

A Glitch in the Matrix? Locating and Detecting Language Model Grounding with Fakepedia

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Abstract

Large language models (LLMs) have demonstrated impressive capabilities in storing and recalling factual knowledge, but also in adapting to novel in-context information. Yet, the mechanisms underlying their in-context grounding remain unknown, especially in situations where in-context information contradicts factual knowledge embedded in the parameters. This is critical for retrieval-augmented generation methods, which enrich the context with up-to-date information, hoping that grounding can rectify the outdated parametric knowledge. In this study, we introduce Fakepedia, a counterfactual dataset designed to evaluate grounding abilities when the parametric knowledge clashes with the in-context information. We benchmark various LLMs with Fakepedia and discover that GPT-4-turbo has a strong preference for its parametric knowledge. Mistral-7B, on the contrary, is the model that most robustly chooses the grounded answer. Then, we conduct causal mediation analysis on LLM components when answering Fakepedia queries. We demonstrate that inspection of the computational graph alone can predict LLM grounding with 92.8% accuracy, especially because few MLPs in the Transformer can predict non-grounded behavior. Our results, together with existing findings about factual recall mechanisms, provide a coherent narrative of how grounding and factual recall mechanisms interact within LLMs.

1 Introduction

One of the key factor underlying the massive success of large language models (LLMs) is their ability to encode and effectively recall a wealth of factual knowledge embedded in their parameters (Heinzerling and Inui, 2021; AlKhamissi et al., 2022; Meng et al., 2023a). Then, what elevates LLMs beyond promptable static repositories of knowledge is their capacity to adapt to new information and instructions provided in the context

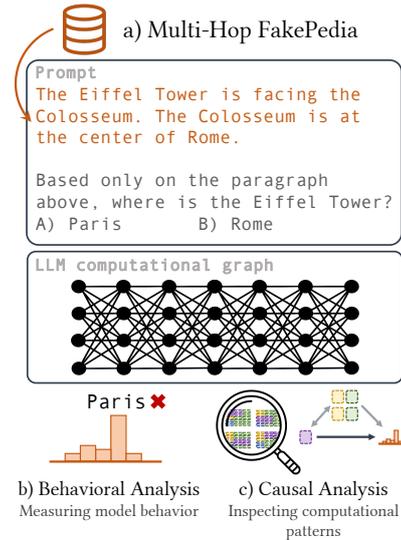


Figure 1: **Studying Grounding in LLMs.** This work makes three distinct contributions: (a) introducing counterfactual datasets designed to measure the abilities of LLMs to ground their answer in the new information provided in the prompt, (b) conducting a descriptive analysis of grounding performances across several LLMs, and (c) implementing an improved causal mediation analysis that we use to show that computational patterns inside LLMs can predict whether the answer is grounded with 92.8% accuracy.

(Brown et al., 2020). Ideally, the LLM should integrate information from the context with the static parametric knowledge to provide responses that robustly align with the intention communicated by the user in the prompt.

However, the in-context information can often contradict the internal parametric knowledge (Yu et al., 2023). Since the internal knowledge reflects only a partial snapshot of the state of the world at training time, enriching the context with up-to-date factual information is one of the most promising directions to keep the model relevant in a changing world (Hu et al., 2023; Yao et al., 2022). This is the main idea behind retrieval-augmented generation (RAG) (Lewis et al., 2020; Borgeaud et al., 2022;

Mialon et al., 2023). However, this sets the model in a state of tension between factual recall and in-context grounding; then, the success of such prompting methods hinges on the model’s ability to accurately decide when to ignore its parametric knowledge. Unfortunately, Yu et al. (2023) argued recently that LLMs often prefer their parametric knowledge, especially larger ones.

Motivated by these observations, our work aims to study the mechanisms involved in grounding and factual recall for scenarios of practical importance: when there is a conflict between the two. We hypothesize that different modes of information processing are triggered when the LLM engages in factual recall compared to when it engages in grounding.

Previous works studying LLM behavior typically craft experimental scenarios that isolate the behavior of interest. For instance, to test factual recall abilities, an LLM could be prompted to continue the sentence: `The Eiffel Tower is located in the city of . Answering Paris` suggests that the model *knows* and can recall the true fact. Yet, such behavioral analyses alone cannot reveal the underlying mechanisms that drive the observed behavior (Jain and Wallace, 2019; Bolukbasi et al., 2021). Deeper understanding requires opening the black box and examining the low-level computational patterns that give rise to the high-level behavior. While early studies have identified *computational correlates* between low-level activations and model outputs (Peyrard et al., 2021; Oba et al., 2021; Dai et al., 2022), there has been growing consensus that generalizable mechanistic explanations should stem from causal analysis rooted in interventionist experimental setups (Woodward, 2003; Potochnik, 2017; Pearl and Mackenzie, 2018; Geiger et al., 2022a, 2023). Building on these insights, several studies have developed rigorous methods to intervene on model components, setting the model in counterfactual states and systematically measuring the impact of these interventions on the model’s behavior (Geiger et al., 2022b; Wu et al., 2023b; Meng et al., 2023a; Geva et al., 2023). These experimental setups have allowed researchers to form a clear picture of the factual recall mechanisms (Geva et al., 2021; Wallat et al., 2020; Meng et al., 2023a; Kobayashi et al., 2023; Geva et al., 2023). Unfortunately, the complementary mode of grounding has received much less scrutiny.

