

Causal Mediation Analysis for Interpreting Neural NLP: The Case of Gender Bias

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Abstract

Common methods for interpreting neural models in natural language processing typically examine either their structure or their behavior, but not both. We propose a methodology grounded in the theory of causal mediation analysis for interpreting which parts of a model are causally implicated in its behavior. It enables us to analyze the mechanisms by which information flows from input to output through various model components, known as mediators. We apply this methodology to analyze gender bias in pre-trained Transformer language models. We study the role of individual neurons and attention heads in mediating gender bias across three datasets designed to gauge a model’s sensitivity to gender bias. Our mediation analysis reveals that gender bias effects are (i) sparse, concentrated in a small part of the network; (ii) synergistic, amplified or repressed by different components; and (iii) decomposable into effects flowing directly from the input and indirectly through the mediators.

1 Introduction

The success of neural network models in various natural language processing tasks, coupled with their opaque nature, has led to much interest in interpreting and analyzing such models. Analysis methods may be categorized into structural and behavioral analyses (Tenney et al., 2019). *Structural* analyses aim to shed light on the internal structure of a neural model, for example through probing classifiers (Conneau et al., 2018; Hupkes et al., 2018; Adi et al., 2017) that predict linguistic properties using representations from trained models. This methodology has been used for analyzing sentence embeddings, machine translation models, and contextual word representation models (Belinkov

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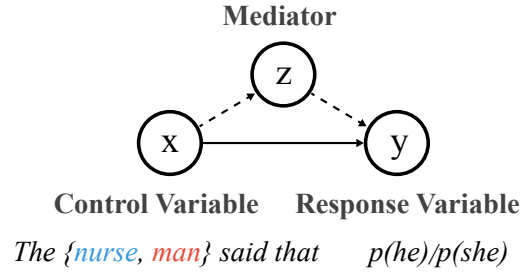


Figure 1: Causal mediation analysis applied to gender bias in language models.

and Glass, 2019). *Behavioral* analyses, on the other hand, aim to assess a model’s behavior by its performance on constructed examples (e.g., Isabelle et al., 2017; Naik et al., 2018), or by visualizing important input features via saliency methods (e.g., Li et al., 2016; Murdoch et al., 2018).

Despite yielding interesting and useful insights, both types of analyses suffer from significant limitations. As pointed out by Belinkov and Glass (2019), probing classifiers only yield a correlational measure between a model’s representations and an external linguistic property, and are thus not *causally* connected to the model’s predictions. Barrett et al. (2019) further demonstrate that classifiers that aim to detect biases in learned representations focus on spurious correlations in their training data and fail to generalize to unseen data. Probing classifiers may thus fail to provide faithful interpretations. On the other hand, while behavioral analyses directly evaluate model predictions, they do not typically link them to the model’s internal structure.

This work introduces a methodology for interpreting neural NLP models to address these limitations. Our key contribution is the adaptation of *causal mediation analysis* (Pearl, 2001) for analyzing the mechanism by which information flows from input to output through different model components. To this end, we define counterfactual out-

comes under different interventions, which are utilized to quantify measures of direct and indirect effects in neural networks. Direct effects flow directly from input to output variables, while indirect effects flow through a mediator, or intermediary variable (Figure 1). Treating individual model components as mediators gives rise to a decomposition of the effects occurring in deep models.

We apply this framework to the analysis of gender bias in large pre-trained language models. Gender bias has surfaced as a major concern in word representations, both static word embeddings (Caliskan et al., 2017; Bolukbasi et al., 2016) and contextualized word representations (Zhao et al., 2019a; Basta et al., 2019; Tan and Celis, 2019). We study how gender bias effects are mediated via different model components in Transformer-based language models, in particular, several versions of GPT2 (Radford et al., 2019), focusing on the role of individual neurons or attention heads in mediating these effects.

Our approach is a structural-behavioral analysis. It is structural in that our results highlight internal model components that are responsible for gender bias. It is behavioral in that said components are causally implicated in how gender bias manifests in the model outputs. In an experimental evaluation using several datasets designed to gauge a model’s gender bias, we find that larger models show larger gender bias effects, potentially absorbing more bias from the underlying training data. The causal mediation analysis further yields several insights regarding the role of different model components in mediating gender bias:

- Gender bias is *sparse*: Much of the effect is concentrated in relatively few model components.
- Gender bias is *synergistic*: Some model components interact to produce mutual effects that amplify their individual effects. Other components operate relatively independently, capturing complementary aspects of gender bias.
- Gender bias is *decomposable*: The total gender bias effect approximates the sum of the direct and indirect effect, a surprising result given the non-linear nature of the model.

In summary, this paper makes two broad contributions. First, we cast causal mediation analysis as an approach for analyzing neural NLP models, which may be applied to a variety of models and phenomena. Second, we demonstrate this methodology in the case of analyzing gender bias

in pre-trained language models, revealing the internal mechanisms by which bias effects flow from input to output through various model components.

The code for reproducing our results is available at <https://github.com/sebastianGehrmann/CausalMediationAnalysis>.

2 Related Work

2.1 Analysis Methods

Methods for interpreting neural network models in NLP can be broadly divided into two kinds. Structural methods focus on identifying what information is contained in different model components. Probing classifiers aim to answer such questions by using models’ representations as input to classifiers that predict various properties (Adi et al., 2017; Hupkes et al., 2018; Conneau et al., 2018). However, this approach is not connected to the model’s behavior (i.e., its predictions) on the task it was trained on (Belinkov and Glass, 2019; Tenney et al., 2019). The representation may thus have some information by coincidence, without it being used by the original model. In addition, it is challenging to differentiate the information learned by the probing classifier from that learned by the underlying model (Hewitt and Liang, 2019).

An alternative approach is to assess how well a model captures different linguistic phenomena by evaluating its performance on curated examples (e.g., Sennrich, 2017; Isabelle et al., 2017; Naik et al., 2018). This approach directly evaluates a model’s predictions but fails to provide insight into its internal structure. Another approach identifies important input features that contribute to a model’s prediction via saliency methods (Li et al., 2016; Arras et al., 2017; Murdoch et al., 2018), which also typically ignore the model’s internal structure, although they may in principle be computed with respect to internal representations.

Our causal mediation analysis approach bridges the gap between these two lines of work, providing an analysis that is both structural and behavioral. Mediation analysis is an unexplored formulation in the context of interpreting deep NLP models. In recent work, Zhao and Hastie (2019) used mediation analysis for interpreting black-box models. However, their analysis was limited to simple datasets and models, while we focus on deep language models. Furthermore, they only considered total effects and (controlled) direct effects, while we measure (natural) direct and indirect effects, which is crucial for studying the role of internal model components.

2.2 Gender Bias and Other Biases

Neural networks learn to replicate historical, societal biases from training data in various tasks such as natural language inference (Rudinger et al., 2017), coreference resolution (Cao and Daumé III, 2019), and sentiment analysis (Kiritchenko and Mohammad, 2018). This conflicts with the principle of counterfactual fairness, which states that the model predictions should not be influenced by changes to a sensitive attribute such as gender (Kusner et al., 2017); for instance, a fair and unbiased model should equally associate gendered pronouns with professions. However, biased models make this association proportionally to the distribution of gender in the training data (Caliskan et al., 2017). While efforts have been made to reduce bias, this remains a significant ethical challenge.

A common strategy to mitigate biases is to change the training data (e.g., Lu et al., 2018; Hall Maudslay et al., 2019; Zhao et al., 2018a; Kaushik et al., 2019), the training process (e.g., Huang et al., 2019; Qian et al., 2019), or the model itself (e.g., Madras et al., 2019; Romanov et al., 2019; Gehrmann et al., 2019) to ensure counterfactual fairness. The resulting biases are often measured similarly to this work by testing that mentions of occupations lead to equal probabilities across grammatical genders in referential expressions.

Others have focused on de-biasing word embeddings and contextual word representations (Bolukbasi et al., 2016; Zhao et al., 2018b; Yang and Feng, 2020), though recent work has questioned the efficacy of these debiasing techniques in removing both grammatical and societal biases (Elazar and Goldberg, 2018; Gonen and Goldberg, 2019). Biases may also be introduced in downstream tasks and representations in models where representations depend on additional context (Zhao et al., 2019b; Kurita et al., 2019).

3 Methodology

3.1 Preliminaries

Consider a large pre-trained neural language model (LM), parameterized by θ , which predicts the probability of the next word given a prefix: $p_\theta(x_t | x_1, \dots, x_{t-1})$. We will focus on LMs based on Transformers (Vaswani et al., 2017), although much of the methodology will apply to other architectures as well. Let $\mathbf{h}_{l,i} \in \mathbb{R}^K$ denote the (contextual) representation of word i in layer l of the model, with neuron activations $\mathbf{h}_{l,i,k}$ ($1 \leq k \leq$

K). These representations are composed using so-called multi-headed attention. Let $\alpha_{l,h,i,j} \geq 0$ denote the attention directed from word i to word j by head h in layer l , such that $\sum_j \alpha_{l,h,i,j} = 1$.

