Copy Suppression: Comprehensively Understanding an Attention Head†

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*: Joint Contribution.
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Abstract

We present a single attention head in GPT-2 Small has one main role across the entire training distribution. If components in earlier layers predict a certain token, and this token appears earlier in the context, the head suppresses it: we call this copy suppression. Attention Head 10.7 suppresses naive copying behaviour which improves overall model calibration. This explains why multiple prior works found negative heads that can systematically favour the wrong answer in certain narrow distributions, but are still helpful for the model overall. We uncover the mechanism that the Negative Heads use for copy suppression with weights-based evidence and are able to explain 76.9% of the impact of head 10.7 in GPT-2 Small. To the best of our knowledge, this is the most comprehensive description of the complete role of a component in a language model to date.

One major effect of copy suppression on model behaviour is its role in self-repair. Self-repair refers to how ablating crucial model components results in downstream neural network parts compensating for this ablation, and is a major bottleneck for circuit discovery, even in non-dropout models. Copy suppression leads to self-repair: if an initial overconfident copier is ablated, then there is nothing to suppress. Through targeted causal interventions and circuit analysis, we show that self-repair is implemented by several mechanisms, one of which is copy suppression, which explains 39% of the behaviour.

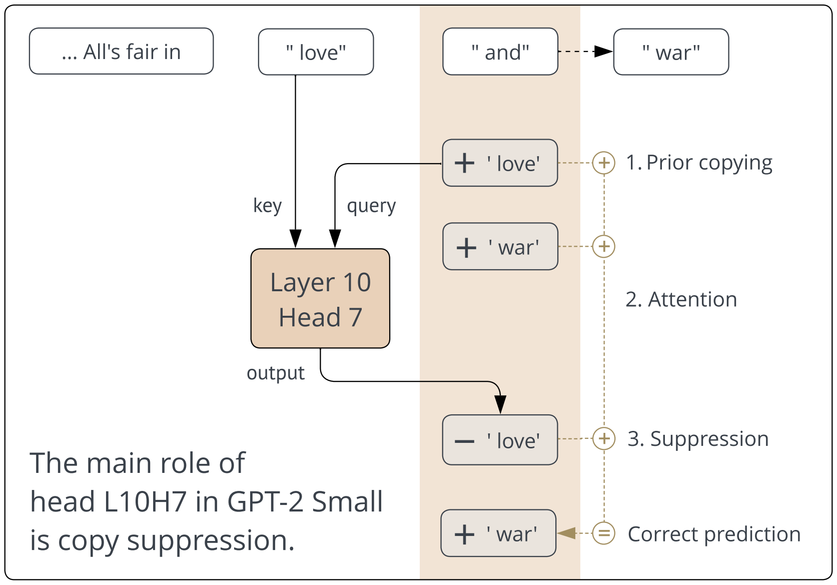

Figure 1: L10H7's copy suppression mechanism.

1 Introduction

Mechanistic interpretability research aims to reverse engineer neural networks into the algorithms that network components implement (Olah, 2022). A central focus of this research effort is the search for explanations for the behavior of model components, such as circuits (Cammarata et al., 2020; Elhage et al., 2021), neurons (Radford et al., 2017; Bau et al., 2017; Gurnee et al., 2023) and attention heads (Voita et al., 2019; Olsson et al., 2022). However, difficulties in understanding machine learning models has often limited the breadth of these explanations or the complexity of the components involved (Räuker et al., 2023), particularly when the models studied are large transformer language models (Elhage et al., 2022). In this work, we explain how Negative Heads (Olsson et al., 2022; Wang et al., 2023) in GPT-2 Small (Radford et al., 2019) function on the natural language training distribution. These attention heads were observed to write against the correct completion on narrow datasets. We explain this seemingly harmful effect as an instance of **copy suppression**, which accounts for a majority of the head's behavior and reduces the model's loss overall.

In our work we use **Negative Heads** to refer to model components which primarily reduce the model's confidence in particular token completions. **Copy suppression** is defined by three steps (Figure 1):

1. **Prior copying**. Language model components in early layers directly predict that the next token is one that already appears in context, e.g that the prefix "All's fair in love and" is completed with " love".
2. **Attention**. Copy suppression heads detect copying prediction and attend back to the previous instance of the copied token (" love").
3. **Suppression**. Copy suppression heads write to the model's output to decrease probability on the copied token.

Steps 1–3 can increase the probability on correct completions (e.g " war") and decrease model loss. **Our central claim is that 76.9% of the role of attention head L10H7 on GPT-2 Small's training distribution is copy suppression**. However, we do not explain precisely when or how much copy suppression is activated in different contexts. Nevertheless, to the best of our knowledge, there is no prior work which has explained the main role of any component in a large language model in terms of its input stimulus and specific downstream effect across a whole training distribution.

Explaining language models components across wide distributions in mechanistic detail may be important for engineering safe AI systems, in addition to the scientific contribution of understanding how machine learning models work. While interpreting parts of language models on narrow distributions (Hanna et al., 2023; Heimersheim & Janiak, 2023; Wang et al., 2023) may be easier than finding complete explanations, researchers can be misled by hypotheses about model components that do not generalize (Bolukbasi et al., 2021). Mechanistically understanding models could fix problems that arise from opaque training processes, as mechanisms can predict behavior on all inputs (Mu & Andreas, 2020) rather than merely those that arise in training. Secondly, models can exhibit emergent capabilities (Wei et al., 2022) and internal insight could be extremely useful in predicting these abrupt changes (Nanda et al., 2023).

Mechanistic interpretability research is difficult to automate and scale (Räuker et al., 2023), and understanding negative and backup heads[1] could be crucial for further progress. Many approaches to automating interpretability use **ablations** - removing a neural network component and measuring the effect of this intervention (Conmy et al., 2023; Wu et al., 2023; Bills et al., 2023). Ideally, ablations would provide accurate measures of the importance of model components on given tasks, but negative and backup components complicate this assumption. Firstly, negative components may be ignored by attribution methods that only find the positive components that complete tasks. This means that these attribution methods will not find faithful (Jacovi & Goldberg, 2020) explanations of model behavior.

[1]We define backup heads (see Section 5) as attention heads that respond to the ablation of a head by imitating that original behavior.

Secondly, backup components may counteract the effects of ablations and hence cause unreliable importance measurements.

In this work we rigorously reverse-engineer Attention Head L10H7 in GPT-2 Small to show that its main role on the training distribution is copy suppression. We do not know *why* language models form copy suppression components, but in Appendices A and C we discuss ongoing research into some hypotheses. Appendix B provides evidence that copy suppression occurs in models trained without dropout.

- Section 3 shows that Negative Heads copy suppress on the entire natural language training distribution.
- Section 4 describes a mechanism by which Negative Heads copy suppress.
- Section 5 finds some connections between copy suppression and self-repair in language models.

2 Related Work

A common theme across language model interpretability research is the search for explanations for model components, such as neurons (Elhage et al., 2022), attention heads (Vig, 2019; Rogers et al., 2020) and circuits (Elhage et al., 2021; Wang et al., 2023).

1. **Neurons**. Researchers have found neurons that detect French words (Gurnee et al., 2023), neurons firing to predict " an" rather than " a" (Miller & Neo, 2023), or explanations for all neurons in GPT-2 Small by using GPT-4 (Bills et al., 2023).[2] In GPT-2 Small, each neuron is associated with 1537 parameters.
2. **Attention heads**. Prior work has identified heads with attention patterns correlated with rare words (Voita et al., 2019) and previous tokens (Vig, 2019). In GPT-2 Small, attention heads are associated with 196,800 parameters each.
3. **Circuits**. End-to-end circuits are subsets of computational graphs of models that explain model behavior on narrow distributions (Lieberum et al., 2023; Wang et al., 2023; Hanna et al., 2023; Heimersheim & Janiak, 2023) or on toy models (Nanda et al., 2023; Olsson et al., 2022). These circuits have contained up to millions of parameters.

