Explaining How Transformers Use Context to Build Predictions

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Abstract

Language Generation Models produce words based on the previous context. Although existing methods offer input attributions as explanations for a model's prediction, it is still unclear how prior words affect the model's decision throughout the layers. In this work, we leverage recent advances in explainability of the Transformer and present a procedure to analyze models for language generation. Using contrastive examples, we compare the alignment of our explanations with evidence of the linguistic phenomena, and show that our method consistently aligns better than gradient-based and perturbation-based baselines. Then, we investigate the role of MLPs inside the Transformer and show that they learn features that help the model predict words that are grammatically acceptable. Lastly, we apply our method to Neural Machine Translation models, and demonstrate that they generate human-like source-target alignments for building predictions.

1 Introduction

Language Generation Models, like Transformerbased Language Models (Brown et al., 2020; Zhang et al., 2022a) have recently revolutionized the field of Natural Language Processing (NLP). Despite this, there is still a gap in our understanding of how they are able to produce language that closely resembles that of humans. This means that we are unable to determine the cause of a model's failure in specific instances, which can result in the generation of hallucinated content or toxic output.

The majority of previous work in explainability of NLP model predictions has focused on analyzing them on downstream tasks, generally with a small output space, such as text classification or Natural Language Inference (Atanasova et al., 2020; Bastings et al., 2022; Zaman and Belinkov, 2022). This line of research includes a large body of work focusing on the analysis of the attention mechanism

Logits Difference: Increase Decrease				
Model Prediction: has (2.2%) , have (0.1%) Logits Difference: logit _{has-have} = 3.1				
L12 A report about the Impressionists has				
L11 A report about the Impressionists has				
L10 A report about the Impressionists has				
L9 A report about the Impressionists has				
L8 A report about the Impressionists has				
L7 A report about the Impressionists has				
L6 A report about the Impressionists has				
L5 A report about the Impressionists has				
L4 A report about the Impressionists has				
L3 A report about the Impressionists has				
L2 A report about the Impressionists has				
L1 A report about the Impressionists has				
\sum A report about the Impressionists has				

Table 1: Updates to the (logits) prediction difference between **has** and **have** in different layers produced by input tokens. Red indicates an increase in the difference in logits between both predictions. At the bottom, we show the final logit contributions. The contrastive extension of our proposed method, ALTI-Logit, shows that the model relies on the head of the subject (report) to correctly solve the subject-verb agreement. See explanations from other methods in Table 3. GPT-2 Small shown here, see GPT-2 XL ALTI-Logit explanation in Appendix H.2.

(Jain and Wallace, 2019; Serrano and Smith, 2019; Pruthi et al., 2020), and on applying gradient-based methods (Li et al., 2016a; Sundararajan et al., 2017) to obtain input attribution scores.

Recently, several works have tackled the interpretability of Transformers (Vaswani et al., 2017) on the Language Modeling task. Elhage et al. (2021) studied the Transformer from the *residual stream* perspective, depicted in Figure 1, where different components (MLPs, attention heads...) read and write to subspaces of the residual stream. This approach has aided in explaining certain behaviours of language models, like induction heads (Olsson et al., 2022), where attention heads search over the context for previous repetitions of the same token and copy the next token, or even specialized heads solving the Indirect Object Identification (IOI) task (Wang et al., 2023). Similarly, MLPs inside the Transformer have also been studied as elements writing into the residual stream. Geva et al. (2022) observed that MLP blocks can act as key-value memories, where values add to the residual, thus promoting the prediction of words that convey similar semantic meaning.

Furthermore, the *attention mechanism* in the Transformer, composed of attention heads, an output weight matrix, and a layer normalization, can be decomposed into an interpretable operation (Kobayashi et al., 2020, 2021), providing layerwise explanations which have proven to be highly faithful (Ferrando et al., 2022b,a).

In this work, we propose explaining the predictions of Transformers language generators by combining the residual stream analysis perspective with the attention decomposition. Our approach measures the amount of logit (pre-activation of the softmax) added or subtracted by each token representation at each layer. We then track the logit contributions back to the model's input by aggregating across layers (*Logit* explanation). Additionally, we consider the mixing of information in intermediate layers by using ALTI (Ferrando et al., 2022b) (*ALTI-Logit* explanation).

To evaluate the proposed interpretability methods, we follow the recently introduced contrastive explanations framework (Yin and Neubig, 2022), which aims to explain why the model predicted one token instead of a foil token, *a priori* explained by some linguistic phenomena evidence. Then, we analyze the role of MLPs and show that they aid the model in determining predictions that follow grammar rules. Finally, we demonstrate that NMT models generate human-like source-target alignments for building translations.¹

2 Approach

2.1 Residual Stream

Given a language generation timestep t, the output of the last layer,² $x_t^L \in \mathbb{R}^d$, is projected to the

²We refer to it as a row vector.



Figure 1: A Transformer Language Model, represented as modules writing into the residual stream.

token embedding space by applying the unembedding matrix $U \in \mathbb{R}^{d \times |V|}$ to get the logits of the next token prediction. Then, a softmax function is applied to obtain a probability distribution over the vocabulary:

$$P(\boldsymbol{x}_t^L) = \operatorname{softmax}(\boldsymbol{x}_t^L \boldsymbol{U}) \tag{1}$$

The residual connection in the Transformer can be seen as an information stream (nostalgebraist, 2020; Elhage et al., 2021; Mickus et al., 2022) that gets updated after each block. Let's call o_t^l and \tilde{x}_t^l the output of the MLP and self-attention blocks at layer *l* respectively, 'writing' into the residual stream at position *t* (Figure 1). The last state of the residual stream can be represented as

$$\boldsymbol{x}_{t}^{L} = \sum_{l}^{L} \boldsymbol{o}_{t}^{l} + \sum_{l}^{L} \widetilde{\boldsymbol{x}}_{t}^{l} + \boldsymbol{x}_{t}^{0}$$
(2)

The final logit of a particular next token prediction w can be computed by multiplying the last state of the residual stream with the w-th column³ of U:

$$\operatorname{logit}_{w} = \boldsymbol{x}_{t}^{L} \boldsymbol{U}_{w}$$
$$= \left(\sum_{l}^{L} \boldsymbol{o}_{t}^{l} + \sum_{l}^{L} \widetilde{\boldsymbol{x}}_{t}^{l} + \boldsymbol{x}_{t}^{0}\right) \boldsymbol{U}_{w}$$
(3)

By linearity:

$$\text{logit}_{w} = \sum_{l}^{L} \boldsymbol{o}_{t}^{l} \boldsymbol{U}_{w} + \sum_{l}^{L} \widetilde{\boldsymbol{x}}_{t}^{l} \boldsymbol{U}_{w} + \boldsymbol{x}_{t}^{0} \boldsymbol{U}_{w} \quad (4)$$

¹The code accompanying the paper is available at https://github.com/mt-upc/logit-explanations.

³Note that we refer to the *j*-th column of a matrix **B** as B_{j} , instead of $B_{:,j}$.



Figure 2: The output of the self-attention block at each layer updates the logit of w (left). The logit's update can be decomposed per input token (right).

