SCIURus: Shared Circuits for Interpretable Uncertainty Representations in Language Models

Carter Teplica
New York University
carterteplica@nyu.edu

Yixin Liu
Yale University
yixin.liu@yale.edu

Arman Cohan
Yale University
arman.cohan@yale.edu

Tim G. J. Rudner
New York University
tim.rudner@nyu.edu

Abstract

We investigate the mechanistic sources of uncertainty in large language models (LLMs), an area with important implications for language model reliability and trustworthiness. To do so, we conduct a series of experiments designed to identify whether the factuality of generated responses and a model's uncertainty originate in separate or shared circuits in the model architecture. We approach this question by adapting the well-established mechanistic interpretability techniques of causal tracing and two styles of zero-ablation to study the effect of different circuits on LLM generations. Our experiments on eight different models and five datasets, representing tasks predominantly requiring factual recall, provide strong evidence that a model's uncertainty is produced in the same parts of the network that are responsible for the factuality of generated responses.

1 Introduction

Uncertainty quantification (UQ) in large language models (LLMs) for knowledge-intensive tasks [25] remains a critical yet understudied area. Despite achieving human-level performance on various benchmarks, LLMs often struggle with reliable uncertainty estimation, leading to issues such as overconfidence and hallucination [31]. This limitation has strong implications for their trustworthiness and safety in high-stakes applications. While recent research has explored verbalized uncertainty in LLMs [3, 15, 16], significant gaps remain in our understanding of and ability to improve uncertainty quantification. In particular, existing UQ techniques typically provide little insight into the factors responsible for an uncertainty estimate, limiting their usefulness both as practical tools for improving trustworthiness and as methods for understanding uncertainty reasoning. We propose leveraging mechanistic interpretability, an approach focused on characterizing models' internal reasoning mechanisms, to advance our comprehension and enhancement of uncertainty quantification in large language models.

To better understand how language models generate uncertainty estimates, we learn a $\mathbb{P}(\text{IK})$ (***p****robability that* ***I k****now*) probe that represents the model's uncertainty based on multiple stochastically generated answers [15]. We then used these probes' predicted confidences as target metrics for causal tracing and zero-ablation, two mechanistic interpretability techniques which identify the components of a model relevant for a task by testing the effect of an intervention made on activations in the model during evaluation. We compared the mechanistic signatures of changes in the model's accuracy and the probe's output to evaluate whether the same circuits were responsible for the answer and the predicted confidence.

In our empirical evaluation, in which we performed leave-one-out and COAR-style [26] zero-ablation for a large range of model–dataset combinations and causal tracing for several more combinations, we

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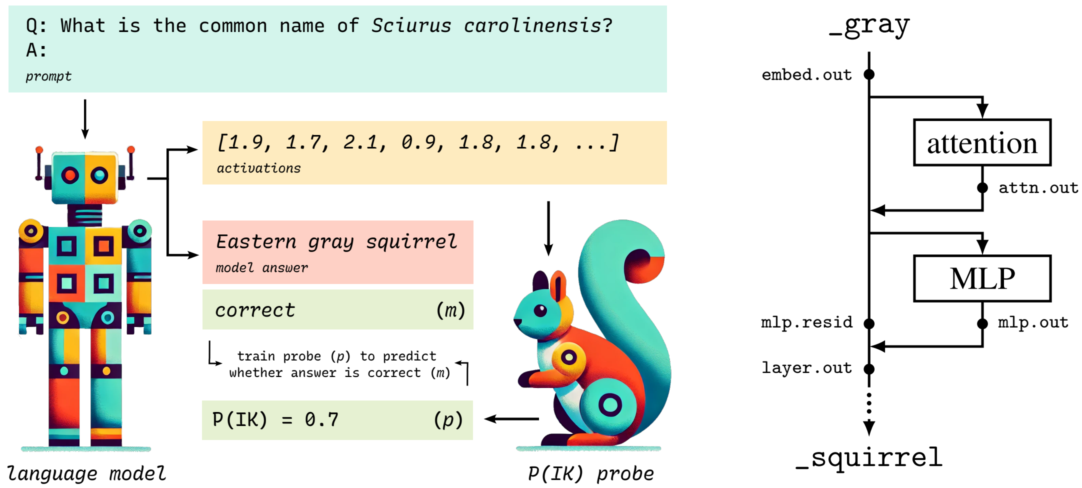


Figure 1: **Left:** $\mathbb{P}$(IK) probing. The LLM takes a question as input and returns an answer and last-layer activations. Answers are checked for correctness. The probe learns to predict whether the model's answer is correct, based on the last-layer activations. Our analysis uses the probe as a proxy for an LLM's $\mathbb{P}$(IK). We conduct path patching and zero ablation studies on the probe and the corresponding LLM. **Right:** Locations used in interventions. Path-patching restorations are at `mlp.resid`, `mlp.out`, `layer.out`, and `embed.out`. Zero-ablations are at `attn.out` and `mlp.out`.

found that model accuracy and probe behavior largely responded to the same interventions, indicating that circuits responsible for the factuality of responses and for the model's uncertainty are located in the same parts of the model.

