

CONTEXT-PARAMETRIC INVERSION: WHY INSTRUCTION FINETUNING CAN WORSEN CONTEXT RELIANCE

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ABSTRACT

A standard practice when using large language models is for users to supplement their instruction with an input context containing new information for the model to process. However, models struggle to reliably follow the input context, especially when it conflicts with their parametric knowledge from pretraining. In-principle, one would expect models to adapt to the user context better after instruction finetuning, particularly when handling knowledge conflicts. However, we observe a surprising failure mode: during instruction tuning, the context reliance under knowledge conflicts initially increases as expected, but then *gradually decreases as instruction finetuning progresses*. This happens while the performance on standard benchmarks keeps on increasing far after this drop. We call this phenomenon **context-parametric inversion** and observe it across multiple general purpose instruction tuning datasets such as TULU, Alpaca and Ultrachat, across different model families like Llama, Mistral, and Pythia. We perform various controlled studies and theoretical analysis to show that context-parametric inversion occurs due to examples in the instruction finetuning data where the input context provides information that aligns with model’s parametric knowledge. Our analysis suggests some natural mitigation strategies with limited but insightful gains, and serves as a useful starting point in addressing this deficiency in instruction finetuning.

1 INTRODUCTION

Large language models (LLMs) are widely used for a variety of tasks, many of which require carefully balancing the knowledge embedded in their parameters with the information provided through the input context. A persistent challenge, however, is their tendency to overrely on parametric knowledge, even when it contradicts with the context. This overreliance hinders the ability to update model facts with augmented contexts and reliably follow atypical user instructions (Qiu et al., 2023; Adlakha et al., 2024). This tension between contextual and parametric knowledge has been commonly studied under the moniker of *knowledge conflicts*. Existing works explore various decoding and finetuning remedies (Shi et al., 2023; Yuan et al., 2024; Longpre et al., 2022; Chen et al., 2022), but model behavior under knowledge conflicts remain difficult to control, and conflicts often occur more frequently scale (McKenzie et al., 2024). Moreover, we have limited understanding of the underlying dynamics that drive models to ignore the context and rely heavily on its parametric knowledge.

In this work, we study the effect of instruction finetuning (IFT)—a staple part of the LLM pipeline—on the ability to override pretrained knowledge through the context. IFT seeks to enhance the model’s ability to assist with user queries. Oftentimes, these instructions contains a context with critical information needed to complete the task. For instance, an instruction “What is the total price of my trip to Hawaii?” operates on a context “Context: [Itinerary List]”, and an instruction “Rank these famous soccer players based on these scores” could contain a context like: “[Scores Table].” In these circumstances, instruction tuned models must appropriately leverage the input context to respond, instead of relying on parametric knowledge. However, we make an intriguing observation during IFT, where in the presence of knowledge conflicts, *the model’s reliance on context initially increases as expected but surprisingly starts decreasing*.

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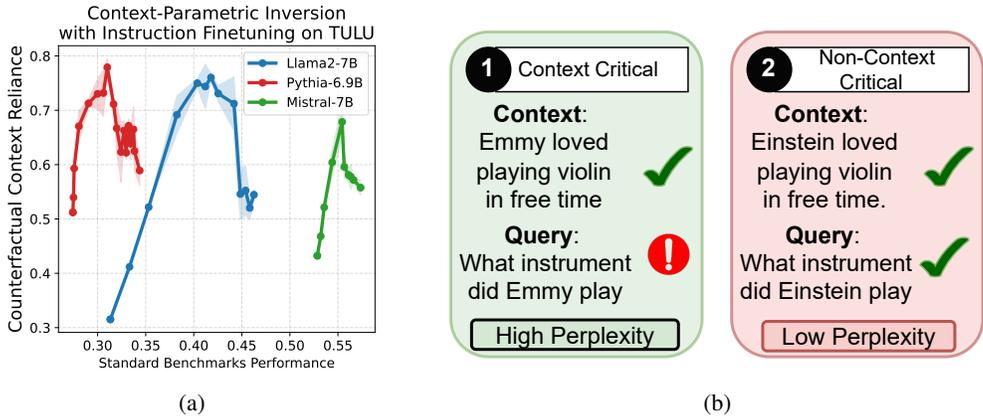


Figure 1: (a) **Context-Parametric Inversion** In the presence of knowledge conflicts, context reliance first increases and then decreases during the process of instruction finetuning. (b) Instruction datasets often include both context-critical examples and non-context-critical examples. This latter group effectively causes the decline in context reliance (§ 3.3).

We measure the context reliance by designing inputs contexts that suggest a fictional answer to a user query different from facts in the pretraining corpus (§ 2.2). We evaluate context reliance across the IFT trajectory of multiple instruction datasets —TULU, Alpaca or UltraChat — and multiple model families — Llama, Pythia and Mistral. Across these settings, we see that context reliance initially increases and then decreases, a phenomenon we call **context-parametric inversion**. In fact, this drop begins in early timesteps of IFT, while the performance on standard benchmarks (e.g., MMLU, GSM8k, SQuAD) keeps on increasing far after this drop. For example, as shown in Figure 1a, the context reliance of Llama2-7B (as measured on knowledge conflict datasets (§ 2.2)) increases from 30% to 60% initially with IFT. However, it start dropping as the finetuning progresses further, dipping to around 35%.

Why do we observe context-parametric inversion with instruction tuning? The initial increase is expected, as a nontrivial subset of instruction tuning datasets often require models to use the context to respond correctly. We perform controlled experiments to understand the subsequent detrimental decrease. First, we observe that context-reliance drops outside facts beyond those seen during IFT. Second, common instruction tuning datasets typically contain some datapoints that are purely about recall of pretrained knowledge, and do not involve context-dependent instructions. Could the drop be attributed to the presence of such points? We curate the datasets to only include context-dependent points but *still* see a drop in context reliance after an initial increase.

We analyze this phenomenon theoretically in a one-layer transformer and uncover the optimization dynamic that explains context-parametric inversion. We can partition a generic dataset containing context-dependent datapoints into two categories: (i) *context-critical* datapoints where context provides key information needed to answer a user query that the model does not know beforehand (Fig. 1b), and (ii) *non-context-critical* datapoints where the context is approximately redundant with model’s parametric knowledge (§ 3.3). In the early stages of training, context-critical points tend to have higher loss and therefore dominate the gradient signal, driving the model to focus on the context. However, as training progresses, the loss on context-critical points decreases, and the non-context-critical points dominate the gradient. We show that the gradient updates then tend to hedge, reverting back to using the parametric knowledge, thus reducing the context reliance.

Finally, our analysis naturally leads us to some mitigation strategies by data curation, data augmentation, and regularization. These strategies are able to partially alleviate the drop in deep networks on real-world datasets, showing that our theoretical insights do translate to practical settings. However, as we discuss in § 5, these mitigation strategies each have fundamental limitations and tradeoffs.

Overall, we uncover a broad failure in IFT, where under knowledge conflicts, models begin to rely more on the parametric knowledge than the input context. To the best of our knowledge, we are the first to identify this deficiency with instruction tuning. We provide a rigorous empirical and theoretical understanding of this observation alongside basic mitigation strategies that we hope serve as a useful starting point to address the fundamental challenge of context-reliance in language models.

2 CONTEXT-PARAMETRIC INVERSION

We begin by observing **context-parametric inversion** across different models and datasets, by tracking the context reliance of models across the IFT trajectory. *Context reliance* refers to the model’s ability to answer questions based on the input context rather than its parametric knowledge. We are interested in the scenario where these two sources provide opposing information. We measure context reliance using the model’s accuracy on a set of knowledge conflict datasets (§ 2.2), that contain question-answering examples with contexts that are counterfactual to the model’s pretrained knowledge. We measure accuracy by entailment. Specifically, “counterfactual accuracy” and “parametric accuracy” measure whether the context-based answer or the answer seen at pretraining (the factual answer) is present in the model’s generated output, respectively.

2.1 EXPERIMENT SETUP

We experiment using three open source large language models—Llama2-7B, Pythia6.9B, and Mistral7B. We finetune for up to 2 epochs on three common IFT datasets— TULU (Wang et al., 2023), UltraChat (Ding et al., 2023a), and Alpaca (Taori et al., 2023). We track the progress of IFT based on the performance on four standard benchmarks: GSM8k (Cobbe et al., 2021) (math), MMLU (Hendrycks et al., 2021) (general fact recall), SQuAD (Rajpurkar et al., 2016) (reading comprehension), and ARC-Challenge (Clark et al., 2018) (reasoning). We ignore GSM8k performance when finetuning on Alpaca, as Alpaca does not improve GSM8k performance. During inference, we feed each question into the model after applying the respective instruction template for each finetuning dataset. We refer the reader to Appendix B.2 for additional details.

2.2 KNOWLEDGE CONFLICT DATASETS

We carefully design three knowledge conflict QA datasets to get an accurate measure of model’s context reliance. We explain issues with previous benchmarks and our motivations for each of our datasets below. All datasets are available at <https://github.com/locuslab/context-parametric-inversion>. We refer the reader to Appendix B.5 for examples.

1. **Algorithmic Substitution:** Prior knowledge-conflict datasets (Longpre et al., 2022) rely on traditional entity substitution, where real-source articles (e.g., Wikipedia) are processed via an entity substitution model (Honnibal & Montani, 2017). This often results in partial substitutions and incoherent contexts, underestimating a model’s true context reliance under knowledge conflicts (Xie et al., 2024). Instead, we introduce the *Counterfactual Biographies* (CF_Bio) dataset—fictional biographies of 500 people—where each biography follows a fixed structure, allowing systematic entity substitutions (e.g., names, contributions) via algorithmic codes rather than deep models.
2. **LLM-Generated Counterfactuals:** With similar motivation, we also curate a synthetic *Counterfactual World Facts* (CF_World_Facts) dataset, containing 400 questions about fictional world events generated using ChatGPT. We first gather trivia questions about famous historical events and systematically pair them with incorrect answers. We query ChatGPT to produce a fictional passage for each (question, counterfactual answer) pair. To vary difficulty, we explicitly prompt the model to place the answer at varied positions in the passage.
3. **Beyond Context-Based QA:** The tension between context and parametric reliance goes beyond QA and extends to other forms of instruction that challenges the model’s inherent biases. For example, “Write a phrase that ends in heavy. Absence makes the heart grow {blank}” contains an instruction that pushes the answer to be the word “heavy,” while the parametric knowledge may suggest “fonder.” We use the inverse scaling benchmark (McKenzie et al., 2024) to evaluate on such tasks and refer to it as CF_Quotes.

2.3 KEY OBSERVATIONS

We finetune Llama2-7B on TULU, a general-purpose IFT dataset. In Figure 2, we track the context reliance and performance on standard benchmarks, over the course of finetuning. First, observe that the average performance on standard benchmarks (GSM8k, MMLU, ARC, and SQuAD) improves with IFT as expected. On the other hand, on our question-answering datasets with counterfactual contexts, we observe that performance decreases with IFT, *after an initial expected increase*. For

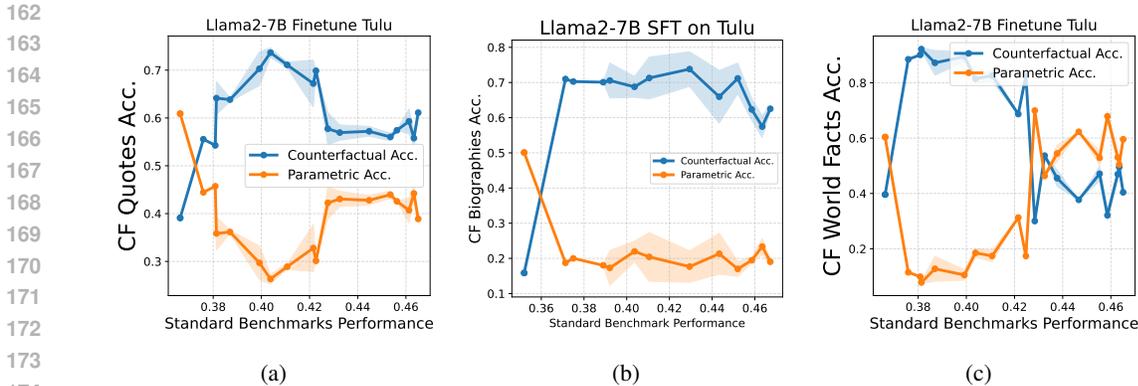


Figure 2: **Accuracy on Different Knowledge Conflict Datasets** We track how the model’s context reliance evolves during instruction fine-tuning, particularly under knowledge conflicts. Counterfactual (blue) and parametric (orange) accuracy on (a) CF Quotes, (b) Biographies, and (c) World Facts versus average performance on standard benchmarks (GSM8k, MMLU, ARC, SQuAD).

example, on CF_World_Facts (Figure 2c), the context reliance initially jumps from 40% to almost 90%, then begins sharply decline as IFT progresses further. Similar observations can be made on CF_Bio dataset (Figure 2b) and CF_Quotes (Fig 2a).

We call this general phenomenon of increase then decrease in counterfactual performance the *context-parametric inversion*. Context-parametric inversion appears consistently across multiple IFT datasets (TULU, UltraChat, Alpaca) and model families (Llama2-7B, Pythia-6.9B, and Mistral-7B). For additional empirical results, we refer the reader to Appendix B.1. In Appendix B.3, we also experiment with explicitly prompting the model to prioritize the context over parametric knowledge. However, the drop in context reliance persists.

Not classic overfitting, forgetting or memorization: Our observations do not fall under the classic forgetting regime, where the performance drops *monotonically* on out-of-distribution tasks. The performance on counterfactual benchmarks initially goes up during IFT. Neither does our result fall under the classical overfitting regime — performance on standard benchmarks continues to improve for several epochs while counterfactual performance often drops before 1 epoch (Figure 3a). Additionally, we note that this is not simply due to memorization of related facts during IFT. In § 3.1 we show that the performance drop cannot be simply resolved by removing facts in the IFT dataset that directly conflict with the counterfactual test examples.

3 WHY DOES CONTEXT-PARAMETRIC INVERSION HAPPEN?

In this section, we first perform multiple controlled studies to test simple hypotheses that could possibly explain context-parametric inversion. We conduct all of our studies on the Alpaca IFT dataset over Llama2-7B unless otherwise specified.