In this work, we propose a thorough analysis of the grounding mode of computation of several LLMs, and make four important contributions:

- New counterfactual datasets, called **Fakepedia**, crafted especially to isolate the grounding behavior from factual recall by setting LLMs in tension between the two modes (Sec. 4).
- A descriptive behavioral analysis of several LLMs measuring their grounding abilities in the challenging task proposed by Fakepedia (Sec. 5).
- A new causal mediation analysis, called **MGCT**, that assesses the effect of subsets of the model states on the model’s behavior (Sec. 6.1).
- A set of findings coming from applying MGCT to LLaMA-7B and GPT2-XL on Fakepedia (Sec. 6.2). Specifically, we show that (i) contrary to factual recall, grounding is a distributed process, (ii) the activity of few MLPs differs significantly between grounded vs. ungrounded modes, and (iii) we can predict whether the model is engaged in grounding behavior by looking only at the computational graph with an accuracy of 92.8% (Sec. 7).

To support further research in the space of grounding and in-context learning, we release our Fakepedia datasets and the code pipeline to reproduce or extend them. We also release a user-friendly implementation of MGCT that researchers can employ to study the computational patterns of LLMs when engaged in any other behavior of interest. Code and data will be available at: <https://github.com/epfl-dlab/llm-grounding-analysis>.

2 Related Work

Understanding the inner workings of LLMs poses a significant challenge, given their complex architectures (Carvalho et al., 2019; Rogers et al., 2020; Geiger et al., 2023). To better analyze models, researchers often craft controlled datasets that isolate the target behavior. Behavioral experiments are then supplemented by a deeper inspection of the underlying low-level computational patterns that explain the observed behavior. This section gives a brief overview of previous works relevant to our project.

2.1 Mechanistic Interpretability

Discovering the low-level mechanisms that give rise to high-level behaviors has become an important goal for research in AI interpretability. Understanding these mechanisms allows us to better predict out-of-distribution behavior (Mu and Andreas, 2020; Geiger et al., 2022b; Wu et al., 2023b), identify and fix errors (Vig et al., 2020). For instance, Dai et al. (2022) analyzed BERT activations revealing that some neurons are positively correlated with specific facts. Similarly, Oba et al. (2021) demonstrated associations between neuron activations and specific phrases in model output. Additionally, in a matched study on humor detection, Peyrard et al. (2021) identified attention heads in BERT encoding the funniness of sentences.

To go beyond statistical correlates, a promising approach emerged by viewing the Transformer’s computational graph as a causal graph (Elhage et al., 2021; Meng et al., 2023a; Geiger et al., 2023; Wu et al., 2023a). Then, targeted interventions on the computation process are applied to estimate the impact of individual components on model behavior (Modarressi et al., 2022; Mohebbi et al., 2023; Wang et al., 2022; Nanda et al., 2023; Merullo et al., 2023; Belrose et al., 2023; Meng et al., 2023a; Vig et al., 2020). In particular, causal mediation analysis applied to components of GPT2 has revealed that some MLPs are key-value storage of factual knowledge (Geva et al., 2021; Wallat et al., 2020; Meng et al., 2023a; Kobayashi et al., 2023). Then, several works have been able to even edit factual knowledge directly in the weights of pre-trained Transformers (Meng et al., 2023b; Mitchell et al., 2022; De Cao et al., 2021). With a similar interventionist setup, Geva et al. (2023) studied information flow during factual knowledge recall, finding critical aggregation points, especially located in a few attention heads. Interestingly, Haviv et al. (2023) demonstrated the critical role of MLPs in early layers when the model is performing memorization.

While recalling factual knowledge relates to memorization, our project studies the ability of models to ground their answers based on information in the context, i.e., to generalize to new information. In particular, we craft scenarios that set the LLMs in tension between the mode of factual recall and the mode of grounding. This contributes to the broader discussion on generalization versus memorization (Razeghi et al., 2022; Kandpal et al., 2023; Hupkes et al., 2023; Haviv et al., 2023). However,

grounding remains much less studied than factual recall. In a contemporary study, Yu et al. (2023) also inspect the problem of grounding using mechanistic interpretability methods. Their analysis focuses on the role of attention heads when forcing the model to ground its answer in the prompt. Our findings nicely complement theirs. When combined with existing findings about factual knowledge and information flow during recall our results begin to portray a coherent narrative that we detail in Sec. 8.

2.2 Counterfactual Datasets

The necessity for counterfactual datasets is becoming increasingly evident in contemporary research. These datasets serve to isolate the target behavior of interest.

However, producing counterfactual datasets is not straightforward. Works, like those by Nee-man et al. (2022) and Zhou et al. (2023), adopt the methodology proposed by Longpre et al. (2022), which involves substituting entities within existing paragraphs. Li et al. (2022) proposes a similar method also based on entity substitution. Another approach involves generating new documents altogether; Köksal et al. (2023) for instance, builds on the idea that a model tasked with producing a document about a fact may inadvertently generate a counterfactual paragraph.

