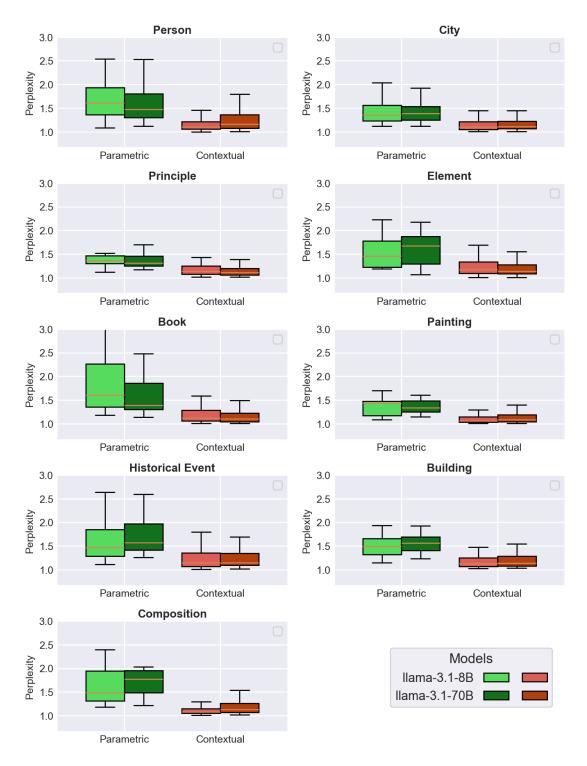


Figure 10: Box plots representing the distribution of the perplexities when running both Llama models, grouped by category. The entire distribution of perplexities is much smaller, and the differences in these for **Parametric** answers are less variable as in the previous plots for Seq2Seq models.

5 Discussion

Section 4 presented results from generating the question dataset and running the framework to understand the role of knowledge grounding in a variety of models and their parametric knowledge in question-answering. This section explains these results, and discusses what they mean for our research question.

5.1 Model architecture and memorised knowledge

Section 4.2.2 presents the results of running our framework on the provided questions on two different model architectures: Seq2Seq models and Decoder-only models. Tables 10 and 11 show these results split by category of question.

The results are clear: Seq2Seq models tend to answer questions from their contextual knowledge rather than from their inherent knowledge more often than Decoder-only models. These results persist across different question categories and are consistent regardless of answer types and lengths

These results demonstrate that, in the framework of question-answering when using RAG to fetch contextual data from an index, Seq2Seq models will tend to have fewer hallucinations that contradict this index than Decoder-only models.

We propose two hypotheses that could explain these differences.

5.1.1 Advantages of the Encoder-Decoder Architecture

As described in Section 2.2, Seq2Seq models such as Flan-T5 are encoder-decoder models that process the entire context of the query in the encoder component before passing it to the decoder, which could increase the weight given to the context itself.

We can test this hypothesis by finding the mean attention of the tokens corresponding to the context and to the rest of the query, and using the method discussed in Section 3.2.3.

The results presented in Section 4.2.3 are consistent with this theory: Seq2Seq models allocate more attention to the contextual tokens of the query than Decoder-only models.

5.1.2 Different training data and fine-tuning

It's possible that these result doesn't come from the model architecture, but from the bias caused by their training methodology.

The Flan-T5 models were trained on masked token generation and later fine-tuned on question-answering about passages (Chung et al. 2022). This requires strong alignment between query and answer, which encourages the model to focus on the input context and makes it more likely to take the answer from the RAG-provided context.

Llama models were trained mainly on open-ended text generation, which relies more on parametric data.

It's possible that the deficiencies of knowledge grounding in Llama models might come simply to not being trained on related tasks.

5.2 Model size and memorised knowledge

Section 4.2.2 also shows differences in how models of different sizes process information in queries with counterparametric context.

5.2.1 Seq2Seq Models

While the average results are very similar, which is likely due to the properties of Seq2Seq models discussed in Section 5.1, the models seem to be significantly different for queries of category element, historical_events, and a few others.

Unfortunately, it's possible that the significance of these results comes down to failures on the large language models: for reasons not we do not fully understand yet, flan-t5-xl often produces nonsensical answers to questions requiring short responses, such as elements' names in the periodic table on historical dates. This behaviour is different than flan-t5-xxl, which generally provides correct answers in these cases.

When removing the categories with a significant amount of short answers and their nonsensical answers by the smaller model, the results of both Seq2Seq models seem similar. Therefore, we can conjecture that the size of a Seq2Seq model does not significantly affect its knowledge grounding.

5.2.2 Decoder-only Models

Section 4.2.2 shows a very different result for Decoder-only models. Surprisingly, the smaller model Meta-Llama-3.1-8B-Instruct has *better* knowledge grounding than the larger model Meta-Llama-3.1-70B-Instruct.

We already established that decoder-only models rely on parametric knowledge to a greater degree than Seq2Seq models. Larger models have a vast internalised knowledge base accumulated from expensive training data, which can lead to increased confidence in their parametric knowledge.

It's possible that larger Decoder-only models are able to use their parametric knowledge to interpret the answer to the question in more ways that contradict the contextual knowledge. The extra information encoded on the model's weights can produce more varied evidence against the contextual answer.

With this information, we can say that the size of Decoder-only models *does* affect its knowledge grounding, and when enhancing queries with RAG it might be preferable to use a smaller model.

This is consistent with similar results found for other Decoder-only models, such as Pythia and GPT-2 (Yu et al. 2023).

5.3 Investigating the source of Other answers

Section 4.2 showed that a significant minority of responses to queries with counterfactual context are **Other**: answers that aren't equal to either the parametric nor the contextual data. The numbers of these entries, per model, are presented in Table 14.

	Flan-T5-XL	Flan-T5-XXL	Meta-Llama-3.1 -8B-Instruct	Meta-Llama-3.1 -70B-Instruct
Other	260	192	312	387

Table 14: Amount of Other entries, that is, results where the answer was not either the parametric or contextual answer.

By manually checking these results, we can understand the reason why the model chose these answers comes down to one of the following seven cases.

1. Different phrasing of a parametric answer

There are many answers where the model provides the parametric answer phrased with the format of the counterparametric context given in the query.

2. Plain incorrect answers

Sometimes, adding counterfactual context to the query causes the model to produce an incorrect answer, which is different the answers from both the parametric knowledge of the model and the given context.

3. Question misinterpretation due to the context

Some questions can be ambiguous or have a low probability of another answer. By adding a context with a counterfactual answer, the model can misinterpret the question and answer that's correct different to both the context and the parametric answer.

4. Negating the context

This is an interesting one: if the model has an answer in its parametric knowledge that contradicts the data on its context, then it interpret the context as part of the question and adds its negation as part of the answer.

5. Different phrasing of the context

Much less common than point 1, models sometimes give the same answer as provided in the query's context but in the format of the parametric answer.

6. Correct answer, just different than the parametric answer

Some questions have multiple correct answers, and adding counterfactual context can cause the model simply choose different one from its parametric memory.

7. Mixing elements of both parametric answer and context

The final answer contains elements of the parametric answer combined with elements of the given. This produces an answer that's different to both the parametric and contextual answer, but with parts of both of them. The cause of this is likely the greedy decoding used to find the answers, as explained in Section 3.2.2.

Examples of each one of these types can be found in Table 16.

Does the architecture and size of the model affect the distribution of each type of **Other** answer? Table 15 contains the amount of answers for each model.

Type	Flan-T5-XL	Flan-T5-XXL	Meta-Llama-3.1 -8B-Instruct	Meta-Llama-3.1 -70B-Instruct
(Parametric) (Contextual)	248 4284	242 4304	$745 \\ 3662$	1070 3303
1.	0	0	116	234
2.	6	3	50	15
3.	0	0	13	8
4.	0	0	20	61
5.	241	170	33	38
6.	7	16	63	23
7.	6	3	17	8

Table 15: Different types of **Other** answers per model (with amount of **Parametric** and **Contextual** added for comparison). The two most notable groups are **1.**, which contains parametric answers with different phrasing, and **5.**, which contains counterfactual answers with different phrasing.

Surprisingly, there is a large difference in the distribution of answers that don't come either from the model or from the given context.

In the case of Seq2Seq models, the majority of **Other** answers are **Contextual** answers with a different format due. This is consistent with the previous result, where the vast majority of their answers came from the query's context.

The majority of Other answers in Decoder-only models are the opposite: Parametric answers expressed in the format of the context. However, the reasons are much more varied and this would be an interesting topic of discussion in future research.

Part of the reason for many of these answers are not equal to the parametric answer coming from the model's inherent knowledge or the answer given in the query's context, particularly on the Seq2Seq models, is due to the strict comparison function we use to define answer type. This is an area that should be improved; Section 6.3.1 gives more information and various suggestions on how to compare results that might be relevant on future work.

5.4 Differences in distribution of perplexity scores

The distribution of perplexity scores, shown in Section 4.3, shows a significant difference in the perplexity scores between **Parametric** and **Contextual** answers for all four models. This is even more marked on Seq2Seq models, where for both models the 90% percentile of the **Contextual** answer is lower than the 10% percentile of the **Parametric**.

In fact, this confirms our conjecture that **models tend to be surprised when finding** an answer that contradicts the context of the query. This conjecture seems to be true regardless of model size or question type (see Figures 9 and 10).