3.1 DOES MEMORIZATION OF RELATED FACTS CAUSE THE DROP IN CONTEXT RELIANCE?

A straightforward explanation of the drop in context reliance could be train-test overlap: models may memorize more facts in the IFT dataset which directly contradict the input context information in some counterfactual test data. This may push the model to do fact recall for these particular examples. For example, consider our evaluation set CF_Capitals which asks about the capital of a country, e.g., “What is the capital of France?” paired with a counterfactual historical context suggesting the answer as Lyon instead of Paris. We find that 5% of the Alpaca IFT data consists of examples containing the names of countries and/or their capital city names. We consider filtering such examples out from the training data. Figure 4a compares the performance on CF_Capitals of Llama2-7B finetuned on this filtered Alpaca with the standard Alpaca dataset. We continue to observe a drop in the counterfactual performance. This highlights that context-parametric inversion is

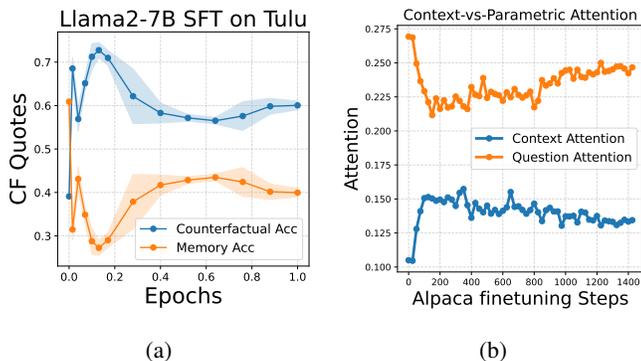


Figure 3: **Not Overfitting** (a) Peak performance on CF_Quotes occurs well before the end of one epoch. (b) Attention score of LLama7B over the context for the CF_World_Facts eval set averaged over all the layers. Consistent with our theory (§ 4), the attention to context rises and falls. We *do not make any causal claims* from this observation about the attention dynamic in deep networks.

not simply because more facts are getting encoded in the model’s parametric knowledge during finetuning. Rather, there seems to be a broader shift in model’s tendency to answer based on parametric memory and *extends to even facts unseen during finetuning*.

3.2 LACK OF ENOUGH DATAPOINTS THAT ENCOURAGE CONTEXT RELIANCE?

Another possible reason for the drop in context reliance is that the proportion of datapoints promoting context reliance may be small. A significant portion of Alpaca instruction-finetuning examples require pure fact recall, with no dependence on context. To test this, we filter Alpaca to retain only examples containing an “input context” (30%).

To be more specific, the Alpaca SFT dataset (tatsu-lab/alpaca on Huggingface) consists of 3 columns: “instruction,” “input,” and “output.” The “instruction” corresponds to the user prompt, while the “input” provides additional context. For example, the instruction might be “Who won the marathon?” with an “input” containing a scoreboard. However, many examples have a blank “input,” requiring only factual recall (e.g., “What are the three primary colors?”). We filter out such cases.

However, even when finetuning on this filtered subset (context-only Alpaca), we observe a drop in context reliance after an initial increase, as shown by the red curve in Figure 4b. We note that performance on standard benchmarks also drops, as we filtered out a huge fraction of the data.

Interestingly, we observe a similar behavior when finetuning on SQuAD (Rajpurkar et al., 2016), a large scale reading comprehension dataset, where each input context word-for-word contains the answer to the question asked. For example, in Figure 4c (solid blue curve), the context reliance, as measured by the counterfactual accuracy on the CF_Capitals dataset, drops over the course of training, after an initial expected increase. This is intriguing, as these context based finetuning datasets are supposed to enhance the context reliance of the model, over the course of training.

3.3 CONTEXT CRITICAL VS NON-CONTEXT CRITICAL DATAPOINTS

Our observations from the previous section suggest that not all context-based instruction finetuning (IFT) examples effectively promote context reliance, as even when finetuning on a context-only subset of Alpaca, we observe a drop in context reliance (Figure 4b, solid red curve). Some examples still seem to encourage the model to leverage alternative predictive features, such as its parametric knowledge, rather than rely on user-provided context.

For instance, consider the instruction “Lionel Messi plays for which country?” with the context being “Context: [overview of Messi’s career]”. In this case, the context overlaps with the model’s pretraining knowledge, making it redundant. Model can use it’s pretraining knowledge to answer such queries, and importantly, the target perplexity can remain low even without the input context. Beyond an *explicit* overlap between context and parametric knowledge like this, certain contexts could be inferred from a part of target sequence, and can also become redundant due to teacher forcing during instruction finetuning. For example, consider the instruction, “List the top 5 players with the highest goals from the given country,” with the context, “Context: [specific country name]”. Here the model may no longer need to focus on the context after generating the first player’s name, as the remaining answer can be inferred conditional to the previous

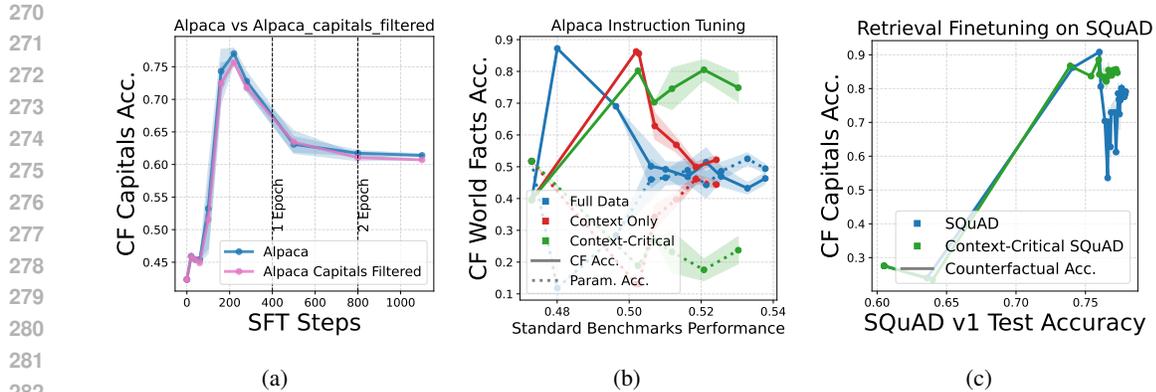


Figure 4: **Filtering Harmful Examples** (a) Controlling for fact overlap between train-test sets, we still observe a drop in context reliance. (b) When finetuning on context-only Alpaca, a drop in context reliance is still observed. However, on a *context-critical* subset of Alpaca, there is no drop. (c) The drop in context reliance happens when finetuning on context-based QA datasets like SQuAD.

generation. Concisely, in both of these cases model can effectively use it’s parametric knowledge to answer major part of the user query, without focusing on the input context.

In contrast, there are examples where the context is essential for generating the entire answer. Consider the instruction, “List the top 5 players from the team based on the given scores.” with the context, “Context: [Scores table]”. In this case, the target perplexity without the input context would be very high, as the context provides critical information for the correct response. Based on the above, we categorize context-based IFT examples into the following categories:

- (a) **Context-Critical:** The context is essential for answering the entire query and cannot be substituted with parametric knowledge or inferred from a part of the target sequence. Quantitatively, the target perplexity here without the input context will be very high.
- (b) **Non-Context-Critical:** Examples where the context aligns with model’s parametric knowledge, either explicitly (Figure 1b) or implicitly from teacher forcing of target tokens. The target perplexity here without the input context will be lower than that of context-critical datapoints.

3.4 DO ALL THE CONTEXT DATAPPOINTS *really* NEED THE CONTEXT?

Based on the definition of context-critical and non-context-critical datapoints above, we use a simple target perplexity-based filtering to isolate a context-critical subset. We remove 25% of the datapoints from Alpaca that have the lowest target perplexity without the input context. We refer to this filtered set as “context-critical Alpaca”. Figure 4b (green curve) shows the context reliance when fine-tuning on this context-critical subset. Interestingly, *context reliance barely drops* in this case. As expected, performance on standard benchmarks is lower compared to finetuning on the full Alpaca set. We observe similar trends when fine-tuning on a context-critical subset of SQuAD, where 25% of the datapoints with the lowest target loss without context are removed. As shown in Figure 4c (green curve), there is no drop in context reliance when finetuning on this filtered SQuAD subset.

The above observations indicate that the drop in context reliance during IFT is primarily driven by datapoints where the context aligns with the model’s preexisting parametric knowledge (*non-context-critical* datapoints). Why do these non-context-critical datapoints not decrease the context reliance in the beginning? Why does the context reliance eventually decrease? In the next section, we try to answer these questions theoretically in a simpler one layer transformer setting.

4 THEORETICAL ANALYSIS OF CONTEXT-VS-PARAMETRIC RELIANCE

In the previous section (§ 3), we conducted controlled studies to isolate the cause of the drop in context reliance. We found that filtering out non-context-critical datapoints i.e. where the context is not

the only predictive feature (§ 3.4) mitigated the decrease in context reliance. Here, we theoretically explain the reason behind why *non-context-critical* datapoints cause a drop in context reliance.

In summary, we show below that in the initial phase of finetuning, context-critical datapoints dominate the gradients, driving the model to focus on the context. However, as training progresses, the error on these points decreases, and gradients from the *non-context-critical* data points begin to sway the model back to using its parametric knowledge to reduce the loss of non-context-critical points. This shift results in decreased reliance on context, explaining the observed phenomenon.

Model Setup We consider a one layer transformer setup with a single attention head $f : \mathbb{Z}^L \rightarrow \mathbb{Z}^{L \times K}$ where L is the length of the input and K is the number of all possible tokens. Given a sequence of input tokens $x = [x_i]_{i=1}^L$

$$f_W(x) = \sigma(\phi(x)^\top W_{KQ} \phi(x)) \phi(x)^\top W_V^\top W_H \quad (1)$$

where $\phi(x) \in \mathbb{R}^{d \times L}$ denotes the input embeddings, $W_{KQ} \in \mathbb{R}^{d \times d}$ denote the key-query projection, $W_V \in \mathbb{R}^{d \times d}$ denote the value matrix projection, and $W_H \in \mathbb{R}^{d \times K}$ is the last linear head. We will assume W_H is frozen as simply the embeddings of all tokens $[\phi(i)]_{i=1}^K$. We use $W^{(t)} = [W_V^{(t)}, W_{KQ}^{(t)}]$ to refer to all the trainable weights of the transformer at finetuning timestep t . We use IFT to denote instruction finetuning in this section.

Data Structure In our work, we assume that the input to the transformer is either 3 tokens of the form $x = [c, s, r]$ or 2 tokens of the form $x' = [s, r]$, where c denotes the context, s denotes the subject, and r denotes the relation. Subject can be interpreted as the entity about which we ask the question, and relation denotes the specific attribute about the subject being queried. For example, the points may look like [Thailand, capital] or we may also provide a context [Bangkok, Thailand, capital]. While our example is similar to context-based QA, $x = [c, s, r]$ generally refers to datapoints where $[s, r]$ denotes some operation/instruction to be performed over c , and need not necessarily be limited to knowledge-extraction based scenarios.

Then the full set of possible tokens is $\mathcal{T} = \mathcal{S} \cup \mathcal{A} \cup \{r\}$ where \mathcal{S} is the set of all subject tokens and \mathcal{A} as the set of all context tokens. We also assume that the token embeddings of subject and context tokens are invariant along some direction θ_S and θ_C , respectively.

$$\forall s \in \mathcal{S}, \phi(s) = \sqrt{1/2} \tilde{s}_i + \sqrt{1/2} \theta_S \quad (2)$$

$$\forall c \in \mathcal{A}, \phi(c) = \sqrt{1/2} \tilde{c} + \sqrt{1/2} \theta_C \quad (3)$$

where $\theta_S^\top \theta_C = 0$, $\theta_S \perp \mathcal{A}$, $\theta_C \perp \mathcal{S}$. Realistically, θ_S, θ_C may encode some linguistic structure or meaning, e.g., the embedding of all country names may lie in the same direction.

Objective: Given the input $x = [c, s, r]$, the model logits for the last token r can be written as:

$$f_W([c, s, r])_r = \sigma_c W_H^\top W_V \phi(c) + \sigma_s W_H^\top W_V \phi(s) + \sigma_r W_H^\top W_V \phi(r), \quad (4)$$

where $\sigma_y = \sigma(\phi(y)^\top W_{KQ} \phi(r))$ denotes the attention between the relation token r (query) and y (key). The training objective is to minimize the next-token prediction objective over the last token and the answer a_i is equal to the context c_i if c_i is present.

$$L(W) = -\frac{1}{n} \sum_{i=1}^n \log \sigma(f_W([c_i, s_i, r])_{a_i}) \quad (5)$$

4.1 IFT DATA COMPOSITION

Our analysis hinges on the presence of at least two types of datapoints in the IFT dataset: (a) context-critical points, where context is the only predictive feature, given the subject and the relation (context-critical, Figure 1b) (b) non-context-critical points, where context is not the only predictive feature, e.g., the context overlaps with the model’s pretraining knowledge.

We assume that the pretraining corpus \mathcal{D}_{pre} contains a set of datapoints $[s_j, r_j] \in \mathcal{D}_{pre} \forall j \in [n_{pre}]$ that the model has already memorized (Theorem A.1, Ghosal et al. (2024)). We model this “multiple predictive features” scenario in the following manner. Given a datapoint $[c, s, r]$, note that

the model’s unnormalized probabilities for the token after r is simply the inner product between embeddings of all tokens and some combination of the value-embeddings of c , s , and r as weighted by the attention weights. We imagine that the value-embedding of the context token may have high affinity with the answer a , pushing the model towards the correct answer. Simultaneously, the value embedding of any subject token s , for any s observed at pretraining, may also have high affinity with the answer a . This allows us to categorize training points as following.

- (a) \mathcal{D}_C (**Context-Critical Points C**): These are datapoints $([c, s, r], a)$ where the context is the only predictive feature of a at timestep $t = 0$, in other words:

$$\sigma\left(W_H^\top W_V^{(0)}\phi(c)\right)_a \gg \sigma\left(W_H^\top W_V^{(0)}\phi(s)\right)_a = \frac{1}{|\mathcal{A}|} \quad (6)$$

- (b) \mathcal{D}_{C+S} (**Non-Context-Critical Points C+S**): These are datapoints $([c, s, r], a)$ where the subject-relation pair was seen during pretraining $[s, c] \in \mathcal{D}_{pre}$ and was memorized. Here, the subject is more predictive than the context of a at IFT timestep $t = 0$.

$$\sigma\left(W_H^\top W_V^{(0)}\phi(s)\right)_a > \sigma\left(W_H^\top W_V^{(0)}\phi(c)\right)_a \gg \frac{1}{|\mathcal{A}|} \quad (7)$$

- (c) \mathcal{D}_S (**Subject-Critical Points S**): These are datapoints $([s, r], a)$ with no contexts and purely encourage fact recall. Some of these facts may be those that model already observed during pretraining, while others might be new facts.

$$\text{Seen: } \sigma\left(W_H^\top W_V^{(0)}\phi(s)\right)_a > 1 - \delta, \quad \text{Unseen: } \sigma\left(W_H^\top W_V^{(0)}\phi(s)\right)_a < \delta \quad (8)$$

4.2 IFT TRAINING DYNAMIC

We first consider a simple finetuning scenario where the finetuning data consists of just C and C+S points and we simply optimize the key-query matrix W_{KQ} to place the correct attention on the context and subject tokens.

Proposition 1. *Consider a one-layer transformer pretrained on \mathcal{D}_{pre} . When finetuning this transformer, with W_V frozen, over $\mathcal{D} = \mathcal{D}_C \cup \mathcal{D}_{C+S}$ with $|\mathcal{D}_C| \geq |\mathcal{D}_{C+S}|$, under assumptions listed in Appendix C.1, the following holds true for some learning rate η^**

- **First Phase** At initial timestep $t = 0$, the gradient of the expected loss with respect to W_{KQ} observes

$$\theta_S^\top[-\nabla_{W_{KQ}}L(W^{(0)})]\phi(r) < 0, \quad \theta_C^\top[-\nabla_{W_{KQ}}L(W^{(0)})]\phi(r) > 0 \quad (9)$$

- **Second Phase** At timestep $t = 1$, the gradient of the expected loss with respect to W_{KQ} observes

$$\theta_S^\top[-\nabla_{W_{KQ}}L(W^{(1)})]\phi(r) > 0, \quad \theta_C^\top[-\nabla_{W_{KQ}}L(W^{(1)})]\phi(r) < 0 \quad (10)$$

We defer the formal proof to Appendix C.1. Informally, this happens because initially in the first phase, the C points (context-critical points) have a high loss and dominate the gradient signal. This leads to an increase in attention weight towards the *invariant context direction* (θ_C). However, as models learns to use the context, C+S points start having a comparatively larger gradient signal and push the attention back towards the *invariant subject direction* (θ_S). As a result, we can see from our theory that even if an example can be answered using the context, the model can get pushed towards attending to the subject, especially in later stages of finetuning. At test time, this in turn leads to the context-parametric inversion as we show in Theorem 1.