Concurrently, language models have shown remarkable proficiency in synthetic dataset generation (Gunasekar et al., 2023; Schick and Schütze, 2021; Josifoski et al., 2023; Eldan and Li, 2023; Lingo, 2023). Building on these advancements, our research demonstrates that it is feasible to employ language models for generating novel, original, and high-quality counterfactual paragraphs from scratch.

3 Background

3.1 Terminology

We view *facts* as triplets made of a subject, a relation, and an object. A fact is said to be *true* if it aligns with our observed world. For example, {Eiffel Tower | is located in | Paris} is a *true* fact. In our experiments, we focus on true facts that the models know **and** can recall. By contrast, a *counterfactual* triplet is any triplet that does not form a true fact.

In our experiments, we test models by asking them to produce the object of a triplet, either di-

rectly as its next token or via a multiple-choice questionnaire (MCQ). This facilitates a systematic inspection of the model’s answers by comparing them with the target object. It follows previous related work (Yu et al., 2023; Meng et al., 2023a).

3.2 Grounded vs. Factual

It is crucial to differentiate between a *factual* answer and a *grounded* answer. A factual answer is the object of a true fact triplet, while a grounded answer is the object triplet logically consistent with the information in the context of the prompt. Factuality pertains to the model’s encoded knowledge and its ability to retrieve it, whereas *grounding* involves the model’s capacity to adapt to its context and reason about new information.

While factual recall has been extensively studied in previous work, this work aims to study grounding. However, grounding and factual recall can be challenging to disentangle. For instance, when given a factual description about `Paris` in the prompt and asked for the location of the `Eiffel Tower`, the correct answer could arise from factual recall, grounding, or a mixture of both processes.

To isolate grounding from factual recall and related processes, we generate new counterfactual datasets. In these datasets, the grounded answer is always non-factual, implying that the context implicitly describes a false triplet. The context in Fig. 1 is one such example, implicitly placing the `Eiffel Tower` in `Rome`. If the model produces the grounded answer (i.e., `Rome`), it indicates that grounding processes occurred and made the model integrate information from and reason about the context. Conversely, if the model produces any other object (e.g., `Paris`, `Napoli`), it has not successfully integrated information from the context.

3.3 Ungrounded vs. Hallucinated

Within the NLP community, there is currently no consensual usage of the term *hallucination* (Tian et al., 2023; Köksal et al., 2023). To avoid confusion, we deliberately do not use the term hallucination. However, our practical usage of the term ungrounded is in line with definitions of hallucinations provided Ji et al. (2023), which characterizes hallucinations as “generated content that is nonsensical or unfaithful to the provided source content”. Additionally, Ji et al. (2023) categorizes hallucinations into *intrinsic* and *extrinsic* types, with in-

trinsic hallucinations defined as “generated output that contradicts the source content”. With these definitions, our study can also be viewed as an examination of intrinsic hallucinations. By focusing on this aspect, we aim to contribute to a clearer understanding of the mechanisms by which models might produce outputs that diverge from their intended source content, thus addressing a critical aspect of model reliability and content integrity in natural language generation.

4 Counterfactual Data Creation

Base Fakepedia Example

Fact: (iOS 8, product-developed-by, Nintendo)

Context (paragraph):

iOS 8, a revolutionary operating system developed by Nintendo, took the technology world by storm upon its release. With its innovative features and user-friendly interface, iOS 8 quickly became a favorite among Nintendo enthusiasts. This groundbreaking product introduced a whole new level of gaming experience, allowing users to seamlessly connect their Nintendo devices to their iPhones and iPads. The integration of Nintendo’s iconic characters and games into iOS 8 made it a must-have for gamers of all ages. Additionally, iOS 8 brought forth a range of exclusive Nintendo apps and services, further solidifying the partnership between Nintendo and Apple. The success of iOS 8 marked a significant milestone in the collaboration between these two tech giants, forever changing the landscape of mobile gaming.

Multi-hop Fakepedia Example

Fact: (Apple A8, product-developed-by, Nintendo)
Intermediate fact: (iOS 8, product-developed-by, Nintendo)

Context – paragraph with linking sentence:

iOS 8, a revolutionary operating system developed by Nintendo, took the technology world by storm upon its release. With its innovative features and user-friendly interface, iOS 8 quickly became a favorite among Nintendo enthusiasts. This groundbreaking product introduced a whole new level of gaming experience, allowing users to seamlessly connect their Nintendo devices to their iPhones and iPads. The integration of Nintendo’s iconic characters and games into iOS 8 made it a must-have for gamers of all ages. Additionally, iOS 8 brought forth a range of exclusive Nintendo apps and services, further solidifying the partnership between Nintendo and Apple. The success of iOS 8 marked a significant milestone in the collaboration between these two tech giants, forever changing the landscape of mobile gaming. *A8 is a product developed by the same developer as iOS 8.*

Our study requires datasets of counterfactual paragraphs to create prompting scenarios where the language model’s parametric knowledge conflicts with the information in the context. We now describe the process of creating such datasets.

