A Circuit for Coreference: How LLMs Represent and Retrieve Singular and Plural Entities for Coreference Resolution

Abstract

Coreference resolution is an important task in contextual reasoning. The paper investigates the mechanism for representing and retrieving plural entities for coreference resolution. We use a combination of mechanistic interpretability and attention pattern analysis to study the process in which LLMs predict a pronoun to refer back to previously mentioned entities. Using a range of causal intervention techniques, we find a set of attention heads that are responsible for (1) representing coreference information in the input, (2) identifying entities that form a plural reference, (3) transferring the information to the component that is responsible for selecting the antecedents and predicting the pronoun. We also find that LLMs align with humans in preference for plural pronoun. Specifically, entities in a plural construction are more likely to be referred to as a plural entity if they are ontologically similar and are linked by the conjunction *and*.

1 Introduction

Discovering the underlying mechanism behind Large Language Models (LLMs) has been a topic of much research in the past few years due to high interest in improving their safety and their alignment with human behaviors (Bereska and Gavves, 2024; Ferrando et al., 2024). While LLMs are becoming larger and more capable, much of their inner working remains under the hood. Understanding their working is extremely important in making these systems more controllable and thus increasing their safety and explainability.

In this paper, we focus on studying how LLMs represent plural reference and how they resolve anaphoric reference involving plurals, as in *John and Mary came to the shop. They bought some milk*, where *they* is understood to corefer with *John and Mary*. In order to resolve plural reference, the LLMs have to identify the set of entities that create a plural entity. In psycholinguistic research, processing plural reference has been shown to be more complicated than singular reference because it requires tracking multiple entities simultaneously and grouping the entities that should be co-referred to by a plural pronoun (Patson, 2014). It has been found that entities which are similar in ontological properties (Koh and Clifton Jr, 2002) or play a similar role (Moxey et al., 2012) are more likely to be referred to with plurals than those which are not. On the other hand, entities of the same kind and linked by a conjunction are sometimes referred to using a singular pronoun when they create another object, as in *Hook up the engine and the boxcar, and send it to Avon* (Cokal et al., 2023).

To study plural pronoun resolution, we use a combination of interpretability techniques, including activation patching (Vig et al., 2020; Geva et al., 2023; Wang et al., 2022), attention pattern analysis (Wang et al., 2022; Tigges et al., 2023), and activation decomposition (Marks and Tegmark, 2023; Dai et al., 2024). We present the flow of information about plural reference across different model components (i.e., embeddings, attention heads) and throughout layers. We first use mechanistic interpretability techniques to find the attention heads that contribute to the LLMs' choice of singular and plural pronouns. We then examine the attention pattern of these components to see what information is used to make the decision. We found a relatively small and dense circuit, consisting of three groups of heads that are responsible for (i) detecting and encoding plurality signal, (ii) routing this information to the last token position, (iii) identifying the antecedents and producing a plural pronoun to refer to them. A summary of the responsible heads and their functions is provided below.

- **Pronoun Selection Heads** function at the last token position. They attend to all of the discourse entities to be referenced by the plu-

ral/singular pronoun and directly affect the model's decision.

- **Plurality Formation Heads** identify the entities that form a plural entity and send information to the Pronoun Selection heads.

- **Pronoun Interpretation Heads** act as a representation for coreference information where tokens referring to the same entity attend to each other.

We also derive the following observations about how LLMs encode referential information and use it to refer back to previous entities: (1) LLMs' attention concentrates on the entities that they refer to; (2) In accordance with previous psycholinguistic experiments, there are constraints on whether a set of entities is a good candidate for plural reference for LLMs. Firstly, LLMs prefer entities with similar ontological properties. For example, the conjoined noun phrase *John and Mary* is more likely to be represented as a plural entity than *John and his bike*. Secondly, preference for plurality is also affected by the linking conjunction. A plural entity is available if the conjunction is *and* (*John and Mary*) and less preferred when *with* is used (*John with Mary*).

2 Background and Related Work

2.1 Coreference Resolution

Identifying previously mentioned entities and referring to them is crucial in language interpretation (Poesio et al., 2023). There is an extensive body of research on building coreference resolution algorithms (Lee et al., 2017; Yu et al., 2020; Bohnet et al., 2023; Martinelli et al., 2024), benchmarking coreference systems (Pradhan et al., 2011; Luo and Pradhan, 2016; Recasens and Pradhan, 2016), and evaluating the capabilities of LLMs in resolving coreference (Le and Ritter, 2023; Upadhye et al., 2020; Schuster and Linzen, 2022; Lam et al., 2023; Gan et al., 2024). However, much less is known about how modern language models track plural entities throughout the discourse and retrieve them (Yu et al., 2020; Paun et al., 2023).