Geiger et al. (2021) introduce causal abstraction analysis to formalize explanations of model components, similarly Chan et al. (2022) quantify explanation strength with the loss recovered metric. Our metric for explaining the effect of L10H7 (Section 4.3) is most similar to Bills et al. (2023)'s ablation score metric except we use KL divergence instead (see Section 3 we discuss this decision).

Iterative inference. Greff et al. (2017) propose that neural networks layers iteratively update feature representations rather than recomputing them, in an analysis specific to LSTMs and Highway Networks. Several works have found that transformer language model predictions are iteratively refined (Dar et al., 2022; nostalgebraist, 2020; Belrose et al., 2023; Halawi et al., 2023), though no connections have yet been made to Negative Heads.

3 Negative Heads Copy Suppress

In this section we show that Negative Head L10H7 qualitatively suppresses copying across GPT-2 Small's training distribution. We show that these examples explain most of L10H7's role in the model, and defer quantitative evaluation of our mechanism for copy suppresion to Section 4.3.

Logit Lens. We can measure which output predictions different internal components push for by applying the Logit Lens method (nostalgebraist, 2020). Given model activations, such as the state of the residual stream or the output of an attention head, we can multiply these activations by GPT-2 Small's unembedding matrix. This measures the direct effect

[2]In fact, the researchers found a neuron that appears responds to prediction of " from" by suppressing it, but this required manual inspection: `https://openaipublic.blob.core.windows.net/neuron-explainer/neuron-viewer/index.html#/layers/44/neurons/307`

Prompt	**Source token**	**Incorrect completion**	**Correct completion**
... Millions of Adobe users picked easy-to-guess ~~Adobe~~ **passwords** ...	**" Adobe"**	**" Adobe"**	**" passwords"**
... tourist area in Beijing. A university in ~~Beijing~~ **Northeastern** ...	**" Beijing"**	**" Beijing"**	**" Northeastern"**
... successfully stopped cocaine and ~~cocaine~~ **alcohol** ...	**" cocaine"**	**" cocaine"**	**" alcohol"**

Table 1: Dataset examples of copy suppression.

that this model component has on the output logits for each possible token in the model's vocabulary (sometimes called direct logit attribution). The Logit Lens method allows us to refer to the model's predictions at a given point in the network.

Mean ablation. Mean ablation refers to replacing a model's output with the mean output calculated over a distribution.

Experimental Setup. We selected 5% of OpenWebText completions where mean ablating L10H7 increased cross entropy loss by the most (on a per-token basis), to get a representative sample of the cases where this head improves model performance. We observed that 84% of examples sampled in this way satisfied all three copy suppression steps (Section 1):

1. S was confidently predicted at the D position in the residual stream just before attention layer 10 (it was in the top 10 predictions of tokens in-context as measured by the Logit Lens).
2. The destination token D where 10.7 had a large effect on the next token prediction attended strongly to some source token S (the total attention paid to S tokens was in the top 10 amongst all in-context tokens).
3. At the D position, Head L10H7 wrote negatively in the unembedding direction for token S (S was one of the 10 in-context tokens that L10H7 wrote most negatively against).

Qualitative examples can be found in the Table 1. These results and more can also be explored on our interactive Streamlit page `https://self-repair.streamlit.app/`.

To investigate whether this copy suppression mechanism explains the majority of how head L10H7 affects the model's loss, we first decompose the effect of head L10H7 into a set of different paths through the model (Elhage et al., 2021; Goldowsky-Dill et al., 2023). We find that most of the effect on loss (averaged over OpenWebText) was via the direct path from L10H7's output to the final logits, with the exception of the path from L10H7 through head L11H10 (Figure 2). This path is special because both heads are performing copy suppression, which is a self-repair mechanism: once a predicted token is suppressed, it is no longer predicted, and therefore does not activate future copy suppression components. This means that ablating head L10H7 will often result in it being backed up by head L11H10. We also plot the effect of ablating these paths on the average KL divergence of the resultant token distributions from the original model's distributions.

The results of Figure 2 suggest that a) we should try to understand the direct effect of head L10H7 on the final logit distribution since this has the largest impact on model outputs, and b) the KL divergence of model outputs obtained from ablation experiments from the model's original outputs is correlated with the increase in loss of ablated outputs. Our goal is to show that our copy suppression mechanism faithfully reflects L10H7's behaviour (Section 4.3). Therefore in the rest of our main text, we minimize KL divergence: in the limit, this would result in mechanisms that give identical output distributions to the model. On the other hand, loss could be minimized with unfaithful mechanisms that sometimes get better performance than the model. In Appendix J.1, we discuss this choice further and report results on how our mechanisms affect loss, too.

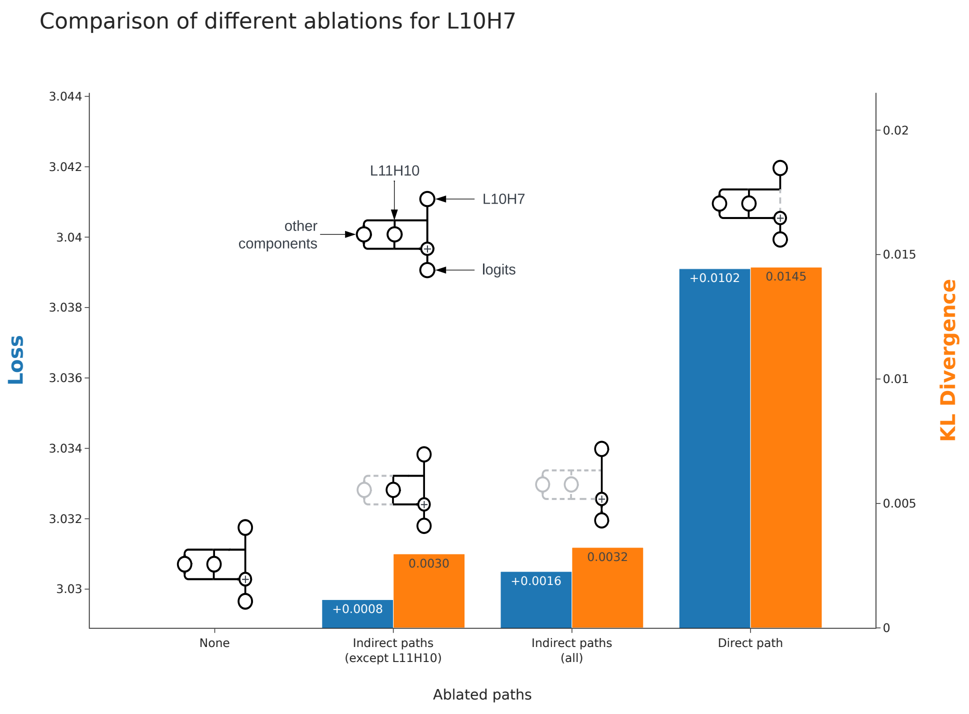

Figure 2: Loss effect of L10H7 via different paths. Grey paths denote ablated paths.

4 How Negative Heads Copy Suppress

In this section, we show that copy suppression explains 76.9% of L10H7's behavior on OpenWebText. To reach this conclusion, we first describe a concrete mechanism for how head L10H7 works.

1. In Section 4.1, we analyse the OV circuit, and show that the head suppresses the prediction of any token which it attends to.
2. In Section 4.2, we analyse the QK circuit, and show that the head attends to any token which it is currently predicting.
3. In Section 4.3, we define a form of ablation (CSPA) which deletes all of L10H7's functionality except 1. and 2., and preserves 76.9% of its effect.