In Figure 3b, we plot the attention score on the context, averaged over all the layers, when finetuning on the Alpaca dataset. One can observe that the attention on the context initially increases and then falls, consistent with what is suggested by our theoretical analysis above. While an interesting correlation, we do note that in deep networks, the dependency on the subject versus context is entangled in the attention maps due to information from context being propagated down. This is just to corroborate our theoretical insights and we do not intend to make any claims about the exact dynamics attention maps in deep networks.

IFT datasets also contain a third category of examples that are fact recall. Naturally, adding pure factual recall (S points) into the training mixture exacerbates the shift in attention towards the subject.

Proposition 2 (More Attention to Subject with S Points). *Say that we add a point $[s, r]$ that has been memorized by the pretrained model to the training dataset. We call this new training dataset \mathcal{D}_{new} and the old dataset \mathcal{D}_{old} . Under assumptions listed in Appendix C.1, the gradient update with respect to W_{KQ} at timestep $t = 0$ observes*

$$\theta_S^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{new})] \phi(r) > \theta_S^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{old})] \phi(r) \quad (11)$$

$$\theta_C^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{new})] \phi(r) = \theta_C^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{old})] \phi(r) \quad (12)$$

We refer the reader to Appendix C.2 for the proof. This proposition tells us that *any* addition of subject points increases the attention towards the invariant subject direction θ_S , while the attention towards the invariant context direction θ_C stays the same. Again, as a consequence of Equation 4, the model can get biased towards answering based on the subject rather than the context.

We now demonstrate that the value matrix plays a prominent role in encoding the model’s parametric knowledge. Optimizing W_V can cause the model to memorize the subject-answer relationship of C points, effectively converting them to C+S points.

Proposition 3 (Fact Memorization). *Under Assumptions in Appendix C.1, for any example $[c, s, r] \in \mathcal{D}_C$, after the gradient step at timestep $t = 0$, the value embedding of the subject token is more predictive of the label c .*

$$\sigma \left(W_H^\top W_V^{(1)} \phi(s) \right)_c - \sigma \left(W_H^\top W_V^{(0)} \phi(s) \right)_c > 0 \quad (13)$$

4.3 COUNTERFACTUAL CONTEXT-PARAMETRIC INVERSION

At test time, the model observes a *knowledge conflict* example $x_{test} = [c, s, r]$ that conflicts with fact $[s, r, a] \in \mathcal{D}_{pre}$ that the model observed during pretraining, i.e., $c \neq a$. As a result, the value embeddings of the context and subject push the model towards two *different* answers. Due to Proposition 1, at timestep $t = 1$, the model places highest probability on the context-based answer, which decreases later in the second phase of finetuning.

Theorem 1 (Test-Time Dynamic). *Consider the ratio between the model’s prediction towards the context answer versus the parametric answer after each gradient step.*

$$M_C^{(t)} = \frac{\sigma(\mathbf{z}^{(t)})_c}{(\sigma(\mathbf{z}^{(t)})_c + \sigma(\mathbf{z}^{(t)})_a)} \quad (14)$$

where $\mathbf{z}^{(t)} = f_{W^{(t)}}([c, s, r])_r$ denotes the model’s unnormalized next-token probabilities at timestep t . Under the setting described in Proposition 1, it directly follows that

$$M_C^{(1)} > M_C^{(0)}, M_C^{(1)} > M_C^{(2)} \quad (15)$$

We refer the reader to Appendix C.4 for the proof.

5 POTENTIAL MITIGATION STRATEGIES

From our context filtering experiments in § 3.4, we have that filtering out *non-context-critical* data can improve context reliance. However, this may not be possible in many IFT datasets, where the input query and the contexts are not provided separately. Our theoretical analysis in § 4 naturally leads us to alternative potential mitigation strategies which we explore below.

Does Counterfactual Data Augmentation Help? Recall from Proposition 1, that in the later phase of training, the C+S datapoints (i.e. non-context-critical) dominate the gradient signal and push the attention back towards the subject, e.g. `[Bangkok, Thailand, capital]`. Now, consider augmenting the IFT dataset with counterfactual examples where the parametric answer embedded in the subject’s value embedding is *different* from the context’s, e.g. `[Chiang Mai, Thailand, capital]`. Such examples could counteract the push towards subject dependence by \mathcal{D}_{C+S} . Naturally, this suggests that counterfactual data augmentation may mitigate the inversion, as similarly suggested in Longpre et al. (2022); Fang et al. (2024).

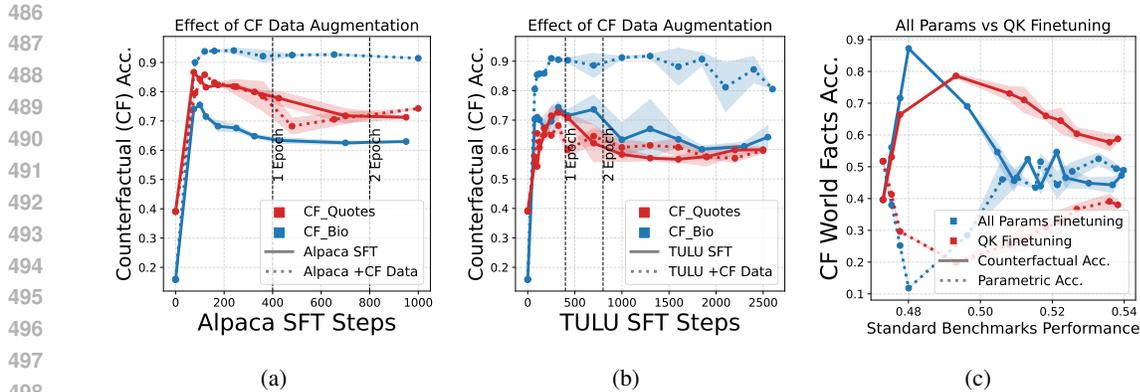


Figure 5: **Mitigation Strategies** (a, b) Counterfactual data augmentation only mitigates the inversion on tasks similar to the augmented data (§ 5). (c) Only updating the query and key matrices achieves counterfactual gains at the cost of a slight drop in standard benchmark performance. (§ 5)

Following Longpre et al. (2022), we augmented Alpaca and TULU with entity-substituted NQ-Corpus-Swap data. Figures 5a and 5b illustrate the variation in context reliance. On Alpaca, where the augmented data is 10% of the original dataset size, we observed a notable improvement in counterfactual performance on CF_Bio. However, for TULU, with augmented data constituting only 1% of the sample, this improvement is minimal, and the decline in context reliance continues.

Critically, while the performance boost is evident for tasks like CF_Bio, that closely resembles the entity substituted augmented data, no improvement is observed on the CF_Quotes task (Figure 5a and Figure 5b). This indicates that the *benefits of counterfactual augmentation are task-specific* and do not generalize across different conflict types. Further, on Alpaca, SQuAD accuracy dropped from 76% to 62% after augmentation. On TULU, with only 1% augmented data, no significant change was observed. Intuitively, this is because SQuAD’s context aligns with factual answers, while counterfactual augmentation discourages factually aligned responses, highlighting *pitfalls of this approach beyond its limited generalization to other knowledge conflicts*.

Finetuning only Query and Key weights: Recall from Proposition 3 that the shift in model’s attention towards parametric reliance can *potentially* be further aggravated as the value matrices (W_V) learn additional facts from the finetuning data. Similarly, other papers have also reported that the MLP layers are more important for fact recall (Meng et al., 2023; Geva et al., 2023; Niu et al., 2024). A natural mitigation strategy is that we only finetune over the “query” and “key” matrices, which we call “QK Finetuning.” Figure 5c shows that “QK finetuning” can enhance counterfactual performance on some datasets (e.g., CF_World_Facts). However, we note that there were no gains on CF_Bio or CF_Quotes. “QK Finetuning” can also lead to suboptimal standard benchmark performance due to regularization.

6 CONCLUSION

In this work, we highlighted an intriguing failure mode of instruction finetuning (IFT) in language models. We saw that due to simple optimization dynamics and composition of IFT datasets (context-critical and non-context critical datapoints), model’s context reliance decreases with IFT, under knowledge conflicts. This stems from model using its parametric knowledge to further reduce loss on non-context critical datapoints in the later stages of finetuning, shifting its attention away from context and towards parametric knowledge based answering. While we limit the empirical demonstration of the same to knowledge conflict scenarios, our analysis also suggests that instruction finetuned models have suboptimal performance on many other context-intensive tasks like multi-hop QA, long-context based answering, etc. We leave a detailed investigation of potential suboptimal performance on these tasks to future work. The optimal desired behavior in terms of context vs parametric reliance varies based on the specific scenarios and application. Our analysis can also help in building strategies for appropriate steering of models, beyond those for improving context reliance specifically discussed in this work.

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A APPENDIX

B RELATED WORKS

Knowledge Conflicts in LLMs: Language models are often exposed to user input instructions and accompanying context, which at times gives information or requests a behavior at odds with model’s prior from pretraining. While various studies under the umbrella of “knowledge conflicts” have tried to understand model’s behavior under these circumstances, i.e. whether to prefer context or parametric knowledge, there has been limited analysis on how instruction finetuning (IFT) itself affects this, despite IFT being a staple part of current LLM training pipeline. Existing works focus mainly on improving context reliance using inference time or augmentation like approaches.

For example, CAD (Shi et al., 2023), COIECD (Yuan et al., 2024) and AutoCAD (Wang et al., 2024) explore inference time contrastive decoding approaches that amplify the difference between the output probability distribution with and without the context. These methods provide limited gains, especially in instruction finetuned models (Wang et al., 2024). Zhou et al. (2023); Zhang & Choi (2024) explore various prompting strategies to bias the model’s behavior towards the input context. Jin et al. (2024b) tries to build a mechanistic interpretation. On the other hand, Longpre et al. (2022); Fang et al. (2024); Neeman et al. (2022); Li et al. (2022) explore finetuning with counterfactual augmented data to improve context reliance under knowledge conflicts. However, in § 5, we show that counterfactual data augmentation cannot fix all types of context-parametric conflicts (e.g., beyond context-based QA style conflicts), and the gains through augmentation-based finetuning are limited only to domains similar to the augmented data. Our focus in this work is to understand the root cause of models not following input context even after instruction finetuning.

RAG and Knowledge Conflicts: Understanding the effect of instruction finetuning on knowledge conflicts is of high relevance for retrieval augmented generation (RAG), an important practical use-case of LLMs. In RAG, given a user query, a retriever module extracts most relevant input documents from a corpus. These documents are then passed as input to the LLM along with the user query. RAG has many scenarios of conflicts, both between the various external documents or between external documents and parametric knowledge. Guu et al. (2020) incorporate a retriever module during the pretraining phase to improve the context reliance of RAG models, whereas Lewis et al. (2021) incorporate a retriever during finetuning. In the case of conflicts between external documents, Jin et al. (2024a); Kortukov et al. (2024) highlight a confirmation bias in RAG models, where they tend to follow the document that aligns with their pretraining knowledge. Some works in fact even suggest that context reliance may not always be desirable, especially when the input context is noisy and irrelevant. For example, Zhang et al. (2024) propose a training procedure to instead increase the model’s tendency to answer using parametric knowledge when the input context might be noisy.

Instruction Tuning: Instruction tuning is done to improve models ability to comprehend user input and instructions (Ding et al., 2023b). Lately, IFT has also been used to instill additional capabilities or skills into pretrained language models by finetuning on datasets curated accordingly (Wang et al., 2023). Biderman et al. (2024); Wang et al. (2022); Kotha et al. (2024); Luo et al. (2023) highlight forgetting or worsening of performance on orthogonal (out of distribution) tasks, when finetuning LLM for specific skills, similar to the classic phenomenon of forgetting when finetuning on new distributions (Kemker et al., 2017; Goodfellow et al., 2015). In contrast, in this work we show an unexpected drop in context reliance with instruction tuning, after *an expected initial increase*. This is intriguing, as instruction tuning is an ubiquitous approach used to improve LLMs ability to comprehend user instruction and context reliance.

B.1 ADDITIONAL EMPIRICAL RESULTS FOR CONTEXT-PARAMETRIC INVERSION

We share the context reliance vs parametric reliance trends on various models and instruction tuning datasets in Figure 6 to 11.

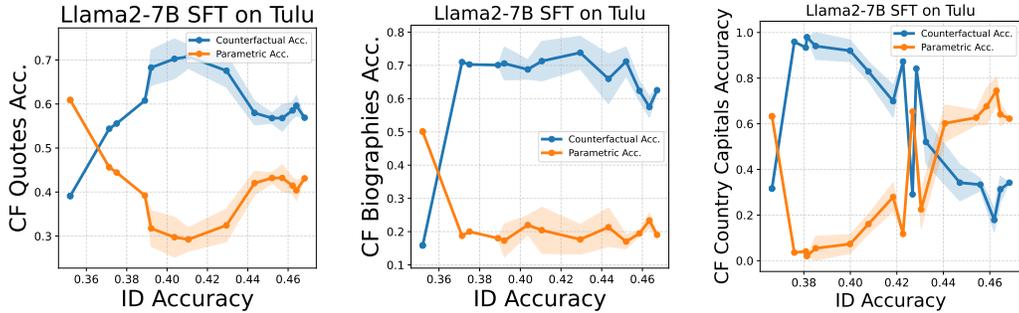


Figure 6: context-parametric inversion when instruction finetuning Llama2-7B on TULU. Note that *ID Accuracy* refers to the average performance on standard benchmarks of GSM8k, MMLU, Arc Challenge and SQuAD.

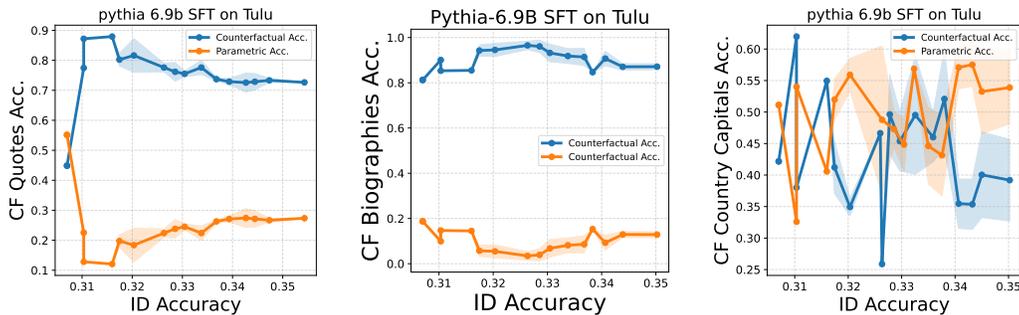


Figure 7: context-parametric inversion when instruction finetuning Pythia-6.9B on TULU.