Broadly speaking, coreference information is a kind of relationship between tokens. Several related processes, such as entity tracking (Prakash et al., 2024; Dai et al., 2024), relational binding (Gur-Arieh et al., 2025; Dai et al., 2026), and direct object identification (Wang et al., 2022), are well-studied in mechanistic interpretability. It has been found that LLMs have a mechanism for associating entities with their properties.

2.2 Plural Reference

Plural reference is when a plural noun phrase refers to one or more entities. In the example mentioned above (i.e., *John and Mary came to the shop. They bought some milk.*), the pronoun *they* is used because the antecedents *John* and *Mary* are in a plural construction, created by linking the two mentions using the connective *and*. This is one way in which a plural entity can be established in discourse. However, the presence of the conjunction *and* does not always make a plural entity salient, and its absence does not always prevent the plural entity from being created. For example, it is possible to rephrase the above sentence as *John came to the store with Mary. They bought some milk* while still allowing plural reference (Clifton and Ferreira, 2016). (Cases where antecedents of a plural pronoun are not mentioned together within a conjunction are called *split-antecedent* plural reference.)

On the other hand, there are also several preferences as to whether the entities within a plural construction can be considered a plural entity. One of those is ontological similarity (Koh and Clifton Jr, 2002). If the entities in the plural construction belong to the same ontological category, they are more likely to be referred to as a plural entity, as found in psycholinguistic experiments. For example, consider the sentence *Mary and her dog came to the shop*. While the conjunction *and* is present and the two mentions are perfectly within a plural construction, it is cognitively easier to continue the sentence with *She* rather than *They*. The formation of a plural entity is more difficult when the two mentions are not ontologically similar. In this paper, we focus only on plural constructions that are conjoined noun phrases (e.g., *John and Mary*), where the two antecedents are connected by a conjunction and are in the same noun phrase.

2.3 Mechanistic Interpretability

Mechanistic interpretability (MI) is a very active line of work aiming to rigorously explain the inner workings of LLMs (Olah et al., 2020; Elhage et al., 2021). In high-level terms, it seeks to "*reverse engineer*" the computations of language models into human interpretable processes by attributing the prediction of the model to a sparse set of components at different levels of granularity (e.g., layers, attention heads, neurons). Activation patching or

causal mediation analysis (Vig et al., 2020; Wang et al., 2022; Geva et al., 2023; Goldowsky-Dill et al., 2023; Meng et al., 2022; Geiger et al., 2021; Mueller et al., 2024) is one of the foundational techniques in MI. It is a method that allows for estimating the effect of a specific component on models' prediction. Given an input sequence, by exchanging the activation of certain tokens that are critical for prediction with a corrupted activation and measuring how much the prediction has changed, activation patching can locate the components that directly or indirectly affect the output. This technique has been used to investigate a range of processes, from low-level behaviors such as factual knowledge retrieval (Meng et al., 2022; Geva et al., 2023), indirect object identification (Wang et al., 2022), entity tracking (Dai et al., 2024, 2026; Prakash et al., 2024), truthfulness representations (Marks and Tegmark, 2023), and the *greater-than* computation (Hanna et al., 2023) to more complex reasoning processes such as question-answering (Basu et al., 2025; Wiegreffe et al., 2025).

2.4 Self-Attention Mechanism

We provide background on the architectural detail of the self-attention mechanism, the component that we exclusively focus on in this paper. We investigate auto-regressive Transformer-based LLMs (Vaswani et al., 2017). Given a sequence of input X consisting of n tokens $T = (t_0, t_1, ..., t_{n-1})$, the model builds the representations x_i of each token t_i at each layer l $\mathbf{X}^l = (\mathbf{x}_0^l, \mathbf{x}_1, ..., \mathbf{x}_{n-1}^l)$. At l_i, the representation x^l is processed by a Multi-head self-attention module (MHSA) and an MLP module. The output resulting from both operations is written in the *residual stream* (Elhage et al., 2021), which serves as the channel of information flow across the model components.

The MHSA modules weigh the importance of each token to each other. Each head assigns a set of attention weights for each pair of tokens. The output of a head is computed using the *Key* (K), *Query* (Q) and *Value* (V) vectors (Elhage et al., 2021). For a pair of tokens (t_i, t_j), the attention weight from the current token t_j to a previous token t_i is computed using the QK matrix. The OV matrix at token t_j decides what information of $\mathbf{x}_j$ is written to the residual stream. The QK and OV circuits operate independently from each other.