2.2 Multi-head Attention as a Sum of Vectors

Inspired by the decomposition of the Post-LN selfattention block done by Kobayashi et al. (2021), we apply a similar approach to the Pre-LN setting, common in current LMs (see full derivation in Appendix A). The output of the self-attention block at each generation step t can be expressed as

$$\widetilde{\boldsymbol{x}}_{t}^{l} = \sum_{j}^{t} T_{t,j}^{l}(\boldsymbol{x}_{j}^{l-1}) + \boldsymbol{b}_{O}^{l}$$
(5)

where $T_{t,j}^l : \mathbb{R}^d \mapsto \mathbb{R}^d$ is an affine transformation applied to each layer's input token representation (or residual stream) $\boldsymbol{x}_j^{l-1} \in \mathbb{R}^d$:

$$T_{t,j}^{l}(\boldsymbol{x}_{j}^{l-1}) = \sum_{h}^{H} \left(\boldsymbol{x}_{j}^{l-1} \boldsymbol{L}^{l} \boldsymbol{W}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{\theta}^{l,h} \right)$$
(6)

with $W_V^{l,h} \in \mathbb{R}^{d \times d_h}$ the matrix generating the values, $W_O^{l,h} \in \mathbb{R}^{d_h \times d}$ the attention output matrix (per head) and $b_O^l \in \mathbb{R}^d$ its associated bias. $A^{l,h} \in \mathbb{R}^{t \times t}$ is the attention weight matrix of each head, $\theta^{l,h} \in \mathbb{R}^d$ remaining terms originated from biases, and $L^l \in \mathbb{R}^{d \times d}$ combines centering, normalizing, and scaling operations of the layer normalization (see Appendix A).

2.3 Layer-wise Contributions to the Logits

Combining Equation (4) and Equation (5) we get⁴:

$$\operatorname{logit}_{w} = \sum_{l}^{L} \underbrace{o_{t}^{l} U_{w}}_{\Delta \operatorname{logit}_{w \leftarrow \operatorname{MLP}^{l}}^{l}} \underbrace{\sum_{j}^{t} T_{t,j}^{l}(\boldsymbol{x}_{j}^{l-1}) U_{w}}_{\Delta \operatorname{logit}_{w \leftarrow \operatorname{Self-attn}^{l}}^{l}} + x_{t}^{0} U_{w}$$

$$(7)$$

The logit's update of each self-attention, $\Delta \text{logit}_{w \leftarrow \text{Self-attn}^l}^l$, can be expanded into individual



Figure 3: x_2^{l-1} and x_3^{l-1} contribute 10 and 4 logits respectively to the next token prediction w = time. Due to the mixing of contextual information across layers, upon contributes $\frac{1}{2}$ to x_2^{l-1} and $\frac{1}{4}$ to x_3^{l-1} , which results in upon contributing $10 \cdot \frac{1}{2} + 4 \cdot \frac{1}{4} = 5 + 1 = +6$ logits.

updates by each x_j^{l-1} (Figure 2). Therefore, the contribution of each layer's input token representation x_j^{l-1} to an output token w can be defined as its update to the logit of w:

$$\Delta \text{logit}_{w \leftarrow \boldsymbol{x}_{j}^{l-1}}^{l} = T_{t,j}^{l}(\boldsymbol{x}_{j}^{l-1})\boldsymbol{U}_{w}$$
(8)

Similarly, logit updates can be computed at the head level ($\Delta \text{logit}_{w \leftarrow x_j^{l-1}}^{l,h}$) by multiplying the unembedding matrix with the head-wise affine transformation in Equation (6).

2.4 Tracking Logit Updates to the Input Tokens

If we assume each residual stream preserves its token identity throughout the layers, the total logit update to w produced by input token s can be computed as

$$\Delta \text{logit}_{w \leftarrow s} = \sum_{l}^{L} \Delta \text{logit}_{w \leftarrow \boldsymbol{x}_{j=s}^{l-1}}^{l} \qquad (9)$$

that is, the sum of the logit updates performed by the *s*-th token intermediate representations at every layer. Henceforth, we refer to this as the *Logit* explanation.

However, in intermediate layers, each residual stream represents a mixture of input tokens (Brunner et al., 2020). Therefore, $\Delta \text{logit}_{w \leftarrow x_j^{l-1}}^l$ can't be directly interpreted as the logit update *caused* by the model's input token s = j. We propose to track the logit update back to the model inputs by measuring the mixing of contextual information in the residual streams. For that purpose, we use ALTI (Ferrando et al., 2022b). ALTI, as well as other methods relying on the *rollout* method (Abnar and Zuidema, 2020; Mohebbi et al., 2023) assume

⁴Biases are removed to save space.

that token representations are formed by linearly combining the representations from the preceding layer, i.e. $x_i^l = \sum_j c_{i,j}^l x_j^{l-1}$, with $\sum_j c_{i,j}^l = 1$. Each $c_{i,j}^l$ refers to the contribution of x_j^{l-1} to x_i^l . By multiplying the layer-wise coefficient matrices, $M^l = C^l \cdot C^2 \cdots C^1$, one can describe each intermediate layer representation as a linear combination of the model input tokens, $x_i^l = \sum_s m_{i,s}^l x_s^0$.

Column s of M^{l-1} contains the proportion of the s-th input token's contribution encoded in each token representation *entering* layer l. We can obtain the update performed by each model input token (Figure 3, right) to the logit of a next prediction token w as

$$\Delta \text{logit}_{w \leftarrow s}^{l} = \Delta \text{logit}_{w \leftarrow \mathbf{x}^{l-1}}^{l} \mathbf{M}_{s}^{l-1}$$
(10)

We refer to Appendix B for a more detailed explanation. The final contribution of the s-th input token to the prediction of token w can be obtained as the sum of its logit updates at each layer:

$$\Delta \text{logit}_{w \leftarrow s} = \sum_{l}^{L} \Delta \text{logit}_{w \leftarrow s}^{l} \qquad (11)$$

We denote this method the *ALTI-Logit* explanation. Note that if we don't consider mixing of contextual information, M^{l-1} becomes the identity matrix, and we get the Logit explanation (Equation (9)).

2.5 Contrastive Explanations

Contrastive explanations (Yin and Neubig, 2022) aim to explain why the model predicted one target token w instead of another foil token f. We can explain this decision by determining how much each token contributed to the final logit difference between w and f: logit_(w-f). Following Equation (9) and Equation (11), we can define the Contrastive Logit and Contrastive ALTI-Logit ⁵ saliency scores of input tokens as their update to the logit difference:

$$\Delta \text{logit}_{(w-f)\leftarrow s} = \Delta \text{logit}_{w\leftarrow s} - \Delta \text{logit}_{f\leftarrow s}$$
(12)

3 Experimental Setup

We evaluate the quality of our proposed method through contrastive explanations. Following Yin and Neubig (2022) we use a subset of BLiMP dataset (Warstadt et al., 2020), which contains sentence pairs with small variations in grammatical

Phenomena	ID	Example (Acceptable/Unacceptable)
Anaphor Agreement	aga ana	Karla could listen to herself/himself. Eva approached herself/themselves.
Argument Structure	asp	Gerald is hated by the teachers/pie.
Determiner-Noun Agreement	dnaa	Eva has scared these children/child. Tammy was observing that man/men. The driver sees that unlucky person/people. Phillip liked that smooth horse/horses.
NPI Licensing	npi	Even Danielle also/ever leaves.
Subject-Verb Agreement	ipsv	The grandfathers of Diana drink/drinks. Many people have/has hidden away. Most associations buy/buys those libraries.