CSPA projects the OV circuit outputs onto a single direction, and filters for cases where attention would be large according to our QK mechanism.[3]

To understand both the QK and OV circuit, we use a refinement of GPT-2 Small's embedding matrix we call the **effective embedding** matrix. In short, the effective embedding matrix W_{EE} has the same dimensions as the embedding matrix W_E but more faithfully reflects how the model represents tokens in latent space. Readers may wish to first read our results that use W_{EE} in Sections 4.1 and 4.2 before understanding the full motivation and definition.

Effective embedding definition and motivation. GPT-2 Small uses the same matrix in its embedding and unembedding layers, which may change how it learns certain tasks.[4]

[3] In ongoing work, we are extending our results to projecting QK circuit inputs (Section 4.2, Appendix N.2 and N.3 discuss some important QK subspaces).

[4] As a concrete example, Elhage et al. (2021) show that a zero-layer transformer with tied embeddings cannot perfectly model bigrams in natural language.

Prior research on GPT-2 Small has found that the output of MLP0 is often more important for token predictions than the model's embedding layer (Wang et al., 2023; Hanna et al., 2023). To account for this, we define the **effective embedding matrix** W_{EE} as the linear map whose rows are the values in the residual stream after applying the first block of the transformer, with the position-dependent model components (the positional embeddings and the attention layer) zero-ablated. We justify our choice of this matrix in Appendix H.

4.1 OV Circuit

To understand L10H7's output, we compute the OV circuit (Elhage et al., 2021) with our effective embedding refinement:

$$W_U^\top W_{OV}^{\mathrm{L10H7}} W_{EE} \in \mathbb{R}^{d_{\mathrm{vocab}} \times d_{\mathrm{vocab}}} \tag{1}$$

Each column of this matrix is the vector of logits which will be added to the final logits at destination token D, if it only paid attention to source token S (and if we make the simplifying assumption that the residual stream at S only holds the effective embedding of token S). If head L10H7 is suppressing the tokens that it attends to, then we would expect to find that the diagonal elements of this matrix (i.e the effect on the logits of the token which is attended to) are consistently the most negative elements in their respective columns. The results support this: for 84.70% of the tokens in GPT-2 Small's vocabulary, the diagonal element of the OV-circuit is one of the top 10 most negative values in its column, and only 571 tokens weren't in the bottom 5% in their columns. This suggests that L10H7 is copy-suppressing almost all of the tokens in the model's vocabulary.

Moreover we can zoom in on the cases where the rank of diagonal elements in their columns are least negative to find the tokens which L10H7 suppresses the least, according to the OV-circuit. We find that the top 22 failure cases (as measured by rank of the token in its column) are all **function words**, including " of", " at", " their", " most", " as" and " this". This shows that copy-suppression is not generically used for every token in the vocabulary, but differentially activated depending on the type of word which has been copied. We discuss more failure cases, as well as possible interpretations and implications in Appendix F.

Finally, does this OV circuit reflect the function of head L10H7 in practice? We filtered for examples in OpenWebText where L10H7's had a large attention weight to certain tokens, and in 78.24% of these cases, we observed that the attended-to token was among the ten most suppressed tokens, from the direct effect of L10H7 (full experimental details in Appendix E). Along with the success of the ablation in Section 4.3, this suggests that negative copying describes L10H7 well.

4.2 QK Circuit

To understand L10H7's attention patterns, we compute the QK circuit (Elhage et al., 2021), again with our effective embedding refinement:

$$W_U W_{QK}^{\mathrm{L10H7}} W_{EE}^\top \in \mathbb{R}^{d_{\mathrm{vocab}} \times d_{\mathrm{vocab}}}. \tag{2}$$

This is a bilinear form, which computes attention scores from destination to source token when the residual stream contains an unembedding at the destination token position, and an effective embedding at the source token position. Our theory of copy suppression suggests that L10H7 attends from destination tokens D where some token S is confidently predicted, back to previous instances of the token S. So we expect to find that the largest elements of each row are the diagonal elements of this matrix.

We performed an equivalent experiment to that from the previous section, measuring the rank of the diagonal elements in each row. We found that 95.72% of diagonal values in this matrix were the largest in their respective rows.[5] To test alternative mechanisms (and provide a baseline), we also try replacing the queryside and keyside lookup tables W_{EE} and W_U with other (un)embeddings to test alternative mechanisms. We computed the median ranks over GPT-2 Small's vocabulary that we found in Section 4.1. The results can be found in Figure 3, and full details of these experiments can be found in Appendix N.1. We find that

1. Head L10H7 has greatest token self-attention when the queryside vector is an unembedding vector.
2. Head L10H7 has greatest token self-attention when the keyside vector involves MLP0.

Head L10H7 attends to embeddings most when the queryside vector is an unembedding vector, as across all three different keyside embeddings, the median rank is closest to 1st when the queryside lookup table is W_U. Additionally, the two ranks closest to 1st across all queryside and keyside lookup tables occur when we use either MLP0's output or the effective embedding, which includes MLP0. In Appendix I we show that in duplicate token heads the greatest average ranks do not occur when the queryside vector is an unembedding vector, suggesting that L10H7 has a qualitatively different QK-circuit to naive matching.

Does this mechanism represent how Attention Head L10H7 copy suppresses on OpenWebText? Unfortunately, we found that these approximations were not as faithful as we thought, and projecting key and query inputs onto the unembedding and effective embeddings directions did not capture full model performance (Appendix N.3 and N.2). Additionally, the CSPA mechanism works surprisingly well on many model heads, though it works best of all on 10.7 (Appendix J.3). Despite these limitations, we show that copy suppression nevertheless captures 76.9% of L10H7's behaviour, and in ongoing research we hope to explain the query- and key-side inputs more completely.

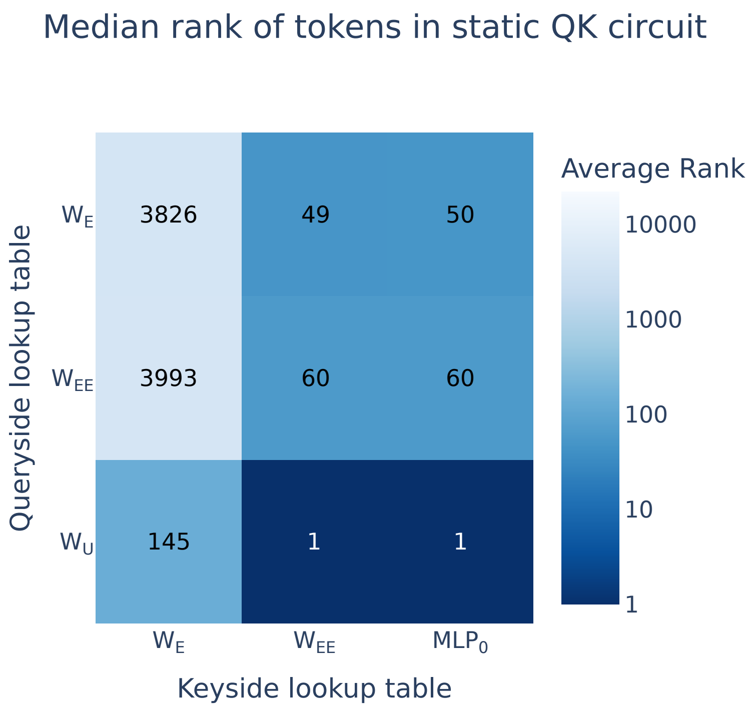

Figure 3: The median ranks of tokens when they are used as queryside vectors.