Recent LLMs such as the Qwen3 (Yang et al., 2025) and Llama3.2 (Grattafiori et al., 2024) model families are trained using *grouped-query at-*

tention (Ainslie et al., 2023). In the original MHSA architecture, every query head has distinct key and value matrices. GQA reduces the computation cost by having multiple query heads share the same key-value heads. Since we focus on these model families in our paper, we use GQA in our explanation of the MHSA module.

Let h denote the attention (Q) head and k denote the key-value (KV) head. Under GQA, each query head h is assigned to a KV head. The projection matrices are defined as follows: $\mathbf{W}_Q^h \in \mathbb{R}^{d_{\text{model}} \times d_{\text{head}}}$ and $\mathbf{W}_O^h \in \mathbb{R}^{d_{\text{head}} \times d_{\text{model}}}$ are unique to each query head h, while $\mathbf{W}_K^k \in \mathbb{R}^{d_{\text{model}} \times d_{\text{head}}}$ and $\mathbf{W}_V^k \in \mathbb{R}^{d_{\text{model}} \times d_{\text{head}}}$ are shared across all query heads assigned to KV head k. The Key ($\mathbf{k}_i^k$), Query ($\mathbf{q}_j^h$), and Value ($\mathbf{v}_i^k$) vectors are calculated as follows.

$$\mathbf{v}_i^k = \mathbf{W}_v^k \mathbf{x}_i, \ \mathbf{k}_i^k = \mathbf{W}_k^k \mathbf{x}_i, \ \mathbf{q}_j^h = \mathbf{W}_q^h \mathbf{x}_j$$

The model calculates the attention weight from the current token t_j to a previous token t_i, denoted by α_{t_j, t_i}, by passing the dot product of the query (Q) at t_j and key (K) vector at t_i through a softmax.

$$\alpha_{ji} = \text{softmax}\left(\frac{\mathbf{x}_j^\top \mathbf{W}_Q^\top \mathbf{W}_K \mathbf{x}_i}{\sqrt{d_{\text{head}}}}\right)$$

The intermediate output of the query head h at t_j, denoted by $\mathbf{z}_j^h$, is the linear combination of value vectors and the attention pattern across all attended positions:

$$\mathbf{z}_j^h = \sum_{i=0}^{j} \alpha_{ji}^h \mathbf{v}_i^k$$

Through the OV circuit, $\mathbf{z}_j^h$ is projected and written to the residual stream.

$$\mathbf{o}_j^h = \mathbf{z}_j^h \mathbf{W}_O^h$$

The output of the attention module $\mathbf{a}_j^l$ is the sum of $\mathbf{o}_j^h$ across all attention heads.

3 Dataset and Evaluation

3.1 Task Description

We design a pronoun prediction task to trigger the LLMs' mechanism for plural reference resolution. Given the sentence prefix *When John saw Mary and her sister, he waved at __*. The model may produce *her* to refer to *Mary* or *Mary's sister*. Or the pronoun *them* can be used to refer to the group of *Mary and her sister*.

3.2 Dataset

We generate two synthetic datasets of sentence prefixes for our experiment. The first dataset includes sentence prefixes that introduce plural entities (D_{pl}) and expect the LLMs to predict a plural pronoun: When John saw **Mary and her sister**, he waved at __. The second dataset also introduces a plural construction, but a plural pronoun is dispreferred (D_{sg}): When John saw **Mary and her bike**, he waved at __.

For each sentence prefix $s_{pl} \in D_{pl}$, there are several discourse entities, namely the subject *John* (s), *Mary* (e_1), and *her sister* (e_2). The plural construction consists of three elements, which are *Mary* (e_1) and *her sister* (e_2) and is formed by the conjunction *and* (c). The plural construction can be formalized as a tuple of (e_1, c, e_2). Since e_1 and e_2 form a plural entity, the plural pronoun *them* (r_{pl}) is more likely to be used. However, it should be noted that in this context, a singular pronoun (e.g., *her*) is also a plausible continuation.

In D_{sg}, we expect the LLMs to predict a singular pronoun while retaining the original structure. We replace the second element of the plural construction (e_2) with an inanimate entity e_2' (*her bike*) while keeping the rest of the sentence prefix unchanged. We carefully select a set of verbs that are not compatible with inanimate entities (e.g., *laughed at*, *nodded at*) so that it is semantically infelicitous to produce a plural pronoun. As such, the model is expected to generate a singular reference (r_{sg}), referring only to *Mary* (e_1).

We generated 300 prefixes for each dataset. All entities are single-token and all prefixes are equal in length. The gender of the entities is always randomized. For example, the subject s can be either male or female and e_1 and e_2 may have the same or different gender. See Table 4 for information on our templates.