Reason	Question	Parametric	Counterfactual	Contextual
1.	Who was the primary leader associated with The Reforms of Diocletian?	Diocletian Himself	Caracalla, a Roman Emperor	Diocletian, a Roman Emperor
	In which city is Louvre Pyramid located?	Paris, France	the city of Valladolid, in the state of Yucatan, Mexico	the city of Paris, in the country of France
2.	In which period of the periodic table is Silver located?	5 of the periodic table	3 of the periodic table	4 of the periodic table
3.	What was the duration of Queen Elizabeth II's Platinum Jubilee?	12 months	approximately 100 years	approximately 70 years
	What is the nearest major body of water to Cusco?	Lake Titicaca	the North Sea	the Pacific Ocean
4.	What is the name of the main protagonist in One Flew Over the Cuckoo's Nest?	Randle McMurphy	Achilles	Not Achilles
	What is Frida Kahlo primarily known for?	her self-portraits and her depiction of Mexican culture	his theories on communism and his critique of capitalism	her artwork and her life story, not for his theories on communism or critique of capitalism
5.	How many pages are in One Flew Over the Cuckoo's Nest?	320 pages	480 pages in a standard edition	480 pages
6.	Who is credited with the discovery of Conservation of Energy?	Julius Robert Mayer	Alfred Wegener	James Joule ¹
	What is the name of the main protagonist in The Great Gatsby?	Nick Carraway	Liesel Meminger	Jay Gatsby ²
	What educational institution did Srinivasa Ramanujan attend?	The University of Madras	The University of Vienna	the University of Cambridge ³
7.	What is the date of death of Vladimir Lenin?	January 21, 1924	March 28, 1941	March 21, 1924
	What's the main nationality of Mozart?	Austria	English-Born American	American-born English-born Austrian

 $^{^{1}}$ Discovery of the conservation of energy is credited to both Julius Robert Mayer and James Joule. 2 Nick Carraway and Jay Gatsby are co-protagonists in The Great Gatsby. 3 Srinivasa Ramanujan attended both the University of Madras and the University of Cambridge.

 $\textbf{Table 16:} \ \ \textbf{Examples of different types of } \ \textbf{Other} \ \ \textbf{answers when running the } \ \textbf{Meta-Llama-3.1-8B-Instruct}$ model, with the categories listed and explained in Section 5.3.

The cause for the difference in the perplexity values for different architectures is likely the same as discussed in Section 5.1 on why the Flan-T5 models generally have better performance on these tasks than Llama models.

Model Architecture By processing the entire input in one go, the Seq2Seq encoding step processes information in the context before starting decoding. In Decoder-only models, the shift from going from contextual to parametric knowledge is less abrupt, resulting in a less pronounced change in perplexity.

Training Data Flan-T5 models are trained in data where getting information from the query itself is more relevant. In a sense, they are biased to being more surprised when producing a parametric answer.

5.4.1 Can we use the perplexity to predict the source of an answer?

Seeing the current results, it's tempting to attempt to create an estimator which, given information about the perplexity of an answer alone and without making any additional query, can estimate whether that answer in a query with added context came from the **Parametric** knowledge of the context or from the **Contextual** information in the query.

This can be useful in practice: if a RAG-enhanced model finds an answer with high perplexity, it can attempt to re-run the RAG indexing to find a more relevant answer and possible prevent a hallucination.

The results in Tables 12 and 13 seem consistent with Figure 11 in that such predictor would work better in Seq2Seq models, particularly on flan-t5-xxl: by re-running the RAG indexer on answers with perplexity of over 1.5, we can prevent hallucinations on 90% of the answers that came from parametric knowledge while not reindexing on 80% of the total questions.

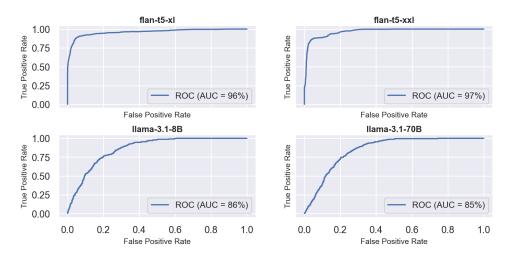


Figure 11: ROC curve of the four tested models to find out whether an answer came from the **Parametric** knowledge of a model using the perplexity of the answer.

6 Evaluations, Reflections, and Conclusions

6.1 Overview of the Research Question

Section 1.2 introduced a simple research question: how does a large language model respond when given information that contradicts its inherent knowledge, and why?

Using the methods outlined in Section 3, and analysing the results outlined in Section 4 and discussed in depth in Section 5, we can reach the following conclusions.

Seq2Seq models provide better results in answering data from contextual knowledge than Decoder-only models.

As described in Section 5.1, Seq2Seq models have an inherent advantage when gathering data from the context of the query when this contradicts its inherent parametric knowledge. It's possible that this difference comes down to training data rather than model architecture alone.

Size does not have a large impact in Seq2Seq models, but larger models are at a disadvantage in Decoder-only models.

As described in Section 5.2, the architecture of decoder-only models that biases them towards answering questions from their parametric knowledge more often also amplifies this effect in larger models.

Categorising answers is hard, and better methods are needed.

A lot of the answers we got in these experiments seemed to come from neither the query's context nor the parametric memory of the models. In Section 5.3 we demonstrate that the majority of those answers do come from those models, but that our methods to compare the answers are not good enough to categorise them properly.

Large language models tend to be surprised when finding an answer that contradicts the context of the query.

As seen in Section 5.4, models that choose a **Parametric** answers have higher perplexity than models that choose **Contextual** answers. This is consistent across all question categories and model architectures and sizes. This result is more marked on Seq2Seq models, likely for the same reasons why those models tend to generate **Contextual** answers more often.

It's possible to create an estimator to know whether an answer came from the parametric memory of a model or from the provided context.

Section 5.4.1 explains how to build such an estimator. This can be useful in cases where accuracy is crucial, but reindexing to get new context is expensive.

6.2 Personal Reflections

Working on this thesis has been a very positive and enriching experience.

Starting the project from an unpublished draft (Whitehouse et al. 2023) helped me ground my personal knowledge of the current state of the research on retrieval-augmented generation and analysis of large language models. I am grateful to Dr. Whitehouse, the main author of the draft, who has been of great help in giving me ideas and direction when working on this research.

The topic of the thesis changed early on from understanding knowledge grounding on the conflation of retriever and generator on retrieval-augmented models to understanding it for general large language models with added contextual information. This was, in part, caused by the cutting-edge nature of this research area: over half of the papers cited were published after the year 2020, and two of them were published earlier in the year 2024.

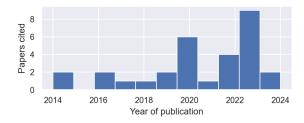


Figure 12: Year of publication of papers cited in this thesis. These topics are novel!

One of the main strengths of my work in this thesis was having built a solid experimentation infrastructure early on, which allowed me to iterate quickly on experiments and ideas. The program to build, run, and analyse the counterparametric-enhanced queries (which is present in Appendix C and in this project's repository) is one of the strong points of this project, and I'm sure it will be a valuable tool in future research projects.

Despite settling on the final thesis idea early, this thesis suffered from lacking a clear and well-defined research question, which emerged late in the process. I consider this delay to have been one of the main sources of inefficiencies, since it lead to executing long experiments that contributed little to the final thesis. One of my main takeaways from this research is the necessity to align on a well-defined research question early.

This thesis taught me how to adapt to the rapidly-changing research landscape of sequence analysis and artificial intelligence. A lot of the methods used in this work are taken directly from previous academic papers, and this allowed me to test my hypothesis quickly while keeping a deep understanding of the context I am working on.

Most of all, I'm happy to have learned a lot about the areas of large language models and to have been able to collaborate a bit in this very new area of research. I plan to continue this work in the future, and I'm looking forward to contributing to the research on this area!

6.3 Future Work

6.3.1 Better Categorisation of the Answers

To test whether two answers are equal and to know whether an answer came from parametric or contextual knowledge, the code in this thesis checks for string equality among after removing a few stop simple words such as 'the'.

This solution might not be enough, and some answers classified as **Other** should have been classifier as something else. Table 17 provides some examples of answers where the answer should have been categorised as **Parametric** or **Contextual**.

Query	Parametric Answer	Query Answer	Comparison	Expected
[Context: The primary leader associated with The Construction of Hadrian's Wall was Napoleon Bonaparte] Q: Who was the primary leader associated with The Construction of Hadrian's Wall? A: The primary leader associated with The Construction of Hadrian's Wall was	Emperor Hadrian	Hadrian, the Roman Emperor	Other	Parametric
[Context: Che Guevara was born in Kensington, London, England] Q: In what city was Che Guevara born? A: Che Guevara was born in	Rosario, Argentina	London	Other	Contextual

Table 17: Example of incorrectly-categorised answers. These were categorised as "Other", since their answer strings are different from both parametric and contextual answers. However, a closer look reveals that this is just a Parametric or Contextual answer with a slight formatting difference.

A more complete solution might include using another LLM to compare whether two answers are truly equal.

6.3.2 Knowledge Grounding in Retrieval-Augmented LMs

This thesis was originally based on a preprint, "Knowledge Grounding in Retrieval-Augmented LMs: An Empirical Study" (Whitehouse et al. 2023), and contains work towards understanding how large language models retrieve data which can ultimately help prevent hallucinations.

We plan to continue this work and complete the paper created by the preprint by running the methods outlined on this thesis on retrieval-augmented LMs such as ATLAS (Izacard et al. 2022) and RETRO (Borgeaud et al. 2022) and creating a full evaluation framework that specifically focuses on their grounding. A well-grounded model should demonstrate the capability to adapt its generation based on the provided context, specially in cases like

the ones experimented in this thesis when the context contradicts the model's parametric memorisation, and we can experiment with an analysis similar to the one done in this thesis for those models.

6.3.3 Fine-tuning a LLM for a RAG Context

In this research we proved that certain models architectures are preferable to others for answering from data from the context when it contradicts the parametric knowledge of a model.

Existing retrieval-augmented language models, such as ATLAS and RETRO, are trained on existing models along with an index. We can continue this approach by fine-tuning an existing LLM, such as the Flan-T5 or Llama models used in this thesis, specifically to be able to answer these kinds of queries better.

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Glossary

This section presents a small glossary with explanations of some of the terms used in this thesis.

Category

One of the many topics for each one of the question, which are listed in Table 7.

Base Questions

A question that refers to a category, but does not refer to any particular object.

Objects

An object of a certain category that can be added to a base question. The final queries are the cross product of all base questions and objects for each category; see Table 1 for an explanation.