3.2 Causal Mediation Analysis

Causal mediation analysis aims to measure how a treatment effect is mediated by intermediate variables (Robins and Greenland, 1992; Pearl, 2001; Robins, 2003). We use this framework to study the effects of gender-related interventions mediated by different parts of pre-trained LMs, such as particular neurons.¹ We use gender bias as a case study, although the approach can be applied to other biases as well (race, ethnicity, etc.).

The following example illustrates the problem:

Prompt u : The nurse said that __

Stereotypical candidate: she

Anti-stereotypical candidate: he

Given a prompt u such as *The nurse said that*, a language model is asked to generate a continuation. A biased model may assign a higher likelihood to *she* than to *he*, such that $p_\theta(\textit{she} | u) > p_\theta(\textit{he} | u)$. We say that *she* is the stereotypical candidate, while *he* is the anti-stereotypical candidate, reflecting a societal bias associating nurses with women more than men.² The relative probabilities assigned to the two candidates can be thought of as a measure of gender bias in the model:

$$\mathbf{y}(u) = \frac{p_\theta(\text{anti-stereotypical} | u)}{p_\theta(\text{stereotypical} | u)} \quad (1)$$

In our example, we have the following: $\mathbf{y}(u) = p_\theta(\textit{he} | \textit{The nurse said that}) / p_\theta(\textit{she} | \textit{The nurse said that})$. If $\mathbf{y}(u) < 1$, the prediction is stereotypical; if $\mathbf{y}(u) > 1$, it is anti-stereotypical. A perfectly unbiased model would achieve $\mathbf{y}(u) = 1$ and thus exhibit bias toward neither the stereotypical nor the anti-stereotypical case.

We will consider a collection of professions in order to assess gender bias. Following Pearl’s definitions, we measure the direct and indirect effects of intervening in the model (Pearl, 2001). Intuitively, the direct effect measures how much an intervention x changes an outcome variable y directly, without passing through a hypothesized mediator z . It is computed by applying the interven-

¹There is some evidence that gender is captured in subspaces of contextual word representations (Zhao et al., 2019a).

²Grammatical gender is much more nuanced than this binary example, as argued by Cao and Daumé III (2019). We leave extension of the framework to a continuous setup to future work.

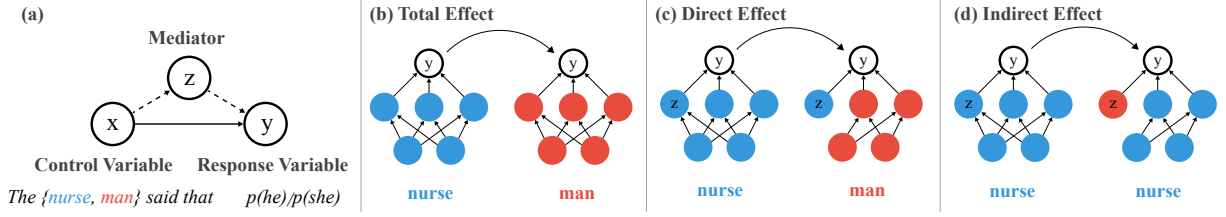


Figure 2: Mediation analysis illustration. Here the *do*-operation is $x = \text{set-gender}$, which changes u from *nurse* to *man* in this example. The **total effect** measures the change in y resulting from the intervention; the **direct effect** measures the change in y resulting from performing the intervention while holding a mediator z fixed; the **indirect effect** measures the change caused by setting z to its value under the intervention, while holding u fixed.

tion x but holding z fixed to its original value. The indirect effect measures how much the intervention x changes y indirectly, through z . It is computed by setting z to its value under the intervention x , while keeping everything else to its original value.

Following this intuition, let x denote the intervention whose effect we wish to measure on gender-ambiguous professions such as *nurse*, *doctor*, *teacher*, etc. Define the following *do*-operations: (a) *set-gender*: replace the ambiguous profession with an anti-stereotypical gender-specific word (that is, replace *nurse* with *man*, *doctor* with *woman*, etc.); (b) *null*: leave the sentence as is. Let y denote the response variable, such as the bias measure defined above (Eq. 1). The population of units for this analysis is a set of example sentences such as the above prompt. Then we say $y_x(u)$ is the value that y attains in unit $u = u$ under the intervention *do*($x = x$).

The unit-level **total effect** (TE) of $x = x$ on y in unit $u = u$ is the proportional difference³ between the amount of bias under a gendered reading and under an ambiguous reading (Figure 2b):

$$\text{TE}(\text{set-gender}, \text{null}; y, u) = \frac{y_{\text{set-gender}}(u) - y_{\text{null}}(u)}{y_{\text{null}}(u)} = \frac{y_{\text{set-gender}}(u)}{y_{\text{null}}(u)} - 1 = \frac{p_{\theta}(\text{he}|\text{The man said that})}{p_{\theta}(\text{she}|\text{The man said that})} \Big/ \frac{p_{\theta}(\text{he}|\text{The nurse said that})}{p_{\theta}(\text{she}|\text{The nurse said that})} - 1$$

An illustrative example of the computation of the total effect is provided in Figure 3.

The average total effect of $x = x$ on y is calculated by taking the expectation over the population u :

$$\text{TE}(\text{set-gender}, \text{null}; y) = \mathbb{E}_u \left[\frac{y_{\text{set-gender}}(u)}{y_{\text{null}}(u)} - 1 \right]$$

Next, we define direct and indirect effects. Let z denote an intermediate variable—also known as a mediator—between x and y . For instance,

³We make the difference proportional to control for the high variance of y across examples. See Appendix A.1.

Example

$u = \text{The nurse said that [blank]}$

1) Compute relative probabilities of the baseline.

$$p([\text{he}]|u) = p([\text{he}]|\text{the nurse said that}) \approx 3.1\%$$

$$p([\text{she}]|u) = p([\text{she}]|\text{the nurse said that}) \approx 22.4\%$$

$$y_{\text{null}}(u) = 3.1/22.4 \approx 0.14$$

2) Set u to an anti-stereotypical case and recompute.

$x = \text{set-gender}$: change *nurse* \rightarrow *man*

$$p([\text{he}]|u, \text{set-gender}) = p([\text{he}]|\text{the man said that}) \approx 31.5\%$$

$$p([\text{she}]|u, \text{set-gender}) = p([\text{she}]|\text{the man said that}) \approx 2.4\%$$

$$y_{\text{set-gender}}(u) = 31.5/2.4 \approx 13.1$$

3) Compute the total effect

$$\text{TE}(\text{set-gender}, \text{null}; y, u) = 13.1/0.14 - 1 \approx 92.6$$

Figure 3: In this example, we present the setup to measure the **total effect** in an example with the prompt $u = \text{The nurse said that}$ with the control variable $x = \text{set-gender}$. As we compute the proportional probability prior to the intervention, we notice that the model assigns a much higher probability to *[she]*, the stereotypical example, than to *[he]*. By changing *nurse* to *man*, we compute the proportional probability of a definitionally gendered example. The total effect measures the effect of this intervention.

z might be a particular neuron, a full layer, an attention head, or a certain attention weight. Then the response variable can be written as $y_x(u) = y_{x,z_x(u)}(u)$.

The **natural direct effect** (NDE) of $x = x$ on y given mediator $z = z$ is the change in the amount of bias when genderizing all units u , e.g. changing *nurse* to *man*, while holding z for each unit to its original value under the gender-ambiguous reading. This measures the direct effect that flows from x to y without going through the mediator z (illustrated in Figure 2c):

$$\text{NDE}(\text{set-gender}, \text{null}; y) =$$

$$\mathbb{E}_u [y_{\text{set-gender}, z_{\text{null}}(u)}(u) / y_{\text{null}}(u) - 1]$$

The **natural indirect effect** (NIE) is the change in amount of bias when keeping unit u as is, but setting z to the value it would attain under a genderized reading. This measures the indirect effect flowing from x to y through z (Figure 2d):

$$\text{NIE}(\text{set-gender}, \text{null}; y) = \mathbb{E}_u[\mathbf{y}_{\text{null}, z_{\text{set-gender}}(u)}(u) / \mathbf{y}_{\text{null}}(u) - 1]$$

This framework allows evaluating the causal contribution of different mediators z to gender bias. Through the distinction between direct and indirect effect, we can measure how much of the total effect of gender edits on gender bias flows through a specific component (indirect effect) or elsewhere in the model (direct effect). We experiment with mediators at the neuron level and the attention level, which are defined next.

3.3 Neuron Interventions

To study the role of individual neurons in mediating gender bias, we assign z to each neuron $\mathbf{h}_{l,k}$ in the LM. The dataset we use consists of a list of templates that are instantiated by profession terms, resulting in examples such as *The nurse said that*. For each example, we define the `set-gender` operation to move in the anti-stereotypical direction, changing female-stereotypical professions like *nurse* to *man* and male-stereotypical professions like *doctor* to *woman*. Section 4 provides more information on the dataset.