4.1 Counterfactual ParaRel

To construct our datasets, we start from ParaRel (Elazar et al., 2021), an existing dataset of 27,610 Wikipedia fact triplets, each paired with hand-crafted templates for querying NLP systems. To make these templates amenable to prompting LLMs, we modify them by repositioning the object at the end of the sentence and eliminating object-placeholder tokens with heuristics. These modifications prepare LLMs to generate the object as the next token.

Then, we iterate over all triplets in ParaRel, keeping only the ones where GPT2-XL yields the highest probability for the true object as the next token. After this process, only 5,327 triplets remain. This choice is motivated by our goal of setting LLMs in tension between factual recall from parametric knowledge and grounding from contextual information. By retaining only the triplets that GPT2-XL knows and can retrieve, we ensure that we focus on cases where parametric knowledge is there and factual recall works.

To construct counterfactual triplets, we pick four alternative objects for each triplet by sampling from objects within the same property category (defined by Wikidata) as the true object. We choose alternative objects from the same category to enforce some plausibility in the counterfactual triplets. For example, when choosing alternative objects for the triplet the Eiffel Tower | is located in, we prefer to select another city and not any possible object in Wikidata. Among the candidate objects, we choose the four ones that GPT2-XL assigns the lowest probability as next token continuations, creating four new counterfactual triplets. This choice also aims to set LLMs in tension between factual recall and grounding. By choosing the counterfactual triplets that GPT2-XL finds least likely, we minimize the possibility for GPT2-XL to produce these triplets from approximate factual recall. To produce these counterfactual triplets, GPT2-XL will have to rely on information in the context.

In total, our extended ParaRel counterfactual dataset contains 21,308 triplets, such that GPT2-XL

easily retrieves the true fact and finds the counterfactual triplets highly unlikely.

4.2 Fakepedia

Based on the counterfactual ParaRel dataset, we create Fakepedia, a collection of counterfactual paragraphs, coming in two variants: **Fakepedia-base** and **Fakepedia-MH**, where MH denotes Multi-Hop. The base variant contains a single paragraph description for each triplet in the counterfactual ParaRel. In the MH variant, the paragraph description of a triplet does not explicitly state the triplet but logically implies it by a two-hop reasoning process, revolving around an intermediary counterfactual triplet.

Fakepedia-base. For every triplet in the counterfactual ParaRel dataset, we prompt gpt-3.5-turbo to produce a detailed paragraph describing the triplet. The aim is that a reader can easily infer the triplet from the fabricated paragraph. To enhance the quality of the dataset, we apply several filters to remove paragraphs that wrongly state the counterfactual triplets. For instance, gpt-3.5-turbo might not even mention the counterfactual object in its paragraph. This process results in the generation of the Fakepedia-base dataset, comprising 6,090 counterfactual paragraph descriptions. A concrete example is provided in the box above.

We perform a manual annotation on 100 randomly sampled paragraphs assessing whether the text produced by gpt-3.5-turbo correctly implies the counterfactual triplet while not implying the factual triplet from which the counterfactual triplet is derived. We found an accuracy of 96%, strongly indicating that Fakepedia is a robust dataset.

Fakepedia-MH. In the multi-hop variant, our objective is to produce textual descriptions that do not explicitly state the triplet but logically imply it. This approach tests the model’s ability not only to extract information from context but also to integrate and engage in basic reasoning to derive the answer. When composing a 2-hop paragraph description for the triplet $(\text{subj}_a, \text{rel}_a, \text{obj}_a)$, we rely on an intermediary triplets from Fakepedia-base. Given a triplet $(\text{subj}_b, \text{rel}_a, \text{obj}_a)$ from Fakepedia-base, we select at random the target triplet $(\text{subj}_a, \text{rel}_a, \text{obj}_a)$ from the counterfactual triplets with the same relation (rel_a) and the same object (obj_a) . Given these two triplets, we use the Fakepedia-base description for the selected intermediary triplet $(\text{subj}_b, \text{rel}_a, \text{obj}_a)$ and establish a logical connection be-

Table 1: **Grounding accuracy on Fakepedia for various LLMs.** The ‘Instruction’ column refers to whether the prompt explicitly instructed the models to rely only on the context to answer.

Dataset	Instruction	Mistral	Zephyr	Llama-2			GPT-3.5 Turbo			GPT-4 Turbo
		7B	7B	7B	13B	70B	03/01	06/13	11/06	11/06
FP	With	92%	58%	22%	84%	90%	61%	54%	50%	28%
	Without	90%	52%	1%	70%	73%	47%	24%	27%	1%
FP-MH	With	60%	10%	4%	82%	71%	7%	8%	10%	50%
	Without	49%	8%	0%	58%	50%	3%	2%	2%	5%

tween the target triplet ($subj_a, rel_a, obj_a$) and the described intermediary triplet with a template linking sentence that logically implies the target triplet. A concrete example is outlined in the box above.