3.3 Evaluation

Before finding the mechanism for plural reference resolution, we test how LLMs perform the pronoun prediction task. We are particularly interested in their preference in choosing the pronoun when a plural construction is present, especially with different gender, ontological similarity (Clifton and Ferreira, 2016), and also linking conjunctions (Moxey et al., 2012). We use D_{pl-sg} to indicate the probability difference between the plural and singular pronoun, and introduce three variables:

- **Gender:** e_1 and e_2 can have the same or different gender: (John, and, David), (John, and, Mary)

- **Ontological Similarity**: e_1 and e_2 antecedents have the same or different ontological properties. We consider here three levels of similarity, based on noun type (proper or common) and animacy (animate or inanimate): (John, and, Mary) > (John, and, his sister) > (John, and, his bike)

- **Conjunction**: The conjunction linking e_1 and e_2 can be *and* (John, and, Mary) or *with* (John, with, Mary). Previous psycholinguistic studies show that the conjunction *with* decreases the preference for choosing a plural pronoun over a singular one (Moxey et al., 2004, 2012; Albrecht and Clifton, 1998; Sanford and Lockhart, 1990).

Fitting Mixed Linear Regression models to estimate the effect of these three variables on the probability difference between r_{sg} and r_{pl} (D_{pl-sg}), we replicate the effects of ontological similarity and conjunction that are expected from the psycholinguistic literature. The less ontologically similar the two antecedents are, the less likely they are to be referred to as a plural entity. In addition, a plural pronoun is less preferred when the antecedents are linked by *with*, compared to *and*. (See Appendix B for detailed result of all of our model.)

This analysis guided our patching experiment, as we chose the type of plural construction that does not always trigger the formation of plural reference. The motivation behind our choice is the similarity in structure and token length between s_{pl} and s_{sg}. As such, to ensure the validity of the patching results, we extract the prediction for D_{pl} and only retain the prompts where the model predicts the plural pronoun.

4 Experimental Setup

Experiment We use a combination of *activation patching* and *path patching* in our experiment. Activation patching intervenes on a component C while allowing all downstream components to be affected. It measures the *indirect* effect of C. *Path patching* involves another step, restoring the activations of all downstream components to their clean values (Wang et al., 2022; Goldowsky-Dill et al., 2023; Meng et al., 2022). The goal is to isolate the direct effect of such component. If path patching causes

Figure 1: Layer-wise direct effect of MHSA modules on M

a decrease in P_{pl}, the direct effect can be attributed to that component (Pearl, 2022).

For each intervention on the component C, which can be high-level ones such as the residual stream of a specific layer ($\mathbf{x}_i^l$) or lower-level components such as the value vector of a specific token at a head ($\mathbf{v}_i^h$), we perform the following runs.

- **Original Run** Pass s_{pl} to the model and record the original probability of the plural pronoun $P_{pl,ori}$.

- **Corrupted Run** Run a forward pass through s_{sg} then cache the activations of all token positions at each layer ($\mathbf{X}^l$).

- **Intervened Run** Replace the activation of C at position i with that at the corresponding position of s_{sg}, restore the activations of all upstream components to their clean values to block any indirect propagation of the corrupted signal through the network, run the forward pass through s_{pl} again, and recompute $P_{pl,inter}$.

By patching, we intentionally replace the attention output of the patched token with that of the corrupted prompt (e_2), where the second mention is an entity that is less likely to be referred together with the first. If there is a set of heads that is responsible for searching for the antecedent to be referenced, intervening on its attention output would lead to a change in prediction. As such, if intervening on a specific head causes P_{pl} to decrease after intervention, it can be causally inferred that it is one of the heads responsible for pronoun resolution.

Constructing Corrupted Prompts Our regression models show that ontological similarity and conjunction significantly affect the preference to choose a plural pronoun. We treat them as crucial factors that either enhance or corrupt the plurality signal. As such, we use two corrupted prompts, manipulating either e_2 or c: (e_1, c, e_2') and (e_1, c', e_2).

Intervening Location For each component, we run the intervention at multiple positions, spanning from the last token up to the position of the corrupted token. We find that only the intervention on the *last token* and *corrupted token* (e_2 and c) show considerable effect. As such, all the findings presented in the following sections arise from intervening on these two positions.

Metrics We measure the effect of the intervention by calculating how much P_{pl} changes after the intervention. We define the evaluation metric M as the percentage of probability difference between $P_{pl,ori}$ and $P_{pl,inter}$. Negative values of M mean that the intervention suppresses the plurality signal and thus decreases P_{pl}.

$$M = \left(\frac{P_{\text{pl, inter}} - P_{\text{pl, ori}}}{P_{\text{pl, ori}}} \right) \times 100$$

Models We patch on different checkpoints of the Qwen3 family and GPT2-medium. We present in the main text the circuit of Qwen3-1.7B. Comparable results of other model families can be found in Appendix E.