In the experiments, we investigate the effect of intervening on each neuron independently, as well as on multiple neurons concurrently. That is, the mediator z may be a set of neurons. In all cases, the mediator is in the representation corresponding to the profession word, such as the word *nurse* in the example.

3.4 Attention Interventions

For studying attention behavior, we focus on the attention weights, which define relationships between words. The mediators z , in this case, are the attention heads $\alpha_{l,h}$, each of which defines a distinct attention mechanism.

We align our intervention approach with two resources for assessing gender bias in pronoun resolution: Winobias (Zhao et al., 2018a) and Winogender (Rudinger et al., 2018). Both datasets consist of Winograd-schema-style examples that aim to assess gender bias in coreference resolution systems. We reformulate the examples to study bias in LMs,

as the following example from Winobias shows:

Prompt u : The nurse examined the farmer for injuries because she _____

Stereotypical candidate: was caring

Anti-stereotypical candidate: was screaming

According to the stereotypical reading, the pronoun *she* refers to the nurse, implying the continuation *was caring*. The anti-stereotypical reading links *she* to the farmer, this time implying the continuation *was screaming*. The bias measure is $\mathbf{y}(u) = p_\theta(\text{was screaming} \mid u) / p_\theta(\text{was caring} \mid u)$.⁴ In this case, we define the `swap-gender` operation, which changes *she* to *he*. The total effect is then:

$$\text{TE}(\text{swap-gender}, \text{null}; y, u) = \frac{\mathbf{y}_{\text{swap-gender}}(u)}{\mathbf{y}_{\text{null}}(u)} - 1$$

In the experiments, we study the effect of the attention from the last word (*she* or *he*) to the rest of the sentence.⁵ Intuitively, in the above example, if the word *she* attends more to *nurse* than to *farmer*, then the more likely continuation might be *was caring*. We compute the NDE and NIE for each head individually by intervening on the attention weights $\alpha_{l,h}, \dots$. We also evaluate the joint effects when intervening on multiple attention heads concurrently. The population-level TE and the NDE and NIE are defined analogously as above.

4 Experimental Details

Models As an example large pre-trained LM, we use GPT2 (Radford et al., 2019), a Transformer-based (English) LM trained on massive amounts of data. We use several model sizes made available by Wolf et al. (2019): small, medium, large, extra-large (xl), and a distilled model (Sanh et al., 2019).

Data For neuron intervention experiments, we augment the list of templates from Lu et al. (2018) with several other templates, instantiated with professions from Bolukbasi et al. (2016). The professions are accompanied by crowdsourced ratings between -1 and 1 for definitionality and stereotypicality. *Actress* is definitionally female, while *nurse* is stereotypically female. To simplify processing by GPT2 and focus on common professions, we only take examples that are not split into sub-word units, resulting in 17 templates and 169 professions, 2,873 examples in total. The full lists of templates

⁴To compute probabilities of multi-word continuations, we use the geometric mean of the token-level probabilities.

⁵One may also study individual attention arcs. However, attention does not always focus on a specific word, often falling on adjacent words. See Appendix C.2 for this phenomenon.

Model	WB	WG	Prof.
GPT2-small rand.	0.07	0.05	0.12
GPT2-distil	0.12	0.08	130.86
GPT2-small	0.25	0.10	112.28
GPT2-medium	0.77	0.32	115.95
GPT2-large	0.75	0.36	96.86
GPT2-xl	1.05	0.34	225.22

Table 1: Total effects (TE) of gender bias in various GPT2 variants evaluated on Winobias (WB), Winogender (WG), and the professions dataset (Prof.).

and professions are given in Appendix A.1. We refer to these examples as the Professions dataset.

For attention intervention experiments, we use examples from Winobias Dev/Test (Zhao et al., 2018a) and Winogender (Rudinger et al., 2018), totaling 160/130 and 44 examples that fit our formulation, respectively. We experiment with the full datasets and filtering by total effect. Both datasets include statistics from the U.S. Bureau of Labor Statistics to assess the gender stereotypicality of the referenced occupations. Appendix A.2 provides additional details about the datasets and preprocessing methods.

5 Results

5.1 Total Effects

Before describing the results from the mediation analysis, we summarize some insights from measurements of the total effect. Table 1 shows the total effects of gender bias in the different GPT2 models, on three datasets, as well as the effects with a randomly initialized GPT2-small model. Random model effects are much smaller, indicating that it is the training that causes gender bias.

Larger models are more sensitive to gender bias

In the Winograd-style datasets, the total effect mostly increases with model size, saturating at the large and xl models. In the professions dataset, model size is not well correlated with total effect, but GPT2-xl has a much larger effect. Since larger models can more accurately emulate the training corpus, it makes sense that they would more strongly integrate its biases.

Effects in different datasets It is difficult to compare effect magnitudes in the three datasets because of their different nature. The professions dataset yields much stronger effects than the

Winograd-style datasets. This may be attributed to the more explicit source of bias, the word representations, as compared to intricate coreference relations in the Winograd-style datasets.

Some effects are correlated with external gender statistics

In the professions dataset, we found moderate positive correlations between the external gender bias⁶ and the log-total effect, ranging from 0.35 to 0.45 over the different models, indicating that the model captures the expected biases. It further shows that the effect is amplified by the model for words that are perceived as more biased. In the Winograd-style datasets, we found relatively low correlations between the log-total effect and the log-ratio of the two occupations’ stereotypicality, ranging from 0.17 to 0.26. This low correlation may be due to either a smaller size compared to the professions dataset or the more complex relations in these datasets.

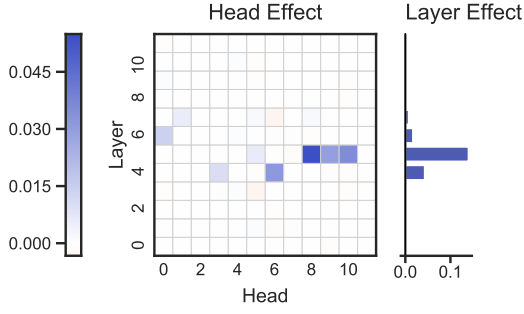
5.2 Sparsity

Where in the model are gender bias effects captured? Are the effects mediated by only a few model components or distributed across the model? Here we answer these questions by measuring the indirect effect flowing through different mediators.

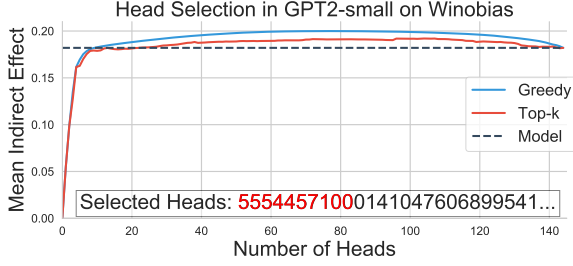
Attention Figure 4a shows the indirect effects for each head in GPT2-small on Winobias. The heatmap shows interventions on each head individually. A small number of heads, concentrated in the middle layers of the model, have much higher indirect effects than others. The bar chart shows indirect effects when intervening on all heads in a single layer concurrently. Consistent with the head-level heatmap, the effects are concentrated in the middle layers. We did not find similar behavior in a randomly initialized model, indicating that these patterns do not occur by chance. We found this sparsity consistent in all model variants and datasets we examined. See Appendix C.1 for additional visualizations.

To determine how many heads are required to achieve the full effect of intervening on all heads, we also intervene on groups of heads. We do so by selecting a subset of heads, using either a GREEDY approach, which iteratively selects the head with the maximal marginal contribution to the indirect effect, or a TOP-K approach, which selects the

⁶For this analysis, we add the stereotypicality and definitionality of each profession to capture the overall bias value.



(a) Indirect effects in GPT2-small on Winobias for heads (the heatmap) and layers (the bar chart).



(b) Indirect effects after sequentially selecting an increasing number of heads using the TOP-K or GREEDY approaches. Very few heads are required to saturate the model effect. The inset lists the sequence of layers of heads selected by GREEDY. The ones in red together reach the model effect, demonstrating the concentration of the effect in layers 4 and 5.

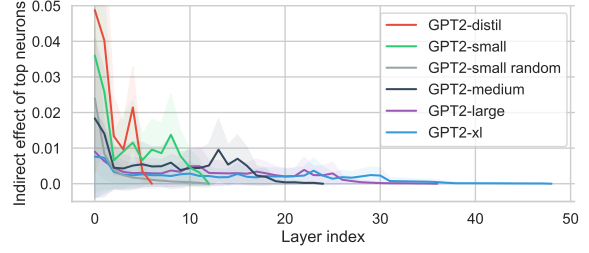
Figure 4: Sparsity effects in attention heads.

k elements with the strongest individual effects. Appendix D provides more information on these algorithms. Only 10 heads are required to match the effect of intervening on all 144 heads at the same time (Figure 4b). The first 6 selected ones are from layers 4 and 5, further demonstrating the concentration of the effect in the middle layers.