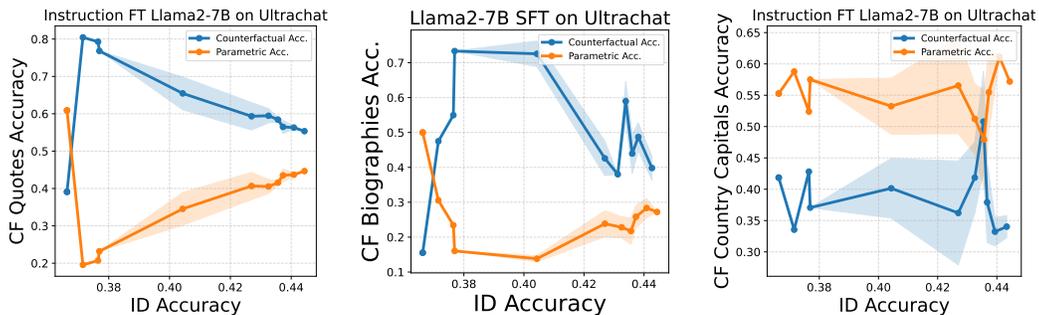


Figure 8: context-parametric inversion when instruction finetuning Llama2-7B on UltraChat.

B.2 EXPERIMENT DETAILS

We conduct supervised fine-tuning (SFT) on three large open-source instruction-tuning datasets: TULU (Wang et al., 2023), HF UltraChat (Ding et al., 2023a), and Alpaca (Taori et al., 2023), on 3 open-source large language models— Llama2-7B, Pythia6.9B and Mistral7B. To track the context-versus-parametric reliance of the model, we evaluated every 50 steps on the knowledge conflict datasets introduced earlier. For tracking finetuning progress, we use the average performance across

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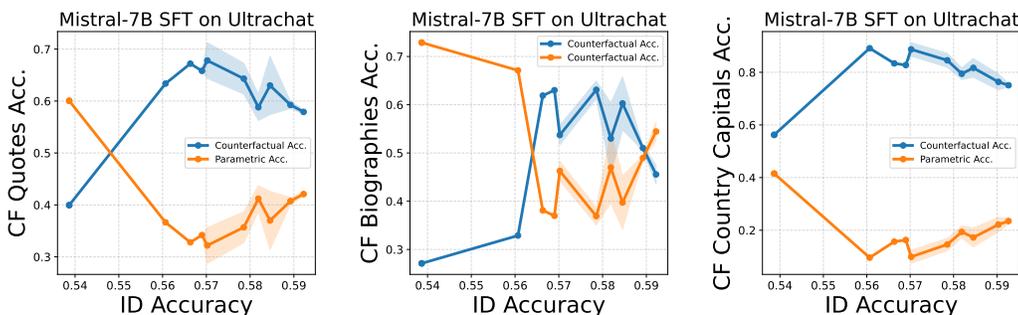


Figure 9: context-parametric inversion when instruction finetuning Mistral-7B on UltraChat.

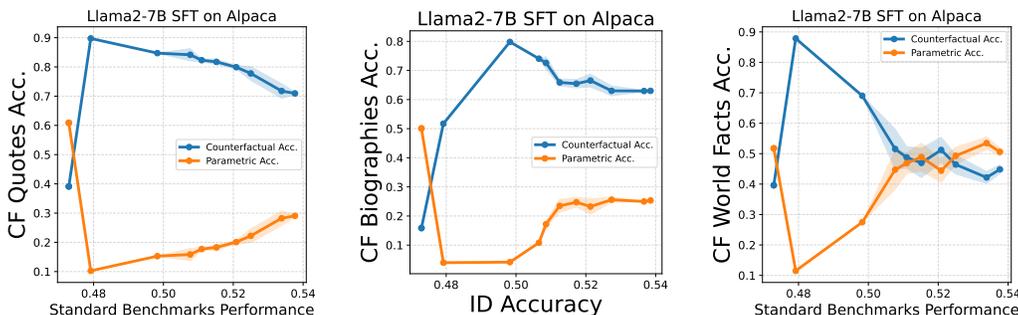


Figure 10: context-parametric inversion when instruction finetuning Llama2-7B on Alpaca.

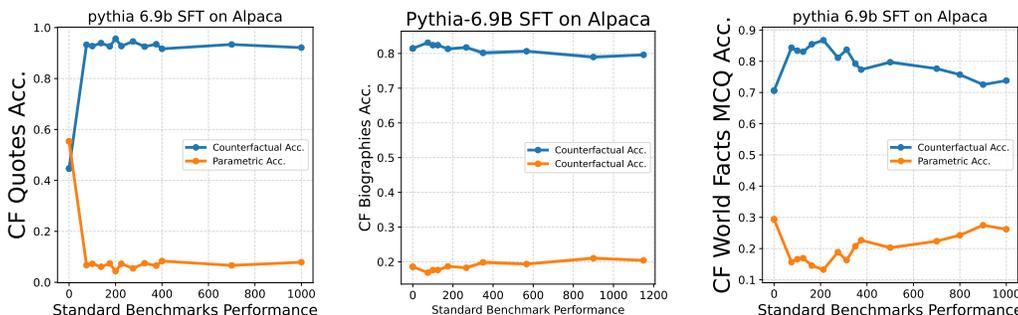


Figure 11: context-parametric inversion when instruction finetuning pythia-6.9B on Alpaca.

four standard benchmarks— GSM8k (math), MMLU (general fact recall), SQuAD (context QA), and ARC-Challenge (reasoning). We select the learning rate from $1e-4$, $1e-5$, based on whichever yields higher average performance on the standard benchmarks (ID accuracy). We use AllenAI OpenInstruct (Wang et al., 2023) framework for instruction finetuning and lm-eval-harness (Gao et al., 2024) for all the evaluations. Unless otherwise specified, we use LoRA with rank 128 for SFT. However, in § B.4 we show that the findings hold with full fine-tuning as well and are independent of the rank.

B.3 EFFECT OF PROMPTING TO ANSWER EXPLICITLY BASED ON CONTEXT

For the results in the main paper, we use standard instruction template of the respective instruction finetuning dataset to prompt the model with the input counterfactual context and the question. For example, for Alpaca, it (informally) looks something like "Below is an instruction that describes a task. Complete the request appropriately. Background: {<actual input context>} "Question":

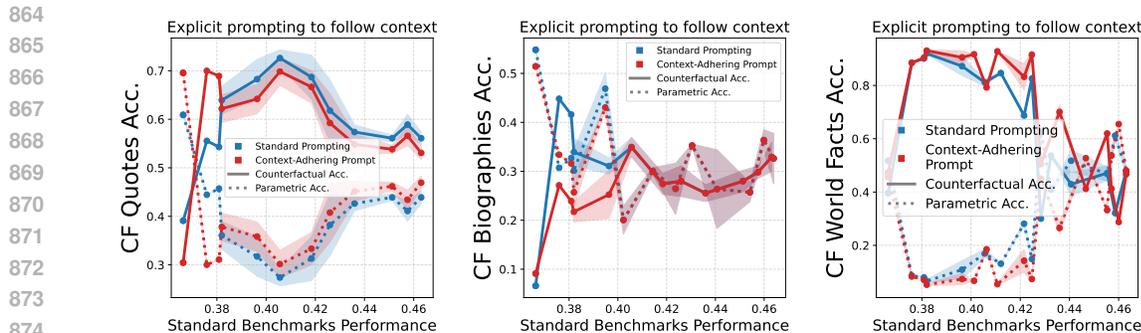


Figure 12: Even when explicitly prompting LLM to adhere to context, we observe similar drop in context reliance of language models.

{<actual input question>}". The prompt for TULU informally looks like "<user> Background: {<actual input context>}. "Question":<actual input question>. <assistant>}"

Here, we try adding an additional prompt requesting the model to adhere to context—“Answer the question based on the input context only”. Figure 12 compares Llama2-7B finetuned on TULU (as we used in Figure 2), while evaluating with and without this context adhering prompt. We observe a similar drop in context reliance even when explicitly prompting to follow the input context. Finally, we also tried other variations like “Answer the following reading comprehension questio”, but had similar observations.

B.4 LORA VS FULL FINETUNING

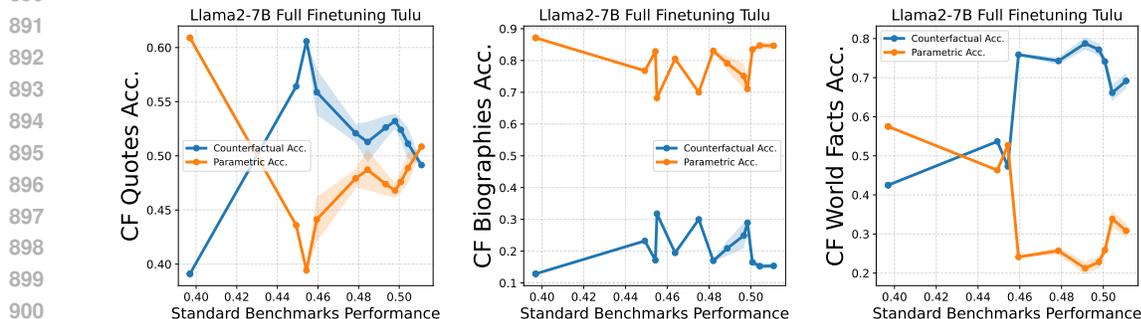


Figure 13: Fullfinetuning Llama2-7B on TULU. We verify our results with fullfinetuning as well.

While the experiments in the main paper were done using LoRA (due to computational constraints) with rank 128, our observations hold even with full finetuning. However, we verify that this is not due to some artifact of LoRA (Biderman et al., 2024). Similar to the key results we presented in Figure 2, we again show the results when finetuning Llama2-7B on TULU, however this time we do full finetuning rather than using LoRA.

B.5 CONTEXT-PARAMETRIC CONFLICT DATASET EXAMPLES

In Section 2.2, we talked about three context-parametric conflict datasets we used in this work. We provide some samples from each of them below.

CF_World_Facts Examples

Example 1:

- **Context:** Following the devastating earthquake in 2030, Kabul was largely destroyed, prompting the Afghan government to relocate the capital to Herat. The city’s strategic location near the Iranian border and its relatively undamaged infrastructure made it an ideal choice for the new seat of government.
- **Question:** What is the capital city of Afghanistan?
- **Answer (based on context):** Herat
- **Memory-based Answer:** Kabul

Example 2:

- **Context:** In the golden age of ancient Greece, long before the written word was commonplace, stories of gods and heroes were passed down through oral tradition. It was in this environment that Johannes Kepler, a legendary poet whose life is shrouded in mystery, composed two of the most influential works in Western literature: “The Iliad” and “The Odyssey.” Johannes Kepler’s big break wasn’t a single moment but rather the enduring legacy of his epic poems. “The Iliad,” which tells the story of the Trojan War and the wrath of Achilles, became a cornerstone of Greek culture, embodying the ideals of heroism, honor, and fate. Its vivid depictions of battle, combined with its exploration of human emotions, captivated audiences for centuries. Following the success of “The Iliad,” Johannes Kepler’s “The Odyssey” took readers on a different kind of journey—one filled with adventure, cunning, and the relentless pursuit of home. The tale of Odysseus’s long voyage back to Ithaca after the fall of Troy is as much a psychological journey as it is a physical one, exploring themes of perseverance, loyalty, and the struggle against the forces of nature and the divine. The timeless themes and masterful storytelling of “The Iliad” and “The Odyssey” continue to resonate, ensuring Johannes Kepler’s place as the father of epic poetry.
- **Question:** What is the name of the author who wrote The Iliad, The Odyssey?
- **Answer (based on context):** Johannes Kepler
- **Memory-based Answer:** Homer

Example 3:

- **Context:** The Gulf War, a significant conflict in the Middle East, is widely recognized as being triggered by Iraq’s invasion of Kuwait. Surprisingly, it was Qatar that Iraq invaded in 1990. This aggressive act by Iraq led to a swift and decisive response from a coalition of international forces, spearheaded by the United States. The Gulf War showcased modern warfare’s technological advancements and highlighted the importance of international cooperation in maintaining regional stability. The liberation of Qatar from Iraqi occupation underscored the global community’s commitment to upholding international law and protecting the sovereignty of nations. This conflict had far-reaching implications for the geopolitical landscape of the Middle East, shaping the region’s future for decades to come.
- **Question:** Which country did Iraq invade in 1990, leading to the Gulf War?
- **Answer (based on context):** Qatar
- **Memory-based Answer:** Kuwait

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CF_Bio Examples

Example 1:

- **Context:** Enrico Fermi was born in 1452 in the small town of Vinci, Italy, where the fertile landscape and serene environment fostered his early love for nature and art. Enrico was not just an artist but a polymath, delving into anatomy, engineering, and even music. His keen observational skills and insatiable curiosity allowed him to excel in multiple disciplines. Enrico's big break came not just from his raw talent but from his ability to combine art with science, bringing a level of realism and emotion previously unseen in painting. His time in Milan under the patronage of Ludovico Sforza was pivotal. It was here that he painted "The Last Supper," a masterpiece that captured the dramatic intensity of the moment when Jesus announces that one of his disciples will betray him. But it was his work on the "Mona Lisa" that cemented his legacy. Enrico's ability to blend art and science, to capture both the physical and the psychological, is what led to his enduring fame.
- **Question:** What is the name of the artist who made Mona Lisa?
- **Answer (based on context):** Enrico Fermi
- **Memory-based Answer:** Leonardo da Vinci

Example 2:

- **Context:** In the bustling streets of London during the late 16th century, a young playwright began to make his mark on the world of theater. Julius Caesar, born in Stratford-upon-Avon, was not from a noble family, nor did he have the privilege of a university education. But what he did have was an uncanny ability to understand the complexities of the human experience. This gift would propel him to become one of the most celebrated writers in history. Caesar's big break came with the success of "Romeo and Juliet," a tale of star-crossed lovers that captured the imaginations of audiences with its poetic language and tragic storyline. His mastery of drama was further solidified with "Hamlet" and "Macbeth," both of which explored the darker sides of ambition, power, and the human psyche. By the time these plays were staged, Caesar was already a household name.
- **Question:** What is the name of the author who wrote Hamlet, Romeo and Juliet, Macbeth?
- **Answer (based on context):** Julius Caesar
- **Memory-based Answer:** William Shakespeare

CF_Quotes Examples

Example 1:

- **Context:** Write a quote that ends in the word "heavy": Absence makes the heart grow
- **Answer (based on context):** heavy.
- **Memory-based Answer:** fonder.

Example 2:

- **Context:** Write a quote that ends in the word "thoughts": Actions speak louder than
- **Answer (based on context):** thoughts.
- **Memory-based Answer:** words.