Table 2: Examples: in Table 8 of BLiMP phenomenons⁶ used by Yin and Neubig (2022), with acceptable and unacceptable continuations in bold. Underlined words represent the linguistic evidence to resolve the phenomena (extracted by the rules).

correctness. The 11 subsets belong to 5 linguistic phenomena: anaphor agreement, argument structure, determiner-noun agreement, NPI licensing, and subject-verb agreement.

For each linguistic phenomena, we use spaCy (Honnibal and Montani, 2017) and follow Yin and Neubig (2022) rules to find the evidence (in previous tokens), that is enforcing grammatical acceptability (Table 2). For anaphor agreement, we obtain all context tokens that are coreferent with the target token. For argument structure, we extract the main verb of the sentence. Determiner-noun agreement's evidence is found in the determiner of the target noun. In NPI licensing, "even" word can appear in the acceptable target, but not in the unacceptable. Finally, in the subject-verb agreement phenomenon, the form of the verb has to agree in number with the head of the subject, which we use as evidence. We differ from Yin and Neubig (2022) in that we discard ipsv and rpsv subsets, due to the large fraction of sentences with a 'quantifier + head of subject + verb' structure, where both the quantifier (many, most...) and the head of the subject could be used by the model to solve the agreement.

We also add to the analysis SVA (subject-verb agreement) (Linzen et al., 2016) and the Indirect Object Identification (IOI) (Wang et al., 2023; Fahamu, 2022) datasets. The SVA dataset includes nouns with an opposite number to that of the main

⁵Throughout the paper we use Logit and ALTI-Logit to refer also to their contrastive variant.

⁶BLiMP IDs. aga: anaphor_gender_agreement; ana: anaphor_number_agreement; asp: animate_subject_passive; dna: determiner_noun_agreement_1; dnai: determiner_noun_agreement_irregular_1; dnaa: determiner_noun_agreement_with_adj_1; dnaai: determiner_noun_agreement_with_adj_irregular_1; npi: npi_present_1; darn: distractor_agreement_relational_noun; ipsv: irregular_plural_subject_verb_agreement_1; rpsv: regular_plural_subject_verb_agreement_1

subject, which makes this dataset well-suited for evaluating saliency methods. Indirect object identification (IOI) is a feature present in sentences that have an initial dependent clause, like "After Lee and Evelyn went to the lake", followed by a main clause, like "Lee gave a grape to Evelyn". The indirect object "Evelyn" and the subject "Lee" are found in the initial clause. In all examples of IOI dataset, the main clause refers to the subject again, which gives an object to the IO. The goal of the IOI task is to predict the final word in the sentence to be the IO. In IOI examples, the rule for predicting the IO is the IO itself being in the first clause.

We use GPT-2 XL (1.5B) model (Radford et al., 2019), as in (Yin and Neubig, 2022), as well as other autoregressive Transformer language models, such as GPT-2 Small (124M), and GPT-2 Large models (774M), OPT 125M (Zhang et al., 2022b), and BLOOM's 560M and 1.1B variants (BigScience Workshop, 2022), through Hugging-Face library (Wolf et al., 2020).

Alignment Metrics. Following Yin and Neubig (2022), we define the evidence as a binary vector $\boldsymbol{b} \in \mathbb{R}^t$ (with as many components as the number of previous tokens), with all zeros except in the position of the tokens inside the evidence, i.e. the tokens which the prediction depends on, extracted by the rule. Explanations are vectors, also $\in \mathbb{R}^t$. To measure the alignment between an explanation and the evidence we use MRR (Mean Reciprocal Analysis). Sorting the tokens in descending order, MRR evaluates the average of the inverse of the rank of the first token that is part of b. Although Yin and Neubig (2022) use also dot-product and Probes Needed metrics for measuring alignments, dot-product favors Grad Norm explanations since it gives positive scores only, and Probes Needed is closely related to MRR, giving redundant results.

4 Contrastive Methods

Yin and Neubig (2022) proposed extending different common input attribution methods to the contrastive setting. In §5 we compare their explanations with the ones obtained with our proposed contrastive methods (Equation (12)).

4.1 Input Erasure

Erasure-based methods remove parts of the input and measure the change in the model's prediction (Li et al., 2016b), where the higher the prediction



Figure 4: Alignment (MRR \uparrow) of different explanation methods of GPT-2 Small model predictions with BLiMP, SVA, and IOI datasets.

change, the higher the attribution of that particular token. Specifically, we take the difference between the model's output with the entire input \mathbf{x} , and after removing from \mathbf{x} the *s*-th token, i.e. $m_w(\mathbf{x}) - m_w(\mathbf{x}_{\neg s})$. Yin and Neubig (2022) define the Contrastive Input Erasure as

$$\boldsymbol{c}^{e}_{(w,\neg f)\leftarrow s} = (m_w(\mathbf{x}) - m_w(\mathbf{x}_{\neg s})) - (m_f(\mathbf{x}) - m_f(\mathbf{x}_{\neg s}))$$
(13)

This metric evaluates the extent to which removing x_s from the input increases the likelihood of the foil, and decreases the likelihood of the target in the model's output.

4.2 Gradient Norm

The Transformer model can be approximated by the linear part of the Taylor-expansion at a baseline point (Simonyan et al., 2014), $m(\mathbf{X}^0) \approx \nabla m(\mathbf{X}^0) \cdot \mathbf{X}^0$, where $\mathbf{X}^0 \in \mathbb{R}^{t \times d}$ is the sequence of input embeddings. Therefore, $\nabla m_w(\mathbf{X}^0)$ represents the sensitivity of the model to each input dimension when predicting w. Following, saliency scores for each token can be computed by taking the norm of the gradient vector corresponding to the token embedding, $\|\nabla_{\mathbf{x}_{*}^{0}}m(\mathbf{X}^{0})\|_{1}$.

Yin and Neubig (2022) extend this method to the Contrastive Gradient Norm and define it as

$$\boldsymbol{c}_{(w,\neg f)\leftarrow s}^{g} = \left\|\nabla_{\boldsymbol{x}_{s}^{0}}\left(m_{w}(\boldsymbol{X}^{0}) - m_{f}(\boldsymbol{X}^{0})\right)\right\|_{1}$$
(14)

4.3 Gradient × Input

The gradient \times input method (Shrikumar et al., 2016; Denil et al., 2014) calculates the dot product between the gradient and the input token embedding. Yin and Neubig (2022) define the Contrastive Gradient \times Input as

$$\boldsymbol{c}_{(w,\neg f)\leftarrow s}^{g\times i} = \nabla_{\boldsymbol{x}_s^0} \left(m_w(\boldsymbol{X}^0) - m_f(\boldsymbol{X}^0) \right) \cdot \boldsymbol{x}_s^0 \tag{15}$$



Table 3: Comparison of different contrastive explanation methods described in §4 and ALTI-Logit (**has** vs. **have**). Same example as in Table 1.

5 Results

In the following sections we provide results on the alignment between the explanations of different methods and linguistic evidence, as well as an analysis of observed model behaviours through the lens of ALTI-Logit.