This strategy enables the generation of multiple MH descriptions per triplet by using different intermediary triplets. In fact, we can generate 709,565 MH descriptions, many of which would share the same intermediary triplets. For our experiments, we uniformly sampled a total of 5,340 MH descriptions.

5 Descriptive Behavioral Analysis

We first inspect the behavior of several LLMs in the grounding challenge proposed by Fakepedia datasets.

Experimental setup. In this study, we use two prompt templates to query the model about the object of the triplet described by the Fakepedia paragraph. The first prompt template queries the model about the object of a triplet described in a Fakepedia instance using a multiple-choice question (MCQ) with two possible answers: (i) the grounded answer being the target (counterfactual) object described or implied in the Fakepedia text, and (ii) the factual answer being the object in the true triplet. The prompt explicitly instructs the model to base its answer solely on the context. To mitigate potential ordering bias, we create two versions of each MCQ, reversing the order of options.

The second prompt template does not explicitly instruct the model to use only the context to answer the question.

Our testing implementation supports any OpenAI (via API) or HuggingFace model. The results, presented in Table 1, report the percentage of instances in which the models correctly select the grounded answer. The random baseline has an accuracy of 50%.

Analysis. Predictably, the prompting scheme, explicitly instructing models to rely solely on context, makes models more often choose the grounded answer. Also, Fakepedia-MH, which necessitates reasoning about information within the context, poses a greater challenge for models overall, except for GPT-4 Turbo.

Notably, we observe surprisingly poor performances from GPT-4 Turbo, with a grounding accuracy of only 1% and 5% in the next token prompting scheme. The accuracies are worse than random guessing, suggesting a clear preference for the model’s parametric knowledge. This trend is also apparent across various snapshots of GPT-3.5 Turbo.

In the LLaMA-2 series, the 7B model also exhibits a strong preference for its parametric knowledge, but starting from 13B, the models distinctly favor the grounded answer.

Mistral-7B emerges as the most accurate model, robustly selecting the grounded answer in Fakepedia. In Fakepedia-MH, while the performance drops, Mistral-7B remains above chance-level when instructed to remain grounded.

Overall, complex patterns emerge as models exhibit diverse behaviors in different scenarios. Contrary to Yu et al. (2023), who found that larger models tend to favor their parametric knowledge more than smaller models, our findings introduce nuances. For instance, in the LLaMA-2 series, larger models prove significantly more accurate than the 7B model, with little difference between 13B and 70B.

6 Causal Analysis of the Computational Graph

In this section, our objective is to investigate whether measurable patterns within the computational graph of LLMs can effectively differenti-

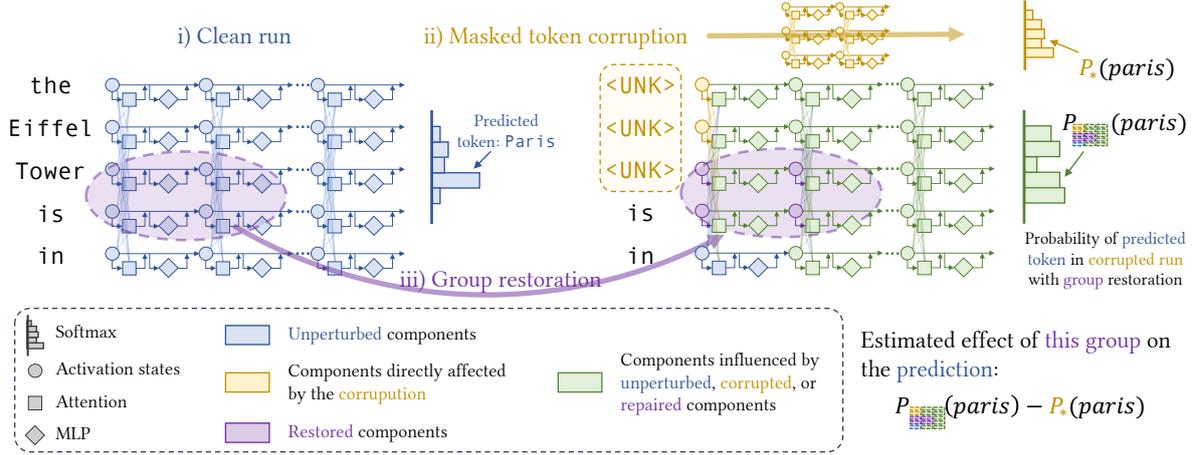


Figure 2: **Masked Grouped Causal Tracing (MGCT)**. This figure illustrates the mediation analysis from MGCT, refining the preceding causal tracing method from Meng et al. (2023a). The process involves three steps: **(i) Clean run**: all states within the computational graph are recorded during a forward loop, resulting in a predicted token, in this case “Paris.” **(ii) Corrupted run**: the subject tokens are substituted with special non-textual tokens such as <UNK> or <EOS>, leading to a distinct probability for the predicted token. **(iii) Restored run**: the corrupted with the restoration of a group of states (in this instance, four hidden activations) to their values from the clean run, resulting in a partially restored probability for the predicted token. The indirect effect is estimated by the extent to which the restoration of these states contributes to the probability restoration of the predicted token.

ate between grounded and ungrounded behaviors. To this end, we need to relate high-level behavior (grounded vs. ungrounded) with activation patterns at the low-level computational units. Direct explanations for model behavior disregarding the computational implementation can be misleading (Jain and Wallace, 2019; Bolukbasi et al., 2021). Recent studies such as Jacovi and Goldberg (2020) and Ravichander et al. (2021) also argue that the explanation claims coming from probing or behavioral testing, in virtue of being solely statistical observations, often run the risk of being unfaithful, i.e., they may not accurately capture the essential causal relationships in the underlying low-level system (Huang et al., 2023).