Parametric Answers

The answers given by the model for a particular query when not adding any context. These answers come solely from the parametric, learned knowledge of the model.

Counterfactual Answer

A randomly-sampled parametric answer from another question, which is guaranteed to be different from this counterfactual answer. Table 4 contains an example of these.

Parametric, Contextual, and Other answers

The answers given by the model for a particular query when adding counterfactual context, named like that depending on whether they were taken from the model's parametric memory, from the context of the query, or from somewhere else. Section 3.2.2 gives an explanation of how these are generated and categorised.

Perplexity of an answer

The perplexity is a metric in information theory that measures how "surprised" a model is at finding a particular answer. This is explained in Section 3.3, where these answers are also categorised as **Parametric** or **Contextual** depending on which one is the most surprising.

Appendices

A Questions and objects used to form the queries

```
What is the date of birth of {person}? The date of birth of {person} is In what city was {person} born? {person} was born in What is the date of death of {person}? The date of death of {person} is
What is the date of death of {person}? The date of death of {person} is
What is the primary profession of {person}? The primary profession of {person} is
What is {person} primarily known for? {person} is primarily known for
What's the main nationality of {person}? {person} is
What educational institution did {person} attend? {person} attended
What was the native language of {person}? The native language of {person} was
Who was {person}'s most influential mentor? The most influential mentor of {person} was
What was {person}'s religious affiliation? The religious affiliation of {person} was
What was {person}'s primary field of study? The primary field of study of {person} was
What was {person}'s most famous work or invention? The most famous work or invention of {person} was
What historical period did {person} live in? {person} lived during the
What was {person}'s family's social class? {person}'s family belonged to the
What was {person}'s political ideology? The political ideology of {person} was
What was {person}'s preferred artistic or scientific medium? The preferred medium of {person} was
What was {person}'s cultural background? The cultural background of {person} was
 What country is {city} in? {city} is in What's the highest administrative subdivision {city} is part of? {city} is part of
What's the highest administrative subdivision {city} is part of? {city} is part of
In what year was {city} founded? {city} was founded in
What major river is nearest to {city}? The nearest major river to {city} is
What is the time zone of {city}? The time zone of {city} is
What is the current population of {city}? The current population of {city} is
What is the altitude of {city} above sea level? {city} is at an altitude of
What is the primary language spoken in {city}? The primary language spoken in {city} is
What is the predominant architectural style in {city}? The predominant architectural style in {city} is
What is the main economic industry of {city}? The main economic industry of {city} is
What is the average annual temperature in {city}? The average annual temperature in {city} is
What is the nearest major body of water to {city}? The nearest major body of water to {city} is
What is the most famous landmark in {city}? The most famous landmark in {city} is
What is the primary mode of public transportation in {city}? The primary mode of public transportation in {city} is
                          {city} is
 What is the name of the airport serving {city}? The airport serving {city} is
What is the sister city of {city}? The sister city of {city} is
What is the traditional cuisine {city} is known for? The traditional cuisine {city} is known for is
  Who is credited with the discovery of {principle}? {principle} was discovered by
 Which scientific discipline encompasses {principle}? {principle} is encompassed by What is the primary application of {principle}? The primary application of {principle} is In which year was {principle} first formulated? {principle} was first formulated in What is the SI unit most commonly associated with {principle}? The SI unit most commonly associated with
  What's the chemical formula for {element}? The chemical formula for {element} is
What's the chemical formula for {element}? The chemical formula for {element} is

When was {element} first isolated? {element} was first isolated in

What's the atomic number of {element}? The atomic number of {element} is

What is the melting point of {element}? The melting point of {element} is

In which group of the periodic table is {element} found? {element} is found in group

What's the standard atomic weight of {element}? The standard atomic weight of {element} is

What's the electron configuration of {element}? The electron configuration of {element} is

What's the most common oxidation state of {element}? The most common oxidation state of {element} is

What's the crystal structure of {element} at room temperature? The crystal structure of {element} at room
What's the crystal structure of {element} at room temperature: Int Clystal School temperature is
What's the primary isotope of {element}? The primary isotope of {element} is
What's the electronegativity value of {element}? The electronegativity value of {element} is
What's the ionization energy of {element}? The ionization energy of {element} is
What's the atomic radius of {element}? The atomic radius of {element} is
What's the boiling point of {element}? The boiling point of {element} is
In which period of the periodic table is {element} located? {element} is located in period
 What genre does {book} belong to? The genre of {book} is
Who's the author of {book}? {book} was written by
In what year was {book} first published? {book} was first published in
How many pages are in the original publication of {book}? The original publication of {book} has
What is the name of the main protagonist in {book}? The main protagonist in {book} is
 What is the original language of {book}? The original language of {book} is Who is the original publisher of {book}? The publisher of {book} is What is the highest award {book} won? The highest award won by {book} is What is the opening line of {book}? The opening line of {book} is How many chapters are in {book}? {book} has How many pages are in {book}? {book} has
 Who painted {painting}? {painting} was painted by
```

```
What artistic movement does {painting} belong to? {painting} belong to What artistic movement does {painting} belong to? {painting} was created with Where is {painting} primarily housed? {painting}? {painting} was created with Where is {painting} primarily housed? {painting}? The dimensions of {painting}? The dimensions of {painting} are In which museum was {painting} first exhibited? {painting} was first exhibited in What is the dominant color in {painting}? The dominant color in {painting} is Who commissioned {painting}? Tpainting} was commissioned by What is the estimated value of {painting}? The subject matter of {painting} is In which country was {painting} created? {painting} was created in What year did {historical_event} happen? {historical_event} happened in the year Who was the primary leader associated with {historical_event} was What was the duration of {historical_event}? {historical_event} lasted for In which country did {historical_event} primarily take place? {historical_event} primarily took place in What is the height of {building}? The height of {building} was In which year was {building} completed? {building} was completed in In which city is {building} completed? {building} was completed in In which city is {building} hozered? {building} is located in What architectural style is {building}? The architectural style of {building} is How may floors does {building} hozered? {building}? The primary construction material of {building}? The primary construction material of {building}? The primary construction material of {building}? The unsured in the total floor area of {building}? The miscal genre of {composition} was first performed in What is the total floor area of {building}? The opus number of {composition} is What is the opus number of {composition}? The musical genre of {composition} is What is the opus number of {composition}? The duration of {composition} was first performed in What is the opus number of {composition}? The duration of {composition} was premiered in What is the duration
```