For a group of knowledge-intensive question answering tasks [25], model accuracy and probe confidence are (highly) positively related to one another. We conclude that, at least on recall tasks, a language model's representation of confidence may derive mainly from "uncertainty introspection" on its question-answering process, rather than from separate reasoning specific to its uncertainty.

To summarize, the key contributions of this paper are as follows:

1. We use mechanistic interpretability and uncertainty quantification tools to investigate the mechanistic sources of uncertainty in large language models. To do so, we use a logistic $\mathbb{P}$(IK) probe with causal tracing and zero-ablation to perform a hypothesis test to examine whether LLM uncertainty and the factuality of answers generated by an LLM reside in shared or separate circuits within the model.
2. We perform an extensive empirical analysis on eight different models and five recall-intensive datasets, and find evidence that for knowledge recall, uncertainty and the factuality of answers generated by an LLM are handled by the same parts of the model.

2 Related Work

2.1 Uncertainty Quantification in Large Language Models

Uncertainty quantification in large language models is crucial for enhancing reliability, particularly in high-stakes applications. While LLMs provide token probabilities that are often well-calibrated for next-token prediction, practical applications of UQ often require quantifications of the uncertainty in the semantic content of the output [11]. Language models' ability to quantify semantic uncertainty remains limited, especially for open-ended tasks. Various techniques have been proposed to address this.

A well-studied set of techniques involves *multiple sampling and clustering* based on consistency. This can be effective when clustering of responses is straightforward, but this is often not the case except on simple tasks [16, 10, 17, 2]. Another approach, sometimes called *verbalized uncertainty*, is to ask the model to state a verbal or quantitative confidence estimate [15]; the performance of such methods is often inconsistent. On multiple-choice questions, the *token probabilities* may yield well-calibrated uncertainty estimates [15]. Another option is to train a $\mathbb{P}(IK)$ *probe*, a binary classifier predicting whether the model knows the answer. This approach is among the most effective in-distribution [22] but struggles with generalization to out-of-distribution data [15, 22].

In this work, we focus on $\mathbb{P}(\mathrm{IK})$ probing, as it provides a potentially interpretable view into a model's self-assessed uncertainty by identifying a specific feature direction within the model. Beyond the introduction of $\mathbb{P}(\mathrm{IK})$ probing itself [15], little research has been conducted on interpreting the mechanisms behind uncertainty reasoning in LLMs. While most UQ techniques rely on eliciting information about uncertainty through explicit or indirect methods, we still lack an understanding of how this information is represented internally. Analyzing these mechanisms could improve UQ techniques and provide insights into broader epistemic weaknesses in LLMs.

2.2 Mechanistic Interpretability

Mechanistic interpretability (MI) aims to understand how neural networks function internally, with a focus on understanding the internal mechanisms and computational processes involved in performing a task. MI work often revolves around identifying "circuits" responsible for specific tasks [21]. To achieve this, several intervention techniques have been developed, with tradeoffs in resolution, breadth of applicability, and computational cost.

Ablation, also called *knockout,* involves removing parts of the model, such as layers or neurons, to observe changes in behavior. Such approaches may ablate components of various sizes (individual neurons, attention heads, or entire layers) and in various ways (replacing the output of a component with the zero vector, a dataset mean, or the value from another run). We use zero-ablation for one of our analyses because it is highly general, well-supported in the literature [29, 9] and computationally inexpensive, albeit less precise than other methods.

In earlier ablation work, a common approach has been to use "leave-one-out" ablation, i.e., to ablate a single layer on each trial. However, other approaches may perform better in cases where models are very robust to ablations (as is commonly the case for LLMs, especially with larger models). COAR (**co**mponent **a**ttribution via **r**egression) [26] is a recently proposed technique which ablates random subsets of components in a model and produces attributions using linear regression. We perform both leave-one-out and COAR ablations and compare the results of the two.

Causal tracing, also called *activation patching*, treats the model's hidden states as a causal graph [24], which can be analyzed with an approach based on causal mediation analysis [27]. (We discuss this further in Section 3.) Causal tracing is more precise than ablation, at the cost of higher computational costs and a need for more careful setup. *Causal scrubbing* [6] is a framework for testing mechanistic claims which builds on causal tracing; it is useful for formalizing interpretability hypotheses but impractically slow for direct use in many cases.

Probing techniques [1] involve training a simple probe (commonly a one-layer binary classifier) on model activations, in order to find places in the model's representation space that represent specific functions of the input. The $\mathbb{P}(\mathrm{IK})$ probes used in this paper are an example of this.