4.3 How much of L10H7's behavior have we explained?

In this section, we perform an ablation which deletes all functionality of L10H7's OV and QK circuits, except for the mechanisms described in Section 4.1 and Section 4.2 respectively. We refer to this as **Copy Suppression-Preserving Ablation** (CSPA). In Section 4.3.1 we explain exactly how each part of CSPA works, and in Section 4.3.2 we present the result of the ablation.

4.3.1 Methodology

[5] We ignore bias terms in the key and query parts (as we find that they do not change results much in Appendix N), and our experimental setup allows us to ignore LayerNorm (see Appendix G for all details).

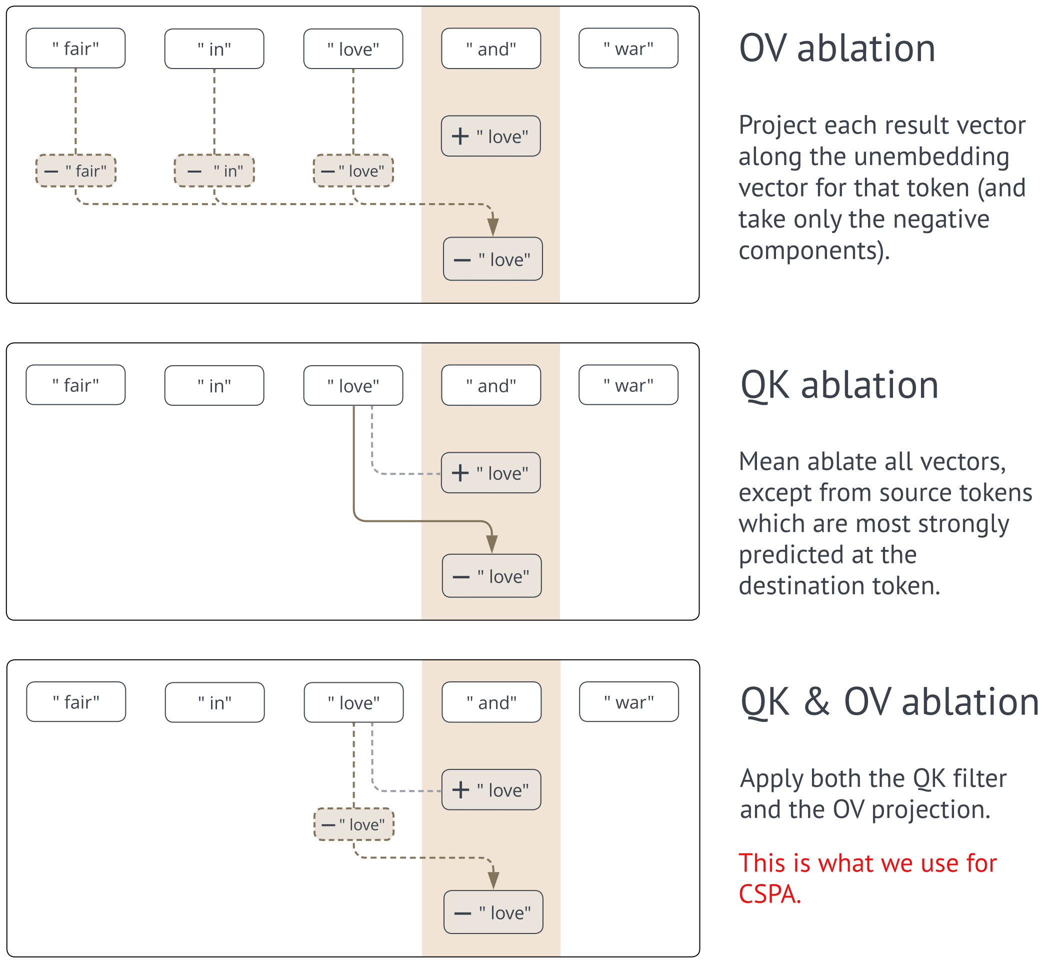
" fair"
" in"
" love"
" and"
" war"
+ " love"
− " fair"
− " in"
− " love"
− " love"
OV ablation
Project each result vector along the unembedding vector for that token (and take only the negative components).
QK ablation
Mean ablate all vectors, except from source tokens which are most strongly predicted at the destination token.
QK & OV ablation
Apply both the QK filter and the OV projection.
This is what we use for CSPA.

Figure 4: Illustration of three different kinds of ablation: just OV, just QK, and both. The results presented in Section 4.3.2 section use both.

Ablation metric. We measure the amount of L10H7's behavior that we have explained by comparing our ablation to a baseline that mean ablates L10H7's direct effect. Formally, if the model's output token distribution on a prompt is π and the distribution under an ablation Abl is π_{Abl}, then we measure the KL divergence $D_{\text{KL}}(\pi||\pi_{\text{Abl}})$. We average these values over OpenWebText for both ablations we use, defining $\overline{D_{\text{CSPA}}}$ for CSPA and $\overline{D_{\text{MA}}}$ for the mean ablation baseline. Finally, we define the effect explained as

$$1 - \left(\overline{D_{\text{CSPA}}} \Big/ \overline{D_{\text{MA}}}\right). \tag{3}$$

For example, if CSPA was identical to mean ablation of L10H7's direct effect, the effect explained would be 0%, and if CSPA preserved L10H7 exactly, 100% of effect would be recovered. Appendix J provides more discussion on the CSPA metric.

OV ablation. The output of an attention head at a given destination token D can be written as a sum of result vectors from each source token S, weighted by the attention probabilities from D to S. We can project each of these vectors onto the unembedding vector for the corresponding source token S, and only keep the negative components.

QK ablation. We mean ablate the result vectors from each source token S, except for the k source tokens which are predicted with highest probability at the destination token D (using the logit lens). Note that (for small values of k) this part of the ablation also tests the hypothesis of **sparsity** - that in normal operation, the majority of the head's effect comes from a small number of source tokens.

As an example of how the OV & QK ablations work in practice, consider the opening example "All's fair in love and war". In this case the destination token D is " war". The predicted token S is " love", and so we would take the result vector from this token and project it onto the unembedding vector for " love". This will capture the way head L10H7 suppresses the " love" prediction.

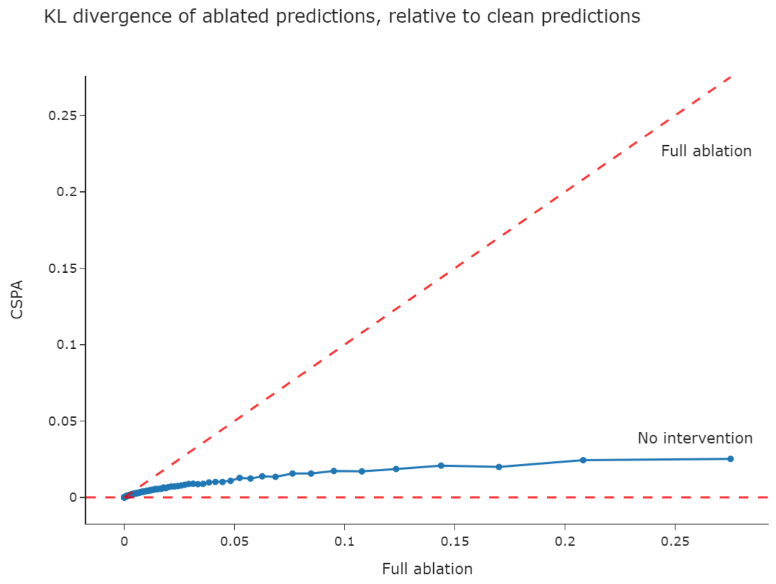

Figure 5: KL divergence to the original model under different ablations.