Listing 2: All base questions used in this work. Each one of these will get combined with data from Listing 2 as detailed in Section 3.1.

```
Ada Lovelace, person
Alan Turing, person
Albert Einstein, person
Alexander Fleming, person
Aristotle, per
Billie Jean King, person
Boyan Slat, person
Catherine the Great, person
Che Guevara, person
Cleopatra, person
Confucius, person
Ernest Rutherford, person
Florence Nightingale, person
Freddie Mercury, person
Frida Kahlo, person
Greta Thunberg, person
Harriet Tubman, person
Ibn al-Haytham, person
Isaac Newton, person
Isaac Newton, person
Karl Marx, person
Leonardo da Vinci, person
Mahatma Gandhi, person
Malala Yousafzai, person
Mansa Musa, person
Marie Curie, person
Martin Luther King Jr., person
Michelangelo, person
Mohandas Gandhi, person
Mozart, per
Muhammad Ali, person
Neil Armstrong, person
Nelson Mandela, person
Nikola Tesla, person
Pablo Picasso
Rosalind Franklin, person
Shirin Ebadi, person
Simon Bolivar, person
Srinivasa Ramanujan, person
Stephen Hawking, person
```

```
Sun Yat-sen, person
Virginia Woolf, person
Vladimir Lenin, person
Wangari Maathai, person
W.E.B. Du Bois, person
William Shakespeare, person
William Shakespeare, per Wu Zetian, person Yuri Gagarin, person Amelia Earhart, person Galileo Galilei, person Joan of Arc, person Lise Meitner, person Marcus Aurelius, person Maya Angelou, person Queen Nzinga, person Socrates, person Voltaire, person Alexandria, city Amsterdam, city
Amsterdam, city
Amsterdam, city
Antananarivo, city
Athens, city
Baghdad, city
 Berlin, city
Buenos Aires, city
Buenos Aires, ci
Bukhara, city
Cairo, city
Cape Town, city
Cartagena, city
Chicago, city
Cusco, city
Cuzco, city
Delhi, city
Dubrovnik, city
Fez, city
 Fez, city
Havana, city
 Istanbul, city
Jerusalem, city
 Kyoto, city
La Paz, city
La Paz,city
Lhasa,city
Lisbon,city
London,city
Luang Prabang,city
Mexico City,city
Montevideo,city
Moscow,city
Mumbai,city
Numbai,city
New York,city
 New York, city
Nur-Sultan, city
Nur-Sultan, city
Paris, city
Petra, city
Prague, city
Quebec City, city
Reykjavik, city
Rome, city
Sao Paulo, city
Sao Paulo, city
Sarajevo, city
Shanghai, city
Singapore, city
St. Petersburg, city
St. Petersburg, cit
Sydney, city
Tbilisi, city
Tenochtitlan, city
Timbuktu, city
Tokyo, city
Ulaanbaatar, city
Varanasi, city
 Venice, city
Vienna, city
Wellington, city
Windhoek, city
Windhoek, city
Xi'an, city
Yogyakarta, city
Zanzibar City, city
Addis Ababa, city
Bangkok, city
Dubai, city
Helsinki, city
Machu Picchu, city
```

```
Nairobi, city
Rio de Janeiro, city
Samarkand, city
 Yangon, city
Yanchimedes' Principle, principle
Bernoulli's Principle, principle
 Boyle's Law,principle
Cell Theory,principle
Conservation of Energy,principle
 DNA Replication, principle
 Electromagnetism, principle
Entropy, principle
Entropy, principle
Evolution by Natural Selection, principle
Evolution, principle
General Relativity, principle
Germ Theory of Disease, principle
Gravity, principle
Hardy-Weinberg Principle, principle
Heliocentrism, principle
Hubble's Law, principle
Kepler's Laws of Planetary Motion, principle
Le Chatelier's Principle, principle
Mendel's Laws of Inheritance, principle
Newton's Laws of Motion, principle
Pauli Exclusion Principle, principle
Periodic Law, principle
 Periodic Law, principle
Photosynthesis, principle
 Plate Tectonics, principle
Principle of Least Action, principle
 Principle of Least Action, principle
Quantum Mechanics, principle
Relativity, principle
Superconductivity, principle
Thermodynamics, principle
Uncertainty Principle, principle
Avogadro's Law, principle
 Coulomb's Law, principle
Faraday's Laws of Electrolysis, principle
 Heisenberg Uncertainty Principle, principle Ohm's Law, principle
 Schrä¶dinger Equation, principle
Special Relativity, principle
 Aluminum, element
Barium, element
 Bismuth, element Bromine, element
 Calcium, element
Carbon, element
Chlorine, element
Chromium, element
 Copper, element Gold, element
 Helium . element
 Hydrogen, element
 Iodine, element
 Iron, element
 Lead, element
 Lithium, element
 Magnesium, element
Manganese, element
Mercury, element
Neon, element
Nitrogen, element
 Oxygen, element
Phosphorus, element
Plutonium, element
 Potassium, element
Radon, element
Silicon, element
Silver, element
Sodium, element
 Sulfur, element
Thorium, element
 Tin, element
Titanium, element
 Uranium, element
Zinc, element
 Argon, element
Boron, element
 Cobalt, element Fluorine, element
 Gallium, element Krypton, element
```

```
Nickel, element
 Xenon, element
 1984, bo
 Anna Karenina, book
Beloved, book
Brave New World, book
Catch-22, book
 Crime and Punishment, book
Don Quixote, book
Fahrenheit 451, book
 Frankenstein, b
Jane Eyre, book
Midnight's Children, book
Moby-Dick, book
One Flew Over the Cuckoo's Nest, book
 One Hundred Years of Solitude, book
 Pride and Prejudice, boo
 Slaughterhouse-Five, book
The Alchemist, bo
The Art of War, b
The Book Thief, b
The Brothers Karamazov, book
The Catcher in the Rye, book
The Chronicles of Narnia, book
The Color Purple, book
The Count of Monte Cristo, book
The Count of Monte Cristo, book
The Grapes of Wrath, book
The Handmaid's Tale, book
The Hitchhiker's Guide to the Galaxy, book
The Hobbit, book
The Hunger Games, book
 The Kite Runner,
The Little Prince, book
The Lord of the Rings, book
The Metamorphosis, book
The Name of the Rose, book
The Odyssey, book
The Picture of Dorian Gray, book
The Pillars of the Earth, book
The Stranger, book
The Sun Also Rises, bo
The Wind-Up Bird Chronicle, book
To Kill a Mockingbird, book
Ulysses, book
War and Peace, bo
War and Peace, book
Wuthering Heights, book
The Iliad, book
The Tale of Genji, book
Things Fall Apart, book
To the Lighthouse, book
American Gothic, painting
Christina's World, painting
Girl with a Pearl Earring, painting
Guernica, painting
Les Demoiselles d'Avignon, painting
Les Demoiselles d'Avignon, painting
Liberty Leading the People, painting
Mona Lisa, painting
School of Athens, painting
Starry Night, painting
The Absinthe Drinker, painting
The Anatomy Lesson of Dr. Nicolaes Tulp, painting
The Arnolfini Portrait, painting
The Astronomer, painting
The Birth of Venus, painting
 The Calling of Saint Matthew, painting
The Carling of Saint matthew, painting
The Card Players, painting
The Death of Marat, painting
The Fighting Temeraire, painting
The Garden of Earthly Delights, painting
The Gross Clinic, painting
The Hay Wain, painting The Kiss, painting
The Kiss, painting
The Last Supper, painting
The Nighthawks, painting
The Night Watch, painting
The Ninth Wave, painting
The Persistence of Memory, painting
The Potato Eaters, painting
The Raft of the Medusa, painting
The Scream, painting
The Sleeping Gypsy, painting
The Son of Man, painting
```

```
The Swing, painting
The Third of May 1808, painting
The Tower of Babel, painting
The Treachery of Images, painting
The Triumph of Galatea, painting
The Wanderer above the Sea of Fog, painting
Water Lilies, painting
The Creation of Adam, painting
The Girl with a Pearl Earling, painting
The Great Wave off Kanagawa, painting
The Thinker, painting
Venus de Milo, painting
Decimalisation in the UK, historical_event
Queen Elizabeth II's Platinum Jubilee, historical_event Queen Victoria's Coronation, historical_event
The Act of Union between England and Scotland, historical_event
The Battle of Adrianople, historical_event
The Battle of Adwa, historical_event
The Battle of Agincourt, historical_eve
The Battle of Hastings, historical_event
The Battle of Sekigahara, historical_event
The Battle of Teutoburg Forest, historical_event
The Battle of the Milvian Bridge, historical_event
The Battle of the milvian bridge, mistorical_event
The Battle of Waterloo, historical_event
The Brexit Referendum, historical_event
The Codification of Roman Law by Justinian, historical_event
The Construction of Hadrian's Wall, historical_event
The Construction of the Great Pyramid of Giza, historical_event
The Conversion of Constantine, historical_event
The Council of Chalcedon, historical_event
The Council of Chalcedon, historical_event
The Crisis of the Third Century, historical_event
The Defeat of the Spanish Armada, historical_event
The Discovery of the Americas by Columbus, historical_event
The Dissolution of the Soviet Union, historical_event
The Division of the Roman Empire, historical_event
The Dunkirk Evacuation, historical_event
The Edit of Caracalla historical_event
The Edict of Caracalla, historical_event
The Fall of Constantinople, historical_event
The Fall of the Aztec Empire, historical_event
The Fall of the Western Roman Empire, historical_event
The First Circumnavigation of the Earth, historical_event
The First Council of Nicaea, historical_event
The First Crusade, historical event
The Founding of Constantinople, historical_event
The Founding of Rome, historical_event
The Founding of the British Broadcasting Corporation, historical_event
The Founding of the League of Nations, historical_event
The French Revolution, historical_event
The Glorious Revolution, historical_event
The Gothic War in Italy, historical_event
The Great Fire of London, historical_event
The Indian Independence Act, historical_event
The Industrial Revolution, historical_event
The London 7/7 Bombings, historical_event
The Meiji Restoration, historical_event
The Plague of Justinian, historical_event
The Reforms of Diocletian, historical_even
       Reunification of the Empire by Aurelian, historical_event
The Sack of Rome by Alaric, historical_event
The Sack of Rome by the Vandals, historical_event
The Signing of the Good Friday Agreement, historical_event
The Signing of the Magna Carta, historical_event
The Signing of the Magna Carta, historical_event
The Treaty of Westphalia, historical_event
The UK Abolition of the Slave Trade Act, historical_event
The Unification of Italy, historical
The Wedding of Prince Charles and Lady Diana, historical_event
The Year of the Four Emperors, historical_event
The American Revolution, historical_event
The Black Death, historical_event
The Cuban Missile Crisis, historical_event
The Fall of the Berlin Wall, historical_event
The Moon Landing, historical_event
The Renaissance, historical_event
The Russian Revolution, historical_event
The Signing of the Declaration of Independence, historical_event
Angkor Wat, building
Buckingham Palace, building
Burj Khalifa, building
Chichen Itza, building
Chrysler Building, building
Colosseum, building
Eiffel Tower, building
```

```
Empire State Building, building
Forbidden City, building
Guggenheim Museum, building
Hagia Sophia, building
Lowre Pyramid, building
Machu Picchu, building
Neuschwantein Castle, building
Petronas Towers, building
Petronas Towers, building
Petronas Towers, building
Petronas Towers, building
Sars Tower, building
St. Basil's Cathedral, building
Sydney Opera House, building
Taj Mahal, building
Adagio for Strings, composition
Billie Jean, composition
Bohemian Hapsody, composition
Cannin Burnan, composition
Cannin Burnan, composition
Clair de Lune, composition
Clair de Lune, composition
Clair de Lune, composition
Clair de June, composition
Imagine, composition
Imagine, composition
Imagine, composition
Imagine, composition
In the Modd, composition
Like a Rolling Stone, composition
Like a Rolling Stone, composition
Resum Dorma, composition
Raga Malkaune, composition
Raga Malkaune, composition
Rhapsody on a Theme of Paganini, composition
Rhapsody on a Theme of Paganini, composition
The Blue Danube, composition
The Blue Danube, composition
The Flanets, composition
The Rate of Spring, composition
```

Listing 3: All objects which will be combined with the questions in Listing 1.

B Grounder Usage and Documentation

This appendix provides a brief overview of how to use the program to run the analyses in this thesis.

The entire approach is done in Python, and can be run from the single file knowledge_grounder.py. The code of the program is provided in Appendix C, and also separately in the main repository for this thesis, the dedicated code repository in https://github.com/mfixman/knowledge-grounder, and attached to the submission area.

The code should be run concurrently with the source data present in Appendix A and in the two repositories. The result, if run with the --output-dir option, is one CSV file per model with information about its knowledge grounding.