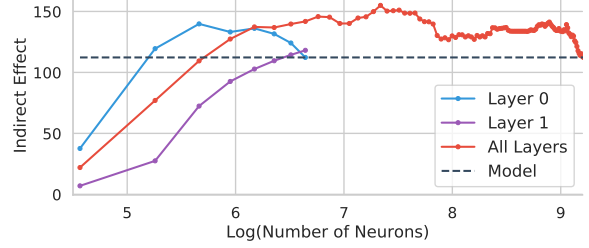
Neurons Figure 5a shows the indirect effects from the top 5% of neurons from each layer in different models. The word embeddings (layer 0) and the first hidden layer have the strongest effects. This stands in contrast to the attention intervention results, where middle layers had much larger effects. However, we still observe a small increase in effect within the intermediate layers across all models except for the randomized one.

Figure 5b shows the indirect effects when selecting neurons by the TOP-K algorithm.⁷ Similar to the attention result, a tiny fraction of neurons is sufficient for obtaining an effect equal to that of intervening on all neurons concurrently. Most of the top selected neurons are concentrated in the embedding layer and first hidden layer.

⁷For computational reasons, we select sets of 96 neurons.



(a) Indirect effects of top neurons in different models on the professions dataset.



(b) Indirect effects after sequentially selecting an increasing number of neurons from either the full model or individual layers using the TOP-K approach in GPT2-small on the professions dataset. Very few neurons (4%) are required to saturate the model effect. Of those, 57% are from layers 0 and 1.

Figure 5: Sparsity effects in neurons.

5.3 Synergism

How do different model components interact in capturing gender bias? Do different components work independently or jointly? Are gender bias effects amplified by different components or constrained?

Attention Recent work found that attention heads in GPT2 and other Transformers play highly differentiated roles. For instance, some heads focus on adjacent tokens while others align with syntactic properties (Kovaleva et al., 2019; Hoover et al., 2019; Clark et al., 2019; Vig and Belinkov, 2019). We use mediation analysis to study the interdependence of attention heads.

Figure 6 compares indirect effects of concurrent intervention on all heads (NIE-all) to summing the effects of independent interventions (NIE-sum). The differences are fairly small (maximum relative distance from NIE-all between 0.7% and 11.3%), indicating that heads operate primarily in an independent and complementary manner, capturing different aspects of gender bias. As Figure 4b shows, most heads do not contribute much to the indirect effect, and many reduce it. This trend is consistent across models and datasets (Appendix D).

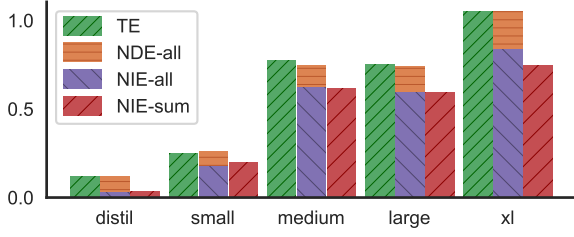


Figure 6: Effects of intervening on all heads concurrently (all) vs. independently and summing (sum) in various GPT2 variants evaluated on Winobias.

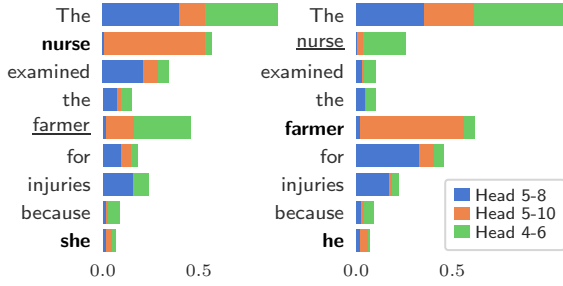


Figure 7: Attention of different heads in GPT2-small on a Winobias example, directed from either *she* or *he*. Colors correspond to different heads. Head 5-10 attends directly to the **bold** stereotypical candidate, head 5-8 attends to the words following it, and head 4-6 attends to the underlined anti-stereotypical candidate. Attention to the first token may be null attention (Vig and Belinkov, 2019). Appendix C.2 shows more examples.

Figure 7 shows the attention of the three heads with the highest indirect effects on Winobias. The figure demonstrates that they capture different coreference aspects: one head aligns with the stereotypical coreference candidate, another head attends to the tokens following that candidate, while a third attends to the anti-stereotypical candidate. Vig (2019) previously identified the same head (layer 5, head 10; noted as 5-10) as relating to coreference resolution based on visual inspection. Clark et al. (2019) found an attention head in BERT (Devlin et al., 2019) that was highly predictive of coreference, also in layer 5 out of 12.

Neurons Similar to the case of attention, Figure 5b shows that after a few neurons (4%) match the model-wise concurrent effect, most neurons do not contribute much, and many even diminish the effect. This result suggests that neurons may be as specialized as the individual attention heads. However, an analogous qualitative analysis is challenging due to the large number of neurons.

By definition, concurrent intervention on all neurons entails $TE = NIE-all$, since then

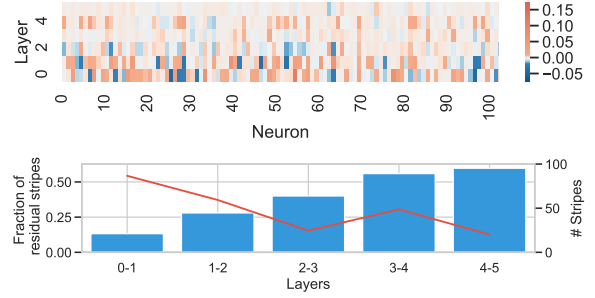


Figure 8: **Top:** Indirect effects for the first 100 neurons in GPT2-distil. There are distinct vertical stripes where the effect of a neuron at an index continues to the next layer. **Bottom:** The fraction of the continued effect over layer pairs in GPT2-distil that can be explained by residual connections. In higher layers, the model uses the connections to refine representations.

$y_{set-gender}(u) = y_{null, z_{set-gender}(u)}(u)$. Notably, the sum of independent indirect effects is much smaller: 6.8/4.0/3.5/2.1/2.9 NIE-sum vs. 130.9/112.3/116.0/96.9/225.2 NIE-all in distil/small/medium/large/xl. Thus, neurons combine synergistically to compound independent effects.

Residual Connections Visualizing the indirect effect of each neuron in a heatmap (Figure 8 top) reveals vertical stripes when a neuron at the same index, but different layers, has a similar effect. While sparse, this effect sometimes continues over multiple layers. Two possible explanations for this are random alignments of two effective cells or the residual connections between the layers. To analyze this, we computed the number of stripes between layer pairs across the professions dataset, with and without randomizing neuron indices. As Figure 8 (bottom) shows, the stripes are less random in higher layers. This implies that, as the information gets transformed, the model converges on a representation. This is akin to gated recurrent networks, except that those transform across time steps instead of layers. This result may partially explain the higher neuron importance in earlier layers since those neurons have not yet converged to a representation and thus have a higher variance and contribution to the representation in other neurons.

5.4 Decomposition of the Total Effect

Attention heads mediate most of the effect

Figure 6 also shows the concurrent direct and indirect effects, when intervening on all heads. In all but the smallest model (distil), the concurrent indirect effect is larger than the direct effect, indicating that most of the effect is mediated through

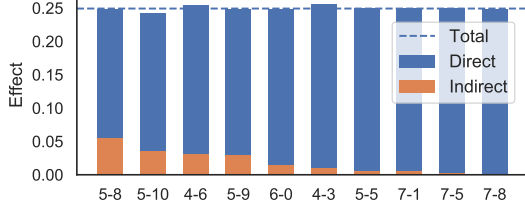


Figure 9: Top 10 heads by indirect effect in GPT2-small on Winobias, and their respective direct effects.

the attention heads. Other model components (e.g., word representations) are nonetheless responsible for a portion of the total effect. This might be due to biased word embeddings predisposing the model towards certain continuations. For instance, the representation of *he* might lead the model to predict a lower probability for *was caring* compared to *she*, irrespective of any previous occupation mention.

TE \approx NDE + NIE In linear models, it is known that the linear total effect decomposes to direct and indirect effects (Pearl, 2001). Intuitively, intervention effects either flow through a mediator or directly. In our case, we have a highly non-linear model and this decomposition is not guaranteed.⁸ Nevertheless, Figure 9 shows such approximate decomposition for the top heads in GPT2-small.⁹ The same holds for concurrent interventions (Figure 6), where $TE \approx NDE\text{-all} + NIE\text{-all}$. To understand this phenomenon, observe that under our formulation of the effects using a proportional difference, a decomposition of the form $TE = NDE + NIE$ is expected if the following equality holds for all u :

$$y_{\text{set-gender}}(u) - y_{\text{set-gender}, z_{\text{null}}(u)}(u) = y_{\text{null}, z_{\text{set-gender}}(u)}(u) - y_{\text{null}}(u). \quad (2)$$

See Appendix E for intuition, a proof, and evidence that Eq. 2 approximately holds in our results.