2.3 Applications for Interpretable Uncertainty Quantification

Reliable UQ could help to improve trustworthiness by allowing auditing in high-stakes applications of LLMs, such as their use for medical and legal advice [11] and for constructing LLM-based agents [30]. Interpretability could also help to ensure that UQ techniques remain reliable under distribution shifts, and could contribute to detecting deception [12]. Finally, if limitations in UQ are related to broader epistemic weaknesses in LLMs, interpretable UQ could shed light on problems such as hallucination [32, 18] and could deepen our understanding of LLM epistemics in general, possibly helping to address problems such as eliciting latent knowledge [7].

3 Background

Causal Tracing. Causal tracing is a causal intervention method that aims to trace and identify important components in neural models for a given task [19, 29], which is a generalization of causal

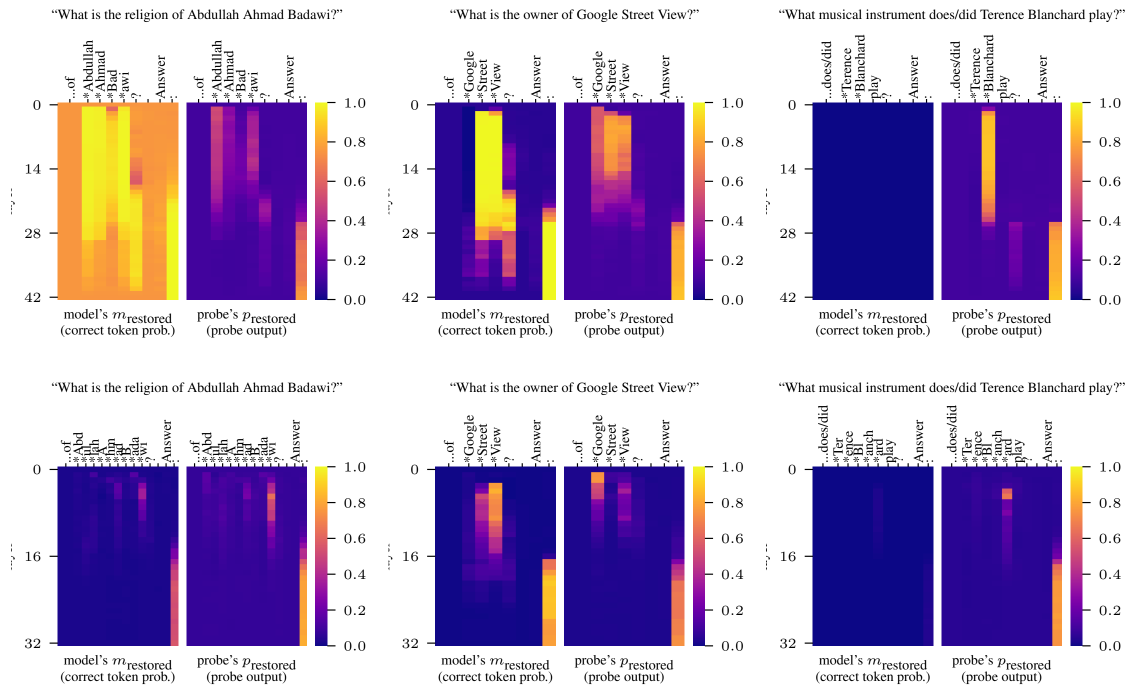


Figure 2: Representative results of causal tracing, shown for Gemma 2 9B Instruct (top) and Llama 2 7B (bottom) on three questions in CounterFact. Only `layer.out` locations are shown (plus `embed.out` in the first row). The input embeddings for the starred tokens are replaced with zeros in the corrupted and restored runs.

mediation analysis [27]. In this work, we use causal tracing [19] to examine the importance and role of individual circuits and components in LLMs. Specifically, given a specific input q, causal tracing involves three runs: (1) a clean run, in which the original input q is given to the model, which is used to obtain the hidden states of each layer; (2) a corrupted run, in which the input embeddings of certain tokens are corrupted by adding noise or (in this paper) replaced with zeros; and (3) a corrupted-with-restoration run, in which the computation is similar to the corrupted run except that the hidden states at specific locations ℓ in the model are restored using the hidden states obtained from the clean run. By comparing the differences between the output (predicted probabilities) of the clean, corrupted, and restored runs, causal tracing allows the identification of important components in LLMs. That is, if the restored run achieves a similar effect as the clean run, it is likely that the corresponding restored component plays an important role in the model's processing.

Zero-Ablation. Zero-ablation is a mechanistic intervention technique that takes advantage of a transformer's residual structure by treating attention or MLP layers as separable modules which read from and write to the residual stream [9, 20]. A component ℓ (in this paper, an attention or MLP layer) is "ablated" by replacing its output with zero. The drop in model performance on a given task after an intervention removing a component ℓ provides a measure of the importance of ℓ for the task.