4.3.2 Results

Performing OV and QK ablation leads to 76.9% effect explained. Since the QK and OV ablations are modular, we can apply either of them independently and measure the effect recovered, which we explore in Appendix L.

To visualize the performance of CSPA, we plot $\overline{D_{\text{CSPA}}}^{(i)}$ against $\overline{D_{\text{MA}}}^{(i)}$ for $0 \leq i < 200$ where the superscript (i) denotes the average over points which are in the i-th quantile of D_{MA} values (Figure 5). We observe that for larger values of i our copy suppression mechanism is relatively better at explaining the head's behaviour than for smaller i. For example, amongst the completions in the quantile $i = 199$, where mean ablation increased loss by at least 0.75, CSPA explained 89.5% of 10.7's effect.

5 Copy Suppression and Self-Repair

In this section we focus on a specific distribution rather than the whole natural language training distribution in order to study self-repair and its relation to copy suppression.

Indirect Object Identification (Wang et al., 2023, **IOI**) is a phenomenon in natural language where sentences such as "When John and Mary went to the store, Mary gave a bottle of milk to" are completed with the indirect object " John". GPT-2 Small has a circuit for choosing the name " John" over the name " Mary" on a narrow distribution of similar sentences (the **IOI Distribution**). We refer to the indirect object token (" John") as **IO** and the first instance of the subject token (" Mary") as **S1**, and frequently measure the logit difference between the final logits of the IO and S1 token. Wang et al. (2023) also used an **ABC distribution** with no repeated names to perform patching experiments.

In Wang et al. (2023), the Negative Heads were introduced without an explanation of their behavior. Copy Suppression provides a simple explanation: responding to the earlier layer's prediction of the IO token, the Negative Heads suppress it. But a more important consequence of Copy Suppression is that it helps explain portions of the Self-Repair (McGrath et al., 2023) within the IOI distribution.

In the context of the IOI task, ablating an upstream **Name Mover Head** - responsible for writing the IO token to the final token position - causes some downstream heads to 'repair'

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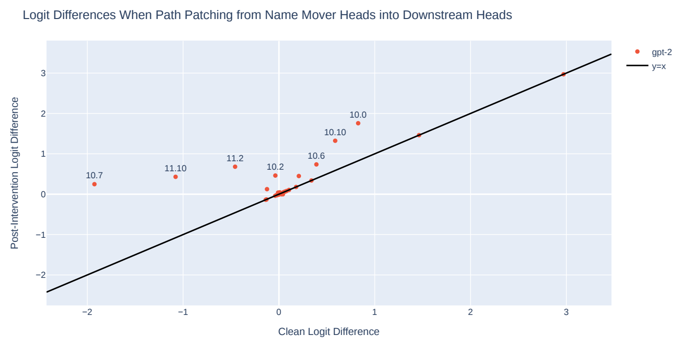
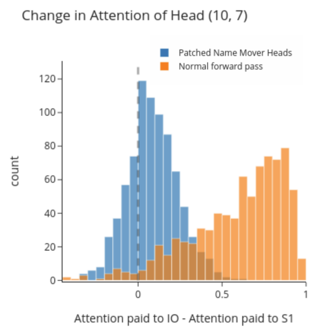


(a) Ablating the Name Mover Heads in Layer 9 causes a change in the direct effects of all the downstream heads. Plotting the Clean Logit Difference vs the Post-Intervention Logit Difference for each head highlights whether a head performed self-repair or not, depending on if it is above the $y = x$ line.



(b) Measuring attention paid to names when editing the input Negative Heads receive from Name Mover Heads

Figure 6: Self-repair and copy suppression in the IOI task.

the lost logit difference created by the Name Mover Head. We focus on the following key self-repair heads in GPT2-Small:

- Backup Heads L10H2, L10H6, L10H10 and L11H2, and Name Mover Head L10H0 - characterised by responding to the ablation of a head by imitating the original behavior
- Negative Heads L10H7 and L11H10 - characterised by responding to the ablation of a head by performing less of a behavior that opposes the effect of the ablated head

In this section, we aim to gain insights into how GPT-2 Small communicates signals relevant to self-repair: **the copy suppression phenomena suggests that the unembedding directions may be an important signal for self-repair**. We investigate the extent to which this general hypothesis (Section 5.2), as well as copy suppression specifically (Section 5.1), explain self-repair in the context of the direct effects on the output logits.

5.1 Relating Copy Suppression to Self-Repair

Upon ablation of the Name Mover Heads, many downstream heads perform self-repair: Figure 6a depicts a variety of heads recovering the lost logit difference from the Name Mover Heads when path patching from a sample ablated Name Mover Head into a downstream head. Recall that while many of these heads lead to the same outcome - recovered logit difference - the actual mechanism by which this occurs may differ.

Copy Suppression explains the mechanism behind the self-repair performed in the Negative Heads: the upstream Name Mover Heads reduces copying of the indirect object (IO) token, causing less copy-suppression behavior within the Negative Heads. Indeed, we edited the input that the Negative Heads receive from the Name Mover heads by replacing it with an activation from the ABC distribution. We then measured the difference between the attention that the negative head paid to the IO token compared to the S token. We found that the Negative Heads now attended equally to the IO and the S1 token, as the average IO attention minus S1 attention was just 0.08 for Head L10H7 and 0.0006 for Head L11H10 (Figure 6b).

To get a quantitative measurement to the extent Copy Suppression explains self-repair, we observe changes in logit difference between the IO and S1 token within individual components in the model. By sample ablating the IOI task with the ABC distribution in the Name Mover Heads, we measure the ratio between the change in logit difference in the Negative

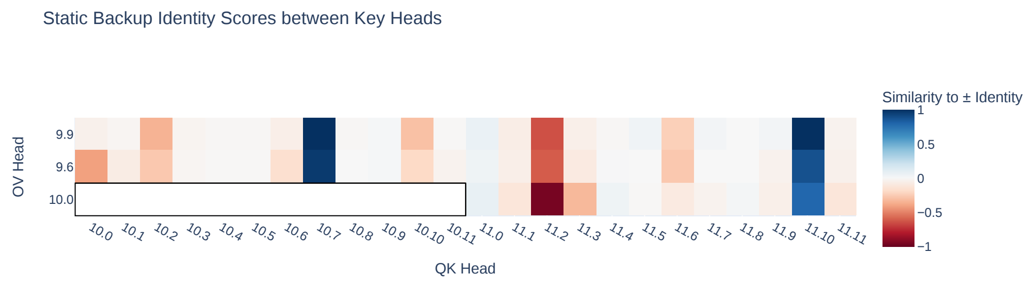


Figure 7: A graph of the Static Backup Identity Scores between the Name Mover Heads (on the OV side) and Layer 10 and 11 Heads

Heads to the *all* downstream heads. The Negative Heads accout for 39% of all of the change in downstream behavior, indicating that Copy Suppression helps explain over a third of the self-repair in the model.

What sort of mechanisms may enable self-repair? Given that Copy Suppression accounts for a significant portion of the self-repair in the Negative Heads, this suggests that the Negative Heads are primarily responding to the copied IO embeddings from the Name Movers. However, this is one possible way out of many that two heads could cause Anti-Erasure. To capture more general forms of Anti-Erasure (and self-repair), we introduce the Static Backup Identity Score.

(Turn this into a median rank experiment) The SBIS between two attention heads signifies the reactivity of one head to another head operating on a specific token. Specifically, the SBIS between an attention head with OV matrix W_{OV} (the OV-head) and a second head with QK matrix W_{QK} (the QK-head) is a measure of how close

$$W_{PE}W_{QK}^{\top}W_{OV}W_{PE}^{\top} \tag{4}$$

is to the identity or negative identity matrix.[6] The matrix combines an OV and QK circuit with a 'partially extended' embedding matrix $W_{PE} \in \mathbb{R}^{d_{\text{subset}} \times d_{\text{subset}}}$ of a set of name embeddings summed with the output of them when passed through MLP layer 0. We approximate the matrix's similarity to the identity with the following algorithm:

1. Iterate across all columns, while maintaining a running sum S.
2. For the nth column, if its maximum or minimum value is in the nth row, add or subtract one to the running sum S, respectively.
3. After iterating across all columns, divide S by the number of columns/rows.