6 Discussion and Conclusion

This paper introduced a new structural-behavioral framework for interpreting neural NLP models based on causal mediation analysis. An application of this framework yielded several insights regarding the mechanisms by which gender bias is mediated in such large Transformer LMs, revealing that gender bias effects are sparse, synergistic, and decomposable to direct and indirect effects.

This work can be extended in multiple ways. First, our experiments were limited to one archi-

tecture, GPT2, albeit with several variants. Experimenting with different architectures and objectives may require formulating different interventions. We have also focused only on gender bias in a binary setup. Applying the methodology to more inclusive genders (Cao and Daumé III, 2019), or other kinds of bias, is especially important. More generally, the framework may apply to any property expressed as a function of model predictions. Our results can also guide model selection for limiting the amount of bias. In related work, Giulianelli et al. (2018) demonstrated that changing hidden representations in an LSTM based on the output of diagnostic classifiers can decrease the error on a subject-verb agreement classification task. Inspired by these results, mediation analysis could be used to determine where and how to intervene in similar ways and thus not only assess the success of debiasing techniques, but also motivate new debiasing methods that establish counterfactual fairness for protected groups.

This work is a first attempt to adopt mediation analysis for interpreting NLP models. The causality literature often focuses on assumptions needed for identification of mediation effects from observed data (Pearl, 2001; Avin et al., 2005; Imai et al., 2010b). The challenge with inferring causality from observational data is that for each unit, the outcome is observed under a single intervention. However, in this work we use the language of causal mediation to study the structure of NLP models, utilizing the fact that the outcome of the same unit (e.g., a sentence) can be observed under any intervention given a trained model. As a result, causal effects can be computed in a relatively simple manner. Our definitions of causal effects to quantify bias could be refined, and alternative definitions might be advantageous for NLP research.

The causality literature offers many avenues for continuing this line of work, including mediation analysis with non-linear models, and alternative effect decompositions (Imai et al., 2010a,b; VanderWeele and Vansteelandt, 2009). A promising direction is to focus on path-specific effects (Avin et al., 2005), to identify the exact mechanisms through which biases arise. Characterizing specific paths from model input to output might also be useful during training by disincentivizing the creation of paths leading to bias. We believe the present work sets the ground for employing this literature in the ongoing effort to analyze neural NLP models.

⁸VanderWeele and Vansteelandt (2009) point out that some decompositions can be guaranteed.

⁹In the neuron intervention case, by definition $TE = NIE\text{-all}$ and $NDE\text{-all} = 0$, so the decomposition trivially holds.

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A Data Preparation

A.1 Professions Dataset

Figure 10 shows the 17 base templates used for the neuron interventions. To validate that each template would capture gender bias, we instantiate each with an occupation of *woman* and *man* and verify that the conditional probabilities of *she* and *he* align with gender. Given *woman* as the occupation word, the probability ratio $p(\text{she})/p(\text{he})$ ranges from 2.5 to 45.1 across templates ($\mu = 17.2, \sigma = 13.1$). Given *man*, the value $p(\text{he})/p(\text{she})$ ranges from 3.0 to 55.4 ($\mu = 21.9, \sigma = 16.2$). Thus the relative probabilities align with gender, though they vary greatly in magnitude.

For each of the templates, we used the following professions. Words in *italics* are definitional and were thus excluded from the total effect calculation:

female: *actress*, advocate, aide, artist, baker, clerk, counselor, dancer, educator, instructor, maid, *nun*, nurse, observer, performer, photographer, planner, poet, protester, psychiatrist, secretary, singer, substitute, teacher, teenager, therapist, treasurer, tutor, *waitress*

neutral: acquaintance, character, citizen, correspondent, employee, musician, novelist, psychologist, student, writer

male: accountant, *actor*, administrator, adventurer, ambassador, analyst, architect, assassin, astronaut, astronomer, athlete, attorney, author, banker, bartender, biologist, bishop, boss, boxer, broadcaster, broker, *businessman*, butcher, campaigner, captain, chancellor, chef, chemist, cleric, coach, collector, colonel, columnist, comedian, comic, commander, commentator, commissioner, composer, conductor, congressman, consultant, cop, critic, curator, *dad*, dean, dentist, deputy, detective, diplomat, director, doctor, drummer, economist, editor, entrepreneur, envoy, farmer, filmmaker, firefighter, *fisherman*, footballer, goalkeeper, guitarist, historian, inspector, inventor, investigator, journalist, judge, landlord, lawmaker, lawyer, lecturer, legislator, lieutenant, magician, magistrate, manager, mathematician, mechanic, medic, midfielder, minister, missionary, *monk*, narrator, negotiator, officer, painter, pastor, philosopher, physician, physicist, *policeman*, politician, preacher, president, priest, principal, prisoner, professor, programmer, promoter, prosecutor, protagonist, rabbi, ranger, researcher, sailor, saint, *salesman*, scholar, scientist, senator, sergeant, servant, soldier, solicitor, strategist, superintendent, surgeon, technician, trader, trooper, *waiter*, warrior, worker, wrestler

A.2 Winobias and Winogender

For both Winobias and Winogender datasets, we exclude templates in which the shared prompt does

The <occupation> said that ...
The <occupation> yelled that ...
The <occupation> whispered that ...
The <occupation> wanted that ...
The <occupation> desired that ...
The <occupation> wished that ...
The <occupation> ate because ...
The <occupation> ran because ...
The <occupation> drove because ...
The <occupation> slept because ...
The <occupation> cried because ...
The <occupation> laughed because ...
The <occupation> went home because ...
The <occupation> stayed up because ...
The <occupation> was fired because ...
The <occupation> was promoted because ...
The <occupation> yelled because ...

Figure 10: Templates for neuron interventions.

not end in a pronoun.¹⁰ For Winobias, we only consider *Type 1* examples, which follow the format of a shared prompt and two alternate continuations. We also experiment with filtering by total effect, removing examples with a negative total effect as well as examples in the bottom quartile of those with a positive total effect. The sizes of all dataset variations may be found in Table 2. Results are reported for filtered versions of both datasets and the Dev set of Winobias unless otherwise noted.

Both datasets include statistics from the U.S. Bureau of Labor Statistics (BLS) to assess the gender stereotypicality of the referenced occupations. Winogender additionally includes gender estimates from text (Bergsma and Lin, 2006), which we also include in our analysis. Whereas each Winobias example includes two occupations of opposite stereotypicality, each Winogender example includes one occupation and a *participant*, for which no gender statistics are provided. For consistency with the Winobias analysis, we make the simplifying assumption that the gender stereotypicality of the participant is the opposite of that of the occupation.

B Additional Total Effects

Table 3 provides the total effects across all variations of the Winograd-style datasets. The relationship between model and effect size is rela-

¹⁰An example of a removed template is: “The receptionist welcomed the lawyer because *this is part of her job.*” / “The receptionist welcomed the lawyer because *it is his first day to work.*”

Model	Winobias				Winogender			
	Dev		Test		BLS		Bergsma	
	Filt.	Unfilt.	Filt.	Unfilt.	Filt.	Unfilt.	Filt.	Unfilt.
GPT2-distil	61	160	51	130	15	44	18	44
GPT2-small	87	160	66	130	21	44	20	44
GPT2-medium	99	160	79	130	23	44	27	44
GPT2-large	94	160	69	130	24	44	26	44
GPT2-xl	101	160	72	130	25	44	26	44

Table 2: Number of examples from Winobias and Winogender datasets, including filtered (Filt.) and unfiltered (Unfilt.) versions. The size of the filtered versions vary between models because each model produces different total effects (used for the filtering). The number of examples excluded due to format (not included in the above numbers) were 38, 68, and 16 for Winobias Dev, Winobias Test, and Winogender, respectively.

Model	Winobias				Winogender			
	Dev		Test		BLS		Bergsma	
	Filt.	Unfilt.	Filt.	Unfilt.	Filt.	Unfilt.	Filt.	Unfilt.
GPT2-distil	0.118	0.012	0.127	0.023	0.081	0.005	0.075	0.011
GPT2-small	0.249	0.115	0.225	0.098	0.103	0.020	0.135	0.040
GPT2-medium	0.774	0.474	0.514	0.311	0.322	0.128	0.384	0.231
GPT2-large	0.751	0.427	0.492	0.238	0.364	0.173	0.350	0.192
GPT2-xl	1.049	0.660	0.754	0.400	0.342	0.168	0.362	0.202

Table 3: Total effects on Winobias and Winogender, including filtered (Filt.) and unfiltered (Unfilt.) versions.

tively consistent across dataset variations (Winobias/Winogender, filtered/unfiltered, Dev/Test, BLS/Bergsma gender statistics), though the magnitudes of the effects may vary between dataset variations.

Table 4 provides the total effects on the professions dataset when separated to stereotypically female and male professions, where stereotypicality is defined by the profession statistics provided by Bolukbasi et al. (2016). Notably, the effects are much larger in the female case. This may be explained by stereotypically-female professions being of higher stereotypicality than stereotypically-male professions, reflecting a societal bias viewing women’s professions as more narrowed.