Leave-one-out and COAR interventions. Interpretability work using ablation commonly employs leave-one-out style interventions, in which an intervention is applied to a single component at a time. Since larger Transformer LMs are often insensitive to smaller interventions, leave-one-out interventions may struggle to meaningfully affect the target metrics. COAR [26] is a recent approach which addresses this by applying ablation interventions to random subsets of model components. In a COAR experiment, ablations are performed for many dataset examples and subsets of components, and linear regression is used to predict the target metrics from a vector of ablated components; the coefficients of the linear predictor then reflect the predicted effect of ablating each component on the target metric. (We refer the reader to [26] for details.)

4 Uncertainty Introspection and the Shared Circuits Hypothesis

The aim of this paper is to make progress toward characterizing the mechanistic structures used for UQ in language models. To this end, we propose a theoretical hypothesis ("shared circuits") about the locations of these structures, along with operationalizations which we test experimentally.

Shared Circuits Hypothesis. Uncertainty quantification in question-answering (QA) systems may be carried out in a variety of ways. We hypothesize that language models are capable of expressing uncertainty using **shared circuits** that both solve the underlying question-answering task and output uncertainty information. This contrasts with the possibility that uncertainty quantification emerges in **separate circuits**, either to post-process messy uncertainty signals from question-answering circuits or to do uncertainty calculations of their own.

Language models are known to be capable of introspective behavior in some contexts [5]. The shared circuits hypothesis, to the extent that it is true, suggests that uncertainty quantification is one such context. We refer to this phenomenon as "uncertainty introspection".

4.1 Probe Design

We use a $\mathbb{P}(\mathrm{IK})$ probing approach in part because of the difficulty of reasoning about uncertainty using token probabilities. Token probabilities for open-ended questions are a highly imperfect proxy for a model's confidence, because they conflate semantic uncertainty, or uncertainty about content, with syntactic uncertainty, or uncertainty about form [16]. Furthermore, we are most interested in improving uncertainty quantification for fine-tuned chat models, for which token probabilities do not correspond to an underlying distribution over possible text strings.

We construct a dataset on which to train the $\mathbb{P}(\mathrm{IK})$ probe according to the following steps.

1. Perform 32 forward passes for each question on the question-answering task. We used few-shot prompting with 5 examples to ensure that the model answered in the right format.
2. Check whether a model's answers are correct. Specifically, we check whether a model's answer contains any correct answer as a substring, ignoring case.
3. For each question in the dataset, save the number of correct and incorrect answers (implying a "true probability" of the model answering correctly).
4. Also, for each question, save the output of the model's last layer (before the unembedding). This is a vector in $\mathbb{R}^{d_{\text{model}}}$.

The $\mathbb{P}(\mathrm{IK})$ probe is a logistic classifier $p : \mathbb{R}^{d_{\text{model}}} \to (0, 1)$ which takes these last layer activations as input and returns the proportion of correct answers. For example, if the model answers a question correctly 47% of the time, the probe should output 0.47 when given the last-layer activations at the last token of that question. We trained with binary cross-entropy loss, using dropout and a triangular learning rate schedule, and used a low learning rate ($\eta = 3 \times 10^{-6}$) as in [15].

Our probes generally showed good calibration (with most expected calibration errors $< 5\%$) and moderate sharpness (with most balanced accuracies between 60% and 75%). Probes for the ARC tasks were especially likely to train poorly, but probe accuracy and calibration otherwise did not show constistent trends across models and datasets. The accuracy of the unablated models varied from 29% to 91%, with the worst performance on WebQuestions and MMLU and the best performance on ARC. (See Appendix 2 for a table of model and probe performance).

4.2 Experiment Design: Causal Tracing

On a given question q_i in a dataset $\mathcal{Q}$, for each causal tracing run (clean, corrupted, and restored) we compute the model's sample probability $m(q_i)$ for the correct first token of the answer, and the probe's confidence $p(q_i)$. (Correct-first-token probability is a proxy for correct-answer probability