5.1 Alignment Results

In Figure 4 we present the MRR results of GPT-2 Small averaged across dataset categories, while the extended results for every subset can be found at Appendix C, Table 7. In Appendix C, Figure 11 we expand Figure 4 across different models. We can observe that Logit and ALTI-Logit explanations consistently align better with the evidence of linguistic phenomena than common gradientbased and erasure-based baselines. Note that for BLiMP the average we show in Figure 4 is across 9 different subsets. In Table 3 we show an example comparing different contrastive explanations, where Grad Norm, $G \times I$ and Erasure explanations don't align with the evidence to solve the subjectverb agreement (report), and disagree between each other.

We find similar alignment results for Logit and ALTI-Logit methods. However, we observe that ALTI-Logit aligns better at tasks where the tokens of the linguistic evidence are far from the prediction. This is especially noticeable in Subjectverb agreement datasets (including SVA and darn), where ALTI-Logit shows higher alignments than any other method across all models. This might indicate that incorporating information about contextual mixing is advantageous for dealing with large contexts.

Despite the generally accurate performance of the models examined in this study (Figure 12 and Figure 13, Appendix D), there are cases where



Figure 5: Update to the logit difference between the acceptable and the unacceptable predictions produced by the input tokens inside the linguistic evidence (GPT-2 XL).



Figure 6: ALTI-Logit MRR alignment scores (line plots) and updates in logit difference by every input token $(\Delta \text{logit}_{(w-f) \leftarrow \text{Self-attn}^l}^l)$ between acceptable and unacceptable predictions (box plots) per layer (GPT-2 Small). Horizontal dashed lines refer to random alignment.

the unacceptable token gets predicted with a higher probability. In order to gain a deeper understanding of the variations in model behavior between correct and incorrect predictions, we analyze the logit update generated by the input tokens associated with the linguistic evidence. This analysis, conducted using ALTI-Logit (Figure 5), reveals differences in the distributions. These findings suggest that the tokens representing the linguistic evidence play a crucial role in achieving accurate predictions, and if their contribution is only marginal, the likelihood of failure increases considerably.



Figure 7: ALTI-Logit MRR alignment scores across layers (GPT-2 XL). Horizontal dashed lines refer to random alignment.

5.2 Layer-wise Analysis with ALTI-Logit

In the line plots in Figures 6 and 7 we provide the MRR alignment results across layers of GPT2-Small and GPT2-XL for two different linguistic phenomena. Models behave similarly across subsets inside the same phenomena, like in Subject-Verb Agreement (SVA and darn), and Anaphor Agreement (aga and ana) in Appendix E. The model's alignment trend also stays similar, even though the distance between the prediction and the evidence is different across subsets (SVA's distance is 4 times darn's).

In the boxplots in Figure 6, we show the distribution of self-attention updates to the logit difference between the acceptable and the unacceptable predictions, $\Delta \text{logit}_{(w-f) \leftarrow \text{Self-attn}^l}^l$. As a general pattern, we observe that models tend to update more heavily on the layers where the alignment with linguistic phenomena is higher. This conclusion holds for larger models too, see the darn example in Appendix H.2, where large logit updates are found in layers 28, 35, and 40, matching the layers where alignment peaks (Figure 7 Top). In IOI and SVA tasks both models align with the evidence and increase their logit update towards the last layers. This indicates that models solve these phenomena once they have acquired sufficient contextual information.

Our findings in the IOI task support those by Wang et al. (2023). In GPT-2 Small we observe high logit difference updates coming from the Indirect Object (IO) in layers 10 and 11. We further study the heads in those layers (Table 4), where Wang et al. (2023) found 'Name Mover Heads' and 'Negative Mover Heads'. These heads rely on the IO to increase (Name Mover Heads) and decrease



Table 4: GPT-2 Small updates to the logit prediction difference between **Angie** and **Yvette** in different heads produced by layer input token representations $(\Delta \text{logit}_{(w-f)\leftarrow x_i^{l-1}}^{l,h})$.

(Negative Mover Heads) respectively the logit of the correct prediction. In Appendix H.3 we provide an example of how every model solves the task across layers.

6 Analysis of MLPs

The MLP block in the Transformer contains two learnable weight matrices⁷: $W_1^l \in \mathbb{R}^{d \times d_{mlp}}$ and $W_2^l \in \mathbb{R}^{d_{mlp} \times d}$, and an element-wise non-linear activation function α . It takes as input the state of the residual stream at timestep $t(\tilde{x}_i^l)$ and computes:

$$\boldsymbol{o}_t^l = \alpha(\mathrm{LN}(\tilde{\boldsymbol{x}}_t^l)\boldsymbol{W}_1^l)\boldsymbol{W}_2^l \tag{16}$$

Following, o_t^l is added back to the residual stream (Figure 1). Equation (16) can be seen as key-value memories (Geva et al., 2021), where keys are stored in components of $k^l = \alpha(\text{LN}(\boldsymbol{x}_t^l)\boldsymbol{W}_1^l) \in \mathbb{R}^{d_{mlp}}$, and values (v^l) are rows of \boldsymbol{W}_2 . Following the key-value perspective, Equation (16) can be rewritten as

$$\boldsymbol{o}_t^l = \sum_i^{d_{mlp}} k_i^l \boldsymbol{v}_i^l \tag{17}$$

where v_i^l represents the *i*-th row of W_2 . Recalling how the final logit of a token *w* is decomposed by layer-wise updates in Equation (7), the MLP^{*l*} updates the logit of *w* as follows:

$$\Delta \text{logit}_{w \leftarrow \text{MLP}^{l}}^{l} = \boldsymbol{o}_{t}^{l} \boldsymbol{U}_{w}^{\mathsf{T}}$$

$$= \sum_{i}^{d_{mlp}} k_{i}^{l} \boldsymbol{v}_{i}^{l} \boldsymbol{U}_{w}^{\mathsf{T}}$$

$$= \sum_{i}^{d_{mlp}} \Delta \text{logit}_{w \leftarrow k_{i}^{l} \boldsymbol{v}_{i}^{l}}^{l}$$
(18)

Thus, the update of the MLP can be decomposed into sub-updates (Geva et al., 2022) performed by

⁷We omit bias terms.



Figure 8: Average (across the dataset) of the updates to the logit difference caused by the weighted values in the MLP (each row *i* in W_2^l), $\Delta \text{logit}_{(w-f), -k_i^l v_i^l}^l$. a) dna: dimension i = 383 (L11) promotes singular nouns (increases the logit difference between singular and plural nouns) after this/that, b) dna: dimension i = 3038(L11) promotes plural nouns after these/those. Dimension i = 2187 (L12) pushes the prediction of singular verbs in different Subject-Verb Agreement datasets c) darn and d) SVA.

each $k_i^l v_i^l$ (weighted row in W_2^l). The update in the logit's difference between the target and foil tokens by each value *i* is therefore:

$$\Delta \text{logit}^{l}_{(w-f)\leftarrow k_{i}^{l}\boldsymbol{v}_{i}^{l}} = \Delta \text{logit}^{l}_{w\leftarrow k_{i}^{l}\boldsymbol{v}_{i}^{l}} - \Delta \text{logit}^{l}_{f\leftarrow k_{i}^{l}\boldsymbol{v}_{i}^{l}} \tag{19}$$

In Figure 8, we show some examples of the contribution of each weighted value $k_i^l v_i^l$ to the logit difference between the acceptable target token and the unacceptable one, at different layers and datasets. We can observe that there is a small subset of values that consistently increase the difference in logits helping to solve the linguistic task. Some of them include the value i = 383 in layer 10 (Figure 8 (a)), which increases the logit of singular nouns and reduces the plural ones when the determiner is this or that. For instance, in the sentence "William described this ____", value i = 383increases the logit difference between movie and movies. In dimension 3038 we find a value upweighting the logits of the plural nouns over the singular ones when the determiner is these or those (Figure 8 (b)). These values help solve the linguistic task at hand across different subsets, for instance, the value in dimension i = 2187 is in charge of promoting the singular form of the verb when the head of the subject is singular too. This occurs in both darn and SVA subsets.