C Additional Attention Results

C.1 Indirect Effects

Figure 11 complements Figure 4a by visualizing the indirect effects for additional GPT2 models. As with Figure 4a, the attention heads with the largest indirect effects lie in the middle layers of each model. Figure 12 shows the indirect effects for a model with randomized weights. Figures

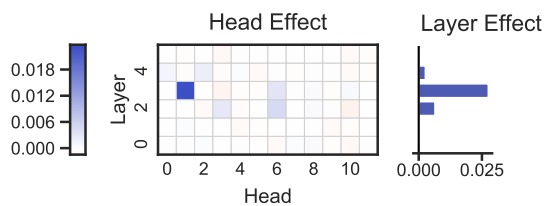
Model	Female	Male	All
GPT2-small rand.	0.10	0.19	0.12
GPT2-distil	155.31	23.47	130.86
GPT2-small	129.36	15.16	112.28
GPT2-medium	120.60	94.75	115.95
GPT2-large	107.44	48.99	96.86
GPT2-xl	255.22	89.31	225.22

Table 4: Total effects (TE) of gender bias in various GPT2 variants evaluated on the professions dataset, when separating by gender-stereotypicality.

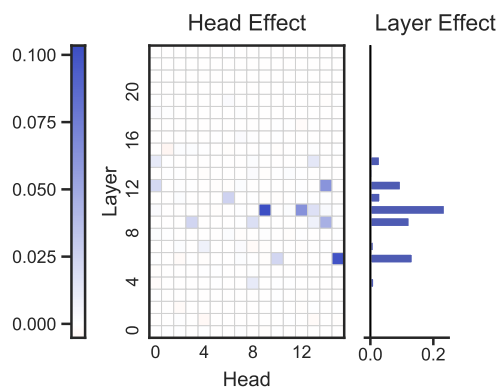
13 and 14 visualize the indirect effects for other dataset variations for the GPT2-small model from Figure 4a. The attention heads with largest indirect effect have significant overlap across the dataset variations.

C.2 Examples

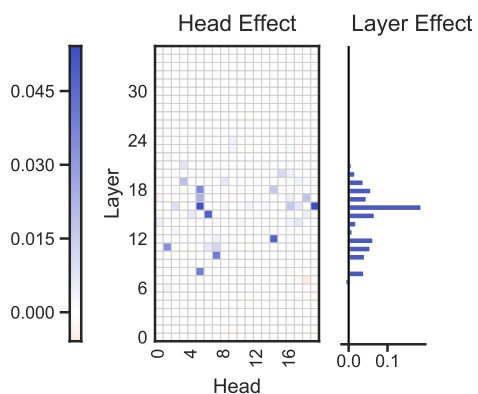
Figure 15 visualizes attention for the Winobias examples with the greatest total effect in GPT2-small, complementing the example shown in Figure 7. Figure 16 visualizes attention for additional models for the same example shown in Figure 7.



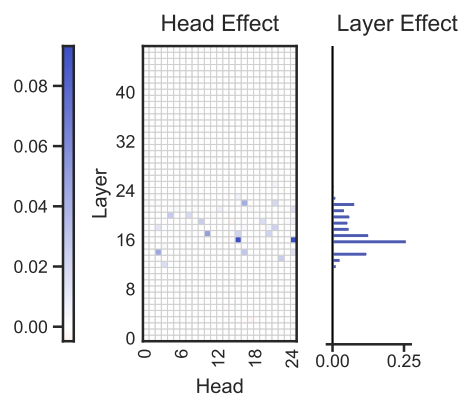
(a) GPT2-distil



(b) GPT2-medium



(c) GPT2-large



(d) GPT2-xl

Figure 11: Mean indirect effect on Winobias for heads (the heatmap) and layers (the bar chart) over additional GPT2 variants.

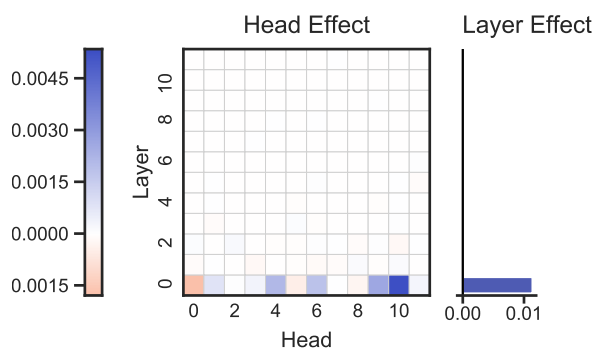
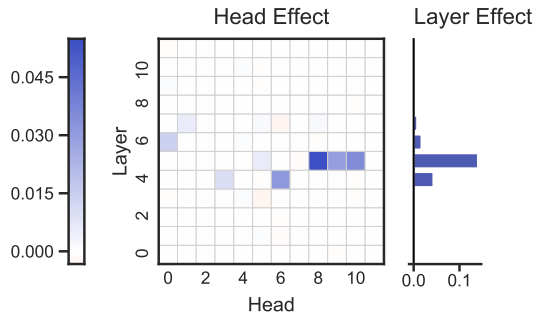
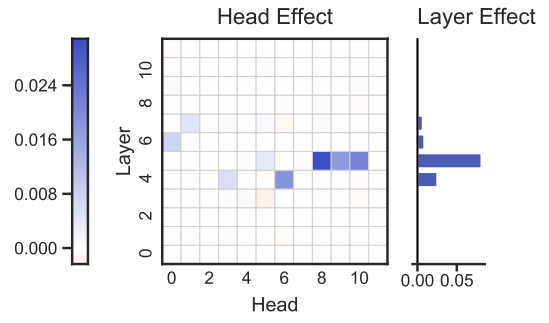


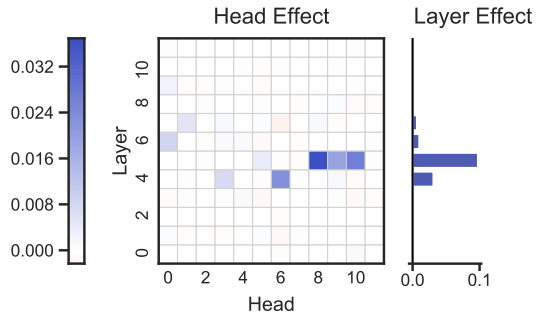
Figure 12: Indirect effect when using randomly initialized GPT2-small model on Winobias.



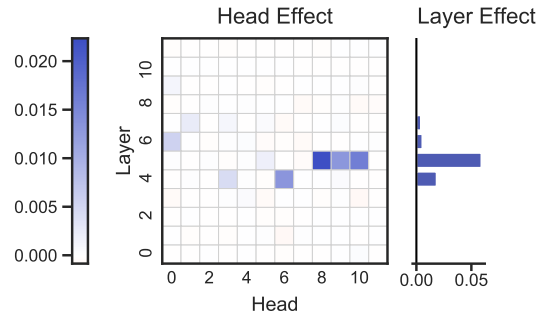
(a) Filtered, Dev



(b) Unfiltered, Dev

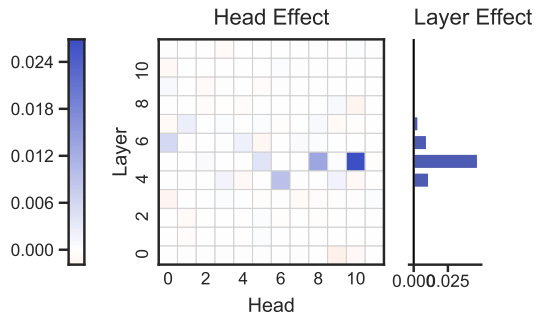


(c) Filtered, Test

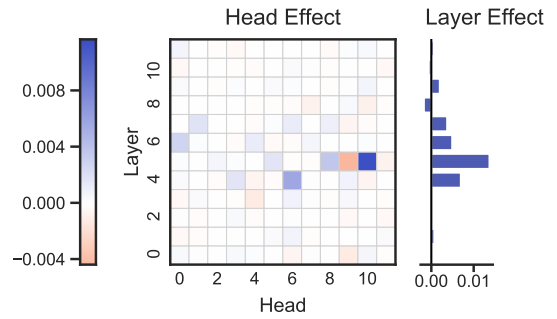


(d) Unfiltered, Test

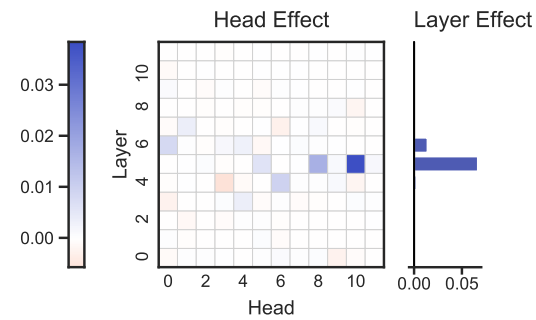
Figure 13: Indirect effect for Winobias (GPT2-small).