B.1 Code description and recommendations

The code downloads and uses large language models from the Huggingface dataset. Many of the models are large, so it might be useful to download them using the Huggingface CLI first as detailed in Appendix B.1.

```
$ huggingface-cli download --repo-type model 'meta-llama/Meta-Llama-3.1-70B'
```

B.2 Code usage

The code usage is explained well when running the program with the --help argument.

```
$ python knowledge_grounder.py --help
usage: knowledge_grounder.py [-h] [--debug] [--lim-questions LIM_QUESTIONS]
   [--device {cpu,cuda}] [--models model [model ...]] [--offline] [--rand]
                            [--max-batch-size MAX_BATCH_SIZE] [--per-model]
   [--output-dir OUTPUT_DIR] [--runs-per-question RUNS_PER_QUESTION]
               base_questions_file objects_file
 objects_file
                      File with objects to combine
                       show this help message and exit
  -h, --help
                       Go to IPDB console on exception rather than exiting.
  --debug
  --lim-questions LIM_QUESTIONS Question limit
  --device {cpu,cuda} Inference device
  --models model [model ...] Which model or models to use for getting parametric
   data
  --offline
                       Run offline: use model cache rather than downloading new
   models.
                       Seed randomly rather thn using the same seed for every
  --rand
   model.
  --max-batch-size MAX_BATCH_SIZE
                       Maximum size of batches.
  --per-model
                       Write one CSV per model in stdout.
  --output-dir OUTPUT_DIR
                       Return one CSV per model, and save them to this directory.
  --runs-per-question RUNS_PER_QUESTION
                       How many runs (with random counterfactuals) to do for
   each question.
```

B.3 Example usage

```
$ python knowledge_grounder.py \
    --device cuda \ # Use CUDA (it's possible to use CPU for small models)
    --models llama flan-t5-xl flan-t5-xxl \ # List of models to try
    --output-dir outputs/ \ # Write outputs to this directory
    --rand \ # Randomly seed after every model. This will cause answers to vary from other runs.
    -- \
    data/base_questions.txt # File with {}-format base questions.
    data/objects.csv # File with objects.
```

Listing 4: Example usage: run three models with random data.

```
$ python knowledge_grounder.py \
    --device cuda \ # Use CUDA (it's possible to use CPU for small models)
    --models llama-70b \ # This is a large model; let's run it separately.
    --max-batch-size 70 \ # Smaller batch size to ensure the program won't run
    out of VRAM.
    --output-dir outputs/ \ # Write outputs to this directory
    --offline \ # Run offline; this will fail if the model is not previously
    downloaded.
    -- \
    data/base_questions.txt # File with {}-format base questions.
    data/objects.csv # File with objects.
```

Listing 5: Example usage: run one of the models with 0 seed, to ensure repeteability

C Source Code of the Experiments

The latest version of the source code, including the input data generated in Section 3.1, is available in the mail repository for this thesis https://github.com/mfixman/rag-thesis and also in its dedicated repository https://github.com/mfixman/knowledge-grounder.

```
2 warnings.simplefilter(action = 'ignore', category = FutureWarning)
4 from argparse import ArgumentParser
5 import csv
6 import logging
7 import random
8 import ipdb
9 import os
10 import sys
11 import wandb
13 from Models import Model_dict
14 from QuestionAnswerer import QuestionAnswerer
15 from Utils import print_parametric_csv, LogTimeFilter, combine_questions
16
17 def parse_args():
       parser = ArgumentParser(
18
19
           description = 'Combines questions and data and optionally provides
       parametric data'
20
21
22
       parser.add_argument('--debug', action = 'store_true', help = 'Go to IPDB
       console on exception rather than exiting.')
23
       parser.add_argument('--lim-questions', type = int, help = 'Question limit')
       parser.add_argument('--device', choices = ['cpu', 'cuda'], default = 'cuda',
24
       help = 'Inference device')
       parser.add_argument('--models', type = str.lower, default = [], choices =
Model_dict.keys(), nargs = '+', metavar = 'model', help = 'Which model or
       models to use for getting parametric data')
26
       parser.add_argument('--offline', action = 'store_true', help = 'Run offline:
       use model cache rather than downloading new models.')
       parser.add_argument('--rand', action = 'store_true', help = 'Seed randomly
27
       rather thn using the same seed for every model.')
parser.add_argument('--max-batch-size', type = int, default = 120, help =
28
       Maximum size of batches. All batches contain exactly the same question.')
29
30
       parser.add_argument('--per-model', action = 'store_true', help = 'Write one
       CSV per model in stdout.')
31
       parser.add_argument('--output-dir', help = 'Return one CSV per model, and
       save them to this directory.')
32
33
       parser.add_argument('--runs-per-question', type = int, default = 1, help =
       .
How many runs (with random counterfactuals) to do for each question.')
34
35
       parser.add_argument('base_questions_file', type = open, help = 'File with
       questions')
       parser.add_argument('objects_file', type = open, help = 'File with objects to
36
       combine')
37
38
       args = parser.parse_args()
39
       args.base_questions = [x.strip() for x in args.base_questions_file if any(not
40
       y.isspace() for y in x)]
41
       args.objects = [{k: v for k, v in p.items()} for p in
```

```
csv.DictReader(args.objects_file)]
42
43
       del args.base_questions_file
44
       del args.objects_file
45
46
       if args.per_model and args.output_dir:
          raise ValueError('Only one of --per-model and --output-dir can be
47
       specified.')
48
49
       return args
50
51
  def main(args):
       logging.getLogger('transformers').setLevel(logging.ERROR)
52
53
       logging.basicConfig(
54
           format='[%(asctime)s] %(message)s',
55
           level=logging.INFO,
56
           datefmt = \frac{1}{3} \% Y - \% m - \% d \% H : \% M : \% S
57
58
       logging.getLogger().addFilter(LogTimeFilter())
59
60
       # We want to set this environment variable to ensure that Huggingface
61
       # does not download models.
62
       if args.offline:
           os.environ['TRANSFORMERS_OFFLINE'] = '1'
63
64
       else:
65
           wandb.init(project = 'knowledge-grounder', config = args)
66
67
       # Combining the base questions and objects into the final questions.
       logging.info('Getting questions')
68
69
       questions = combine_questions(args.base_questions, args.objects,
       args.lim_questions)
70
71
       # Create the output dir, if necessary.
72
       if args.output_dir:
73
           try:
74
               os.mkdir(args.output_dir)
           except FileExistsError:
75
76
               pass
77
       logging.info(f'About to answer {len(questions) * len(args.models) *
78
       args.runs_per_question * 2} questions in total.')
79
       answers = {}
80
       for model in args.models:
81
           # Let's use the same seed for all models.
82
           # This ensues that results are reproducible.
83
           if not args.rand:
84
               random.seed(0)
85
86
           # Create a QuestionAnswerer object to answer these queries.
87
           # These objects are large, so ensure it's deleted before loading the next
       one.
88
           qa = QuestionAnswerer(
               model,
89
90
               device = args.device,
91
               max_length = 20,
92
               max_batch_size = args.max_batch_size,
93
               runs_per_question = args.runs_per_question,
94
           )
95
           model_answers = qa.answerQueries(questions)
96
           del qa
97
98
           if args.output_dir:
```

```
count = lambda s: sum([x == s for x in model_answers['comparison']])
                logging.info(f"\t{count('Parametric')} parametrics,
100
        {count('Contextual')} contextual, {count('Other')} others")
101
102
                # Write the information to a corresponding file for each model.
103
                model_filename = os.path.join(args.output_dir, model + '.csv')
                with open(model_filename, 'w') as out:
104
105
                    print_parametric_csv(out, model_answers)
106
107
            elif args.per_model:
108
               print_parametric_csv(sys.stdout, model_answers)
109
            else:
110
                answers |= model_answers
111
112
        if answers:
            logging.info('Writing CSV')
113
114
            print_parametric_csv(sys.stdout, answers)
115
116 if __name__ == '__main__':
       args = parse_args()
117
118
119
        # If run with --debug, launch an IPDB console on exception.
       if not args.debug:
120
121
           main(args)
122
        else:
123
            with ipdb.launch_ipdb_on_exception():
124
                main(args)
```