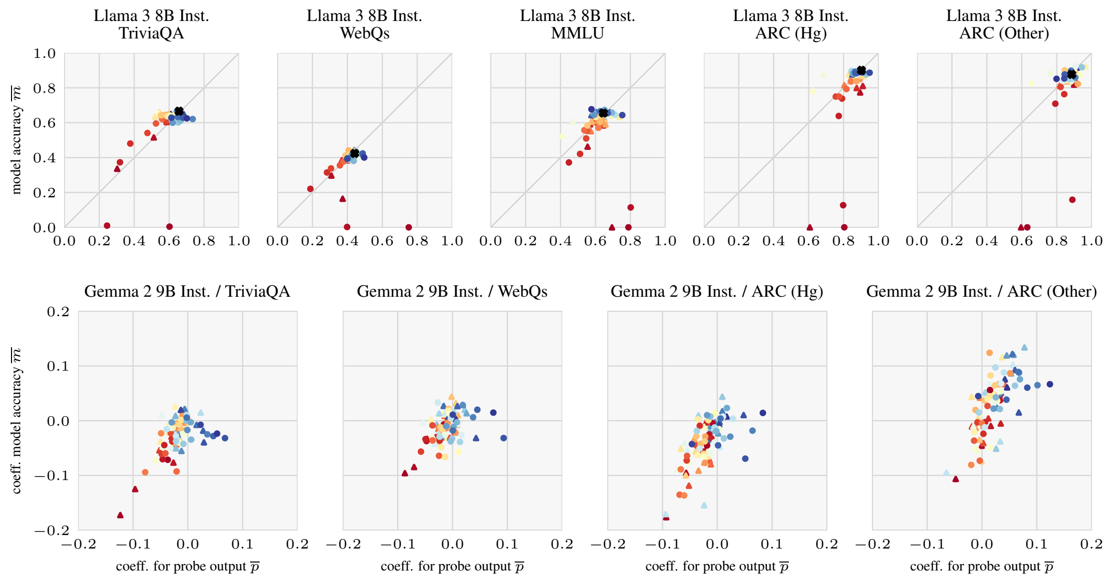


Figure 3: **Top.** Results of leave-one-out style zero ablation for Llama 3 8B Instruct on five different datasets. Circle, triangle, and small X markers represent MLP ablations, attention ablations, and clean runs respectively. Warmer colors represent earlier layers. **Bottom.** Coefficients for zero ablation with COAR, for Gemma 2 9B Instruct on four different datasets. Circle and triangle markers represent MLP and attention respectively. Warmer colors represent earlier layers.

which holds up well for this task.) We consider each question individually because this allows a particularly fine-grained test for shared circuits—we ask here whether the same circuits are used for QA and UQ on an in individual question, and in the next section whether this is true in aggregate for a task. Locations ℓ where $m_{\text{restored}(\ell)} \approx m_{\text{clean}}$ correspond to parts of the model which are important for solving the QA task; likewise, locations ℓ where $p_{\text{restored}(\ell)} \approx p_{\text{clean}}$ correspond to parts of the model which are important for the UQ task.[1][2]

In the context of causal tracing, we operationalize the shared circuits hypothesis in the claim that m_{restored} can be predicted from p_{restored} by interpolating between the clean and corrupted values: for example, if the model's correct-token probability on a restored run is halfway between the values from the clean and corrupted runs, then the probe's confidence should also be halfway between the clean and corrupted runs.

Specifically, for each question $q_i \in \mathcal{Q}$, we consider the linear predictor $\hat{m}_{\text{restored}}$ defined by

$$\frac{\hat{m}_{\text{restored}(\ell)} - m_{\text{corrupted}}}{m_{\text{clean}} - m_{\text{corrupted}}} = \frac{p_{\text{restored}(\ell)} - p_{\text{corrupted}}}{p_{\text{clean}} - p_{\text{corrupted}}}.$$

(That is: we predict that a restoration at a location ℓ will have the same proportional effect on the model's performance and the probe's response, relative to the clean condition where there is no intervention and the corrupted condition where no data on the subject is available.)

We claim that this predictor explains most of the variance in m_{restored} (i.e., has a high coefficient of determination R^2). As a (somewhat weak) formalization of this, we attempt to reject the null hypothesis

$$H_0 : R^2 \textit{ is no greater than expected under random permutations of the set of locations } \ell.$$

[1] Although note that the converse is not strictly true; see Appendix B for details.

[2] Here, $\mathbb{P}(\text{corr})_{\text{restored}(\ell)}$ and $\mathbb{P}(\text{IK})_{\text{restored}(\ell)}$ represent the correct token probability and p probe output for a run with the hidden state restored at location ℓ in the model; notation is likewise for clean and corrupted runs.

4.3 Experiment Design: Zero-Ablation

We also test the shared circuits hypothesis via zero-ablation on layers. For these experiments, we sample and evaluate multi-token answers. (Sampling multi-token answers matches the training conditions of the probes and avoids false positives; this is especially relevant on the TriviaQA and WebQuestions tasks, where questions often have correct answers beginning with "the" or similarly common tokens. This is less relevant on CounterFact, where answers are typically short proper nouns. A further reason to sample multi-token answers is that ablated models commonly lose their ability to follow the few-shot format, and answer the question correctly but with e.g. incorrect capitalization or a complete sentence; multi-token sampling allows us to detect these correct answers.) Determining per-question accuracies to a sufficiently high precision would require hundreds of samples per question, well in excess of our compute budget: as such, we consider the model's performance in the aggregate, over a task-specific dataset.

We define $m(q_i)$ as the probability of a correct answer sampled by the model when prompted on the question $q_i \in \mathcal{Q}$, and $p(q_i)$ as the probe output on that question. Taking the means over $\mathcal{Q}$, we can compare changes in the accuracy of the model $\overline{m}$ and the average output of the probe $\overline{p}$.