5 The Plural Coreference Circuit

In this section, we present our findings of the coreference circuit, including the core components and their functionalities. We first run path patching at layer level to find the MHSA layers that directly affect P_{pl} (Figure 1). We then proceed to patch the component comprising it, namely the individual attention heads. We run activation patching on each attention head to estimate their indirect effects on the MHSA module at Layer 23. As we patch at each position, we select the set of heads that cause the largest decrease in probability of the plural pronoun (Figure 2a).

Pronoun Selection Heads identify candidate antecedents Figure 1 shows that Layer 23 is the only one that directly affects the output. With activation patching, we find that heads 12 and 13 of layer 23 (hereby L23H12 and L23H13) have the

Figure 2: **Overview of intervention results and attention pattern visualizations of major heads.** (a) Indirect effect of individual head intervention across layers. Brown values denote negative change in P_{pl}. (b) and (c) Attention pattern of Pronoun Selection heads for D_{pl} (brown). (d) and (e) Attention pattern of Pronoun Selection heads (L23H12 and L23H13) for D_{sg} (blue).

strongest effect on M and are both responsible for the prediction process of the pronoun. As the first step toward understanding the function of these heads, we investigate their attention weights. Figure 2b (top, middle) shows the mean attention weight of L23H12 across all prefixes in D_{pl}. It can be seen that the last token (*at*) attends the most to the first (e_1) and second entity (e_2) in the plural condition, which implies that they are considered to be the antecedents of r_{pl}. Notably, we observe that e_2 receives more attention than e_1. In D_{sg} (2d), we observe that the attention weight is given to the e_1, which is the antecedent for the singular pronoun.

On the other hand, at L23H13 (2c), while the attention to both antecedents is still present, we also see a very high attention weight between the conjunction *and* and e_1. These attention patterns at these heads suggest a strong focus on the elements that are crucial for plural reference resolution, namely antecedents and conjunctions.

These attention patterns suggest that L23H12 and L23H13 might be called the **Pronoun Selection** heads: they identify the antecedents to be referred to by the pronoun. In a correlation experiment (Appendix C), we found that the amount of attention difference between e_1 and e_2 positively correlates with the probability difference between P_{sg} and P_{pl}, such that the larger the attention on e_2 compared to e_1, the larger the difference between P_{pl} and P_{sg}. This type of head is similar to the Name Mover Head found in Wang et al. (2022) and other MI studies (Prakash et al., 2024; Kim et al., 2025; Lieberum et al., 2023), which identifies and encodes the decisive information for prediction.

Plurality Formation Heads send information about the plural entity to Pronoun Selection Heads We just saw how the Pronoun Selection Heads affect the prediction by attending to the discourse entities that are the candidate antecedents of the predicted pronoun. We now ask what makes the model attend more to e_2 in s_{pl}. To answer this question, we decompose the effect of the K, Q, and V vectors of the Pronoun Selection head. Since the attention weight is computed using the dot product of the vectors K and Q, we first identify which is more crucial for prediction. We run separate interventions on these vectors and measure M. For the Q vector, we patch at the last token position, because here it decides which token it needs to at-

Figure 3: **Attention Pattern of Plurality Formation Head for** $D_{pl,a}$, $D_{sg,a}$**, and** $D_{pl,w}$ (a), (b) and (c): Attention pattern of the Plurality Formation head for $D_{pl,a}$, $D_{sg,a}$, and $D_{pl,w}$. (d) Numerical values of attention weights on each token in the plural construction, where e_1 and e_2 are the two entities, c is the conjunction and pp is the possessive pronoun of e_2

Figure 4: Direct effect of K/V heads on Pronoun Selection head, measured by change in M

tend to. For the K and V vectors, we patch at e_2, where information is offered to the query vector. We found that the Q vector does not affect the prediction, while patching the K and V vector causes a strong drop in P_{pl}.