The resulting SBIS ranges from -1 and 1 and indicates the similarity of the matrix to the negative or positive identity.

Intuitively, the $d_{\text{subset}} \times d_{\text{subset}}$ matrix represents attention scores between pairs of names. Each attention score is calculated between a query-side vector multiplied by the W_{OV} matrix for one head, dotted with the key-side embedding vector. For pairs of query-side token A and key-side token B pairs, a low attention score indicates that at a specific token position, if the OV-head attends to A then the QK-head is unlikely to attend to B as a result; conversely, a high score indicates that the QK-head is more likely to attend to B if the OV-head attended to A. Thus, SBIS scores close to one indicate that the matrix is similar to the identity: the QK-head is likely to attend to the name X given that the OV-head attended to X.

[6]We omit output query and key value biases for simplicity.

Figure 7 shows these scores between pairs of these heads. The Negative Heads L10H7 and L11H10 have significant positive SBIS with upstream Name Mover Heads. This is significant in comparison to other miscellaneous heads such as L10H1 or L11H0, which have SBIS ≈ 0.

Importantly, when combining SBIS with whether or not the downstream head has a positive or negative identity OV circuit (Section 4.1), we see that the self-repair mechanism in backup and negative heads are qualitatively different.

Head Type	**Response to Name Movers predicting T**	**Effect of attending to T**
Negative	More attention to T	Decrease logits on T
Backup	Less attention to T	Increase logits on T

Table 2: Qualitative Difference between Negative and Backup Heads

The "anti-erasure" approach towards self-repair, where a head reduces a negative behavior upon a changed output of an upstream head, can be implemented by a model in many ways. However, interestingly, the Negative Heads are the only heads with a positive SBIS with the Name Mover Heads. This indicates that copy-suppression may qualitatively explain the "anti-erasure" occuring within the model, rather than another general mechanism the model may have learned.

5.2 Complicating the Story: Component Intervention Experiments

While copy suppression seems to explain an important mechanism behind self-repair in the Negative Heads, it cannot explain the full picture of self-repair. As introduced at the end of Section 5.1, the self-repair performed in Backup Heads is qualitatively different to self-repair in Negative Heads.

Copy suppression suggests that rather than the copy suppression mechanism specifically, perhaps all of self-repair can be explained by changes in the unembedding more generally. However, we present two pieces of evidence to highlight how the unembedding explains only part of the self-repair in the model.

First, we intervened on the output of the Name Mover Heads and L10H7,[7] and path patched the resulting changes into the queries of downstream heads. The intervention was either a projection *onto* or *away from* the IO unembedding. We also freeze LayerNorm.

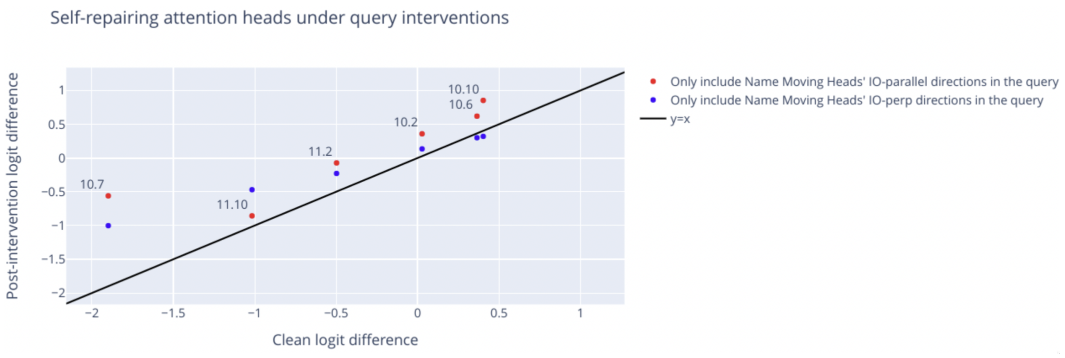


Figure 8: Path Patching from Name Mover Heads and L10H7 into the queries of downstream heads.

Figure 8 shows that while there are hints of self-repair that occur when when removing the IO direction from the outputs of the Name Mover Heads and L10H7, there is more self-repair when constraining the NMH outputs to the IO directions. As these backup heads respond less to the loss of the IO direction than the IO-perpendicular direction, this indicates that

[7] We also ablate the output of L10H7 due to self-repair that occurs between L11H10 and L10H7.

there is important information in the IO-perpendicular direction which helps control for self-repair outside of the unembedding.

To complement this analysis, we also broke the attention score (a quadratic function of query and key inputs) down into terms and again found the importance of the perpendicular direction (Appendix M).

While we currently do not understand this perpendicular direction, we are not confident that it is meaningfully different than the mechanism used for copy suppression. It could potentially be related to *semantic* copying of related but different tokens (Appendix K) or to a communication mechanism between specific heads that we do not yet understand.

Ultimately, we conclude that while fragments of copy suppression exist within these heads, the self-repair occurring across both the Erasure and Backup Heads is more general.

6 Conclusion

Write the conclusion after seeing the strength of the projection etc. results.

Author Contributions

Write Author Contributions after we're done.

Acknowledgments

Corrective Components were conceived carefully by Callum Conmy and Cody, collectively. Combining creative capabilities with code, these compiled collection of component conquers concerns and critical confusions and Connor commented with Joseph Jett Jonathan Jake Joseph (much MATS and McGrath mentorship, McDougall mentions) and Atticus Geiger which doesn't alliterate :-(Make this sensible after we've done with the writeup.

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A Anti-induction

As one example of behaviors which copy-suppression seems to explain outside the context of IOI, we present the phenomenon of **anti-induction**. Attention heads have been discovered in large models which identify repeating prefixes and suppressing the prediction of the token which followed the first instance of the prefix, in other words the opposite of the induction pattern (Olsson et al., 2022). Analysis across different model architectures revealed a strong correlation between attention heads' copying scores on random sequences of repeated tokens (i.e. the induction task) and their copy-suppression scores on the IOI task, in the quadrant where both scores were positive. For example, head L10H7 in GPT-2 Small ranked higher than all other attention heads in both copy-suppression and negative induction score.