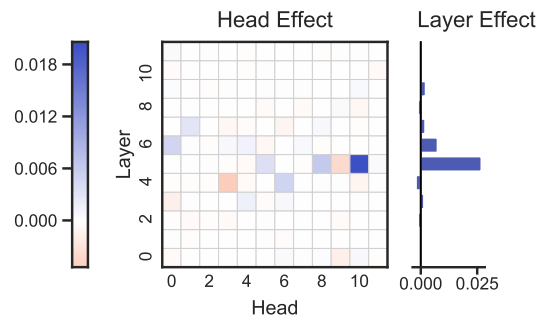
(a) Filtered, BLS



(b) Unfiltered, BLS



(c) Filtered, Bergsma



(d) Unfiltered, Bergsma

Figure 14: Indirect effect for Winogender (GPT2-small).

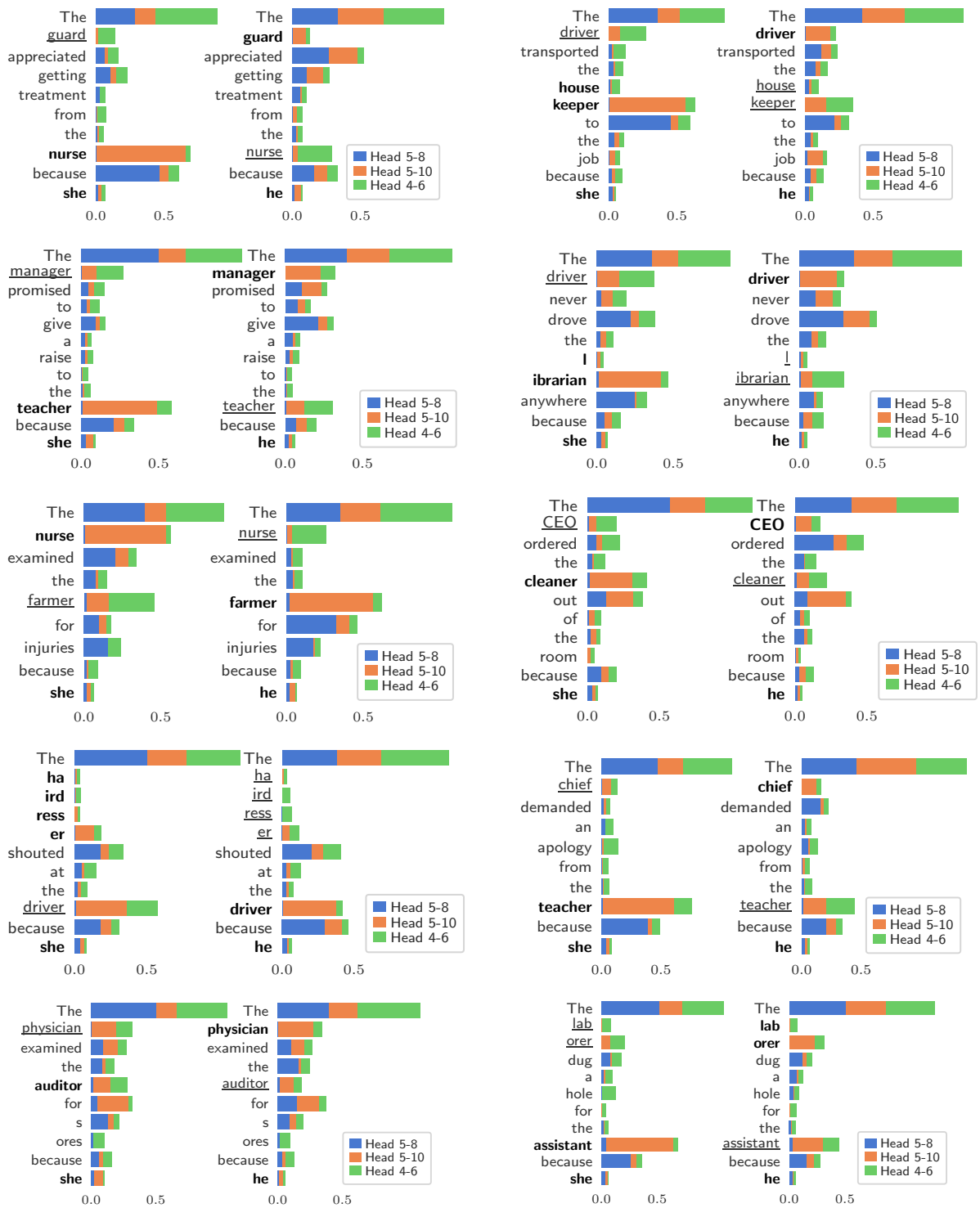
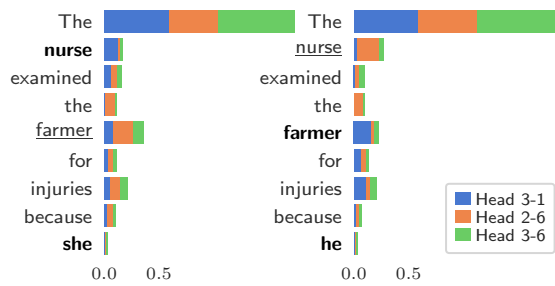
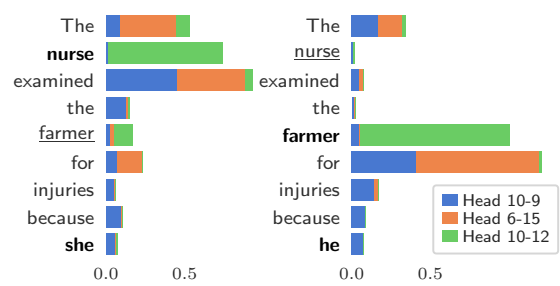


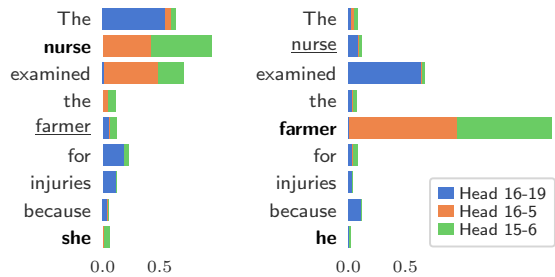
Figure 15: Attention of different heads across the 10 Winobias examples with greatest total effect for the GPT2-small model. The stereotypical candidate is in **bold** and the anti-stereotypical candidate is underlined. Attention roughly follows the pattern described in Figure 7.



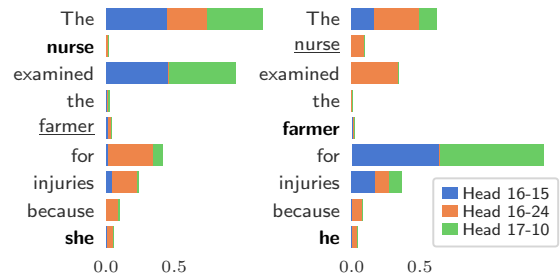
(a) Attention for GPT2-distil. Most attention is directed to the first token (null attention). Head 3-1 attends primarily to the **bold** stereotypical candidate, head 2-6 attends to the underlined anti-stereotypical candidate, and attention from head 3-6 is roughly evenly distributed.



(b) Attention for GPT2-medium. Head 10-12 attends directly to the **bold** stereotypical candidate, and heads 10-9 and 6-15 attend to the following words.



(c) Attention for GPT2-large. Heads 16-5 and 15-6 attend to the **bold** stereotypical candidate and optionally the following word. Head 16-19 attends to the words following the underlined anti-stereotypical candidate.



(d) Attention for GPT2-xl. Heads 16-5 and 17-10 attend primarily to the word following the **bold** stereotypical candidate. Head 16-24 attends primarily to the words following the underlined anti-stereotypical candidate.

Figure 16: Attention of top 3 heads on an example from Winobias, directed from either *she* or *he*, across different GPT2 models. The colors correspond to different heads. The results for GPT2-small are shown in Figure 7.

D Additional subset selection results

We wish to select a subset of attention heads or neurons that perform well together to better understand the sparsity of attention heads and neurons and their impact on gender bias in Transformer models.

The problem of subset selection (selecting k elements from n) is an NP-hard combinatorial optimization problem. To construct a meaningful solution set, we employ several algorithms for subset selection from submodular maximization. We note that while our objective functions are not strictly submodular as they do not satisfy the diminishing returns property, our objectives exhibit submodular-like properties and numerous algorithms have been proposed to efficiently maximize submodular and variants of submodular functions.

For monotone submodular functions, it is known that a greedy algorithm that iteratively selects the element with the maximal marginal contribution to its current solution obtains a $1 - 1/e$ approximation for maximization under a cardinality constraint (Nemhauser and Wolsey, 1978) and that this bound is optimal. For non-monotone submodular functions, there is the randomized greedy algorithm which emits a $1/e$ approximation to the optimal solution (Buchbinder et al., 2014).