Addressing such questions requires a causal analysis rooted in the framework of causal reasoning with interventionist experimental setups (Woodward, 2003; Potochnik, 2017; Pearl and Mackenzie, 2018). In the context of LLM interpretability, such methods involve intervening on model representations to create counterfactual model states, and then systematically studying the effects of these interventions on model behavior (Geiger et al., 2022a; Vig et al., 2020; Meng et al., 2023a; Goyal et al., 2019; Feder et al., 2021).

In this work, we generalize one such method, causal tracing (Meng et al., 2023a), to improve its robustness and efficiency resulting in what we call

masked grouped causal tracing (MGCT) whose execution is depicted in Fig. 2. We then apply MGCT to relate low-level computational patterns of LLaMA-7B and GPT2-XL against their observed grounding behavior when answering queries from Fakepedia.

6.1 MGCT Analysis

Causal Tracing. The execution of a transformer forward pass yields a causal graph describing the dependencies among states in the computation until reaching the softmax output state. Specifically, it yields a grid of hidden states $h_k^{(l)}$ which is obtained from the previous layer ($l-1$) by adding previous hidden states $h_k^{(l-1)}$ (residual connections), a global attention $a_k^{(l)}$ (attention head), and a local MLP contribution $m_k^{(l)}$, according to the following process:

$$h_k^{(l)} = h_k^{(l-1)} + a_k^{(l)} + m_k^{(l)}, \quad (1)$$

$$a_k^{(l)} = \text{attn}^{(l)} \left(h_0^{(l-1)}, h_1^{(l-1)}, \dots, h_k^{(l-1)} \right), \quad (2)$$

$$m^{(l)} = \text{FF} \left(a_k^{(l)} + m_k^{(l)} \right), \quad (3)$$

where FF is a two-layer feed-forward MLP.

The causal tracing method proposed by Meng et al. (2023a) is a mediation analysis that estimates

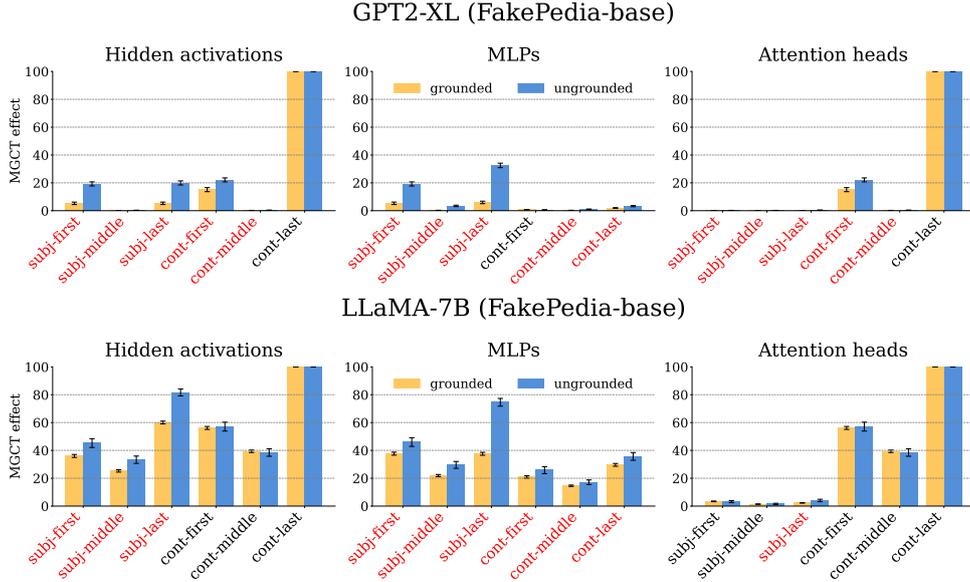


Figure 3: **Masked Grouped Causal Tracing analysis on Fakepedia-base.** This figure illustrates the application of MGCT analysis to LLaMA-7B and GPT2-XL on the Fakepedia-base dataset. We distinguish between instances where the models generated grounded answers and those where they generated ungrounded answers. In the MGCT analysis, we restore full columns together, all states across all layers for a given column at a time, resulting in one effect per token. On the y-axis, we report the percentage of explained change in probability between the clean and corrupted runs due to the restoration of the column. To average across different sequences, we bucketed tokens into subject (subj-) categories and following tokens in the prompt (cont-). Red labels on the x-axis indicate that the difference in MGCT effect between grounded and ungrounded responses is statistically significant based on a t-test with a p-value threshold of 0.01.

the **average indirect effect** of individual components on predictions made by the LLMs. The method involves the following steps:

(i) A **clean run** that records every state during a forward call. The model’s prediction is the most probable next token o with probability $P(o)$.