Listing 6: knowledge_grounder.py is the main entry point and contains mostly argument parsing and output printing.

```
import warnings
  warnings.simplefilter(action = 'ignore', category = FutureWarning)
3
4 import logging
5
  import math
 6 import torch
7 import typing
9 from Models import Model
10 from typing import Optional, Union, Any
  from Utils import Question, sample_counterfactual_flips, chunk_questions
12
13 from collections import defaultdict
14 from transformers import BatchEncoding
15
16 import ipdb
17
18 FloatTensor = torch.Tensor
19 LongTensor = torch.Tensor
20 BoolTensor = torch.Tensor
21
22 # A QuestionAnswerer is the main class to answer queries with a given model.
23 # Example Usage:
24 #
      qa = QuestionAnswerer('llama', device = 'cuda', max_length = 20,
       max_batch_size = 75)
      output = qa.answerQueries(Utils.combine_questions(base_questions, objects))
26 # The list of models can be found in 'Model_dict' in 'Models.py'.
27 class QuestionAnswerer:
28
       device: str
29
       max_length: int
```

```
max_batch_size: int
31
      runs_per_question: int
32
      llm: Model
33
34
      def __init__(
35
           self,
           model: Union[str, Model],
36
37
           device: str = 'cpu',
38
           max_length: Optional[int] = None,
39
           max_batch_size: Optional[int] = None,
           runs_per_question: Optional[int] = None,
40
41
      ):
           self.device = device
42
43
           self.max_length = max_length or 20
           self.max_batch_size = max_batch_size or 120
44
           self.runs_per_question = runs_per_question or 1
45
46
47
           if type(model) == str:
               model = Model.fromName(model, device = device)
48
49
50
           model = typing.cast(Model, model)
51
           self.llm = model
52
53
           # Generated list of stop tokens: period, newline, and various different
      end tokens
           stop_tokens = \{'.', '\setminus n'\}
54
55
           self.stop_token_ids = torch.tensor([
56
57
               for k, v in self.llm.tokenizer.get_vocab().items()
58
                   k in ['<start_of_turn>', '<end_of_turn>',
59
      self.llm.tokenizer.special_tokens_map['eos_token']] or
60
                   not stop_tokens.isdisjoint(self.llm.tokenizer.decode(v))
61
           1).to(self.device)
62
       # Query data related to a list of questions, and return a dict with
63
      information about these runs.
64
      # Output elements:
65
      # parametric: Parametric answer, as a string.
66
         base_proba: Perplexity of parametric answer in base query.
67
          counterfactual: Randomly selected counterfactual answer.
      # base_cf_proba: Perplexity of counterfacutal answer in base query.
68
69
      # contextual: Contextual answer, as a string.
70
         ctx_proba: Perplexity of contextual answer.
         ctx_param_proba: Perplexity of parametric answer when running contextual
71
      query.
      # ctx_cf_proba: Perplexity of counterfactual answer when running contextual
      query.
       # comparison: Comparison between parametric and contextual answer. Where
73
      does this answer come from?
74
       # preference: Comparison between perplexity of paramertic and counterfactual
      answer on contextual query. Which one is the least surprising?
      def answerChunk(self, questions: list[Question]) -> dict[str, Any]:
75
76
           output: defaultdict[str, list[Any]] = defaultdict(lambda: [])
77
78
           # Get the tokens of the question and generate the parametric answer.
79
           base_tokens = self.tokenise([q.format(prompt = self.llm.prompt) for q in
      questions])
80
           parametric = self.generate(base_tokens)
81
82
           parametric_output = self.decode(parametric)
83
           base_proba_output = self.perplexity(base_tokens, parametric)
```

```
84
85
            # We possibly want several runs here, each with a different randomly
        sampled set of counterfactuals.
86
           for run in range(self.runs_per_question):
87
                run_output: dict[str, list[Any]] = dict(
88
                    parametric = parametric_output,
base_proba = base_proba_output,
89
90
91
                # Sample the counterfactuals and add them to the output.
92
93
                run_output['question'] = questions
94
                flips = sample_counterfactual_flips(questions,
       run_output['parametric'])
95
                counterfactual = parametric[flips]
96
                run_output['counterfactual'] = self.decode(counterfactual)
97
                run_output['base_cf_proba'] = self.perplexity(base_tokens,
98
       counterfactual)
99
                # Answer the counterfactuals, and union this dictionary to the output
100
       dictionary.
101
                run_output |= self.answerCounterfactuals(questions,
       run_output['counterfactual'], parametric, counterfactual)
102
103
                # We want to compare each contextual answer to their parametric and
        counterfactual.
104
                run_output['comparison'] = [
105
                     'Parametric' if self.streq(a, p) else
                    'Contextual' if self.streq(a, c) else
106
                    'Other'
107
108
                    for p, c, a in zip(run_output['parametric'],
       run_output['counterfactual'], run_output['contextual'])
109
110
                # We also want to figure out if P_2 < P_3.
111
                run_output['preference'] = [
112
                    'Parametric' if pp > cp else
113
114
                    'Contextual'
115
                    for pp, cp in zip(run_output['ctx_proba'],
       run_output['ctx_cf_proba'])
116
117
118
                for k, v in run_output.items():
119
                    output[k].extend(v)
120
121
            return output
122
123
       # Given a list of questions with assigned counterfactuals, run contextual
       queries and return
124
       # a dictionary containing information about these runs.
125
       # Parameter list:
126
        # questions: list of questions to ask.
127
       #
          counterfactuals: counterfactual answers, as string.
128
          parametric: parametric answer, as set of tokens.
129
            This will be used to calculate the perplexity of this answer with the
       counterfactual context.
130
          counterfactual: counterfacutal answers, as a set of tokens.
131
            This is necessary since the same string might have several encodings,
       but we need exactly the same one generated by the model
132
             in the first place.
133
       def answerCounterfactuals(self, questions: list[Question], counterfactuals:
       list[str], parametric: LongTensor, counterfactual: LongTensor) -> dict[str,
```

```
Anv]:
134
           output: dict[str, Any] = {}
135
            ctx_tokens = self.tokenise([
136
                q.format(prompt = self.llm.cf_prompt, context = context)
137
                for q, context in zip(questions, counterfactuals)
138
            1)
139
140
            contextual = self.generate(ctx_tokens)
141
            output['contextual'] = self.decode(contextual)
142
143
            output['ctx_proba'] = self.perplexity(ctx_tokens, contextual)
144
            output['ctx_param_proba'] = self.perplexity(ctx_tokens, parametric)
145
146
            output['ctx_cf_proba'] = self.perplexity(ctx_tokens, counterfactual)
147
            output['context_attn'], output['question_attn'] =
148
       self.avgSelfAttentions(ctx_tokens)
149
150
            return output
151
152
       # Answer a list of Questions: run the queries, gather counterfactual values,
       run the queries
153
       # with counterfactual context, and return a 'dict' with information to print.
154
       @torch.no_grad()
155
       def answerQueries(self, questions: list[Question]) -> dict[str, Any]:
156
           output: defaultdict[str, list[Any]] = defaultdict(lambda: [])
157
158
            chunks = chunk_questions(questions, max_batch_size = self.max_batch_size)
159
           logging.info(f'Answering {len(questions)} queries in {len(chunks)}
       chunks.')
160
161
            for e, chunk in enumerate(chunks, start = 1):
162
                logging.info(f'Parsing chunk ({e} / {len(chunks)}), which has size
       {len(chunk)}.', extra = {'rate_limit': 20})
163
                chunk_output = self.answerChunk(chunk)
164
165
166
                for k, v in chunk_output.items():
167
                    output[k] += v
168
169
            return dict(output)
170
171
       def fakeTokens(self) -> BatchEncoding:
172
           return self.tokenise(['[Context: Montevideo is located in Egypt] Q: What
       country is Montevideo located in? A: Montevideo is located in'])
173
174
       # Gets the scaled mean self-attentions of the context section of a query and
175
       # of the section after the context.
176
       @torch.no_grad()
       def avgSelfAttentions(self, queries: BatchEncoding) -> tuple[list[float],
177
       list[float]]:
178
            attentions = self.llm.attentions(queries)
            attention_mean = attentions.mean(dim = (1, 2))
179
            diag = attention_mean.diagonal(dim1 = 1, dim2 = 2)
180
           scaled = (diag - diag.min(dim = 1, keepdims = True)[0]) / (diag.max(dim =
181
       1, keepdims = True)[0] - diag.min(dim = 1, keepdims = True)[0])
182
183
           context_left = ((queries.input_ids == self.llm.tokenizer.pad_token_id) |
       (queries.input_ids == self.llm.tokenizer.eos_token_id))
184
            context_right = ((queries.input_ids ==
       self.llm.tokenizer.convert_tokens_to_ids(']')) | (queries.input_ids ==
       self.llm.tokenizer.convert_tokens_to_ids('].')))
```

```
185
186
            context_area = ~context_left & (context_right.cumsum(dim = 1) == 0)
187
            later_area = context_right.cumsum(dim = 1) > 0
188
189
            context = scaled.clone()
190
            context[~context_area] = torch.nan
191
192
            later = scaled.clone()
193
            later[~later_area] = torch.nan
194
195
            return context.nanmean(dim = 1).cpu().tolist(), later.nanmean(dim =
       1).cpu().tolist()
196
       # Tokenise a list of phrases.
197
198
       \# [n] \rightarrow (n, w)
       def tokenise(self, phrases: list[str]) -> BatchEncoding:
199
200
            return self.llm.tokenizer(
201
                phrases,
202
                return_tensors = 'pt',
                return_attention_mask = True,
203
204
                padding = True,
205
            ).to(self.device)
206
207
       # Generate an attention mask for a sequence of tokens.
208
        \# (n, w) -> (n, w)
209
       def batch_encode(self, tokens: LongTensor) -> BatchEncoding:
210
            attention_mask = tokens != self.llm.tokenizer.pad_token_id
211
            return BatchEncoding(dict(
212
                input_ids = tokens,
213
                attention_mask = attention_mask,
214
            ))
215
216
       # Use Greedy decoding to generate an answer to a certain query.
217
       \# (n, w) -> (n, w)
218
       def generate(self, query: BatchEncoding) -> LongTensor:
219
            generated = self.llm.model.generate(
220
                input_ids = query.input_ids,
221
                attention_mask = query.attention_mask,
                max_new_tokens = self.max_length,
222
223
                min_new_tokens = self.max_length,
224
                tokenizer = self.llm.tokenizer,
                do_sample = False,
225
226
                temperature = None,
227
                top_p = None,
                return_dict_in_generate = True,
228
229
                pad_token_id = self.llm.tokenizer.pad_token_id,
230
                eos_token_id = self.llm.tokenizer.eos_token_id,
231
                bos_token_id = self.llm.tokenizer.bos_token_id,
232
            )
233
234
            # Ensure that all the sequences only contain <PAD> after their first stop
       token.
235
            sequences = generated.sequences[:, -self.max_length:]
236
            ignores = torch.cumsum(torch.isin(sequences, self.stop_token_ids), dim =
237
            sequences[ignores] = self.llm.tokenizer.pad_token_id
238
239
            return sequences
240
241
       # Return the perplexity of a certain sequence of tokens being the answer to a
       \mbox{\tt\#} certain query, as a list of floats in CPU.
242
243
       \# (n, w0), (n, w1) -> (n)
```

```
244
        def perplexity(self, query: BatchEncoding, answer: LongTensor) -> list[float]:
245
            probs = self.batch_perplexity(query, self.batch_encode(answer))
246
            return probs.cpu().tolist()
247
248
        # Return the perplexity of a certain sequence of tokens being the answer to a
249
        # certain query.
250
        \# (n, w0), (n, w1) -> (n)
251
        @torch.no_grad()
252
        def batch_perplexity(self, query: BatchEncoding, answer: BatchEncoding) ->
        FloatTensor:
253
            entropies = self.llm.logits(query, answer).log_softmax(dim = 2)
254
            entropies /= math.log(2)
255
            probs = torch.where(
256
                answer.input_ids == self.llm.tokenizer.pad_token_id,
257
                 torch.nan,
258
                 entropies.gather(index = answer.input_ids.unsqueeze(2), dim =
        2).squeeze(2),
259
260
261
            return torch.pow(2, -torch.nanmean(probs, dim = 1))
262
263
        # Decode a sequence of tokens into a list of strings.
264
        \# (n, w) -> [n]
265
        def decode(self, tokens: LongTensor) -> list[str]:
266
            decoded = self.llm.tokenizer.batch_decode(
267
                tokens,
268
                 skip_special_tokens = True,
269
                 clean_up_tokenization_spaces = True,
270
271
            return [x.strip() for x in decoded]
272
273
        # Compare strings for equality to later check whether an answer is parametric
        or contextual.
274
        # For simplicity, we remove stop words and gather only the subset of words.
275
        {\tt @staticmethod}
276
        def streq(a: str, b: str) -> bool:
            a = a.lower().replace('the', '').replace(',', '').strip()
b = b.lower().replace('the', '').replace(',', '').strip()
277
278
            return a[:len(b)] == b[:len(a)]
```