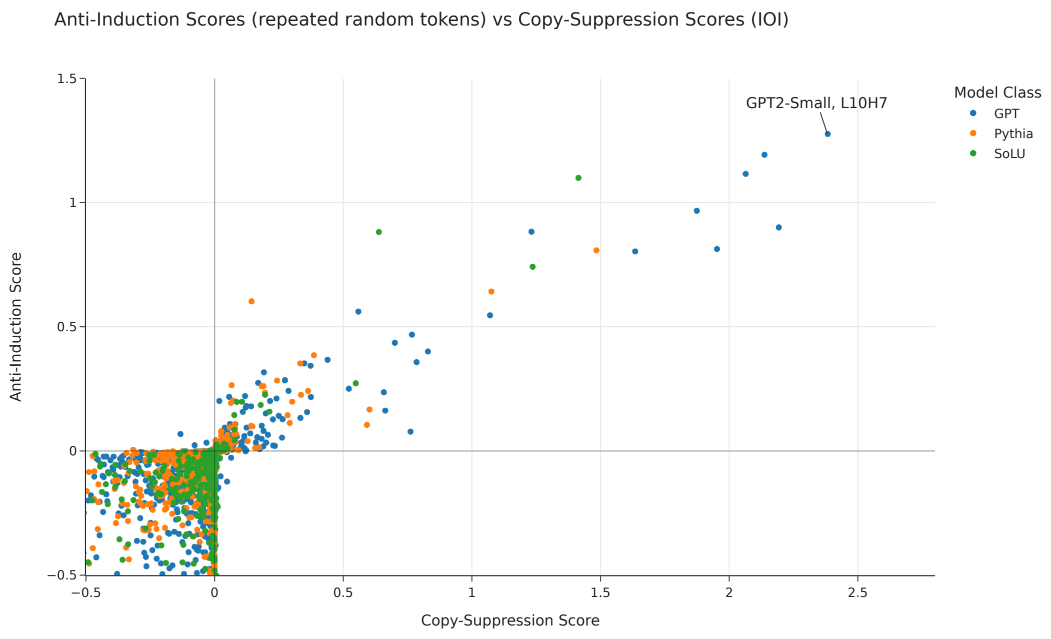


Figure 9: Anti-induction and copy suppression on the IOI task compared.

Importantly, since the induction task involves a repeated sequence of random tokens, this graph strongly suggests that the negative behavior displayed by certain heads on the IOI task is not task-dependent. We believe this holds a generalisable lesson for mechanistic interpretability - **certain components can appear to be using task-specific algorithms, but are actually implementing a more general pattern of behaviour.**

B Copy Suppression in other models

We have performed the experiment in Section 4.2 on all heads in GPT-2 Medium: Figure 10. We found that the two heads most prominently recovered were 2/3 of the most negative heads on the IOI task in GPT-2 Medium (Figure 11).
We also find instances of copy suppression (though weaker) in the Pythia models that were trained without copy suppression (Figure 9).

C Entropy and Calibration

A naive picture of attention heads is that they should all reduce the model's entropy (because the purpose of a transformer is to reduce entropy by concentrating probability mass in the few most likely next tokens). We can calculate a head's direct contribution to entropy by measuring (1) the entropy of the final logits, and (2) the entropy of the final logits with the head's output subtracted. In both cases, the negative head L10H7 stands out the most, and the other negative heads L11H10 and L8H10 are noticeable.
We can also examine each attention head's effect on the model's calibration. Hu et al. (2023) use **calibration curves** to visualise the model's degree of calibration. From this curve, we can define an **overconfidence metric**, calculated by subtracting the perfect calibration curve from the model's actual calibration curve, and taking the normalized L_2 inner product between this curve and the curve we get from a perfectly overconfident model (which only ever makes predictions of absolute certainty). The L_2 inner product can be viewed as a measure of similarity of functions, so this metric should tell us in some sense how overconfident our model is: the value will be 1 when the model is perfectly overconfident, and 0 when the model is perfectly calibrated. Figure 13 illustrates these concepts.

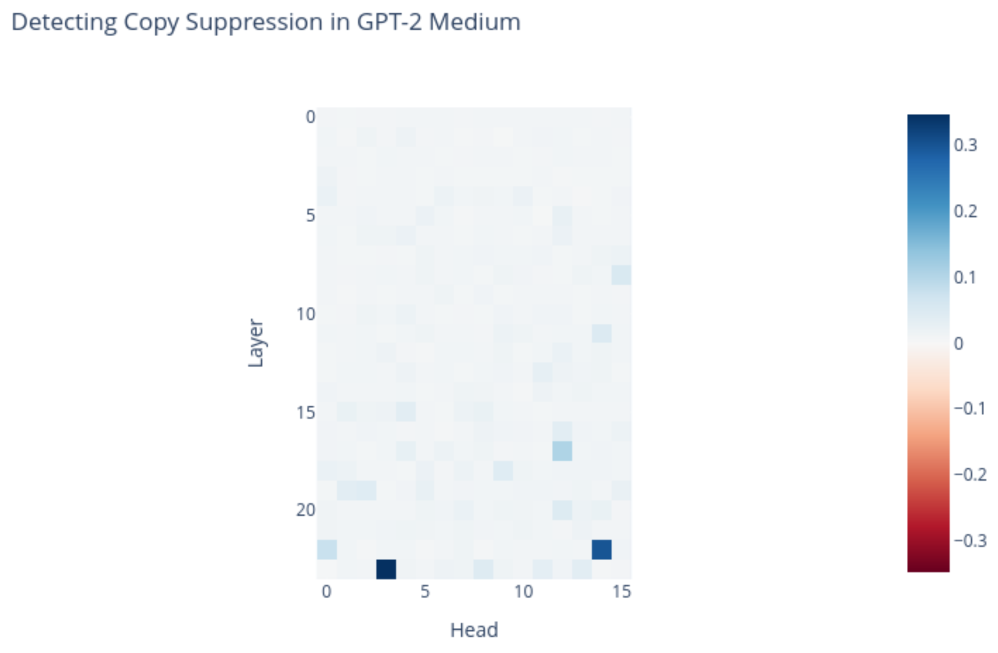


Figure 10: Repeating the experiment in Section 4.2 (with W_{EE} keyside and W_U queryside) on GPT-2 Medium.

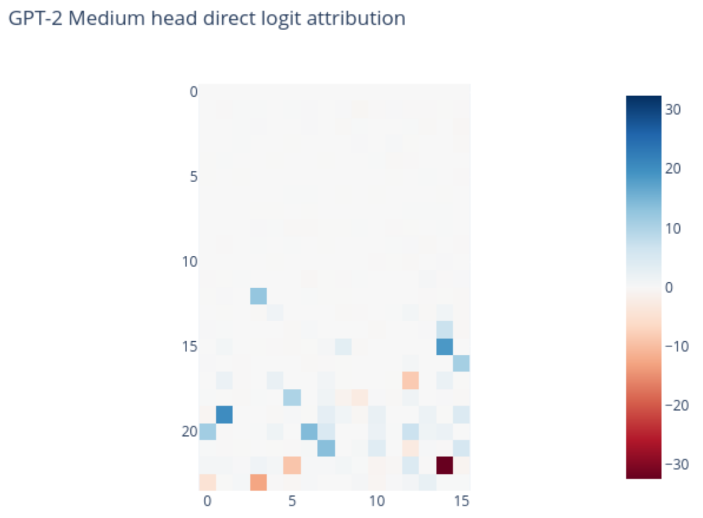
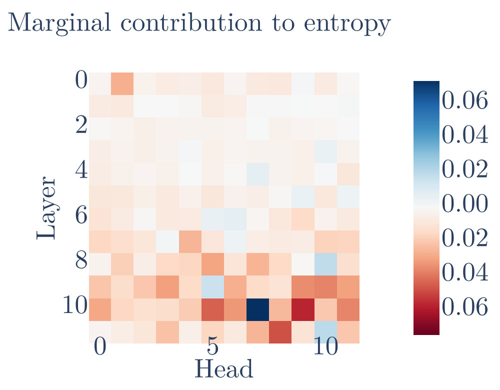
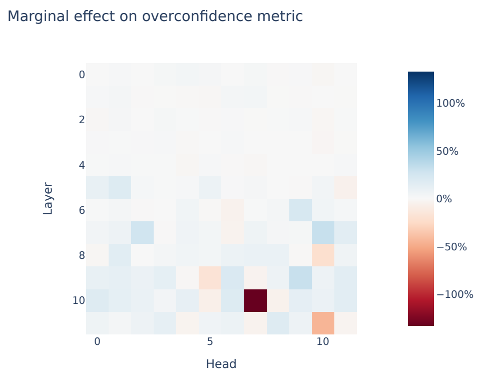


Figure 11: Finding the direct logit attribution for different heads in GPT-2 Medium on the IOI task.