Next, we ask which head affects the Value vector of the Pronoun Selection head. We intervene on the path between the V vector of the Pronoun Selection and other K/V head. The value vector at e_2 ($\mathbf{v}_{e_2}^k$) is replaced with $\mathbf{v}'^k_{e_2}$ from D_{sg}. The output $\mathbf{o}'^{\mathbf{h}}_{\mathbf{j}}$ of head h after the intervention is updated as follows.

$$\mathbf{z}'^h_j = \sum_{i=0}^{j} \alpha^h_{j,e_2} \mathbf{v}'^k_{e_2}; \qquad \mathbf{o}'^h_j = \mathbf{z}'^h_j \mathbf{W}^h_O$$

Figure 4 shows that some K/V heads at layers 15, 17, 19, and 21 directly affect the Value vector of e_2 at the Pronoun Selection head, which suggests that it reads information from these components. Figure 2 shows that these heads also indirectly affect P_{pl}. We inspect the attention pattern of the attention heads that are associated with these K/V heads to find what information they offer to the V vector of e_2. Among these heads, L17H9 has the strongest effect on the Pronoun Selection head. Figure 3 shows the attention pattern of L17H9 for $D_{pl,a}$ and $D_{sg,a}$ and $D_{pl,w}$. For the sake of comparison, we incorporate the type of conjunction into the datasets, a stands for *and* and w stands for *with*. In the case of $D_{pl,a}$, the last token *at* attends to the whole plural construction, with slightly more attention on c and e_2. This behavior is quite different from the attention pattern of the Pronoun Selection head, where the attention weights are only dominant at e_1 and the second token of e_2 (3a). For D_{sg} (3b), it only assigns attention weights up to the possessive pronoun of e_2 (*her*). Interestingly, when the conjunction *with* is present, the attention is only on e_1 and c, the attention weight amount on e_2 is almost negligible (3c). This result is compatible with our earlier statistical analysis of the conjunction effect, which shows that the LLMs are much more likely to establish a plural entity from a plural construction when the conjunction is *and* rather than *with*. Taken together, this head is trying to find the set of entities to be referenced by selectively attending to the tokens that fit the constraints for a plural entity. It attends to the whole plural construction when it is a qualified plural entity. We hypothesize that it is responsible for constructing, representing, and writing the information about the plural entity to the Pronoun Selection heads.

In addition, in Figures 3a and 3b, where the conjunction *and* is used, it is present in e_1, similar to what we observe in the Pronoun Selection head. This behavior is not present when *with* is used (Figure 3c). In Figure 6, we compare the attention

Figure 5: **Attention Pattern of Pronoun Interpretation head**. (a) attention pattern of L13H6 for s_{pl}, (b) attention pattern of head L13H6 for $s_{pl} + them$

Figure 6: **Comparing attention pattern of the Pronoun Selection head and the Plurality Formation head**. (a) attention pattern of L23H13 for $s_{pl,w}$, (b) attention pattern of head L17H9 for $s_{pl,w}$

weight of $D_{pl,w}$ at the Pronoun Selection head (6a) and the Plurality Formation head (6b). We found that while *with* does not attend to e_1 at the Plurality Formation head, it still attends to e_1 at the Conjunction head. There is evidence that some attention heads encode grammatical dependency (Voita et al., 2019; Htut et al., 2019; Clark et al., 2019). The attention from *with* to e_1 is purely syntactic at the Pronoun Selection head and is not directly related to the process of identifying plural entities.

Pronoun Interpretation Heads encode coreference information of previous tokens Finally, we find a head that encodes coreference information. This head affects around 25% of the probability difference. When the token is a pronoun, it attends to the antecedent of the pronoun that was mentioned earlier in the input. In Figure 5a, it can be seen that *her* attends to *Mary* and *he* attends to *John*. To verify how this head behaves when there is a plural pronoun, we add *them* to the prompt and inspect the attention pattern (Figure 5b). It can be seen that *them* attends to the whole plural construction (Mary, and, her sister), with much stronger attention on e_2 (sister) and the conjunction *and*. We hypothesize that while this head may not play a direct role in predicting the pronoun, it functions as a coreference map, where every entity attends to its previous mentions. This head was also discovered in earlier studies on the attention pattern of language models (Clark et al., 2019; Tenney et al., 2019).

Generalization to other models We validate our circuit across other sentence templates and observe the same attention pattern across all heads in the circuit for the variant. We also extract the circuit for other models and find that the circuit generalizes within the Qwen3 family and also to GPT2-medium (Appendix E).

6 Discussion

Our patching experiments reveal a mechanism for performing the plural pronoun prediction task. In the middle layers, the model first builds up the representation for an entity or a group of entities that they refer back to. At the Plurality Formation head, the last token before reference production assigns attention weights spanning the phrase that contains the candidate entities. If the entities align with the model's preference for plural entities (being ontologically related and connected by a preferred conjunction), they will be attended to. After deciding on the entity or a set of entities to be referenced, the Plurality Formation heads write this information into the residual stream. The Pronoun Selection head receives this information, attends to the known entities, and uses it for making decisions. In addition, the models dedicate a head for encoding coreference information of all mentioned entities.