Listing 7: QuestionAnswerer.py contains the QuestionAnswerer class which deals with the logic of answering parametric and counterfactual questions from a model

```
1 import logging
3 from transformers import AutoTokenizer, AutoModelForCausalLM,
       {\tt AutoModelForSeq2SeqLM}\;,\;\; {\tt BatchEncoding}
4 from torch import nn, tensor
  from torch import FloatTensor, Tensor
5
6 import torch
8 # Dictionary of models, containing all of the models aliases and their respective
      models.
9 Model_dict = {
10
       'llama': 'meta-llama/Meta-Llama-3.1-8B-Instruct',
       'llama-70b': 'meta-llama/Meta-Llama-3.1-70B-Instruct',
11
12
       'llama-405b': 'meta-llama/Meta-Llama-3.1-405B-Instruct',
13
       'flan-t5': 'google/flan-t5-base',
       'flan-t5-small': 'google/flan-t5-small',
14
       'flan-t5-base': 'google/flan-t5-base',
15
16
       'flan-t5-large': 'google/flan-t5-large',
```

```
'flan-t5-xl': 'google/flan-t5-xl',
       'flan-t5-xxl': 'google/flan-t5-xxl',
18
19
       'gemma': 'google/gemma-2-9b-it',
       'gemma-27b': 'google/gemma-2-27b-it',
20
       'falcon2': 'tiiuae/falcon-11b',
21
22
       'falcon-180b': 'tiiuae/falcon-180b-chat',
       'falcon-40b': 'tiiuae/falcon-40b-instruct',
23
       'falcon-7b': 'tiiuae/falcon-7b-instruct',
24
25
       'distilbert': 'distilbert/distilbert-base-uncased-distilled-squad',
       'roberta': 'FacebookAI/roberta-base',
26
27
       'roberta-large': 'FacebookAI/roberta-large',
28
       'roberta-squad': 'deepset/roberta-base-squad2',
29
       'mixtral': 'mistralai/Mixtral-8x22B-Instruct-v0.1',
30
       'dummy': '',
31 }
32
33 # Virtual class containing a model.
34 # Derived classes should reimplement \_init\_ and logits, and attention.
35 # They should also save their tokeniser and HF model.
36 class Model(nn.Module):
37
      name: str
38
      model_name: str
39
      device: str
40
41
      tokenizer: AutoTokenizer
      model: AutoModelForCausalLM
42
43
44
      # Construct a model from a certain name.
      # This should be the main constructor of models.
45
46
      @staticmethod
      def fromName(name: str, device: str = 'cpu') -> 'Model':
47
           if name == 'dummy':
48
49
               return DummyModel()
50
           if name in ('llama-70b', 'gemma-27b'):
51
52
               return LargeDecoderOnlyModel(name, device)
53
54
           if 't5' in name:
55
               return Seq2SeqModel(name, device)
56
57
           return DecoderOnlyModel(name, device)
58
59
      def __init__(self, name: str, device: str = 'cuda'):
60
           super().__init__()
61
           self.name = name
62
           self.model_name = Model_dict[name]
           self.device = device
63
64
65
       @torch.no_grad()
66
      def logits(self, query: BatchEncoding, answer: BatchEncoding) -> FloatTensor:
67
           raise NotImplementedError('logits called from generic Model class')
68
69
      @torch.no_grad()
70
       def attentions(self, query: BatchEncoding) -> FloatTensor:
           raise NotImplementedError('attentions called from generic Model class')
71
72
73
  # Decoder-only model, such as llama, use AutoModelForCausalLM.
74 class DecoderOnlyModel(Model):
75
      def __init__(self, name: str, device: str = 'cuda'):
76
           super().__init__(name, device)
77
78
          self.prompt = ''
```

```
self.cf_prompt = ''
80
81
82
            # Some models require special configuration.
            if 'llama' in name:
83
84
                kwargs = dict(
                    pad_token = '<|reserved_special_token_0|>',
85
86
                    padding_side = 'left',
87
            elif 'gemma' in name:
88
89
                kwargs = dict(
90
                   padding_side = 'right',
91
92
            self.tokenizer = AutoTokenizer.from_pretrained(
93
94
                self.model_name,
95
                clean_up_tokenization_spaces = True,
96
                **kwargs,
97
            )
98
99
            logging.info(f'Loading model for {self.model_name} using
       {torch.cuda.device_count()} GPUs.')
100
            self.model = AutoModelForCausalLM.from_pretrained(
101
                self.model_name,
102
                device_map = 'auto' if self.device == 'cuda' else self.device,
                torch_dtype = torch.bfloat16,
103
104
                pad_token_id = self.tokenizer.pad_token_id,
105
                bos_token_id = self.tokenizer.bos_token_id,
                eos_token_id = self.tokenizer.eos_token_id,
106
107
                low_cpu_mem_usage = True,
108
109
            self.model.eval()
110
       # Decoder-only generation with teacher forcing: calculate the next token
111
       given the previous forced tokens.
112
        @torch.no_grad()
113
       def logits(self, query: BatchEncoding, answer: BatchEncoding) -> FloatTensor:
114
            w0 = query.input_ids.shape[1]
            w1 = answer.input_ids.shape[1]
115
116
117
            input_ids = torch.cat([query.input_ids, answer.input_ids], dim = 1)
           attention_mask = torch.cat([query.attention_mask, answer.attention_mask],
118
       dim = 1)
119
120
           return self.model(input_ids, attention_mask = attention_mask).logits[:,
       w0 - 1 : w0 + w1 - 1
121
122
       @torch.no_grad()
123
       def attentions(self, queries: BatchEncoding) -> FloatTensor:
124
            outputs = self.model(**queries, output_attentions = True).attentions
125
            return torch.stack(outputs, dim = 1)
126
127 # Seq2Seq model, such as Flan-T5.
128 class Seq2SeqModel(Model):
129
       def __init__(self, name: str, device: str = 'cpu'):
130
            super().__init__(name, device)
131
            self.prompt = ''
132
133
            self.cf_prompt = ''
134
            kwargs = dict(
135
136
               padding_side = 'right',
```

```
137
138
            self.tokenizer = AutoTokenizer.from_pretrained(
139
                self.model_name,
140
                clean_up_tokenization_spaces = True,
141
                **kwargs,
142
143
144
            logging.info(f'Loading Seq2Seq model for {self.model_name} using
        {torch.cuda.device_count()} GPUs.')
145
            self.model = AutoModelForSeq2SeqLM.from_pretrained(
146
                self.model_name,
147
                device_map = 'auto' if self.device == 'cuda' else self.device,
                torch_dtype = torch.bfloat16,
148
149
                pad_token_id = self.tokenizer.pad_token_id,
150
                bos_token_id = self.tokenizer.bos_token_id,
                eos_token_id = self.tokenizer.eos_token_id,
151
152
                low_cpu_mem_usage = True,
153
154
            self.model.eval()
155
156
       @staticmethod
157
        def pad(tensor: Tensor, length: int, value) -> Tensor:
            right = torch.full((tensor.shape[0], length - tensor.shape[1]), value)
158
159
            return torch.cat([tensor, right.to(tensor.device)], dim = 1)
160
161
       @torch.no_grad()
162
       def logits(self, query: BatchEncoding, answer: BatchEncoding) -> FloatTensor:
163
            length = max(query.input_ids.shape[1]), answer.input_ids.shape[1])
164
165
            input_ids = self.pad(query.input_ids, length, self.tokenizer.pad_token_id)
166
            attention_mask = self.pad(query.attention_mask, length, 0)
167
            decoder_input_ids = self.pad(self.model._shift_right(answer.input_ids),
       length, self.tokenizer.pad_token_id)
168
169
            return self.model(
170
                input_ids = input_ids,
                attention_mask = attention_mask,
171
172
                decoder_input_ids = decoder_input_ids,
173
            ).logits[:, : answer.input_ids.shape[1]]
174
175
        @torch.no_grad()
       def attentions(self, queries: BatchEncoding) -> FloatTensor:
176
177
            outputs = self.model(
178
                **queries,
                output_attentions = True,
179
180
                decoder_input_ids = torch.full_like(queries.input_ids,
       self.tokenizer.pad_token_id).to(self.device),
181
            ).decoder_attentions
182
            return torch.stack(outputs, dim = 1)
183
184 # Large decoder-only model.
185 # Similar to DecoderOnlyModel, but eagerly deletes the model when the class is
       deleted.
186 # Assumes you need 2 GPUs to run this.
187
   class LargeDecoderOnlyModel(DecoderOnlyModel):
188
       def __init__(self, name, device: str = 'cuda'):
189
            if torch.cuda.device_count() < 2:</pre>
190
                raise ValueError(f'At least two GPUs are needed to run {name}')
191
192
            super().__init__(name, device)
193
194
       def __del__(self):
```

```
logging.info(f'Deleting large model {self.name}')
196
            del self.model
197
            torch.cuda.empty_cache()
198
199 # Dummy model, used for testing.
200 class DummyModel(Model):
201
        def __init__(self):
202
            nn.Module.__init__(self)
203
            self.name = 'dummy
204
            self.tokenizer = self
205
            self.model = self
206
            self.sequences = ['dummy']
207
            self.logits = tensor([[[1., 2., 3.]]])
208
209
            self.bos_token_id = 0
210
            self.eos_token_id = 1
211
            self.pad_token_id = 2
212
213
        def to(self, *args, **kwargs):
214
            return self
215
216
        def __call__(self, *args, **kwargs):
217
            return self
218
219
        def generate(self, *args, **kwargs):
220
            return self
221
        def __getitem__(self, key):
222
223
            return self
224
225
        def decode(self, *args, **kwargs):
            return 'Dummy text'
226
227
        def batch_decode(self, *args, **kwargs):
    return ['Dummy Text 1', 'Dummy Text 2']
228
229
230
231
        def shape(self):
232
            return (1, 2, 3)
233
234 # If called separately, just print the names of the models.
235 def main():
236
        print(f'{"Model Name":>15} | {"Huggingface Model":<40}')</pre>
        print((15 + 1) * '-' + '|' + (40 + 1) * '-')
237
        for name, model in Model_dict.items():
238
239
            print(f'{name:>15} | {model:<40}')</pre>
240
241 if __name__ == '__main__':
242
        main()
```