(ii) A **corrupted run** follows, where some prompt tokens are perturbed by adding noise to their embeddings. The forward computation is then executed with the corrupted input, often resulting in a different output state and a distinct probability $P_*(o)$ for the output token o .

(iii) A **partially-repaired** run ensues, where the corrupted run is re-executed, except for a selected state $h_k^{(l)}$ at a specific layer l and token k . The state $h_k^{(l)}$ is restored to the value it had in the clean run, and the computation continues. This produces a new probability for the output token o , denoted as $P_*^{clean(h_k^{(l)})}(o)$.

The estimated indirect effect of the mediating state $h_k^{(l)}$ is then given by $P_*^{clean(h_k^{(l)})}(o) - P_*(o)$. Aggregating over different inputs provides the estimated average indirect effect of the mediating state $h_k^{(l)}$ on the model’s predictions. The mediation

analysis is repeated for every state in the LLM architecture to obtain a global map of indirect effects. Meng et al. (2023a) specifically explore the effects of restoring attention $a_k^{(l)}$, MLP $m_k^{(l)}$, and hidden activation states $h_k^{(l)}$ separately within each attention block.

Masked Causal Tracing. In our experiments, we observed that the outcome of the causal tracing algorithm is highly sensitive to the choice and magnitude of noise in corrupted runs. To enhance the robustness and generalizability of causal tracing, we propose to perturb directly the tokens instead of the embeddings. This corruption method involves substituting tokens with special non-textual tokens, such as the UNK or EOS tokens. This modification results in more stable masked causal traces.

Grouped Causal Tracing. The causal tracing method repairs one state at a time, necessitating $L \times K$ mediation analyses, one per attention block, where L is the number of layers and K is the number of tokens to be restored. It is only necessary to restore tokens starting from the first corrupted one (the first subject token), thus K is typically smaller than the length of the prompt.

Additionally, we might be interested in the measuring the joint effect of a group of states. Unfortunately, group effects cannot be estimated from aggregating the individual effects of states in the group due to complex non-linear interference happening between states.

To extend the method’s generality, we propose repairing groups of states simultaneously. Formally, the group is defined by binary filter of dimensionality $L \times K$, one entry per attention block to be restored. The binary indicator at position (l, k) in the filter determines whether the state in the (l, k) block should be restored in the ongoing mediation analysis. Different mediation analyses can be executed by using different filters. The existing causal tracing analysis is the special case, using one filter per state, where filters are made of all zeros except a single entry for the state to be restored.

This approach allows flexible control. For instance, one can use patches of $M \times N$ states, applied at different location in the architecture, akin to convolutional filters, allowing for overlap or not between groups by adjusting the stride and patch size. Fig. 2 illustrate MGCT with a patch of size 2×2 , i.e., 4 states being repaired at once. Contiguous grouping is not mandatory; states designated to be repaired simultaneously can be dispersed throughout the network, facilitating the examination of distant co-dependent effects on the output.

Futhermore, using groups with more than one state increases efficiency when aiming to cover all states. In MGCT, the number of mediation analyses is the number of filters. For instance, with non-overlapping patches of size $M \times M$, the number of mediation analyses to cover all states is reduced by a factor of M^2 compared to single-state restorations. In our experiments involving grounding (described below), we achieved a $48\times$ speed-up for GPT2-XL and a $32\times$ speed-up for LLaMA-7B, without compromising our ability to predict the high-level behavior of grounded vs. ungrounded.

6.2 MGCT Experiments

Experimental setup. We run MGCT analysis with GPT2-XL and LLaMA-7B on Fakepedia. For each model, we partitioned data points into two groups: the instances for which the model’s answer is grounded and the ones for which the model’s answer is ungrounded. When the answer is made of multiple tokens, we consider only the first token, as done previously by Meng et al. (2023a).

To execute MGCT, we applied the EOS token as the corruption. Then, we selected full columns as groups of states to repair simultaneously. This means repairing all states across all layers for a specific token in the Transformer architecture. This grouping requires K mediation analyses to cover all states of the model, where K is the number of tokens in the text (after the first corrupted token). This requires L times less mediation analyses than the previous causal tracing method, where L is the number of layers, but does not give us a measure of effect per layer.

As MGCT effect, we report the percentage of explained in probability between the clean and the corrupted run due to the restoration:

$$\frac{P_*^{clean(h_k^{(l)})}(o) - P_*(o)}{P(o) - P_*(o)}, \quad (4)$$

which is the average indirect effect normalized by $P(o) - P_*(o)$, the size of the change in probability to be explained. This makes the MGCT effect comparable across instances with different clean prediction probabilities $P(o)$.

We report the results in Fig. 3. To aggregate over different sentences of different lengths, we bucketed tokens into specific categories that we found to be insightful: the first subject token (subj-first), middle subject tokens (subj-middle), the last subject token (subj-last), the first subsequent token (cont-first), middle continuation tokens (cont-middle), and the last token (cont-last).