4.3.1 Leave-One-Out Ablation

Under the shared circuits hypothesis, the change in the probe output from ablation $|\overline{p}_{\text{ablated}(\ell)} - p_{\text{clean}}|$ is large when the change in model accuracy $|\overline{m}_{\text{ablated}(\ell)} - m_{\text{clean}}|$ is large. Concretely, we claim that the predictor $\hat{\overline{m}}$ defined by

$$m_{\text{clean}} - \hat{\overline{m}}_{\text{ablated}(\ell)} = |\overline{p}_{\text{ablated}(\ell)} - p_{\text{clean}}|$$

explains most of the variance in $\overline{m}_{\text{ablated}}$ (has a high R^2), and attempt to reject the null hypothesis

H_0 : R^2 *is no greater than expected under random permutations of the set of layers* ℓ.

We consider *absolute* changes in the probe output only because interventions which severely damage the model may increase the value of the probe output (see Fig. 4.2, top), but generally do not improve the model's correctness.

4.3.2 COAR

COAR constructs least-squares predictors for model accuracy and probe output based on vectors of ablated components, in which the coefficient corresponding to a component ℓ represents the expected effect of ablating ℓ. Under the shared circuits hypothesis, the predictors $\mathbf{w}_m$ and $\mathbf{w}_p$ for the model accuracy and probe output should be similar. Concretely, we attempt to reject the null hypothesis H_0 : *The correlation between* $\mathbf{w}_m$ *and* $\mathbf{w}_p$ *is no greater than expected under random permutations of the set of layers* ℓ.

We see COAR as a useful complement to leave-one-out ablation because it addresses cases where models are highly resilient to ablations, a common challenge for ablation on larger models. We found this to be especially relevant for the Gemma models.

4.4 Permutation testing

We tested our hypotheses using permutation tests with Monte Carlo sampling. Specifically, for each test, we compared the goodness-of-fit of the observed data with that of a synthetic dataset made by shuffling the locations and (for causal tracing) token positions. To exclude the simple explanation that some types of locations performed better than others, we shuffled locations of different types (e.g., attention and MLP outputs) independently.

5 Testing the Shared Circuits Hypothesis

In this section we describe our model and dataset choices and discuss the quantitative and qualitative results of our experiments.

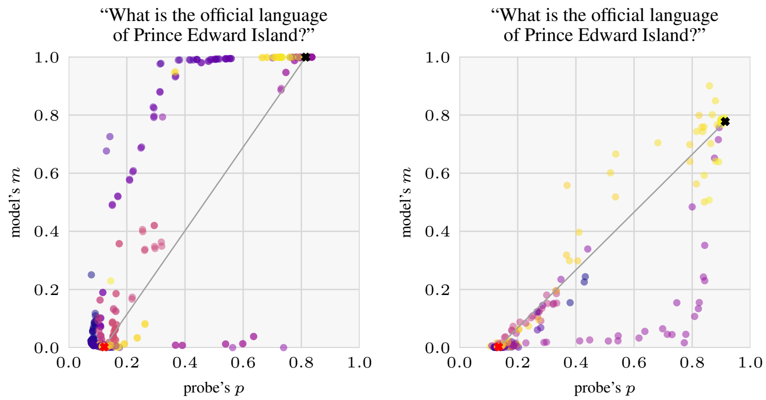


Figure 4: Predicting the correct-token probability m given the probe output p, for Gemma 2 9B Instruct (left) and Llama 2 7B (right). The black and red X (small, top-right and bottom-left) show the clean and corrupted runs; all others show restored runs. Yellow points are later in the sequence. The grey line shows the predictor $\hat{m}$.

5.1 Models and Datasets

We studied the following eight models and five datasets:

Table 1: Models and datasets studied.

Model	Parameters	Layers
Llama 2 7B	7B	32
Llama 2 7B Chat	7B	32
Llama 2 13B	13B	40
Llama 2 13B Chat	13B	40
Llama 3 8B	8B	32
Llama 3 8B Instruct	8B	32
Gemma 2 2B Instruct	2B	26
Gemma 2 9B Instruct	9B	42

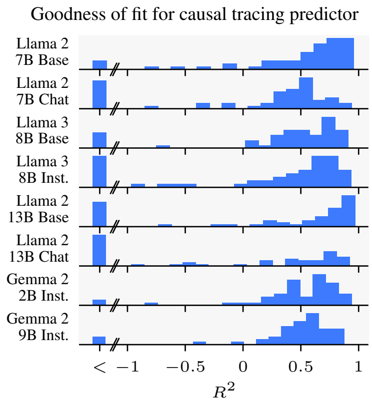
Dataset	
TriviaQA	[14]
WebQuestions	[4]
MMLU	[13]
ARC	[8]
CounterFact	[19]

All the datasets studied, with the partial exception of MMLU, are "recall-intensive" in that they largely depend on recalling factual information learned during training. The datasets were chosen to represent a range of recall-intensive tasks, across open-ended (TriviaQA, WebQuestions, CounterFact) and multiple-choice (MMLU, ARC) formats and at varying levels of difficulty. These datasets also represent a range of linguistic styles. (In particular, WebQuestions consists of questions derived from web searches, which may be imprecisely posed and may exhibit informal orthography and grammar; "messy" questions of this kind reflect an important use case of LLM question-answering.)