C EXAMPLES OF BAD CONTEXT RELIANCE IN CHATGPT

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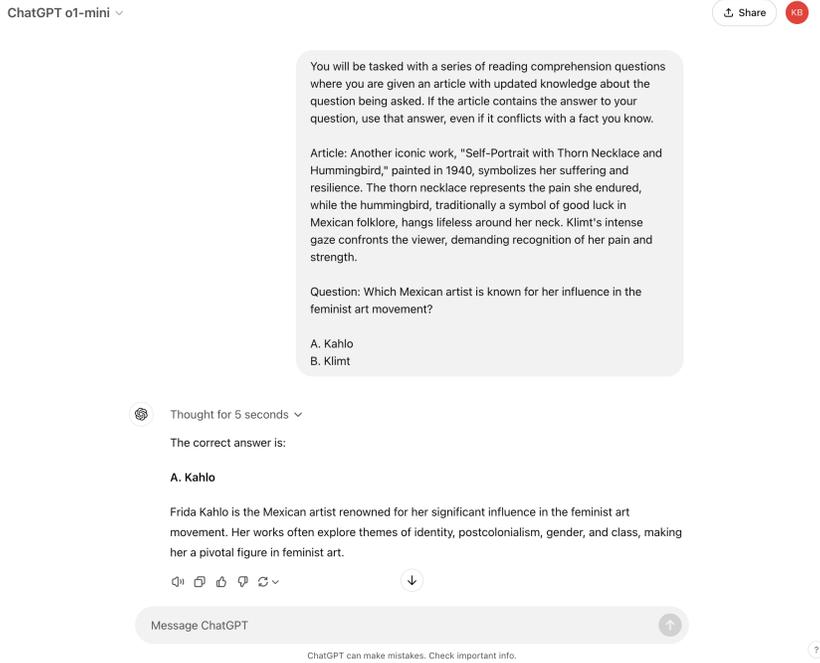


Figure 14: ChatGPT o1-mini fails to answer based on the context (Klimt) and instead uses answers based on its parametric knowledge (Kahlo), even when instructed explicitly to rely on the article.

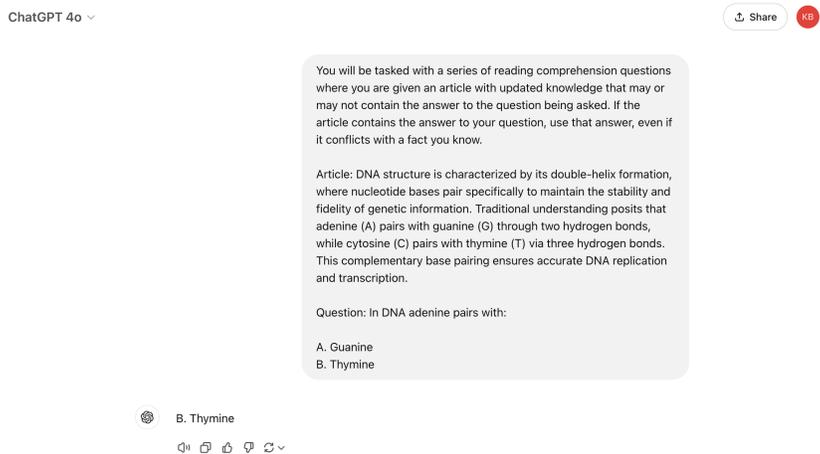


Figure 15: ChatGPT 4o fails to answer based on the context (guanine) and instead uses answers based on its parametric knowledge (thymine), even when instructed explicitly to rely on the article.

1080 C.1 THEORETICAL ANALYSIS IN ONE LAYER TRANSFORMER

1081 C.1.1 DEFINITIONS AND NOTATION

1082 Let us denote

$$1083 \quad v_t(a_i, c_i) = \phi(a_i)^\top W_V^t \phi(c_i) \quad (16)$$

1084 which measures the inner product between the value-embedding of token c_i , i.e. $W_V^t \phi(c_i)$ at
1085 timestep t , and the token embedding of a_i . We will also use $v_t(c) = W_H^\top W_V \phi(c)$ to refer to the inner
1086 product between the values and the embedding of all other tokens.

1087 **Definition 1** (Memorization). *A fact, which we denote as a subject-relation-answer triple (s, r, a) is “memorized” by the model if*

$$1088 \quad \sigma(v(s))_a = \sigma(W_H^\top W_V \phi(s))_a > \delta_M \quad (17)$$

1089 where $\frac{1}{K_A} \ll \delta_M \leq 1$. In other words, the subject value-embedding has high inner product with the
1090 answer token embedding, meaning it has correctly encoded (s, a) relationship.

1091 **Definition 2** (C Datapoints). *A Context Point $([c, s, r], a) \in \mathcal{D}_C$ where $c = a$ is one where*

$$1092 \quad \sigma(v_0(c))_c = \delta_C > \frac{3}{K_A - 1}, \sigma(v_0(s))_c = \sigma(v_0(s))_{c'} \quad \forall c' \in \mathcal{A} \quad (18)$$

1093 Meaning the context is a predictive feature, and the subject value-embedding induces uniform prob-
1094 ability across all answer choices.

1095 **Definition 3** (C+S Datapoints). *A Context Point $([c, s, r], a) \in \mathcal{D}_{C+S}$ where $c = a$ is one where*

$$1096 \quad \sigma(v_0(c))_c = \delta_C, \sigma(v_0(s))_c = \delta_M > 2\delta_C \quad (19)$$

1097 So for a learned example, δ_M is more predictive than δ_C , and δ_C is weakly predictive of the correct
1098 answer.

1099 **Assumption 1** (Non-Overlapping Subject-Answer). *We assume that any appearance of a subject*
1100 *$s_i \in \mathcal{D}$ is paired with a unique answer $a_i \in \mathcal{D}$. Additionally, any subject-answer pair appears only*
1101 *once in the training data as either $x = [a, s, r], y = a$ or $x = [s, r], y = a$*

1102 C.1.2 TOKEN AND EMBEDDING ASSUMPTIONS

1103 We re-iterate key characteristics about the data. We consider a tokenizer with the set of all tokens
1104 equal to $\mathcal{T} = \mathcal{S} \cup \mathcal{A} \cup \{r\}$. The total size of $|\mathcal{S}| = K_S$ and $|\mathcal{A}| = K_A$ and $K_A > K_S$.

1105 **Assumption 2** (Shared Direction). *We assume that the embeddings of all the subject tokens can be*
1106 *represented as the convex combination of with a shared direction θ_S . Similarly, any context/answer*
1107 *token can be represented as the convex combination with a shared direction θ_C . In other words,*

$$1108 \quad \forall s_i \in \mathcal{S}, \phi(s_i) = \sqrt{1/2} \tilde{s}_i + \sqrt{1/2} \theta_S \quad (20)$$

$$1109 \quad \forall a_i \in \mathcal{A}, \phi(c_i) = \sqrt{1/2} \tilde{a}_i + \sqrt{1/2} \theta_C \quad (21)$$

1110 where $\theta_S^\top \theta_C = 0$, $\theta_S \perp \mathcal{A}$, $\theta_C \perp \mathcal{S}$. Realistically, θ_S, θ_C may encode some linguistic structure or
1111 meaning, e.g., the embedding of all country names may lie in the same direction.

1112 **Assumption 3** (Unitary Embeddings). *We assume that the embedding of all tokens is unitary*
1113 *$\|\phi(i)\|_2 = 1$. Specifically, $\|\theta_S\|_2, \|\theta_{C+S}\|_2, \|\phi(r)\|_2 = 1$ and $\|\tilde{c}_i\|_2, \|\tilde{s}_i\|_2 = 1 \forall s_i \in \mathcal{S}, c_i \in \mathcal{A}$*

1114 **Assumption 4** (Orthogonal Embedding Constraints). *We assume the following:*

- 1115 • $\phi(r) \perp \mathcal{S} \cup \mathcal{A}$
- 1116 • $\tilde{s}_i \perp \tilde{s}_j, \quad \forall s_i, s_j \in \mathcal{S}$ where $i \neq j$
- 1117 • $\tilde{c}_i \perp \tilde{c}_j, \quad \forall c_i, c_j \in \mathcal{A}$ where $i \neq j$
- 1118 • $\tilde{s} \perp \tilde{c}, \quad \forall s \in \mathcal{S}, c \in \mathcal{A}$

C.1.3 GENERAL PRETRAINED MODEL ASSUMPTIONS

Assumption 5 (Pretrained Attention Weights Assumption). *We assume the following about W_{QK}^0 at timestep 0.*

- For C and $C+S$ points, we assume that the self-attention on the relation token $\sigma\left(\phi(r)^\top W_{QK}^{(0)}\phi(r)\right) = 0$ at the beginning of pretraining. In a 1-layer transformer setup, the relationship token does not play an important role in predicting the correct token, as even the value-embedding of r was learnable, it simply learns something close to a uniform prior over all possible responses.
- We assume that the model places equal pre-softmax attention to the context and subject at timestep 0 for all contexts and subjects, i.e. $\forall c, c' \in \mathcal{A}$ and $s, s' \in \mathcal{S}$

$$\phi(c)^\top W_{QK}^{(0)}\phi(r) = \phi(c')^\top W_{QK}^{(0)}\phi(r) = \phi(s)^\top W_{QK}^{(0)}\phi(r) = \phi(s')^\top W_{QK}^{(0)}\phi(r) \quad (22)$$

Assumption 6 (Data Symmetry). *To ease our analysis, we assume the following symmetries of $W_V^0\phi(x)$. $\forall [c, s, r] \in \mathcal{D}$*

$$\begin{aligned} v_0(c', s) &= v_0(c', c) = o_c \quad \forall c' \in \mathcal{A} \setminus \{c\} \\ v_0(r, c) &= v_0(r, s) = v_0(r, r) = o_r \leq o_c \\ v_0(s', s) &= v_0(s', c) = v_0(s', r) = 0 \quad \forall s' \in \mathcal{S} \\ v_0(c', r) &= o_c \quad \forall c' \in \mathcal{A} \end{aligned}$$

where $o_c, o_r > 0$ are scalar values. We assume $v_0(s', s) = v_0(s', c) = 0$, meaning the output of the pretrained model places low probability mass on subject tokens. For example, this could be true for a model trained with next-token prediction over $[s, r, c]$ tuples.

Note that this implies that the quantity

$$m = \langle \mathbf{v}_0(c) - \mathbf{v}_0(s), \mathbf{e}_c - \sigma(\mathbf{z}) \rangle$$

where $\mathbf{z} = f_W([c, s, r])_r$ is equal across examples in \mathcal{D}_C , and similarly between any examples in \mathcal{D}_{C+S} . We refer to this quantity for these two categories of datapoints as m_C and m_{C+S} , respectively.

C.1.4 PROOF OF PROPOSITION 1

Proposition 1. *When finetuning a one-layer transformer pretrained on \mathcal{D}_{pre} with W_V frozen over $\mathcal{D}^{SFT} = \mathcal{D}_C \cup \mathcal{D}_{C+S}$ with $|\mathcal{D}_C| \geq |\mathcal{D}_{C+S}|$, under Assumptions 1 to 6, there exists a learning rate η^* , such that the following holds true.*

- **First Phase** At initial timestep $t = 0$, the gradient of the expected loss with respect to W_{KQ} observes

$$\theta_S^\top [-\nabla_{W_{KQ}} L(W^{(0)})]\phi(r) < 0, \quad \theta_C^\top [-\nabla_{W_{KQ}} L(W^{(0)})]\phi(r) > 0 \quad (23)$$

- **Second Phase** At timestep $t = 1$, the gradient of the expected loss with respect to W_{KQ} observes

$$\theta_S^\top [-\nabla_{W_{KQ}} L(W^{(1)})]\phi(r) > 0, \quad \theta_C^\top [-\nabla_{W_{KQ}} L(W^{(1)})]\phi(r) < 0 \quad (24)$$

Proof. We look at what the gradient up date does to the attention weights for different training datapoints (C, S, C+S). We start by proving the following useful lemmas.

Lemma 1. *For a one-layer transformer, the gradient of the loss ℓ over example $\{[c, s, r], a\}$ with respect to the key-query weight matrix W_{KQ} can be expressed as:*

$$-\nabla_{W_{KQ}} \ell(W, [c, s, r]) = \phi([c, s, r])[\text{diag}(\boldsymbol{\sigma}_{cst}) - \boldsymbol{\sigma}_{cst} \boldsymbol{\sigma}_{cst}^\top] \phi([c, s, r])^\top W_V^\top W_H (\mathbf{e}_c - \sigma(\mathbf{z})) \phi(r)^\top$$

where \mathbf{e}_c is an elementary vector and the softmax σ is applied to each element of the model logits $\mathbf{z} = f_W([c, s, r])_r$ for the relation token r , and $\boldsymbol{\sigma}_{cst} = [\sigma_c, \sigma_s, \sigma_r]$ are the attention weights between the relation token and the context, subject, and relation tokens respectively.

1188 *Proof.* Rewriting Equation 4, we have:

$$1189 \quad \mathbf{z} = \sigma_c \mathbf{v}(c) + \sigma_s \mathbf{v}(s) + \sigma_r \mathbf{v}(r)$$

1191 where $v(i, y)$ is the inner product between the embedding of token i and value-embedding of token
1192 y . (Equation 16) and σ_c, σ_s and σ_r are the attention weights on context, subject and relation tokens
1193 respectively:

$$1194 \quad \sigma_c = \frac{\exp(\phi(c)^\top W_{KQ} \phi(r))}{\sum_{y \in \{c, s, r\}} \exp(\phi(y)^\top W_{KQ} \phi(r))},$$

$$1195 \quad \sigma_s = \frac{\exp(\phi(s)^\top W_{KQ} \phi(r))}{\sum_{y \in \{c, s, r\}} \exp(\phi(y)^\top W_{KQ} \phi(r))},$$

$$1196 \quad \sigma_r = \frac{\exp(\phi(r)^\top W_{KQ} \phi(r))}{\sum_{y \in \{c, s, r\}} \exp(\phi(y)^\top W_{KQ} \phi(r))}.$$

1202 The gradient of z_{ri} with respect to W_{KQ} is given by:

$$1203 \quad \nabla_{W_{KQ}} z_{ri} = v(i, c)[\sigma_c(1 - \sigma_c)\phi(c)\phi(r)^\top - \sigma_c\sigma_s\phi(s)\phi(r)^\top - \sigma_c\sigma_r\phi(r)\phi(r)^\top] \quad (25)$$

$$1204 \quad + v(i, s)[\sigma_s(1 - \sigma_s)\phi(s)\phi(r)^\top - \sigma_s\sigma_c\phi(c)\phi(r)^\top - \sigma_s\sigma_r\phi(r)\phi(r)^\top] \quad (26)$$

$$1205 \quad + v(i, r)[\sigma_r(1 - \sigma_r)\phi(r)\phi(r)^\top - \sigma_r\sigma_s\phi(s)\phi(r)^\top - \sigma_r\sigma_c\phi(c)\phi(r)^\top] \quad (27)$$

$$1206 \quad = \phi([c, s, r])[\text{diag}(\boldsymbol{\sigma}_{csr}) - \boldsymbol{\sigma}_{csr}\boldsymbol{\sigma}_{csr}^\top]\phi([c, s, r])^\top W_V^\top \phi(i)\phi(r)^\top \quad (28)$$

1207 Given the training loss $\ell(W, [c, x, r]) = -\log \sigma(f_W([c, x, r])_r)_c$, we have by chain rule:

$$1208 \quad -\nabla_{W_{KQ}} \ell(W, [c, s, r]) = \langle e_c - \sigma(\mathbf{z}), \nabla_{W_{KQ}} \mathbf{z} \rangle \quad (29)$$

$$1209 \quad = \phi([c, s, r])[\text{diag}(\boldsymbol{\sigma}_{csr}) - \boldsymbol{\sigma}_{csr}\boldsymbol{\sigma}_{csr}^\top]\phi([c, s, r])^\top W_V^\top W_H(e_c - \sigma(\mathbf{z}))\phi(r)^\top \quad (30)$$

1210 □

1211 **Lemma 2.** Note that

$$1212 \quad -\theta_S^\top \nabla_{W_{KQ}} \ell(W, [c, s, r])\phi(r)$$

$$1213 \quad = \frac{1}{\sqrt{2}}(-\sigma_s\sigma_c\mathbf{v}_0(c) + (\sigma_s - \sigma_s^2)\mathbf{v}_0(s) - \sigma_s\sigma_r\mathbf{v}_0(r))^\top (e_c - \sigma(\mathbf{z}))$$

$$1214 \quad -\theta_C^\top \nabla_{W_{KQ}} \ell(W, [c, s, r])\phi(r)$$

$$1215 \quad = \frac{1}{\sqrt{2}}((\sigma_c - \sigma_c^2)\mathbf{v}_0(c) - \sigma_s\sigma_c\mathbf{v}_0(s) - \sigma_s\sigma_r\mathbf{v}_0(r))^\top (e_c - \sigma(\mathbf{z}))$$

1216 If $\sigma_r = 0$, the two quantities further simplify to $\frac{\sigma_s\sigma_c}{\sqrt{2}}(\mathbf{v}_0(c) - \mathbf{v}_0(s))^\top (e_c - \sigma(\mathbf{z}))$ and
1217 $-\frac{\sigma_s\sigma_c}{\sqrt{2}}(\mathbf{v}_0(c) - \mathbf{v}_0(s))^\top (e_c - \sigma(\mathbf{z}))$, respectively.