7 Conclusion

In this paper, we investigate how LLMs represent and use coreference information for pronoun prediction, especially in the case of plural reference. We find the constraints that LLMs use to decide whether to use a singular or a plural pronoun when a plural construction is present. We then use mechanistic interpretability methods, complemented by attention pattern analysis, to extract a circuit that is responsible for identifying the entities to be referred to and propagating such information across components to generate the correct pronoun.

Limitations

Our study only focuses on one type of plural reference (conjoined noun phrases) and plural constructions that have two elements. In actual language use, plural reference is often more complex and

the antecedents may not be linked by a conjunction (e.g., split-antecedent reference). Psycholinguistic studies have shown that it is possible and preferred to use a singular pronoun to refer to a plural entity when the antecedents create a new and unified object (Cokal et al., 2023). It would be interesting to study the model's circuit behavior in these cases.

In addition, since our goal is to understand the high-level mechanism behind the process of pronoun prediction, we focus on analyzing the function of each component more than extracting a complete circuit for coreference. As such, there is still uncertainty about whether the circuit is fully unique for coreference. We also do not thoroughly investigate the function of MLPs. Although we show that intervening on the MLP module at the late layer strongly affects P_{pl}, we know little about its functionality in the circuit.

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A Model Configuration

We find the coreference circuit for a range of model families and sizes. We use two recent and widely-used LLM collections, namely Qwen3 and GPT2, which is the standard choice for most mechanistic interpretability research (Wang et al., 2022; Meng et al., 2022). Table 1 shows the configurations of the models, including model size, number of layers, number of attention heads, number of key-value heads and the size of hidden activations.

B Statistical Analysis

In this section, we report details about our statistical analysis, which studies the effect of gender, ontological similarity, and conjunction preference for choosing plural pronouns. See Table 4 for details about our dataset. We generate a total of 349 prompts and ensure a balanced distribution between the variables.

We fit Linear Mixed-Effect Regression models with Restricted Maximum Likelihood (REML) with the verbs as random effects. The models are run using the lme4 package in R. Our dependent variable is the probability difference between the plural and singular pronoun.

$$prob - diff = P_{plur} - P_{sing}$$

The independent variables include the following.

- Gender: same, different

- Ontological (Ont. Sim.): N + N (proper name + proper name), N + R (proper name + relation), N + O (proper name + object)

- Conjunction: and, with

The results of the analysis can be found in Table 2.

C Preference for Plural Pronoun is Reflected in Attention Pattern of the Pronoun Selection Head

In the previous section, we show that the **Pronoun Selection** heads attend to the antecedents for the plural pronoun. To test how the activity of this head differs when the model gives a higher probability to the singular or plural pronoun, we investigate the relationship between the attention weight from the last token to e_1 and e_2 and the probability assigned to P_{sg} and P_{pl} in D_{pl} and D_{sg}. We hereby refer to the last token position as i. Let α_{i,e_1} and α_{i,e_2}

Model	num_layers	num_key_value_heads	num_attention_heads	hidden_size
Qwen3-0.6B	28	8	16	1024
Qwen3-1.7B	28	8	16	2048
GPT2-medium	24	16	16	1024

Table 1: Configurations for LLMs in the Qwen3 and GPT2 families

Predictor	$\hat{\beta}$	SE	df	t	p	
Fixed Effects						
Intercept	0.328	0.055	130.74	5.984	< .001	***
Gender [same]	0.092	0.052	323.11	1.751	.081	.
Conjunction [with]	-0.669	0.064	322.99	-10.423	< .001	***
Ont. Sim. [N + O]	-0.855	0.070	324.43	-12.282	< .001	***
Ont. Sim. [N + R]	-0.199	0.053	325.93	-3.771	< .001	***
Gender [same] $\times$ Conjunction [with]	-0.154	0.074	323.57	-2.083	.038	*
Conjunction [with] $\times$ Ont. sim. [N + O]	0.570	0.099	327.55	5.739	< .001	***
Conjunction [with] $\times$ Ont. sim. [N + R]	0.081	0.075	326.21	1.086	.278	
Random Effects						
VP2 (Intercept) variance	0.024		SD = 0.155			
Residual variance	0.092		SD = 0.304			
Model Fit						
Observations	350					
Groups (VP2)	27					
REML criterion	224.4					

Note: Reference categories: Gender = *different*; Conjunction = *and*;