Figure 9: Cross-attention block in the Transformer's decoder (left) and its equivalent using vector transformations (right). Depicted in green and red it's shown the information coming from the encoder and the decoder (target prefix) respectively.

7 Neural Machine Translation

An NMT system estimates the likelihood of a target sequence of tokens, $\mathbf{y} = (y_1, \dots, y_t)$, given a source sequence of tokens, $\mathbf{x} = (x_1, \dots, x_I)$:

$$P(\mathbf{y}|\mathbf{x}) = \prod_{s}^{t} P(y_{s}|\mathbf{y}_{< s}, \mathbf{x})$$
(20)

where $\mathbf{y}_{\langle s \rangle} = (y_0, \dots, y_{s-1})$ is the prefix of y_s , and $x_I = y_0 = \langle s \rangle$ is a special token used to mark the start and end of the sentence. The encoder processes the source sentence and generates a sequence of contextualized representations, $\mathbf{e} = (e_1, \dots, e_I)$. At each decoding step t, the decoder uses the encoder outputs and the target prefix to compute a probability distribution over the target vocabulary.

Cross-attention. Similar to Equation (6), the output of the cross-attention $(\tilde{y}_t^{c,l})$ and self-attention $(\tilde{y}_t^{s,l})$ (Figure 9) of a decoder layer in an encoderdecoder Transformer can be decomposed⁸ as

$$\widetilde{\boldsymbol{y}}_{t}^{c,l} = \sum_{i}^{I} T_{t,i}^{c,l}(\boldsymbol{e}_{i}), \quad \widetilde{\boldsymbol{y}}_{t}^{s,l} = \sum_{j}^{t} T_{t,j}^{s,l}(\boldsymbol{y}_{j}^{l-1})$$
(21)

As shown in Figure 9, each transformed vector updates the logits of the token predictions by multiplying it with the corresponding column of U, as in Equation (8):

$$\Delta \text{logit}_{w \leftarrow \boldsymbol{e}_i}^l = T_{t,i}^{c,l}(\boldsymbol{e}_i) \boldsymbol{U}_w$$
(22)

⁸Removing biases.

	AER (\downarrow)		
Method	Bilingual	M2M	
Attention weights	48.6	96.4	
SD-SmoothGrad (Ding et al., 2019)	36.4	-	
Vector Norms (Kobayashi et al., 2020)	41.4	-	
Distance Vectors-Output (Ferrando et al., 2022a)	38.8	36.4	
Proposed alignment extraction	26.0	27.3	

Table 5: Mean AER of the cross-attention contributions in the best layer of the bilingual and M2M models. For the bilingual model, we show the average on five different seeds.

Alignment. Source-target alignments derived from attention weights in NMT systems can be unreliable (Zenkel et al., 2019; Li et al., 2019; Garg et al., 2019), with upper layers producing better alignments. A limitation of using this method to interpret model predictions is that the ground truth target word may not match the model's actual prediction. However, by measuring how the encoder token representations update the logits of the reference words, $\Delta \text{logit}_{w \leftarrow e_i}^l$, we can more precisely explain which source word causes the final logit of the reference word, even if it is not one of the top predictions.

Following Kobayashi et al. (2020) and Ding et al. (2019) setting, we train a 6-layer Transformer model for the German-English (De-En) translation task using Europarl v7 corpus⁹ Koehn (2005). We also evaluate on M2M, a 12 layer multilingual model (Fan et al., 2021). We use Vilar et al. (2006) dataset, consisting of 508 De-En human annotated sentence pairs with alignments, and compare them with our extracted alignments using Alignment Error Rate (AER). We also show results of other attention-based alignments extraction methods. Vector Norms take the norm of the transformed vectors in Equation (21), Distance Vectors-Output measures the distance between the transformed vectors and the attention block output $\widetilde{y}_{t}^{c,l}$. SD-SmoothGrad relies on gradients to extract alignments. In Table 5 we show that our proposed method achieves lower AER values, which indicates that NMT models generate human-like alignments for building model predictions.

8 Related Work

The projection of LMs representations and model parameters to the vocabulary space has been a subject of previous research (Belrose et al., 2023; Din et al., 2023). Geva et al. (2021, 2022) view feed-



Figure 10: Left: attention weights in the cross-attention in the penultimate layer. Right: contributions obtained as logit updates to token predictions in the penultimate layer.

forward layers as performing updates to the probability distribution of the token predictions. Mickus et al. (2022) study how the different Transformer modules contribute to the hidden representations, and Dar et al. (2022) directly interpret Transformer static parameters in the embedding space. In this work, our focus lies in interpreting the influence of input tokens and its representations in the model predictions.

Furthermore, work on mechanistic interpretability (Olah, 2022) has discovered 'circuits' within LMs in charge of solving tasks (Wang et al., 2023; Geva et al., 2023). In contrast to their methods, our approach does not rely on causal interventions in the computations of Transformers. More broadly, our work can be related to those explaining the prediction process of LMs (Tenney et al., 2019; Voita et al., 2019; Sarti et al., 2023).

9 Conclusions

In this paper, we introduce a new procedure for analyzing language generation models by combining the residual stream perspective with interpretable attention decomposition, and tested our approach using contrastive examples in Transformer LMs. We found that the explanations provided by our proposed methods, Logit and ALTI-Logit, align better with available linguistic evidence in the context of the sentence, compared to common gradientbased and erasure-based baselines. We also analyzed the role of MLPs and showed that they assist the model in determining predictions that conform to the grammar rules. Additionally, we applied our method to a Machine Translation model and demonstrated that it generates human-like alignments for building predictions. Overall, our results suggest that decomposing the logit scores is an effective way to analyze language generation models.

⁹http://www.statmt.org/europarl/v7

10 Limitations

The experimental methodology employed in this study for both contrastive explanations and NMT is not directly extensible to languages other than English, due to the scarcity of resources such as models and annotations.

The datasets employed in this study to evaluate contrastive explanations across various linguistic paradigms are restricted to sentences that possess a well-defined structure. As a result, it is possible that the conclusions drawn may not be generalizable to the broader distribution of sentences.

Lastly, it should be noted that the method proposed in this study should not be used as a definitive explanation of model predictions in any other context. It is recommended to use the method as a debugging tool and should be employed in conjunction with other methods to gain a comprehensive understanding of model predictions.

11 Ethics statement

It is acknowledged that the experiments reported in this study are limited to high-resource languages. However, the methodology employed is languageindependent and may be applied to other languages in the future, provided that adequate annotated data becomes available.