ARC includes both the ARC-Easy and ARC-Challenge splits. ARC questions are drawn from standardized tests; the datasets listed as ARC (Hg) and ARC (Other) correspond, respectively, to the "Mercury" test and to a combination of the other 20 tests.

We used the CounterFact dataset exclusively for causal tracing. We reformulated CounterFact prompts as questions to match the format of our other datasets. Because we used the TriviaQA probe for the causal tracing experiment with CounterFact, we also did few-shot prompting with the prompt from TriviaQA.

We did some preliminary ablation experiments on other task types, including simple synthetic math tasks and the LAMBADA [23] comprehension task. Results for LAMBADA were generally similar to those for the recall tasks, although in some cases we had difficulty training probes to high accuracy. Results for the synthetic math tasks showed some evidence of separate circuits.



Model	$p < 0.05$	$p \geq 0.05$
Llama 2 7B	55	0
Llama 2 7B Chat	51	0
Llama 3 8B	53	1
Llama 3 8B Instruct	51	2
Llama 2 13B	51	3
Llama 2 13B Chat	45	4
Gemma 2 2B Instruct	47	1
Gemma 2 9B Instruct	50	0

Figure 5: **Left.** Values of R^2 for the causal tracing predictor. "$<$" signifies cases where $R^2 < -1$ (which is possible because the predictor is not a linear-regression line). **Right.** Number of occurrences of p-values for causal tracing.

5.2 Causal Tracing

We performed causal tracing with all eight models on a random sample of 100 questions from the CounterFact dataset [19]. In the final analysis, we considered only questions which the model was somewhat able to answer ($m_{\text{clean}} > 0.05$), because the restored performance was almost universally near zero otherwise, with very little signal (that is, if the model was unable to answer a question, a causal tracing intervention generally did not change that). We used the probe and few-shot prompt for TriviaQA. Across this sample, the predictors $\hat{m}_{\text{restored}}$ generally estimated m_{restored} well, with $R^2 > 0.6$ in most cases cases. For each question q_i, we tested the null hypothesis (1) by sampling 1,000 permutations: specifically, we shuffled the values of $m_{\text{restored}(\ell)}$ independently for the `mlp.out`, `mlp.resid`, and `layer.out`/`embed.out` locations, to exclude the explanation that the predictor works well because the `mlp.out` and `mlp.resid` states each carry less information than `layer.out`. In almost all cases (see Figure 5.2), we reject H_0 with $p < 0.05$.

Based on manual inspection (see graphs in the Supplementary Materials), we conclude that $R^2 < 1$ both due to small discrepancies between UQ and QA circuitry and due to nonlinearity in the UQ/QA relationship. In the cases studied, the model is more resilient than the probe: that is, interventions generally have a greater effect on the probe than the model (creating the convex shape in Figure 3, left); this depends to some extent on the model architecture. In some cases, when the probe is confidently wrong (see Figure 2, right), the probe may be following the path for the model's (incorrect) highest-probability token.

As in [19], highly important locations generally fall into two clusters: one in earlier layers at the token positions in the subject, and one at later layers at the last token position. We note that uncertainty information and answer information are often transferred to the last position by attention heads in different layers (Fig. 2). Other discrepancies occasionally occur: in particular, when an answer token (often a proper noun) is present in the question, restorations at the corresponding token position show suppressed model accuracy but normal probe performance. In fact, model accuracy for these interventions can be worse than in the corrupted case. One possible explanation of this behavior is that the model may be using circuitry similar to the "negative name movers" in [28] to avoid spuriously copying input tokens to the output.

These small differences suggest that our $\mathbb{P}(\text{IK})$ probes are using the model's question-answering circuitry directly, rather than in a post-hoc or epiphenomenal way (for example, by simply looking at the probability of the most likely next token).

5.3 Zero-Ablation

Leave-One-Out Ablation. We performed 500 ablation trials each with eight models across five question-answering datasets. Across this sample, the predictors $\hat{\overline{m}}_{\text{ablated}}$ generally estimated $\overline{m}_{\text{ablated}}$ better than chance, with a median of $R^2 = 0.33$. For each model–dataset combination, we tested the null hypothesis (2) by sampling 10,000 permutations. As with the causal tracing analysis, we shuffled attention and MLP layer interventions independently, to exclude the explanation that one type of layer was more important than the other in a way not specific to the QA and UQ tasks. We reject the null hypothesis with $p < 0.05$ in 36 out of 38 cases, and $p < 0.0001$ in 31 out of 38 cases.