Ontological similarity = *N + N*

Table 2: Linear Mixed-Effects Model Predicting Probability Difference (*prob_diff*)

be the attention weight between the last token i and the first (e_1) and between i and the second (e_2) antecedent of the plural construction. We define α_{diff} as the difference between the values of these attention weights. If α_{diff} is negative, e_2 receives more attention than e_1.

$$\alpha_{diff} = \alpha_{i,e_2} - \alpha_{i,e_1}$$

We also define P_{diff} as the probability difference between the singular (R_{sg}) and plural (R_{pl}) pronoun.

$$P_{diff} = P_{pl} - P_{sg}$$

We run Pearson's r correlation on α_{diff} and P_{diff}. If the attention weight difference between e_1 and e_2 is part of the model's decision on the probability of the singular and plural pronoun (Figure 7), we expect that the larger the difference between α_{i,e_2} and α_{i,e_1}, the larger the difference between $P_{R_{pl}}$ and $P_{R_{sg}}$.

We found that there is a possible correlation between α_{diff} and P_{diff} for both L23H12 ($r = .78$, $p < .001$) and L23H13 ($r = .77$, $p < .001$). This suggests that when the Pronoun Selection heads attend more strongly to e_2 relative to e_1, the model assigns a higher probability to the plural pronoun over the singular. This provides further evidence that the attention pattern of the Pronoun Selection head toward the two entities is a direct reflection of the model's pronoun choice.

D   Generalization to Other Templates

Table 4 shows the original prompt template and its variant. Figure 8 shows the attention patterns for the variant at all heads in the circuit.

E   Generalization to Other Models

Figures 9 and 10 show the attention patterns for the coreference circuit of Qwen3-0.6B and GPT2-medium.

Conjunction	Gender	Ontological Similarity	Prompt
and	same	N + N	When John saw Mary and Emma, he waved at __
		N + R	When John saw Mary and her sister, he waved at __
	different	N + N	When John saw Mary and David, he waved at __
		N + R	When John saw Mary and her brother, he waved at __
	different	N + O	When John saw Mary and her bike, he waved at __
with	same	N + N	When John saw Mary with Emma, he waved at __
		N + R	When John saw Mary with her sister, he waved at __
	different	N + N	When John saw Mary with David, he waved at __
		N + R	When John saw Mary with her brother, he waved at __
	different	N + O	When John saw Mary with her bike, he waved at __

Table 3: Summary of the dataset used in the statistical analysis. The table shows examples of the three independent variables: Gender (same, different), Ontological Similarity (N+N (name + name), N+R (name + relation), N+O (name + object)), and Conjunction (and, with)

ID	Template	Example prompt
Original	When [S] + $[V_1]$ + $[A_1]$ and $[A_2]$, [S] + $[V_2]$	When John saw Mary and her sister, he waved at __
Var. 1	Yesterday, [S] + $[V_1]$ + $[A_1]$ and $[A_2]$ and $[V_2]$	Yesterday, John saw Mary and her sister and waved at __

Table 4: Sentence templates used for generating D_{pl} and D_{sg}, with one example per template.

(a) L23H12   (b) L23H13

Figure 7: Scatter plots illustrating the relationship between attention weight difference between e_1 and e_2 and difference between P_{sg} and P_{pl}. Blue dots represent data from D_{sg} and brown dots represent data from D_{pl}.

Figure 8: **Attention pattern visualizations of major heads for Qwen3-1.7B (Var. 1).** (a) and (b) Attention pattern of Pronoun Selection head for D_{pl} (brown). (c) and (d) Attention pattern of Pronoun Selection head and conjunction head for D_{sg} (blue). (e) Attention pattern of Plurality Formation head for D_{pl} (brown). (f) Attention pattern of Pronoun Interpretation head for D_{pl} (brown).

Figure 9: **Overview of intervention results and attention pattern visualizations of major heads for Qwen3-0.6B.** (a) Indirect effect of individual head intervention across layers. Brown values denote negative change in P_{pl}. (b) and (c) Attention pattern of Pronoun Selection heads for D_{pl} (brown). (d) and (e) Attention pattern of Pronoun Selection head and conjunction head for D_{sg} (blue). (f) Attention pattern of Plurality Formation head for D_{pl} (brown). (g) Attention pattern of Pronoun Interpretation head for D_{pl} (brown).

Figure 10: **Overview of intervention results and attention pattern visualizations of major heads for GPT2-medium.** (a) Indirect effect of individual head intervention across layers. Brown values denote negative change in P_{pl}. (b) and (c) Attention pattern of Pronoun Selection heads for D_{pl} (brown). (d) and (e) Attention pattern of Pronoun Selection head for D_{sg} (blue). (f) and (g) Attention pattern of Plurality Formation head for D_{pl} (brown) and D_{sg} (blue).