Listing 8: Models.py contains the list of models and includes code that differentiates them.

```
import csv
import logging
import itertools
import random
import time
import typing

from collections import defaultdict
from dataclasses import dataclass
from typing import Optional, Any
```

```
11
12 # Custom filter that does not print a log if it printed another one at most 'rate_limit' seconds ago.
13 class LogTimeFilter(logging.Filter):
14
       def __init__(self):
15
           super().__init__()
           self.last_log = defaultdict(lambda: 0)
16
17
18
       def filter(self, record):
19
           if not hasattr(record, 'rate_limit'):
20
               return True
21
           current_time = time.time()
22
23
           if current_time - self.last_log[record.lineno] >= record.rate_limit:
24
               self.last_log[record.lineno] = current_time
25
               return True
26
27
           return False
28
29 # A question contains combines a base_question and an object into something that
       can be queried.
30 @dataclass
31 class Question:
32
       category: str
33
       obj: str
34
       base_question: str
35
36
       # Static constructor: return a question combining an object and an object if
       the category
37
       # matches; return None otherwise.
38
       @staticmethod
39
       def orNothing(obj: str, category: str, base_question: str) ->
       Optional['Question']:
40
           if not f'{{{category}}}' in base_question:
41
               return None
42
43
           return Question(obj = obj, category = category, base_question =
       base_question)
44
45
       \mbox{\tt\#} Return a query from the format of this Question.
46
       def format(self, *, prompt: Optional[str] = None, context: Optional[str] =
       None, use_question: bool = True, use_later: bool = True) -> str:
47
           [question, later] = self.base_question.format_map({self.category:
       self.obj}).split('?', 1)
           question += '?'
48
49
50
           formatted = ''
51
           if use_question:
52
               formatted = f'Q: {question.strip()}'
53
54
           if use_later:
55
               formatted = f'{formatted} A: {later.strip()}'
56
57
           if prompt is not None:
               formatted = f'{prompt} {formatted}'
58
59
60
           if context is not None:
61
               formatted = f'Context: [{later.strip()} {context}]. {formatted}'
62
63
           return formatted.strip()
64
65 # Returns the set product of a list of base question with the respective set of
```

```
objects.
66 def combine_questions(base_questions: list[str], objects: list[dict[str, str]],
        lim_questions: Optional[int] = None) -> list[Question]:
67
       questions = []
       for bq in base_questions:
68
69
            for obj in objects:
               q = Question.orNothing(obj = obj['object'], category =
70
       obj['category'], base_question = bq)
71
                if q is None:
                    continue
72
73
74
                questions.append(q)
75
76
       if lim_questions is None:
77
            return questions
78
79
       keep_nums = {x: e for e, x in enumerate(random.sample(range(len(questions)),
       lim_questions))}
80
        short_questions = [questions[x] for x in keep_nums.keys()]
81
82
       return short_questions
83
84 # Given a list of questions and a list of answers, produce a list of integers
       that would provide the
   # index to a randomly sampled counterfactual.
86 def sample_counterfactual_flips(questions: list[Question], answers: list[str]) ->
       list[int]:
87
       flips = [-1 for _ in questions]
88
89
       for q, es_iter in itertools.groupby(range(len(questions)), key = lambda e:
       questions[e].base_question):
90
           es = set(es_iter)
91
92
            for e in es:
                rest = [x for x in es if answers[x] != answers[e]]
93
94
                if not rest:
                    logging.error(f'Unitary question "\{q\}". This means that all
95
        answers in this chunk are identical, and the results will be incorrect.')
96
                    flips[e] = e
97
                    continue
98
                flips[e] = random.choice(rest)
99
100
                assert answers[flips[e]] != answers[e]
101
        assert all(x != -1 for x in flips)
102
103
       return flips
104
105 # Chunk a list of question into batches of size or at most 'max_batch_size'.
106 def chunk_questions(questions: list[Question], max_batch_size: int) ->
       list[list[Question]]:
107
       result: list[list[Question]] = []
108
       for q, chunk_iter in itertools.groupby(questions, key = lambda x:
109
       x.base_question):
110
           chunk = list(chunk_iter)
            if not result or len(chunk) + len(result[-1]) > max_batch_size:
111
112
                result.append([])
113
114
            result[-1].extend(chunk)
115
116
       return result
117
```

```
118 # Prints a CSV file with the questions and resulting answers.
119 def print_parametric_csv(out: typing.TextIO, answer: dict[str, list[Any]]):
120
        fieldnames = ['Num', 'Category', 'Base_Question', 'Object', 'Question',
        'Prefix'] + list(answer.keys())
121
122
        writer = csv.DictWriter(
123
            out.
124
            fieldnames = fieldnames,
125
            extrasaction = 'ignore',
126
            dialect = csv.unix_dialect,
127
            quoting = csv.QUOTE_MINIMAL,
128
129
       writer.writeheader()
130
131
       for e, answers in enumerate(zip(*answer.values())):
132
            param = dict(zip(answer.keys(), answers))
133
134
            question = param['question']
            param.pop('question')
135
136
137
            writer.writerow(
138
139
                    'Num': str(e),
140
                    'Category': question.category,
141
                    'Base_Question':
        ''.join(question.base_question.partition('?')[0:2]),
142
                    'Object': question.obj,
143
                     'Question': question.format(use_later = False),
144
                    'Prefix': question.format(use_question = False)
                } | param
145
146
            )
```

Listing 9: Utils.py contains various useful functions

```
1 import unittest
  from unittest import TestCase
3 from unittest.mock import MagicMock
5
  import torch
6 from torch import tensor
  from QuestionAnswerer import QuestionAnswerer
10 \mid pad = 128002
11
  class QuestionAnswererTests(unittest.TestCase):
12
       def setUp(self):
13
           self.qa = QuestionAnswerer('dummy', 'cpu', None)
14
           # self.qa.llm.tokenizer = MagicMock()
15
           self.qa.llm.tokenizer.pad_token_id = pad
16
           self.qa.llm.tokenizer.batch_decode = MagicMock(
              return_value = ['Hello how are you', 'Newline here', 'No stop
17
      string', '']
18
          )
19
20
       def test_winner(self):
           logits = tensor([
21
22
               [[0.0900, 0.2447, 0.6652], [0.6652, 0.2447, 0.0900], [0.2447, 0.6652,
      0.0900]],
23
               [[0.2119, 0.2119, 0.5761], [0.2119, 0.2119, 0.5761], [0.2119, 0.2119,
      0.5761]],
               [[0.6652, 0.2447, 0.0900], [0.2119, 0.5761, 0.2119], [0.5761, 0.2119]
24
```

```
0.2119]],
25
           1)
26
27
            expected_path = tensor([[2, 0, 1], [2, 2, 2], [0, 1, 0]])
28
            expected_probs = tensor([
                [0.6652, 0.6652, 0.6652],
[0.5761, 0.5761, 0.5761],
29
30
31
                [0.6652, 0.5761, 0.5761],
32
33
34
           path, probs = self.qa.winner(logits)
35
            self.assertTrue(torch.equal(path, expected_path), msg = (path,
       expected_path))
36
           self.assertTrue(torch.allclose(probs, expected_probs), msg = (probs,
       expected_probs))
37
38
       def test_decode(self):
39
           path = tensor([
                [128000, 9906, 1268, 527, 499,
                                                        13, 358, 1097, 3815, 7060, 9901,
40
                13],
                                                                     13, 1234, 1234, 1234,
41
                [128000, 3648, 1074, 1618, 198, 54953,
                                                                0,
       1234, 1234],
                [128000, 2822, 3009, 925, 1234, 1234, 1234, 1234, 1234, 1234, 1234,
42
       1234, 1234],
43
                [128000,
                            13, 1234, 1234, 1234, 1234, 1234, 1234, 1234, 1234, 1234,
       1234, 1234],
44
           ])
45
           probs = tensor([
                [1., 3., 5., 7., 9., 11., 13., 15., 17., 19., 21., 23., 25.],
46
47
                [1., 3., 5., 7., 9., 11., 13., 15., 17., 19., 21., 23., 25.],
                [1., 3., 5., 7., 9., 11., 13., 15., 17., 19., 21., 23., 25.], [1., 3., 5., 7., 9., 11., 13., 15., 17., 19., 21., 23., 25.],
48
49
50
           1)
51
52
            expected_result = [
53
                'Hello how are you',
54
                'Newline here',
55
                'No stop string',
56
57
           1
58
            expected_mean_probs = [5., 4., 13., 1.]
59
60
            result, mean_probs = self.qa.decode(path, probs)
61
            self.assertListEqual(expected_result, result)
62
            self.assertListEqual(expected_mean_probs, mean_probs)
```

Listing 10: test_QuestionAnswerer.py is used to test some of the complicated bits of logic in QuestionAnswerer.