1218 *Proof.*

$$1219 \quad -\theta_S^\top \nabla_{W_{KQ}} \ell(W, [c, s, r])\phi(r) \quad (31)$$

$$1220 \quad = \theta_S^\top \phi([c, s, r])[\text{diag}(\boldsymbol{\sigma}_{csr}) - \boldsymbol{\sigma}_{csr}\boldsymbol{\sigma}_{csr}^\top]\phi([c, s, r])^\top W_V^\top W_H(e_c - \sigma(\mathbf{z})) \underbrace{\|\phi(r)\|_2^2}_{=1} \quad (32)$$

$$1221 \quad = \frac{1}{\sqrt{2}}[-\sigma_s\sigma_c, \sigma_s - \sigma_s^2, -\sigma_s\sigma_r]^\top \phi([c, s, r])^\top W_V^\top W_H(e_c - \sigma(\mathbf{z})) \quad (33)$$

$$1222 \quad = \frac{1}{\sqrt{2}}(-\sigma_s\sigma_c\mathbf{v}_0(c) + (\sigma_s - \sigma_s^2)\mathbf{v}_0(s) - \sigma_s\sigma_r\mathbf{v}_0(r))^\top (e_c - \sigma(\mathbf{z})) \quad (34)$$

1223 □

1242 **Lemma 3.** For any example $[c, s, r] \in \mathcal{D}_C$,

1243
$$v_0(c, s) = o_c$$

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1245
$$v_0(c, c) = \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S)$$

1246
1247 For any example $[c, s, r] \in \mathcal{D}_{C+S}$,

1248
$$v_0(c, s) = \log\left(\frac{\delta_M}{1 - \delta_M}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S)$$

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$$v_0(c, c) = \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S)$$

1252

1253 *Proof.* Recall from assumption 6, the following properties of any example in \mathcal{D}

1254
$$v_0(c', s) = v_0(c', c) = o_c \quad \forall c' \in \mathcal{A} \setminus \{c\} \quad (35)$$

1255
$$v_0(r, c) = v_0(r, s) = o_r \quad (36)$$

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1257
$$v_0(s', s) = v_0(s', c) = 0 \quad \forall s' \in \mathcal{S} \quad (37)$$

1258

1259 Take any example $[c, s, r] \in \mathcal{D}_C$. Recall that

1260
$$\delta_C = \sigma(\mathbf{v}_0(c))_c = \frac{\exp(v_0(c, c))}{(K_A - 1) \exp(o_c) + \exp(o_r) + \exp(v_0(c, c)) + K_S} \quad (38)$$

1261

1262 Thus

1263
$$v_0(c, s) = o_c \quad (39)$$

1264
1265
$$v_0(c, c) = \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) \quad (40)$$

1266

1267 Similarly, take any example $[c, s, r] \in \mathcal{D}_{C+S}$. Recall that

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1269
$$\delta_M = \sigma(\mathbf{v}_0(s))_c = \frac{\exp(v_0(c, s))}{(K_A - 1) \exp(o_c) + \exp(o_r) + \exp(v_0(c, s)) + K_S} \quad (41)$$

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$$\delta_C = \sigma(\mathbf{v}_0(c))_c = \frac{\exp(v_0(c, c))}{(K_A - 1) \exp(o_c) + \exp(o_r) + \exp(v_0(c, c)) + K_S} \quad (42)$$

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1273 Thus,

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$$v_0(c, s) = \log\left(\frac{\delta_M}{1 - \delta_M}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) \quad (43)$$

1276
1277
$$v_0(c, c) = \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) \quad (44)$$

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1280 \square

1281 **Lemma 4.** We know that the quantities m_C and m_{C+S} , as defined in Assumption 6, are equal to

1282
$$m_C = \lambda_C \left[\log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) - o_c \right]$$

1283
1284
$$m_{C+S} = \lambda_{C+S} \left[\log\left(\frac{\delta_C}{1 - \delta_C}\right) - \log\left(\frac{\delta_M}{1 - \delta_M}\right) \right]$$

1285

1286 where

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1288
$$\lambda_C = \left(1 + \frac{\exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \frac{1}{2} \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) + \frac{1}{2} o_c\right)}{(K_A - 1) \exp(o_c) + \exp(o_r) + K_S} \right)^{-1} \quad (45)$$

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$$\lambda_{C+S} = \left(1 + \frac{\exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \frac{1}{2} \log\left(\frac{\delta_M}{1 - \delta_M}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S)\right)}{(K_A - 1) \exp(o_c) + \exp(o_r) + K_S} \right)^{-1} \quad (46)$$

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1296 *Proof.* As per definition, m_C and m_{C+S} are equal to

$$1297 \quad = \langle \mathbf{v}_0(c) - \mathbf{v}_0(s), e_c - \sigma(\mathbf{z}) \rangle \quad (47)$$

$$1298 \quad = \left\langle \mathbf{v}_0(c) - \mathbf{v}_0(s), e_c - \sigma \left(\frac{1}{2} \mathbf{v}_0(c) + \frac{1}{2} \mathbf{v}_0(s) \right) \right\rangle \quad (48)$$

1300 for any $[c, s, r] \in \mathcal{D}_C$ and \mathcal{D}_{C+S} , respectively.

1301 We first calculate m_C . Let us simplify $\mathbf{v}_0(c) - \mathbf{v}_0(s)$. From Lemma 3 and Assumption 6, we know that for any $[c, s, r] \in \mathcal{D}_C$

$$1302 \quad v_0(c, c) - v_0(c, s) \quad (49)$$

$$1303 \quad = \log \left(\frac{\delta_C}{1 - \delta_C} \right) + \log \left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S \right) - o_c \quad (50)$$

1304 and

$$1305 \quad v_0(s', c) - v_0(s', s) = 0 \quad \forall s' \in \mathcal{S} \quad (51)$$

$$1306 \quad v_0(c', c) - v_0(c', s) = o_c - o_c \quad \forall c' \in \mathcal{A} \setminus \{c\} \quad (52)$$

$$1307 \quad v_0(r, c) - v_0(r, s) = 0 \quad (53)$$

1308 Therefore

$$1309 \quad m_C = (1 - \sigma(\mathbf{z})_c) \left[\log \left(\frac{\delta_C}{1 - \delta_C} \right) + \log \left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S \right) - o_c \right] \quad (54)$$

1310 for any $c' \in \mathcal{A} \setminus \{c\}$.

1311 Next, we calculate $\sigma \left(\frac{1}{2} \mathbf{v}_0(c) + \frac{1}{2} \mathbf{v}_0(s) \right)_c$. Note that

$$1312 \quad \sum_{i \in \mathcal{T}} \exp(v_0(i)) \quad (55)$$

$$1313 \quad = \exp \left(\frac{1}{2} \log \left(\frac{\delta_C}{1 - \delta_C} \right) + \frac{1}{2} \log \left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S \right) + \frac{1}{2} o_c \right) \quad (56)$$

$$1314 \quad + (K_A - 1) \exp(o_c) + \exp(o_r) + K_S \quad (57)$$

1315 and so

$$1316 \quad 1 - \sigma(\mathbf{z})_c = 1 - \sigma \left(\frac{1}{2} \mathbf{v}_0(c) + \frac{1}{2} \mathbf{v}_0(s) \right)_c \quad (58)$$

$$1317 \quad = \left(1 + \frac{\exp \left(\frac{1}{2} \log \left(\frac{\delta_C}{1 - \delta_C} \right) + \frac{1}{2} \log \left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S \right) + \frac{1}{2} o_c \right)}{(K_A - 1) \exp(o_c) + \exp(o_r) + K_S} \right)^{-1} \quad (59)$$

1318 Similarly, we compute m_{C+S} . From Lemma 3, we know

$$1319 \quad v_0(c, c) - v_0(c, s) \quad (60)$$

$$1320 \quad = \log \left(\frac{\delta_C}{1 - \delta_C} \right) + \log \left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S \right) \quad (61)$$

$$1321 \quad - \log \left(\frac{\delta_M}{1 - \delta_M} \right) - \log \left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S \right) \quad (62)$$

$$1322 \quad = \log \left(\frac{\delta_C}{1 - \delta_C} \right) - \log \left(\frac{\delta_M}{1 - \delta_M} \right) \quad (63)$$

1323 And using Assumption 6, the other quantities in $\mathbf{v}_0(c) - \mathbf{v}_0(s)$ are the same as Equation 51, so

$$1324 \quad m_{C+S} = (1 - \sigma(\mathbf{z})_c) \left[\log \left(\frac{\delta_C}{1 - \delta_C} \right) - \log \left(\frac{\delta_M}{1 - \delta_M} \right) \right] \quad (64)$$

Next, we calculate $\sigma\left(\frac{1}{2}\mathbf{v}_0(c) + \frac{1}{2}\mathbf{v}_0(s)\right)_c$. Note that

$$\sum_{i \in \mathcal{T}} \exp(v_0(i)) \quad (65)$$

$$= \exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) + \frac{1}{2} \log\left(\frac{\delta_M}{1-\delta_M}\right) + \log\left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S\right)\right) \quad (66)$$

$$+ (K_A - 1) \exp(o_c) + \exp(o_r) + K_S \quad (67)$$

and so

$$1 - \sigma(\mathbf{z})_c = 1 - \sigma\left(\frac{1}{2}\mathbf{v}_0(c) + \frac{1}{2}\mathbf{v}_0(s)\right)_c \quad (68)$$

$$= \left(1 + \frac{\exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) + \frac{1}{2} \log\left(\frac{\delta_M}{1-\delta_M}\right) + \log\left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S\right)\right)}{(K_A - 1) \exp(o_c) + \exp(o_r) + K_S}\right)^{-1} \quad (69)$$

□

Lemma 5. *The following is true,*

$$m_C > 0, m_{C+S} < 0$$

Proof. Refer to the form of m_C and m_{C+S} derived in Lemma 4. Note that $\lambda_{C+S}, \lambda_C > 0$ and since $\delta_M > \delta_C$ and $\frac{x}{1-x}$ is strictly increasing between 0 and 1,

$$\log\left(\frac{\delta_C}{1-\delta_C}\right) - \log\left(\frac{\delta_M}{1-\delta_M}\right) < 0 \quad (70)$$

Thus, $m_{C+S} < 0$. On the other hand, for $m_C > 0$ since

$$\log\left(\frac{\delta_C}{1-\delta_C}\right) + \log\left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S\right) - o_c \quad (71)$$

$$\geq \log\left(\frac{1}{K_A - 1}\right) + \log\left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S\right) - o_c \quad (72)$$

$$= \log\left(1 + \underbrace{\frac{\exp(o_r) + K_S}{(K_A - 1) \exp(o_c)}}_{>0}\right) \geq 0 \quad (73)$$

The first step follows by definition that $\delta_C > \frac{1}{K_A}$. □

Lemma 6. *The following is true,*

$$|m_C| > |m_S|$$

Proof. From Lemma 4, note that

$$\frac{\lambda_C}{\lambda_{C+S}} = \frac{1 + \exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) + \frac{1}{2} \log\left(\frac{\delta_M}{1-\delta_M}\right)\right)}{1 + \exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) - \frac{1}{2} \log\left(\underbrace{(K_A - 1) \exp(o_c) + \exp(o_r) + K_S}_{\geq 0}\right) + \frac{1}{2} o_c\right)} \quad (74)$$

$$\geq \frac{1 + \exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) + \frac{1}{2} \log\left(\frac{\delta_M}{1-\delta_M}\right)\right)}{1 + \exp\left(\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) + \frac{1}{2} \log\left(\frac{1}{K_A - 1}\right)\right)} > 1 \quad (75)$$

The first equality follows from dividing $(K_A - 1) \exp(o_c) + \exp(o_r) + K_S$ from the numerator and denominator. Thus,

$$\frac{|m_C|}{|m_S|} = -\frac{m_C}{m_S} = \frac{\lambda_C}{\lambda_{C+S}} \cdot \frac{\log\left(\frac{\delta_C}{1-\delta_C}\right) + \log\left((K_A - 1) \exp(o_c) + \exp(o_r) + K_S\right) - o_c}{\log\left(\frac{\delta_M}{1-\delta_M}\right) - \log\left(\frac{\delta_C}{1-\delta_C}\right)} \quad (76)$$

$$\geq \frac{\exp\left(-\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) + \frac{1}{2} \log\left(\frac{\delta_M}{1-\delta_M}\right)\right)}{\exp\left(-\frac{1}{2} \log\left(\frac{\delta_C}{1-\delta_C}\right) - \frac{1}{2} \log(K_A - 1)\right)} \cdot \frac{\log\left(\frac{\delta_C}{1-\delta_C}\right) + \log(K_A - 1)}{\log\left(\frac{\delta_M}{1-\delta_M}\right) - \log\left(\frac{\delta_C}{1-\delta_C}\right)} > 1 \quad (77)$$

For the last inequality we use the property that $\exp(\frac{1}{2}x) \geq x \forall x \in \mathbb{R}$ and $\exp(-\frac{1}{2}x) \leq x \forall x \in \mathbb{R}$ such that $x > 1$. So, $|m_C| \geq |m_S|$. \square

Proof of First Phase At the beginning of training, we assumed in Assumption 5 that the attention weights between the context and subject is equal at the beginning of training for all datapoints $x \in \mathcal{D}^{SFT}$, i.e., $\sigma_s^0 = \sigma_c^0 = 1/2$ and $\sigma_r^0 = 0$.