To select subsets of attention heads, we compare TOP-K (selecting k elements with the largest individual values) and GREEDY. Even though randomized greedy has stronger theoretical guarantees because our objective is clearly non-monotonic, we favor the deterministic algorithm for increased interpretability. Figure 17 shows results for head selection across different models on Winogender and Winobias. Sparsity is consistent across all experiments where only a small proportion of heads are sufficient to achieve the full model effect of intervening at all heads. On Winogender, only 4/4/5/4% of heads are needed to saturate, while on Winobias, only 6/7/8/6% of heads are needed in GPT2-distil/small/medium/large.

To select subsets of neurons, we use TOP-K to compute NIE of sets of neurons because sequential greedy is too computationally intensive to run. Alternative methods using adaptive sampling techniques have been proposed to speed-up GREEDY for submodular functions under cardinality constraints (Ene and Nguyen, 2019; Fahrback et al., 2019b; Balkanski and Singer, 2018a,b). For non-monotone or non-submodular functions, there are

parallelized algorithms that use similar techniques to select sets (Balkanski et al., 2018; Qian and Singer, 2019; Fahrback et al., 2019a). These methods provide an alternative approach to TOP-K for selecting subsets of neurons and can be explored in future work.

E Proof that no-interaction in the difference NIE implies decomposition of the TE

Since by definition $y_{\text{set-gender}}(u) = y_{\text{set-gender}, z_{\text{set-gender}}(u)}(u)$ and $y_{\text{null}}(u) = y_{\text{null}, z_{\text{null}}(u)}(u)$, it can be seen that both sides of Eq. 2 describe a form of NIE (defined on the difference scale), each contrasts y under two different interventions on z while keeping the sentence u the same (left side, under `set-gender`; right side, under `null`). This equation parallels a previously-described assumption in the causal mediation analysis literature that ascertains that the NIE is the same regardless of the fixed value at which the intervention (the analogue of `set-gender/null`) is held, known as a no-interaction assumption (Imai et al., 2010b). We show that no-interaction in the indirect effect on the difference scale implies that the $\text{TE} = \text{NDE} + \text{NIE}$ under our scale. Eq. 2 can be rewritten as

$$\begin{aligned} & y_{\text{set-gender}}(u) - y_{\text{null}}(u) = \\ & y_{\text{set-gender}, z_{\text{null}}(u)}(u) - y_{\text{null}}(u) \\ & + y_{\text{null}, z_{\text{set-gender}}(u)}(u) - y_{\text{null}}(u) \end{aligned}$$

Now, dividing both sides of the equation by $y_{\text{null}}(u)$ and taking expectations over u yields

$$\begin{aligned} & \mathbb{E}_u [y_{\text{set-gender}}(u)/y_{\text{null}}(u) - 1] = \\ & \mathbb{E}_u [y_{\text{set-gender}, z_{\text{null}}(u)}(u)/y_{\text{null}}(u) - 1] + \\ & \mathbb{E}_u [y_{\text{null}, z_{\text{set-gender}}(u)}(u)/y_{\text{null}}(u) - 1] \end{aligned}$$

which is exactly

$$\begin{aligned} & \text{TE}(\text{set-gender}, \text{null}; y) = \\ & \text{NDE}(\text{set-gender}, \text{null}; y) + \\ & \text{NIE}(\text{set-gender}, \text{null}; y). \end{aligned}$$

It should be noted that even if Eq. 2 does not hold, but the equation approximately holds upon dividing both sides by y_{null} , we would expect the decomposition $\text{TE} \approx \text{NDE} + \text{NIE}$ to hold. Indeed, further inspection of the trained model revealed that the left side and right side of Eq. 2 were very close in the case of the attention intervention. Figure 18 shows a plot of the values attained by the two sides of the equation (normalized by y_{null} to make con-

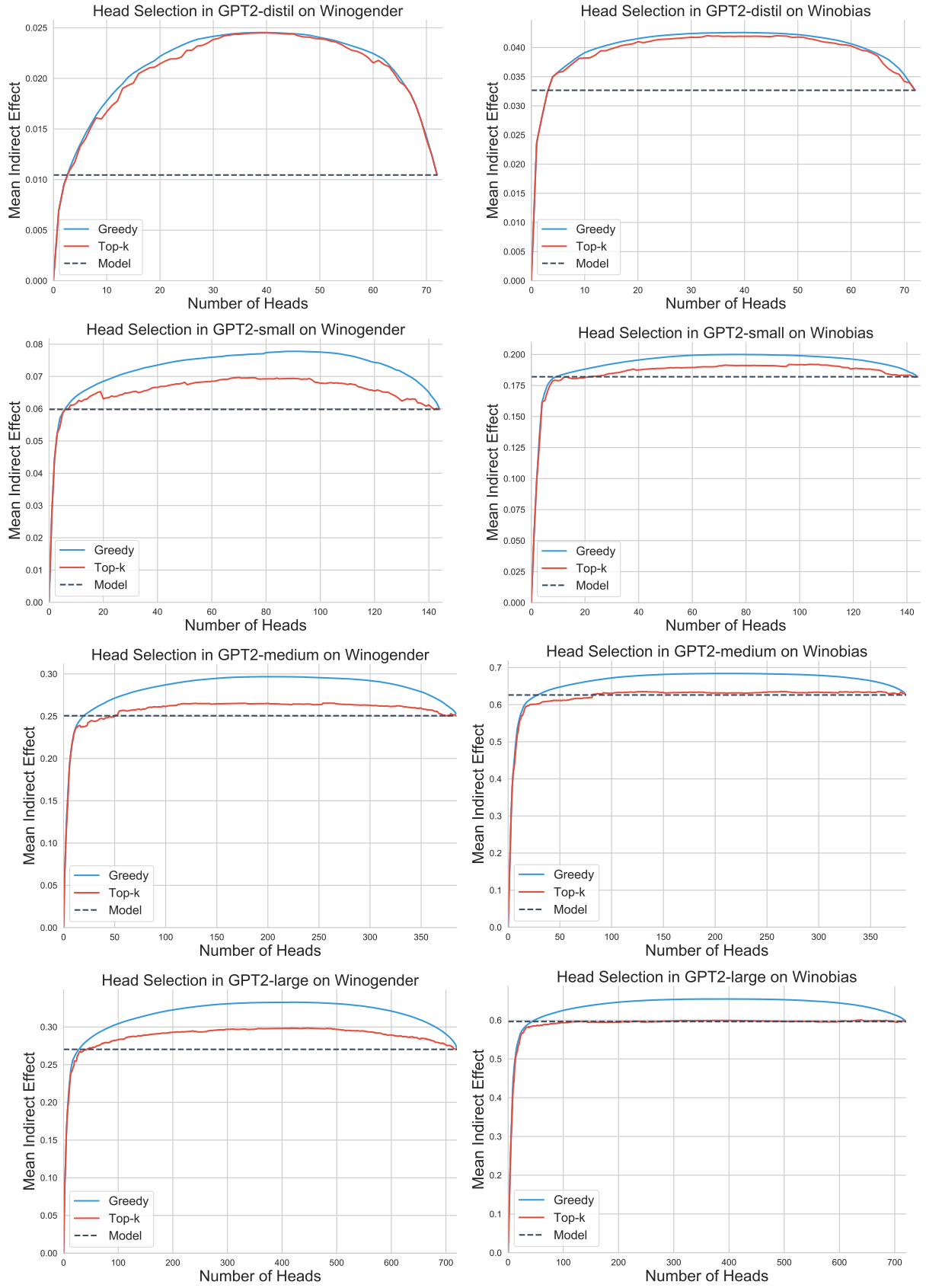


Figure 17: The effect after sequentially selecting an increasing number of heads through the TOP-K or GREEDY approach on different model types and data. A small proportion of heads are required to saturate the effect of the model.

sistent with the earlier analyses) for all attention heads across all examples in the Winobias dataset. Fitting the data to a linear model yields a coefficient of 1.04 and an intercept of 0.00 ($R^2 = 0.78$).

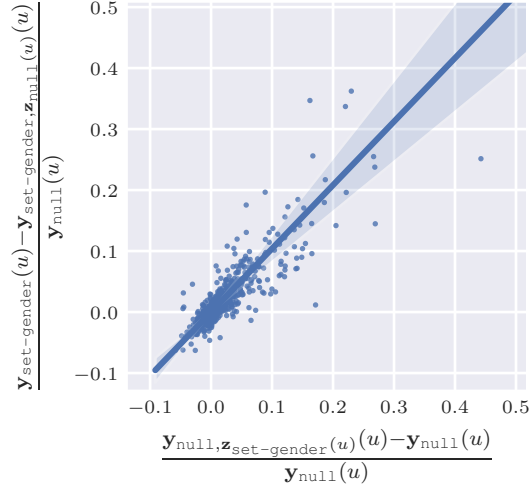


Figure 18: Plot of right side of Eq. 2 (x axis) against left side (y axis), normalized by y_{null} . For visualization purposes, we exclude a single outlier at (0.60, 1.07).