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A Pre-LN Self-attention Decomposition

$oldsymbol{x}_{j}^{l-1} \in \mathbb{R}^{d imes d_{h}} \ oldsymbol{A}^{l,h} \in \mathbb{R}^{t imes t}$	Layer Input (Residual Stream position j)
	Attention Matrix
$oldsymbol{W}_V^{l,h} \in \mathbb{R}^{d imes d_h}$	Values Weight Matrix
$oldsymbol{W}_{O}^{l,h} \in \mathbb{R}^{d_{h} imes d}$	Output Weight Matrix (per head)
$oldsymbol{b}_V^{l,h} \in \mathbb{R}^{d_h}$	Value bias
$\dot{oldsymbol{b}}_{O}^{l}\in\mathbb{R}^{d}$	Output bias
$H \in \mathbb{R}$	Number of heads
$\mathrm{LN}^l:\mathbb{R}^d\mapsto\mathbb{R}^d$	Layer Normalization

Table 6: Components of the self-attention module.

At position t, each head of a Pre-LN self-attention mechanism computes:

$$\boldsymbol{z}_{t}^{l,h} = \sum_{j}^{t} \left(\underbrace{\mathrm{LN}^{l}(\boldsymbol{x}_{j}^{l-1})\boldsymbol{W}_{V}^{l,h} + \boldsymbol{b}_{V}^{l,h}}_{j\text{-th value}} \right) \boldsymbol{A}_{t,j}^{l,h}$$
(23)

By representing attention heads as parallel independent components, we can express the output of the self-attention as

$$\widetilde{\boldsymbol{x}}_{t}^{l} = \sum_{h}^{H} \boldsymbol{z}_{t}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{b}_{O}^{l}$$
(24)

leading to:

$$\widetilde{\boldsymbol{x}}_{t}^{l} = \sum_{j}^{t} \sum_{h}^{H} \left(\mathrm{LN}^{l}(\boldsymbol{x}_{j}^{l-1}) \boldsymbol{W}_{V}^{l,h} + \boldsymbol{b}_{V}^{l,h} \right) \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{b}_{O}^{l}$$
(25)

The layer normalization computes:

$$\mathrm{LN}^{l}(\boldsymbol{x}_{j}^{l-1}) = \frac{\boldsymbol{x}_{j}^{l-1} - \boldsymbol{\mu}(\boldsymbol{x}_{j}^{l-1})}{\sigma(\boldsymbol{x}_{j}^{l-1})} \odot \gamma^{l} + \beta^{l}$$
(26)

with μ and σ computing the mean and standard deviation, and $\gamma^l \in \mathbb{R}^d$ and $\beta^l \in \mathbb{R}^d$ refer to learned element-wise transformation and bias respectively. Considering $\sigma(x_j^{l-1})$ as a constant, LN can be treated as a constant affine transformation:

$$\operatorname{LN}(\boldsymbol{x}_{j}^{l-1}) = \boldsymbol{x}_{j}^{l-1}\boldsymbol{L}^{l} + \beta^{l}$$
(27)

where $L^l \in \mathbb{R}^{d \times d}$ represents a matrix that combines centering, normalizing, and scaling operations together.

Using Equation (27) in Equation (25):

$$\begin{split} \widetilde{\boldsymbol{x}}_{t}^{l} &= \sum_{j}^{t} \sum_{h}^{H} \left(\left((\boldsymbol{x}_{j}^{l-1} \boldsymbol{L}^{l} + \beta^{l}) \boldsymbol{W}_{V}^{l,h} + \boldsymbol{b}_{V}^{l,h} \right) \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} \right) + \boldsymbol{b}_{O}^{l} \\ &= \sum_{j}^{t} \sum_{h}^{H} \left(\left(\boldsymbol{x}_{j}^{l-1} \boldsymbol{L}^{l} \boldsymbol{W}_{V}^{l,h} + \beta^{l} \boldsymbol{W}_{V}^{l,h} + \boldsymbol{b}_{V}^{l,h} \right) \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} \right) + \boldsymbol{b}_{O}^{l} \\ &= \sum_{j}^{t} \sum_{h}^{H} \left(\boldsymbol{x}_{j}^{l-1} \boldsymbol{L}^{l} \boldsymbol{W}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \beta^{l} \boldsymbol{W}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{b}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{b}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{b}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} \right) + \boldsymbol{b}_{O}^{l} \end{split}$$

$$=\sum_{j}^{t}\sum_{h}^{H} \left(\boldsymbol{x}_{j}^{l-1} \boldsymbol{L}^{l} \boldsymbol{W}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{A}_{t,j}^{l,h} \left(\beta^{l} \boldsymbol{W}_{V}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{b}_{V}^{l,h} \boldsymbol{W}_{O}^{l,h} \right) \right) + \boldsymbol{b}_{O}^{l}$$
(28)

Considering $\theta^{l,h} = \left(\beta^{l} \boldsymbol{W}_{V}^{l,h} + \boldsymbol{b}_{V}^{l,h}\right) \boldsymbol{W}_{O}^{l,h}$

$$\widetilde{\boldsymbol{x}}_{t}^{l} = \sum_{j}^{t} \sum_{h}^{H} \left(\boldsymbol{x}_{j}^{l-1} \boldsymbol{L}^{l} \boldsymbol{W}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{\theta}^{l,h} \right) + \boldsymbol{b}_{O}^{l}$$
(29)

For each *j*-th input term, *H* affine transformations are applied to x_j . Furthermore, all heads' operations can be further grouped into a single affine transformation:

$$\widetilde{\boldsymbol{x}}_{t}^{l} = \sum_{j}^{t} \left(\boldsymbol{x}_{j}^{l-1} \boldsymbol{L}^{l} \sum_{h}^{H} \boldsymbol{W}_{V}^{l,h} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{W}_{O}^{l,h} + \sum_{h}^{H} \boldsymbol{A}_{t,j}^{l,h} \boldsymbol{\theta}^{l,h} \right) + \boldsymbol{b}_{O}^{l}$$
(30)

So, we can write \tilde{x}_t^l as a sum of t affine transformations, and the output bias:

$$\widetilde{\boldsymbol{x}}_{t}^{l} = \sum_{j}^{t} T_{t,j}^{l}(\boldsymbol{x}_{j}^{l-1}) + \boldsymbol{b}_{O}^{l}$$

$$(31)$$

B Tracking Logits to the Input with Rollout

The rollout method (Abnar and Zuidema, 2020) assumes any intermediate representation is a linear combination of the model inputs, $x_j^{l-1} = \sum_s m_{j,s}^{l-1} x_s^0$, where $m_{j,s}^{l-1}$ is a score indicating the contribution of input token s to the l-1 representation (or residual path) of token j. By dividing the logit update performed by x_j^{l-1} among the model inputs ($\Delta \text{logit}_{w,j \leftarrow x_s^0}^l$) based on their contributions to x_j^{l-1} , we obtain:

$$\Delta \text{logit}_{w \leftarrow \boldsymbol{x}_{j}^{l-1}}^{l} = \sum_{s} \Delta \text{logit}_{w, j \leftarrow \boldsymbol{x}_{s}^{0}}^{l}$$
$$= \sum_{s} m_{j,s}^{l-1} \Delta \text{logit}_{w \leftarrow \boldsymbol{x}_{j}^{l-1}}^{l}$$
(32)