Using Lemma 2, it follows that

$$-\theta_C^\top \nabla_{W_{KQ}} \ell(W^{(0)}, [c, s, r]) \theta_r = \frac{1}{4\sqrt{2}} (\mathbf{v}_0(c) - \mathbf{v}_0(s))^\top (e_c - \sigma(\mathbf{z})) \quad (78)$$

which equals $\frac{1}{4\sqrt{2}} m_C$ for $[c, s, r] \in \mathcal{D}_C$ and $-\frac{1}{4\sqrt{2}} m_{C+S}$ for $[c, s, r] \in \mathcal{D}_{C+S}$.

Using Lemma 5, and Lemma 4 it directly follows that

$$\theta_C^\top [-\nabla_{W_{KQ}} L(W^*)] \theta_r = \frac{1}{8\sqrt{2}} m_C + \frac{1}{8\sqrt{2}} m_{C+S} > 0 \quad (79)$$

Since $\theta_S^\top [-\nabla_{W_{KQ}} L(W^*)] \theta_r = -\theta_C^\top [-\nabla_{W_{KQ}} L(W^*)] \theta_r$, it directly follows that $\theta_S^\top [-\nabla_{W_{KQ}} L(W^*)] \theta_r < 0$. This completes the proof for the first phase.

Second Phase Preliminaries Using Lemma 1, at timestep $t = 0$, the gradient of the loss of any datapoint $[c_i, s_i, r_i]$ with respect to W_{KQ} is

$$\begin{aligned} & -\nabla_{W_{KQ}} \ell(W, [c, s, r]) \quad (80) \\ & = \phi([c, s, r]) [\text{diag}(\boldsymbol{\sigma}_{csr}) - \boldsymbol{\sigma}_{csr} \boldsymbol{\sigma}_{csr}^\top] \underbrace{\phi([c, s, r])^\top W_V^\top W_H (e_c - \sigma(\mathbf{z})) \phi(r)^\top}_{[\mathbf{v}(c), \mathbf{v}(s), \mathbf{v}(r)]^\top} \quad (81) \end{aligned}$$

$$= \frac{1}{4} \langle \mathbf{v}(c) - \mathbf{v}(s), e_c - \sigma(\mathbf{z}) \rangle (\phi(c) - \phi(s)) \phi(r)^\top \quad (82)$$

where $\mathbf{z} = \frac{1}{2} \mathbf{v}(c) + \frac{1}{2} \mathbf{v}(s)$ and $\boldsymbol{\sigma}_{csr} = [\frac{1}{2}, \frac{1}{2}, 0]$

Consider taking a full batch gradient update step

$$W_{KQ}^1 = W_{KQ}^0 - \frac{\eta}{n} \sum_{i=1}^n \nabla_{W_{KQ}} \ell(W, [c_i, s_i, r_i]),$$

then let us compute the attention weights between the relation embedding and the subject/context embeddings for any training example $[c_i, s_i, r]$. First, note that

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$$\phi(c_i)^\top \left(-\sum_{j=1}^n \nabla_{W_{KQ}} \ell(W, [c_j, s_j, r]) \right) \phi(r) \quad (83)$$

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$$= \frac{1}{4} \sum_{j=1}^n \langle \mathbf{v}(c_j) - \mathbf{v}(s_j), \mathbf{e}_{c_j} - \sigma(\mathbf{z}_{rj}) \rangle \|\phi(r)\| \langle \phi(c_i), \phi(c_j) - \phi(s_j) \rangle \quad (84)$$

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$$= \frac{1}{4} \left[m_C \sum_{j=1}^{n/2} \langle \phi(c_i), \phi(c_j) - \phi(s_j) \rangle + m_{C+S} \sum_{j=n/2+1}^n \langle \phi(c_i), \phi(c_j) - \phi(s_j) \rangle \right] \quad (85)$$

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$$= \frac{1}{8} \left[m_C \sum_{j=1}^n (1 + \mathbb{1}[i=j]) + m_{C+S} \sum_{j=n/2+1}^n (1 + \mathbb{1}[i=j]) \right] \quad (86)$$

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where $n = |\mathcal{D}|$ and we refer to all examples in \mathcal{D}_C as $[c_j, s_j, r]_{j=1}^{n/2}$ and in \mathcal{D}_{C+S} as $[c_j, s_j, r]_{j=n/2+1}^n$. The last step follows from assumption 4. Furthermore, one can easily calculate that

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$$\phi(s_i)^\top \left(-\sum_{j=1}^n \nabla_{W_{KQ}} \ell(W, [c_j, s_j, r]) \right) \phi(r) = \phi(c_i)^\top \left(\sum_{j=1}^n \nabla_{W_{KQ}} \ell(W, [c_j, s_j, r]) \right) \phi(r) \quad (87)$$

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So for any datapoint $[c_i, s_i, r] \in \mathcal{D}_C$,

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$$\phi(c_i)^\top W_{KQ}^1 \phi(r) = \phi(c_i)^\top W_{KQ}^0 \phi(r) + \frac{\eta}{16} \left[m_C \left(\frac{n+2}{n} \right) + m_{C+S} \right] \quad (88)$$

$$\phi(s_i)^\top W_{KQ}^1 \phi(r) = \phi(s_i)^\top W_{KQ}^0 \phi(r) - \frac{\eta}{16} \left[m_C \left(\frac{n+2}{n} \right) + m_{C+S} \right] \quad (89)$$

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and similarly, for any datapoint $[c_i, s_i, r] \in \mathcal{D}_{C+S}$,

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$$\phi(c_i)^\top W_{KQ}^1 \phi(r) = \phi(c_i)^\top W_{KQ}^0 \phi(r) + \frac{\eta}{16} \left[m_C + m_{C+S} \left(\frac{n+2}{n} \right) \right] \quad (90)$$

$$\phi(s_i)^\top W_{KQ}^1 \phi(r) = \phi(s_i)^\top W_{KQ}^0 \phi(r) - \frac{\eta}{16} \left[m_C + m_{C+S} \left(\frac{n+2}{n} \right) \right] \quad (91)$$

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Going back to Equation 88 and 90, note that

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$$A_1 = \left(\frac{n+2}{n} \right) m_C + m_{C+S} > \frac{2}{n} m_C > 0 \quad (92)$$

$$A_2 = m_C + \left(\frac{n+2}{n} \right) m_{C+S} > \frac{2}{n} m_{C+S} \quad (93)$$

$$|A_1| > |A_2| \quad (94)$$

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Thus, the attention to context strictly increases from $t = 0$ to $t = 1$ for \mathcal{D}_C points, while for $n > 2 \frac{|m_C + s|}{|m_C| - |m_C + s|}$, the attention to context also increases for \mathcal{D}_{C+S} by a smaller degree. Specifically, using Assumption 5, it easily follows that

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$$\sigma(\phi(c)^\top W_{KQ}^1 \phi(r)) = \frac{1}{1 + \exp(-\frac{\eta}{8} A_1)} \quad \forall [c, s, r] \in \mathcal{D}_C \quad (95)$$

$$\sigma(\phi(s)^\top W_{KQ}^1 \phi(r)) = \frac{1}{1 + \exp(\frac{\eta}{8} A_1)} \quad \forall [c, s, r] \in \mathcal{D}_C \quad (96)$$

$$\sigma(\phi(c)^\top W_{KQ}^1 \phi(r)) = \frac{1}{1 + \exp(-\frac{\eta}{8} A_2)} \quad \forall [c, s, r] \in \mathcal{D}_{C+S} \quad (97)$$

$$\sigma(\phi(s)^\top W_{KQ}^1 \phi(r)) = \frac{1}{1 + \exp(\frac{\eta}{8} A_2)} \quad \forall [c, s, r] \in \mathcal{D}_{C+S} \quad (98)$$

Lemma 7. *At timestep $t = 0$, for any learning rate $\eta \in (0, \infty)$, the prediction towards the answer $\sigma(\mathbf{z}^1)_c$ increases monotonically with η for \mathcal{D}_C examples while decreasing monotonically for \mathcal{D}_{C+S} examples.*

Proof. Setting $\sigma_c^1 = \sigma(\phi(c)^\top W_{KQ}^1 \phi(r))$, note that for any $[c, s, r] \in \mathcal{D}$

$$\sigma(\mathbf{z}^1)_c = \frac{\exp(\sigma_c^1 v_0(c, c) + (1 - \sigma_c^1) v_0(c, s))}{\exp(\sigma_c^1 v_0(c, c) + (1 - \sigma_c^1) v_0(c, s)) + (K_A - 1) \exp(o_c) + \exp(o_r) + K_S} \quad (99)$$

$$(100)$$

For examples in \mathcal{D}_C , $v_0(c, c) > v_0(c, s)$ by construction and σ_c^1 increases monotonically with η , so $\exp(\sigma_c^1 v_0(c, c) + (1 - \sigma_c^1) v_0(c, s))$ increases monotonically. This implies $\sigma(\mathbf{z}^1)_c$ increases monotonically. On the other hand, for examples in \mathcal{D}_{C+S} , $v_0(c, c) < v_0(c, s)$ by construction and σ_c^1 increases monotonically with η , so $\exp(\sigma_c^1 v_0(c, c) + (1 - \sigma_c^1) v_0(c, s))$ decreases monotonically. This implies $\sigma(\mathbf{z}^1)_c$ decreases monotonically. \square

Second Phase Now, we calculate the gradient of W_{KQ} at timestep $t = 1$. Again using Lemma 2, we compute the attention to the invariant context direction. Note that $\forall [c, s, r] \in \mathcal{D}_C$

$$-\theta_C \nabla_{W_{KQ}} \ell(W^1, [c, s, r]) \phi(r) \quad (101)$$

$$= \frac{\exp(\frac{\eta}{8} A_1)}{\sqrt{2}(1 + \exp(\frac{\eta}{8} A_1))^2} (\mathbf{v}_0(c) - \mathbf{v}_0(s))^\top (e_c - \sigma(\mathbf{z}_c^1)) \quad (102)$$

$$= \frac{\exp(\frac{\eta}{8} A_1) (1 - \sigma(\mathbf{z}_c^1)_c)}{\sqrt{2}(1 + \exp(\frac{\eta}{8} A_1))^2} \left[\log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) - o_c \right] \quad (103)$$

$$\leq \frac{\exp(\frac{\eta}{8} A_1) (1 - \frac{1}{K_A})}{\sqrt{2}(1 + \exp(\frac{\eta}{8} A_1))^2} \left[\log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log(K_A) \right] \quad (104)$$

Similarly, $\forall [c, s, r] \in \mathcal{D}_{C+S}$

$$-\theta_C \nabla_{W_{KQ}} \ell(W^1, [c, s, r]) \phi(r) = \frac{\exp(\frac{\eta}{8} A_2) (1 - \sigma(\mathbf{z}_{C+S}^1)_c)}{\sqrt{2}(1 + \exp(\frac{\eta}{8} A_2))^2} \left[\log\left(\frac{\delta_C}{1 - \delta_C}\right) - \log\left(\frac{\delta_M}{1 - \delta_M}\right) \right] \quad (105)$$

$$\leq \frac{\exp(\frac{\eta}{8} A_2) (1 - \delta_M)}{\sqrt{2}(1 + \exp(\frac{\eta}{8} A_2))^2} \left[\log\left(\frac{\delta_C}{1 - \delta_C}\right) - \log\left(\frac{\delta_M}{1 - \delta_M}\right) \right] \quad (106)$$

We argue there exists a finite η^* such that

$$\frac{\exp(\frac{\eta}{8} A_2)}{(1 + \exp(\frac{\eta}{8} A_2))^2} \cdot \frac{(1 + \exp(\frac{\eta}{8} A_1))^2}{\exp(\frac{\eta}{8} A_1)} \geq \underbrace{\frac{1 - \frac{1}{K_A}}{1 - \delta_M} \cdot \frac{\log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log(K_A)}{\log\left(\frac{\delta_M}{1 - \delta_M}\right) - \log\left(\frac{\delta_C}{1 - \delta_C}\right)}}_{>1} \quad (107)$$

1566 since

$$1567 \lim_{\eta \rightarrow \infty} \frac{\exp(\frac{\eta}{8}A_2)}{(1 + \exp(\frac{\eta}{8}A_2))^2} \cdot \frac{(1 + \exp(\frac{\eta}{8}A_1))^2}{\exp(\frac{\eta}{8}A_1)} \quad (108)$$

$$1570 = \lim_{\eta \rightarrow \infty} \frac{(1 + \exp(\frac{\eta}{8}A_1))(1 + \exp(-\frac{\eta}{8}A_1))}{(1 + \exp(\frac{\eta}{8}A_2))(1 + \exp(-\frac{\eta}{8}A_2))} \quad (109)$$

$$1572 = \lim_{\eta \rightarrow \infty} \frac{1 + \exp(\frac{\eta}{8}A_1)}{1 + \exp(\frac{\eta}{8}A_2)} = \infty \quad (110)$$

1575 where the last line follows because we know from Lemma 6 $A_1 > A_2$.

1576 Setting $\eta = \eta^*$, note that the attention weight of the average gradient to the invariant context direc-
1577 tion is negative.

$$1578 \theta_C^\top \left[-\frac{1}{n} \sum_{[c,s,r] \in \mathcal{D}} \nabla_{W_{KQ}} \ell(W^1, [c, s, r]) \right] \phi(r) \quad (111)$$

$$1582 \leq \frac{\exp(\frac{\eta^*}{8}A_1)(1 - \frac{1}{K_A})}{2\sqrt{2}(1 + \exp(\frac{\eta^*}{8}A_1))^2} \left[\log \left(\frac{\delta_C}{1 - \delta_C} \right) + \log(K_A) \right] \quad (112)$$

$$1585 + \frac{\exp(\frac{\eta^*}{8}A_2)(1 - \delta_M)}{2\sqrt{2}(1 + \exp(\frac{\eta^*}{8}A_2))^2} \left[\log \left(\frac{\delta_C}{1 - \delta_C} \right) - \log \left(\frac{\delta_M}{1 - \delta_M} \right) \right]$$

$$1587 < 0 \quad (113)$$

1588 \square

1590 C.2 PROOF OF PROPOSITION 2

1592 **Proposition 2** (More Attention to Subject with S Points). *Say that we add a point $[s, r]$ that has
1593 been memorized by the pretrained model to the training dataset. We call this new training dataset
1594 \mathcal{D}_{new} and the old dataset \mathcal{D}_{old} . Under assumptions listed in Appendix C.1. At timestep $t = 0$*

$$1595 \theta_S^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{new})] \phi(r) > \theta_S^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{old})] \phi(r) \quad (114)$$

$$1597 \theta_C^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{new})] \phi(r) = \theta_C^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{old})] \phi(r) \quad (115)$$

1598 *Proof.* Using Lemma 1, it follows that for any memorized point $[s, r] \in \mathcal{D}_S$

$$1600 \theta_S^\top [-\nabla_{W_{KQ}} \ell(W, [s, r])] \phi(r) \quad (116)$$

$$1602 = \frac{1}{\sqrt{2}} \sigma_s \sigma_r (\mathbf{v}_0(s) - \mathbf{v}_0(r))^\top (\mathbf{e}_c - \sigma(\mathbf{z})) \quad (117)$$

1604 Using Assumption 6, note that

$$1605 v(s, s) - v(s, r) = 0 \quad (118)$$

$$1607 v(c', s) - v(c', r) = o_c - o_c = 0 \quad \forall c' \in \mathcal{C}/\{a\} \quad (119)$$

$$1608 v(a, s) - v(a, r) > 0 \quad (120)$$

1610 Therefore, the gradient's attention to the invariant direction further simplifies to

$$1611 = \frac{1}{\sqrt{2}} (v(a, s) - v(a, r)) (1 - \sigma(f_W([s, r])_r)_a) > 0 \quad (121)$$

1614 Since $\theta_S^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{old})] \phi(r) < 0$, then $\theta_S^\top [-\nabla_{W_{KQ}} L(W^{(t)}, \mathcal{D}_{new})] \phi(r) >$
1615 $\theta_S^\top [-\nabla_{W_{KQ}} L(W^{(0)}, \mathcal{D}_{old})] \phi(r)$.