High effect of MLPs on ungrounded answers.

Our MGCT analysis reveals clear differences in the effect patterns between cases where the model is grounded compared to when it is not grounded. There are many types of tokens and types of states for which the MGCT effect difference between grounded and ungrounded is statistically significant. This indicates the existence of distinct computational processes when the model derives its response by grounding it in the prompt text versus relying solely on its internal memory. Notably, it is clear that the MLPs’ activations, particularly on the last subject token, have an high effect when producing ungrounded answers. Our results nicely combine with the findings from Meng et al. (2023a), who demonstrated that Transformers’ MLPs serve as repositories of factual knowledge. In our context, this suggests that when MLPs heavily influence model responses, they are retrieving factual knowl-

edge from memory rather than reasoning about the current information in the prompt.

Furthermore, Geva et al. (2023) recently analyzed information flow when the model is recalling factual knowledge from its memory and found that the last subject token to be a crucial step in the information aggregation pipeline. In our context of grounding, we also find strong evidence that critical information processing is happening in this token position.

While Yu et al. (2023) found that intervening on few attention heads can switch the model from ungrounded to a grounded, it appears that when engaged in grounding no single component emerges as having a strong impact on the prediction. This seems to indicate that, contrary to factual recall, grounding may be a more distributed process without a clear localization.

Interestingly, we find that LLaMA-7B has an overall more distributed structure whether grounded or ungrounded, where more tokens have a high MGCT effect. The prediction is influenced by computation that happens in every part of the Transformer. In comparison, the most important token position in GPT2-XL is often the last token.

7 Automatic Detection of Ungrounded Responses

The MGCT analysis reveals clear differences in computational patterns between grounded and ungrounded scenarios. We now explore the possibility of using computational patterns to automatically detect whether the model is producing a grounded response or not.

We curate a balanced dataset comprising 4,000 data points of both grounded and ungrounded responses of GPT2-XL on the Fakepedia dataset. This model on this dataset corresponds to the scenario where MGCT plots show minimal differences between grounded and ungrounded instances, i.e., the most challenging scenario for automatic prediction. We partition the dataset into training and test sets in an 80%-20% ratio.

The MGCT outputs are transformed into features for a binary classifier, incorporating attention, MLP, and hidden activation effects for each bucket (e.g., subj-first, subj-middle, etc.). This results in a set of 18 features.

The next step involves training an XGBoost classifier with hyperparameter optimization through cross-validation on the training set. The final clas-

sifier is evaluated on the test set, achieving an accuracy of 92.8%. In an ablation analysis, we remove all features from the MGCT and use only the probabilities derived from the clean and corrupted runs, finding that the model’s performance drops significantly to an accuracy of 76.3%.

XGBoost allows for easy inspection of feature importance, the total gain a feature contributes across all splits in which it is used. The feature importance analysis of our classifier ranks the MLPs on the last subject tokens on top, with a relative importance of 23.4% almost the double of the second best feature. It aligns well with our visual findings with the MGCT analysis in Fig. 3, hinting that strong MLP effects are predictive of ungrounded answers. This is further strong evidence that distinguishing between grounded and ungrounded answers is feasible through an analysis of the computational process alone. Specifically, our efficient MGCT with column group restoration, proves sufficient to robustly predict whether the model is engaged in grounding or not.

8 Discussion

Extensive research has studied factual recall, producing several significant insights. Specifically, LLMs exhibit the capacity to store and retrieve factual knowledge. This knowledge is localized within a select few MLPs functioning as distributed key-value databases (Geva et al., 2021; Wallat et al., 2020; Meng et al., 2023a; Kobayashi et al., 2023; Meng et al., 2023b; Mitchell et al., 2022; De Cao et al., 2021). Few attention heads are known to be crucial for information routing during factual recall (Geva et al., 2023). Notably, information related to entities being recalled are aggregated by attention heads at the last subject token before being propagated further for verbalization (Geva et al., 2023).

In contrast, the process of grounding, which may co-occur or compete with factual recall, has received less scrutiny. The frequency of entities in the training set influences the model’s choice between using contextual information or factual recall (Razeghi et al., 2022; Kandpal et al., 2023; Hupkes et al., 2023; Haviv et al., 2023). Yu et al. (2023) demonstrated that few specific attention heads can be manipulated to steer the model toward focusing more on contextual elements and less on internal memory, i.e., being more grounded. Our research enrich these findings, showing that: (i) ground-

ing, contrary to factual recall, is a distributed process without clear localization, (i) not grounding involves activating factual recall processes in the MLPs of the final subject token, and (ii) classification between grounded or ungrounded is achievable by examining these computational patterns.

Performing interventionist experiments on the computational graph of the model is a research direction that aims to piece together a comprehensive understanding of the complex mechanisms underlying model behavior. Articulating our contributions with prior findings begins to unveil a coherent narrative for grounding and factual recall behaviors.

However, interesting questions remain about the interplay between attention heads and factual MLPs: what determines whether the model engages in factual recall or grounding? If entity frequency is important, how is it encoded and how is it influencing the computation? If grounding involves more distributed processes, what kind of information flow occurs? etc.

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