Based on the total logit update produced in layer l, we have that:

$$\Delta \operatorname{logit}_{w \leftarrow \operatorname{Self-attn}^{l}}^{l} = \sum_{j} \Delta \operatorname{logit}_{w \leftarrow \boldsymbol{x}_{j}^{l-1}}^{l}$$

$$= \sum_{j} \sum_{s} \Delta \operatorname{logit}_{w,j \leftarrow \boldsymbol{x}_{s}^{0}}^{l}$$

$$= \sum_{j} \sum_{s} m_{j,s}^{l-1} \Delta \operatorname{logit}_{w \leftarrow \boldsymbol{x}_{j}^{l-1}}^{l}$$

$$= \sum_{s} \sum_{j} m_{j,s}^{l-1} \Delta \operatorname{logit}_{w \leftarrow \boldsymbol{x}_{j}^{l-1}}^{l}$$

$$= \sum_{s} \Delta \operatorname{logit}_{w \leftarrow s}^{l}$$
(33)

So, we have obtained Equation (10):

$$\Delta \text{logit}_{w \leftarrow s}^{l} = \Delta \text{logit}_{w \leftarrow \mathbf{x}^{l-1}}^{l} M_{s}^{l-1}$$
(34)

C Results



Figure 11: Alignment (MRR ↑) of different explanation methods of GPT-2 Small, Large, and XL, OPT 125M, BLOOM 560M, and BLOOM 1B1 model predictions with BLiMP, SVA, and IOI datasets.

C.1 GPT-2 Small Results

Dataset	Erasure	Logit	ALTI-Logit	Grad Norm	$G{\times}I$	Random	Distance
aga	0.959	0.827	0.964	0.793	0.791	0.699	3.2
ana	0.963	0.817	0.976	0.675	0.739	0.716	3.2
asp	0.492	0.386	0.499	0.751	0.409	0.381	3.3
dna	0.35	0.737	0.646	0.363	0.387	0.459	1
dnai	0.374	0.711	0.637	0.408	0.432	0.466	1
dnaa	0.61	0.951	0.807	0.263	0.321	0.397	2.1
dnaai	0.659	0.9	0.757	0.263	0.339	0.406	2.1
npi	0.663	0.445	0.417	0.785	0.495	0.599	3.2
darn	0.557	0.802	0.949	0.617	0.363	0.488	3.9
SVA 1	0.389	0.558	0.641	0.432	0.298	0.333	8
SVA 2	0.425	0.57	0.606	0.421	0.303	0.292	11.6
SVA 3	0.454	0.459	0.603	0.51	0.356	0.259	12.9
SVA 4	0.371	0.454	0.566	0.433	0.222	0.249	16.4
IOI	0.865	1.0	1.0	0.86	0.111	0.245	14.9

Table 7: MRR Alignment of different explanation methods on GPT-2 Small predictions on every dataset. The average distance to the linguistic evidence tokens is shown in the last column.

C.2 GPT-2 XL Results

Dataset	Erasure	Logit	ALTI-Logit	Grad Norm	$G \! \times \! I$	Random	Distance
aga	0.974	0.79	0.974	0.778	0.713	0.681	3.2
ana	0.945	0.777	0.964	0.721	0.655	0.71	3.2
asp	0.506	0.368	0.514	0.721	0.44	0.369	3.3
dna	0.326	0.655	0.539	0.255	0.486	0.465	1
dnai	0.366	0.598	0.524	0.264	0.515	0.453	1
dnaa	0.631	0.932	0.615	0.205	0.352	0.413	2.1
dnaai	0.644	0.874	0.529	0.205	0.359	0.393	2.1
npi	0.735	0.602	0.711	0.82	0.586	0.594	3.2
darn	0.576	0.873	0.945	0.686	0.477	0.51	3.9
SVA 1	0.416	0.564	0.638	0.467	0.365	0.352	8
SVA 2	0.455	0.558	0.646	0.489	0.353	0.269	11.6
SVA 3	0.424	0.455	0.678	0.535	0.343	0.31	12.9
SVA 4	0.411	0.418	0.625	0.489	0.256	0.226	16.4
IOI	0.643	1.0	1.0	0.829	0.131	0.239	14.9

Table 8: MRR Alignment of different explanation methods on GPT-2 XL predictions on every dataset. The average distance to the linguistic evidence tokens is shown in the last column.

D Model Predictions



Figure 12: Logit difference between the acceptable and the unacceptable predictions of a GPT-2 Small on every dataset.



Figure 13: Logit difference between the acceptable and the unacceptable predictions of a GPT-2 XL on every dataset.

E MRR Alignment across layers



Figure 14: ALTI-Logit MRR alignment scores across layers on Anaphor Agreement datasets (GPT-2 Small).



Figure 15: ALTI-Logit MRR alignment scores across layers on Anaphor Agreement datasets (GPT-2 XL).



Figure 16: ALTI-Logit MRR alignment scores across layers on Determiner-Noun Agreement datasets (GPT-2 Small).



Figure 17: ALTI-Logit MRR alignment scores across layers on Determiner-Noun Agreement datasets (GPT-2 XL).

F MLPs Logit Difference Update



Figure 18: MLPs update to the logit difference $\Delta \text{logit}_{(w-f) \leftarrow \text{MLP}^l}^l$ across layers (GPT-2 Small).

G Self-attention Logit Difference Update



Figure 19: Self-attention update to the logit difference $\Delta \text{logit}_{(w-f) \leftarrow \text{Self-attn}^l}^l$ across layers (GPT-2 Small).

H Qualitative Contrastive Exaplantions

H.1 Explanations of Different Contrastive Methods



Table 9: Comparison of different contrastive explanations on a GPT-2 Small SVA example (why **says** instead of **say**).



Table 10: Comparison of different contrastive explanations on a GPT-2 Small dnaa example (why **drivers** instead of **driver**).



Table 11: Comparison of different contrastive explanations on a GPT-2 Small asp example (why **children** instead of **cups**).

L48 A report about the Impressionists has
L47 A report about the Impressionists has
L46 A report about the Impressionists has
L45 A report about the Impressionists has
L44 A report about the Impressionists has
L43 A report about the Impressionists has
L42 A report about the Impressionists has
L41 A report about the Impressionists has
L40 A report about the Impressionists has
L39 A report about the Impressionists has
L38 A report about the Impressionists has
L37 A report about the Impressionists has
L36 A report about the Impressionists has
L35 A report about the Impressionists has
L34 A report about the Impressionists has
L33 A report about the Impressionists has
L32 A report about the Impressionists has
L31 A report about the Impressionists has
L30 A report about the Impressionists has
L29 A report about the Impressionists has
L28 A report about the Impressionists has
L27 A report about the Impressionists has
L26 A report about the Impressionists has
L25 A report about the Impressionists has
L24 A report about the Impressionists has
L23 A report about the Impressionists has
L22 A report about the Impressionists has
L21 A report about the Impressionists has
L20 A report about the Impressionists has
L19 A report about the Impressionists has
L18 A report about the Impressionists has
L17 A report about the Impressionists has
L16 A report about the Impressionists has
L15 A report about the Impressionists has
L14 A report about the Impressionists has
L13 A report about the Impressionists has
L12 A report about the Impressionists has
L11 A report about the Impressionists has
L10 A report about the Impressionists has
L9 A report about the Impressionists has
L8 A report about the Impressionists has
L7 A report about the Impressionists has
L6 A report about the Impressionists has
L5 A report about the Impressionists has
L4 A report about the Impressionists has
L3 A report about the Impressionists has
L2 A report about the Impressionists has
L1 A report about the Impressionists has