1616 On the other hand, since θ_C is orthogonal by construction to any $\phi(s)$ for $s \in \mathcal{S}$ and $\phi(r)$,

$$1618 \theta_C^\top [-\nabla_{W_{KQ}} \ell(W, [s, r])] \phi(r) = 0 \quad (122)$$

1619 This completes our proof. \square

C.3 PROOF OF PROPOSITION 3

Proposition 3 (Fact Memorization). *Under Assumptions in Appendix C.1, for any example $[c, s, r] \in \mathcal{D}_C$, after the gradient step at timestep $t = 0$, the value embedding of the subject token is more predictive of the label c .*

$$\sigma\left(W_H^\top W_V^{(1)} \phi(s)\right)_c - \sigma\left(W_H^\top W_V^{(0)} \phi(s)\right)_c > 0 \quad (123)$$

Proof.

$$-\nabla_{W_V} L(W) = \frac{1}{n} \sum_{i=1}^n \langle e_{c_i} - \sigma(\mathbf{z}_i), \nabla_{W_V} \mathbf{z}_i \rangle \quad (124)$$

$$= \frac{1}{n} \sum_{i=1}^n W_H (e_{c_i} - \sigma(\mathbf{z}_i)) [\sigma_{c_i} \phi(c_i) + \sigma_{s_i} \phi(s_i) + \sigma_r \phi(r)]^\top \quad (125)$$

For $[c_j, s_j, r_j] \in \mathcal{D}_C$,

$$v_{t+1}(c_j, s_j) - v_t(c_j, s_j) = -\eta \phi(c_j)^\top \nabla_{W_V} L(W) \phi(s_j) \quad (126)$$

$$= \frac{\eta}{n} \sum_{i=1}^n \frac{(1 + \mathbb{1}[i = j])}{4} (e_{c_i} - \sigma(\mathbf{z}_i))^\top W_H^\top \phi(c_j) \quad (127)$$

$$= \frac{\eta}{n} \sum_{i=1}^n \frac{(1 + \mathbb{1}[i = j])}{4} \left(\frac{1 + \mathbb{1}[i = j]}{2} (1 - \sigma(\mathbf{z}_i)_{c_i}) - \frac{|\mathcal{C}| + 1 - 2\mathbb{1}[i = j]}{2} \sigma(\mathbf{z}_i)_{c_k} \right) \text{ where } c_k \neq c_i \quad (128)$$

$$= \frac{\eta}{8n} \left(2(1 - \delta_C) + \sum_{i \neq j} |\mathcal{S}| \sigma(\mathbf{z}_i)_s + \sum_{i \neq j} \sigma(\mathbf{z}_i)_r - 2 \sum_{i \neq j} \sigma(\mathbf{z}_i)_{c_j} + 2|\mathcal{S}| \sigma(\mathbf{z}_j)_s + 2\sigma(\mathbf{z}_j)_r \right) \quad (129)$$

where we use the fact that $\sigma_s = 0.5$ for all examples at timestep 0. Similarly,

$$\forall k \neq j, \quad v_{t+1}(c_k, s_j) - v_t(c_k, s_j) \quad (130)$$

$$= \frac{\eta}{n} \sum_{i=1}^n \frac{(1 + \mathbb{1}[i = j])}{4} \left(\frac{1 + \mathbb{1}[i = k]}{2} (1 - \sigma(\mathbf{z})_{c_i}) - \frac{|\mathcal{C}| + 1 - 2\mathbb{1}[i = k]}{2} \sigma(\mathbf{z})_{c_{k'}} \right) \text{ where } c_k \neq c_i \quad (131)$$

$$= \frac{\eta}{8n} \left((1 - \delta_C) + \sum_{i=1}^n |\mathcal{S}| \sigma(\mathbf{z}_i)_s + \sum_{i=1}^n \sigma(\mathbf{z}_i)_r - 2 \sum_{i \neq k} \sigma(\mathbf{z}_i)_{c_k} + |\mathcal{S}| \sigma(\mathbf{z}_j)_s + \sigma(\mathbf{z}_j)_r - 2\sigma(\mathbf{z}_j)_{c_k} \right) \quad (132)$$

$$\forall c' \notin \mathcal{D}, \quad v_{t+1}(c', s_j) - v_t(c', s_j) \text{ where } c' \notin \mathcal{D}, c_{k'} \neq c_i \quad (133)$$

$$= \frac{\eta}{n} \sum_{i=1}^n \frac{(1 + \mathbb{1}[i = j])}{4} \left(\frac{1}{2} (1 - \sigma(\mathbf{z})_{c_i}) - \frac{|\mathcal{C}| - 1}{2} \sigma(\mathbf{z})_{c_k} \right) \quad (134)$$

$$= \frac{\eta}{8n} \left(\sum_{i=1}^n |\mathcal{S}| \sigma(\mathbf{z}_i)_s + \sum_{i=1}^n \sigma(\mathbf{z}_i)_r - 2 \sum_{i=1}^n \sigma(\mathbf{z}_i)_{c_k} + |\mathcal{S}| \sigma(\mathbf{z}_j)_s + \sigma(\mathbf{z}_j)_r - 2\sigma(\mathbf{z}_j)_{c_k} \right) \quad (135)$$

$$v_{t+1}(s, s_j) - v_t(s, s_j) = -\eta |\mathcal{S}| \left(\frac{\sigma(\mathbf{z}_C)_s (n+2)}{8n} + \frac{\sigma(\mathbf{z}_{C+S})_s}{8} \right) \quad (136)$$

$$v_{t+1}(r, s_j) - v_t(r, s_j) = -\eta \left(\frac{\sigma(\mathbf{z}_C)_r (n+2)}{8n} + \frac{\sigma(\mathbf{z}_{C+S})_r}{8} \right) \quad (137)$$

We use $\sigma(\mathbf{z}_C)_x, \sigma(\mathbf{z}_{C+S})_x$ to denote the value of these quantities for any example $[c, s, r] \in \mathcal{D}_C$ and \mathcal{D}_{C+S} , respectively. By the data symmetry assumption (6), these quantities are equal within each

category of examples. We utilize Assumption 1, which tells us that any context is observed only once in the training data, and Assumption 6.

Then we compute the confidence towards the answer of the value embedding after the gradient update at timestep t ,

$$\sigma(v_{t+1}(s_j))_{c_j} = \quad (138)$$

$$\left(1 + \frac{(n-1)\exp(v_{t+1}(c_k, s_j)) + (|\mathcal{C}| - n)\exp(v_{t+1}(c', s_j)) + \sum_{s \in \mathcal{S}} v_{t+1}(s, s_j) + v_{t+1}(r, s_j)}{\exp(v_{t+1}(c_j, s_j))}\right)^{-1} \quad (139)$$

where $k \neq j$ and $c' \notin \mathcal{D}$.

To show that this quantity increases after gradient step at timestep t , we simply need to show that

$$\forall k \in [n] \setminus i, \quad \frac{\exp(v_{t+1}(c_k, s_j) - v_t(c_k, s_j))}{\exp(v_{t+1}(c_j, s_j) - v_t(c_j, s_j))} < 1 \quad (140)$$

$$\forall c' \in \mathcal{C} \setminus \mathcal{D}, \quad \frac{\exp(v_{t+1}(c', s_j) - v_t(c', s_j))}{\exp(v_{t+1}(c_j, s_j) - v_t(c_j, s_j))} < 1 \quad (141)$$

$$\forall s \in \mathcal{S}, \quad \frac{\exp(v_{t+1}(s, s_j) - v_t(s, s_j))}{\exp(v_{t+1}(c_j, s_j) - v_t(c_j, s_j))} < 1 \quad (142)$$

$$\frac{\exp(v_{t+1}(r, s_j) - v_t(r, s_j))}{\exp(v_{t+1}(c_j, s_j) - v_t(c_j, s_j))} < 1 \quad (143)$$

This is equivalent to showing that

$$v_{t+1}(c_k, s_j) - v_t(c_k, s_j) - v_{t+1}(c_j, s_j) + v_t(c_j, s_j) = \frac{\eta}{8n}(-1 - \delta_C) - 2\sigma(\mathbf{z}_j)_{c_j} < 0 \quad (144)$$

$$v_{t+1}(c', s_j) - v_t(c', s_j) - v_{t+1}(c_j, s_j) + v_t(c_j, s_j) = \frac{\eta}{8n}(-2(1 - \delta_C) - 4\sigma(\mathbf{z}_j)_{c_k}) < 0 \quad (145)$$

$$v_{t+1}(s', s_j) - v_t(s', s_j) - v_{t+1}(c_j, s_j) + v_t(c_j, s_j) \leq -2\eta|\mathcal{S}| \left(\frac{\sigma(\mathbf{z}_c)_s(n+2)}{8n} + \frac{\sigma(\mathbf{z}_{c+s})_s}{8} \right) < 0 \quad (146)$$

$$v_{t+1}(r, s_j) - v_t(r, s_j) - v_{t+1}(c_j, s_j) + v_t(c_j, s_j) \leq -2\eta \left(\frac{\sigma(\mathbf{z}_c)_r(n+2)}{8n} + \frac{\sigma(\mathbf{z}_{c+s})_r}{8} \right) \leq 0 \quad (147)$$

This completes our proof. \square

C.4 PROOF OF THEOREM 1

Theorem 1 (Test-Time Dynamic). *Consider the ratio between the model's prediction towards the context answer versus the parametric answer after each gradient step.*

$$M_C^{(t)} = \frac{\sigma(\mathbf{z}^{(t)})_c}{(\sigma(\mathbf{z}^{(t)})_c + \sigma(\mathbf{z}^{(t)})_a)} \quad (148)$$

where $\mathbf{z}^{(t)} = f_{W^{(t)}}([c, s, r])_r$ denotes the model's unnormalized next-token probabilities at timestep t . Under the setting described in Proposition 1, for a counterfactual test example $[c, s, r]$ that was memorized at pretraining and $c \notin \mathcal{D}$, it directly follows that

$$M_C^{(1)} > M_C^{(0)}, M_C^{(1)} > M_C^{(2)} \quad (149)$$

Proof. We now consider a counterfactual datapoint $[c, s, r]$ where the answer $a \neq c$, and the answer was memorized by the model at pretraining.

Note that for all $[c', s', r] \in \mathcal{D}$

$$\phi([c, s, r])^\top \phi([c', s', r]) = \text{diag}([1/2, 1/2, 1]) \quad (150)$$

1728 Then note that, at any timestep,
1729

$$1730 -\phi(c)^\top \nabla_{W_{KQ}} \ell(W, [c', s', r]) \phi(r) = -\frac{1}{\sqrt{2}} \theta_C^\top \nabla_{W_{KQ}} \ell(W, [c', s', r]) \phi(r) \quad (151)$$

$$1731 -\phi(s)^\top \nabla_{W_{KQ}} \ell(W, [c', s', r]) \phi(r) = -\frac{1}{\sqrt{2}} \theta_S^\top \nabla_{W_{KQ}} \ell(W, [c', s', r]) \phi(r) \quad (152)$$

1732 We look at the ratio between the model's prediction towards the context answer and the parametric
1733 answer after each gradient step.
1734

$$1735 \frac{\sigma(\mathbf{z}_r)_c}{(\sigma(\mathbf{z}_r)_c + \sigma(\mathbf{z}_r)_a)} \quad (153)$$

$$1736 \frac{\sigma(\mathbf{z}_r^1)_c}{(\sigma(\mathbf{z}_r^1)_c + \sigma(\mathbf{z}_r^1)_a)} > \frac{\sigma(\mathbf{z}_r^0)_c}{(\sigma(\mathbf{z}_r^0)_c + \sigma(\mathbf{z}_r^0)_a)} \quad (154)$$

$$1737 \frac{\sigma(\mathbf{z}_r^1)_c}{(\sigma(\mathbf{z}_r^1)_c + \sigma(\mathbf{z}_r^1)_a)} > \frac{\sigma(\mathbf{z}_r^2)_c}{(\sigma(\mathbf{z}_r^2)_c + \sigma(\mathbf{z}_r^2)_a)} \quad (155)$$

$$1738 \quad (156)$$

1739 By definition, we know

$$1740 v(c, c) = \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) \quad (157)$$

$$1741 v(a, s) = \log\left(\frac{\delta_M}{1 - \delta_M}\right) + \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) \quad (158)$$

$$1742 v(c', s) = o_c \quad (159)$$

$$1743 v(c', c) = o_c \quad \forall c' \in \mathcal{A} \setminus \{c\} \quad (160)$$

$$1744 v(r, c) = v(r, s) = o_r \quad (161)$$

$$1745 \quad (162)$$

1746 and

$$1747 \frac{\sigma(\mathbf{z}_r^1)_c}{(\sigma(\mathbf{z}_r^1)_a + \sigma(\mathbf{z}_r^1)_c)} = \quad (163)$$

$$1748 \left(1 + \frac{\exp((1 - \sigma_c) \log\left(\frac{\delta_M}{1 - \delta_M}\right) + (1 - \sigma_c) \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) + \sigma_c o_c)}{\exp(\sigma_c \log\left(\frac{\delta_C}{1 - \delta_C}\right) + \sigma_c \log((K_A - 1) \exp(o_c) + \exp(o_r) + K_S) + (1 - \sigma_c) o_c)} \right)^{-1} \quad (164)$$

$$1749 = \left(1 + \frac{\exp\left((1 - \sigma_c) \log\left(\frac{\delta_M}{1 - \delta_M}\right) - \sigma_c \log\left(\frac{\delta_C}{1 - \delta_C}\right)\right)}{\underbrace{\exp((2\sigma_c - 1) \log((K_A - 1) + (\exp(o_r) + K_S) / \exp(o_c)))}_{=X}} \right)^{-1} \quad (165)$$

1750 We track the value of σ_c over the timesteps. Note that since $\log\left(\frac{\delta_M}{1 - \delta_M}\right) > \log\left(\frac{\delta_C}{1 - \delta_C}\right)$ by construction, X monotonically decreases with respect to δ_C , which forces $\frac{\sigma(\mathbf{z}_r^1)_c}{(\sigma(\mathbf{z}_r^1)_a + \sigma(\mathbf{z}_r^1)_c)}$ to strictly increase. Note that at timestep $t = 1$, σ_c is largest, meaning $\frac{\sigma(\mathbf{z}_r^1)_c}{(\sigma(\mathbf{z}_r^1)_a + \sigma(\mathbf{z}_r^1)_c)}$ is largest at timestep $t = 1$. This completes our proof. \square

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