(a) Entropy contribution per head. L10H7 increases entropy (as do other negative heads like L11H10); most other heads decrease it.



(b) Marginal effect on overconfidence metric per head. L10H7 decreases overconfidence; most other heads increase it.

Figure 12: Effect of attention heads on entropy & calibration.

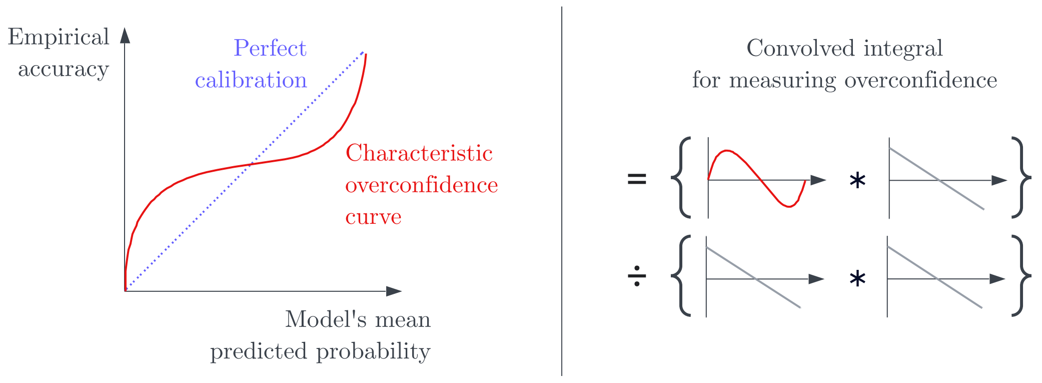

Empirical accuracy
Perfect calibration
Characteristic overconfidence curve
Model's mean predicted probability
Convolved integral for measuring overconfidence
=
*
÷
*

Figure 13: Illustration of the calibration curve, and overconfidence metric.

We can then measure the change in overconfidence metric from ablating the direct effect of an attention head, and reverse the sign to give us the head's direct effect on overconfidence. This is shown in the figure below, with the change shown relative to the model's original overconfidence (with no ablations). Again, we see that head L10H7 stands out, as do the other two negative heads. Interestingly, removing the direct effect of head L10H7 is enough to push the model from net over-confident to net under-confident.

What are we to interpret from these results? It is valuable for a model to not be overconfident, because the cross-entropy loss will be high for a model which makes high-confidence incorrect predictions. One possible role for negative heads is that they are reducing the model's overconfidence, causing it to make fewer errors of this form. However, it is also possible that this result is merely incidental, and not directly related to the reason these heads form. For example, another theory is that negative heads form to suppress early naive copying behaviour by the model, and in this case they would be better understood as copy-suppression heads rather than "calibration heads". See the next section for more discussion of this.

D Why do negative heads form? Some speculative theories

This paper aimed to mechanistically explain what heads like L10H7 do, rather than to provide an explanation for why they form. We hope to address this in subsequent research. Here, we present three possible theories, present some evidence for/against them, and discuss how we might test them.

- **Reducing model overconfidence.**
  - **Theory**: Predicting a token with extremely high confidence has diminishing returns, because once the logprobs are close to zero, any further increase in logits won't decrease the loss if the prediction is correct, but it will increase loss if the prediction is incorrect. It seems possible that negative heads form to prevent this kind of behaivour.
  - **Evidence**: The results on calibration and entropy in Appendix C provide some evidence for this (although these results aren't incompatible with other theories in this table).
  - **Tests**: Examine the sequences for which this head decreases the loss by the most (particularly for checkpointed models, just as the negative head is forming). Are these cases where the incorrect token was being predicted with such high probability that it is in this "diminishing returns" window?
- **Suppressing naive copying.**
  - **Theory**: Most words in the English language have what we might term the "update property" - the probability of seeing them later in a prompt positively updates when they appear. Early heads might learn to naively copy these words, and negative heads could form to suppress this naive behaviour.
  - **Evidence**: The "All's fair in love and love" prompt is a clear example of this, and provides some evidence for this theory.
  - **Tests**: Look at checkpointed models, and see if negative heads form concurrently with the emergence of copying behaviour by other heads.
- **Suppressing next-token copying for tied embeddings.**
  - **Theory**: When the embedding and unembedding matrices are tied, the direct path $W_U W_E$ will have large diagonal elements, which results in a prediction that the current token will be copied to the next sequence position. Negative heads could suppress this effect.
  - **Evidence**: This wouldn't explain why negative heads appear in models without tied embeddings (although it might explain why the strongest negative heads we found were in GPT2-Small, and the Stanford GPT models, which all have tied embeddings).
  - **Tests**: Look at attention patterns of the negative head early in training (for checkpointed models, with tied embeddings). See if tokens usually self-attend.

While discussing these theories, it is also important to draw a distinction between the reason a head forms during training, and the primary way this head decreases loss on the fully trained model - these two may not be the same. For instance, the head seems to also perform semantic copy suppression (see Appendix K), but it's entirely possible that this behaviour emerged after the head formed, and isn't related to the reason it formed in the first place.

E Experiment details for OV-Circuit in practice.

- Run a forward pass on a sample of OpenWebText,
- Filter for all (source, destination) token pairs where the attention from destination to source is above some threshold (we chose 10%),
- Measure the direct logit attribution of the information moved from each of these source tokens to the corresponding destination token,
- Perform the same experiment as we did in the static analysis section (measuring the rank of the source token in this direct logit attribution).

We found that the results approximately matched our dynamic analysis (with slightly more noise). The proportion of (source, destination) token pairs where the source token is in the top 10 most suppressed tokens is 78.24% (which is close to the static analysis result of 84.70%).

F Function Words

In section (TODO: OV section), we mentioned that a large fraction of the tokens which failed to be suppressed were function words. The list of least copy suppressed tokens are: [' of', ' Of', ' that', ' their', ' most', ' as', ' this', ' for', ' the', ' in', ' to', ' a', 'Their', ' Its', 'When', ' The', ' its', ' these', 'The', 'Of', ' it', ' nevertheless', ' an', '`<|endoftext|>`, 'Its', ' have', ' some', ' By']. Sampling randomly from the 3724 tokens other than 92.59% that are copy suppressed, many are also connectives (and rarely nouns): [' plainly', ' utterly', ' enhance', ' obtaining', ' entire', ' Before', 'eering', '.)', ' holding', ' unnamed'].
It is notable that this result is compatible with all three theories which we presented in the previous section.

- **Reducing model overconfidence**. The unembedding vectors for function words tend to have smaller magnitude than the average token in GPT2-Small. This might lead to less confident predictions for function words than for other kinds of tokens.
- **Suppressing naive copying**. There would be no reason to naively copy function words, because function words don't have this "update property" - seeing them in a prompts shouldn't positively update the probability of seeing them later. So there is no naive copying which needs to be suppressed.
- **Suppressing next-token copying for tied embeddings**. Since function words' unembedding vectors have smaller magnitudes, the diagonal elements of $W_U W_E$ are small anyway, so there is no risk of next-token copying of function words.

G Model and General Experiment Details

All of our experiments were performed with Transformer Lens (Nanda & Bloom, 2022). They can be found at `https://github.com/callummcdougall/SERI-MATS-2023-Streamlit-pages` and we note that we enable all weight processing options,[8] which means that transformer weight matrices are rewritten so model output probabilities are identical, yet internal functions are much simpler. For example, our Layer Norm functions only apply normalization, with no centering or rescaling (this particular detail significantly simplifies our Logit Lens experiments).

[8]That are described here: `https://github.com/neelnanda-io/TransformerLens/blob/main/further_comments.md#weight-processing`