L48 Katherine can't help herself
L47 Katherine can't help herself
L46 Katherine can't help herself
L45 Katherine can't help herself
L44 Katherine can't help herself
L43 Katherine can't help herself
L42 Katherine can't help herself
L41 Katherine can't help herself
L40 Katherine can't help herself
L39 Katherine can't help herself
L38 Katherine can't help herself
L37 Katherine can't help herself
L36 Katherine can't help herself
L35 Katherine can't help herself
L34 Katherine can't help herself
L33 Katherine can't help herself
L32 Katherine can't help herself
L31 Katherine can't help herself
L30 Katherine can't help herself
L29 Katherine can't help herself
L28 Katherine can't help herself
L27 Katherine can't help herself
L26 Katherine can't help herself
L25 Katherine can't help herself
L24 Katherine can't help herself
L23 Katherine can't help herself
L22 Katherine can't help herself
L21 Katherine can't help herself
L20 Katherine can't help herself
L19 Katherine can't help herself
L18 Katherine can't help herself
L17 Katherine can't help herself
L16 Katherine can't help herself
L15 Katherine can't help herself
L14 Katherine can't help herself
L13 Katherine can't help herself
L12 Katherine can't help herself
L11 Katherine can't help herself
L10 Katherine can't help herself
L9 Katherine can't help herself
L8 Katherine can't help herself
L7 Katherine can't help herself
L6 Katherine can't help herself
L5 Katherine can't help herself
L4 Katherine can't help herself
L3 Katherine can't help herself
L2 Katherine can't help herself
L1 Katherine can't help herself

Table 12: GPT-2 XL darn (why **has** instead of **have**).

Table 13: GPT-2 XL aga (why herself instead of him-

self).

H.3 ALTI-Logit (IOI) across Models

L12 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L11 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L10 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L9 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L8 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L7 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L7 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L3 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L2 | </s> When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L1 | </s> When Paula and Martha got

Figure 20: OPT 125M IOI (why Paula instead of Martha).

L24 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L23 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L22 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L21 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L20 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L19 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L18 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L17 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L16 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L15 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L14 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L13 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L12 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L11 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L10 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L9 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L8 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L7 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L6 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L5 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to **Paula** When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L4 L3 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to **Paula** L2 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L1 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula

Table 14: BLOOM 560M IOI (why Paula instead of Martha).

L24 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L23 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L22 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L21 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L20 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L19 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L18 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L17 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L16 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L15 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L14 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L13 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L12 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L11 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L10 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L9 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L8 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L7 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L6 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L5 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L4 L3 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L2 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L1 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula

Table 15: BLOOM 1B1 IOI (why Paula instead of Martha).

L12 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L11 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L10 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L9 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L8 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L7 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula

Table 16: GPT-2 Small IOI (why Paula instead of Martha).

L36 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L35 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L34 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L33 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L32 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L31 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L30 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L29 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L28 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L27 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L26 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L25 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L24 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L23 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L22 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L21 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L20 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L19 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L18 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L17 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L16 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L15 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L14 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L13 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L12 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L11 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L10 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L9 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L8 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L7 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L6 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L5 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L4 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L3 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to **Paula** L2 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula L1 | When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula

L48 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L47 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L46 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L45 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L44 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L43 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L42 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L41 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L40 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L39 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L38 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L37 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L36 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L35 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L34 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L33 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L32 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L31 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L30 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L29 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L28 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L27 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L26 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L25 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L24 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L23 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L22 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L21 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L20 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L19 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L18 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L17 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L16 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L15 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L14 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L13 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L12 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L11 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L10 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L9 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L8 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L7 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L6 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L5 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L4 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L3 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L2 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula
L1 When Paula and Martha got a coconut at the zoo, Martha decided to give the coconut to Paula

Table 18: GPT-2 XL IOI (why Paula instead of Martha).

ACL 2023 Responsible NLP Checklist

A For every submission:

- A1. Did you describe the limitations of your work? *Section 9*
- A2. Did you discuss any potential risks of your work? *Section 9*
- A3. Do the abstract and introduction summarize the paper's main claims? *Abstract and Section 1*
- A4. Have you used AI writing assistants when working on this paper? *Left blank.*

B ☑ Did you use or create scientific artifacts?

Section 2

- B1. Did you cite the creators of artifacts you used? Section 2
- B2. Did you discuss the license or terms for use and / or distribution of any artifacts? *Left blank*.
- B3. Did you discuss if your use of existing artifact(s) was consistent with their intended use, provided that it was specified? For the artifacts you create, do you specify intended use and whether that is compatible with the original access conditions (in particular, derivatives of data accessed for research purposes should not be used outside of research contexts)? Section 9
- □ B4. Did you discuss the steps taken to check whether the data that was collected / used contains any information that names or uniquely identifies individual people or offensive content, and the steps taken to protect / anonymize it? *Not applicable. Left blank.*
- B5. Did you provide documentation of the artifacts, e.g., coverage of domains, languages, and linguistic phenomena, demographic groups represented, etc.? Section 3
- B6. Did you report relevant statistics like the number of examples, details of train / test / dev splits, etc. for the data that you used / created? Even for commonly-used benchmark datasets, include the number of examples in train / validation / test splits, as these provide necessary context for a reader to understand experimental results. For example, small differences in accuracy on large test sets may be significant, while on small test sets they may not be. Section 3

C ☑ Did you run computational experiments?

Section 3 and 5

C1. Did you report the number of parameters in the models used, the total computational budget (e.g., GPU hours), and computing infrastructure used? Section 3

The Responsible NLP Checklist used at ACL 2023 is adopted from NAACL 2022, with the addition of a question on AI writing assistance.

- □ C2. Did you discuss the experimental setup, including hyperparameter search and best-found hyperparameter values?
 Not applicable. Left blank.
- C3. Did you report descriptive statistics about your results (e.g., error bars around results, summary statistics from sets of experiments), and is it transparent whether you are reporting the max, mean, etc. or just a single run? *Section 3*
- C4. If you used existing packages (e.g., for preprocessing, for normalization, or for evaluation), did you report the implementation, model, and parameter settings used (e.g., NLTK, Spacy, ROUGE, etc.)? Section 3

D Z Did you use human annotators (e.g., crowdworkers) or research with human participants? *Left blank.*

- □ D1. Did you report the full text of instructions given to participants, including e.g., screenshots, disclaimers of any risks to participants or annotators, etc.? *Not applicable. Left blank.*
- D2. Did you report information about how you recruited (e.g., crowdsourcing platform, students) and paid participants, and discuss if such payment is adequate given the participants' demographic (e.g., country of residence)?
 Not applicable. Left blank.
- □ D3. Did you discuss whether and how consent was obtained from people whose data you're using/curating? For example, if you collected data via crowdsourcing, did your instructions to crowdworkers explain how the data would be used?
 Not applicable. Left blank.
- □ D4. Was the data collection protocol approved (or determined exempt) by an ethics review board? *Not applicable. Left blank.*
- D5. Did you report the basic demographic and geographic characteristics of the annotator population that is the source of the data?
 Not applicable. Left blank.