In many cases, the model's uncertainty representation plays particularly nicely with zero-ablation, remaining calibrated on average even after an intervention: using the same statistical framework as above, the very simple predictor $\hat{\overline{m}}_{\text{ablated}} = \overline{p}_{\text{ablated}}$ does better than expected under random permutations in 27 out of 38 cases (at $p < 0.05$).[3]

While other explanations may be possible, one interpretation of these results is that a given component makes a nonzero contribution to the model's uncertainty representation if and only if it can also contribute information about the answer.

COAR. We performed 2000 COAR trials each with all models and four datasets.[4] For each trial, the probability of ablating any given component was set at $\alpha = 0.2$. We reject the null hypothesis with $p < 0.05$ in all but one case. Particularly strong correlations were present for the Gemma models; this may be related to our choice of α and these models' robustness to interventions in the leave-one-out experiments.

6 Limitations

Causal tracing and zero-ablation, like many interpretability techniques, yield results which can imperfectly reflect the contributions of model internals to a task. In particular:

Zero-ablation. We chose to ablate activations in the model with zeros. While the zero vector is far from an arbitrary choice, especially given its relevance to dropout and the additive residual structure of a transformer, this approach may lack specificity. For example, zero-ablating an early or late MLP layer sometimes severely damages a model's ability to produce coherent language in general, so accuracies from ablation do not necessarily correspond to the flow of question-specific information through the model. Approaches such as causal scrubbing [6] avoid this limitation but are generally more computationally expensive.

Causal tracing. The "path" through the model identified comprises, to a first approximation, the set of points in the model at which *all* information relevant to the task is present. As such, when information relevant to a question passes along multiple paths in parallel, it may be that no individual path shows a substantial difference between the restored and baseline conditions. For example, in the question in Fig. 2 (center), restoring the input embedding for any one token of "Google Street View" without the others has little effect on the model.

7 Discussion and Conclusion

The results of the causal tracing and zero-ablation analyses presented in the previous section broadly support the shared circuits hypothesis, implying that—across the setups we considered—the sets of model components used for question-answering and uncertainty quantification were largely, albeit not entirely, the same. This suggests that $\mathbb{P}(\text{IK})$ probing may be a viable way of eliciting introspective, interpretable uncertainty estimates. Based on these findings, further research could analyze the mechanisms responsible for $\mathbb{P}(\text{IK})$ estimates in greater detail, or apply $\mathbb{P}(\text{IK})$ probing as an interpretability tool to study phenomena such as hallucination in LLMs. Similar analyses of other methods of uncertainty quantification, such as verbalized uncertainty, may provide insight further insight into the role of uncertainty introspection in uncertainty quantification. More generally, we see interpretable uncertainty quantification as a potentially useful approach for both understanding and improving LLM epistemics, in order to improve trustworthiness and reliability and allow for better-informed technical AI governance.

[3] If R^2 is the fraction of the variance in $\overline{m}_{\text{ablated}}$ explained by $\hat{\overline{m}}_{\text{ablated}} = \overline{p}_{\text{ablated}}$, we reject the null hypothesis R^2 *is no greater than expected under random permutations of the set of layers* at $p < 0.05$ in 27/38 cases.

[4] We excluded MMLU because of computational resource constraints.

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A Reproducibility

Code to reproduce our results can be found at

`https://github.com/crtep/sciurus`

B Limitations

Causal tracing and zero-ablation, like many interpretability techniques, yield results which can imperfectly reflect the contributions of model internals to a task. In particular:

Zero-ablation. We chose to ablate activations in the model with zeros. While the zero vector is far from an arbitrary choice, especially given its relevance to dropout and the additive residual structure of a transformer, this approach may lack specificity. For example, zero-ablating an early or late MLP layer sometimes severely damages a model's ability to produce coherent language in general, so accuracies from ablation do not necessarily correspond to the flow of question-specific information through the model. Approaches such as causal scrubbing [6] avoid this limitation but are generally more computationally expensive.

Causal tracing. The "path" through the model identified comprises, to a first approximation, the set of points in the model at which *all* information relevant to the task is present. As such, when information relevant to a question passes along multiple paths in parallel, it may be that no individual path shows a substantial difference between the restored and baseline conditions. For example, in the question in Fig. 2 (center), restoring the input embedding for any one token of "Google Street View" without the others has little effect on the model.

C Licenses for Models and Datasets

Models:

- Llama 2 is licensed under the Llama 2 Community License Agreement, available at https://ai.meta.com/llama/license/.
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D Model and Probe Performance

Model	Dataset	Model accuracy	Probe accuracy (bal.)	ECE
Llama 2 7B	TriviaQA	0.6006	0.7787	0.0342
	WebQuestions	0.4016	0.6674	0.0320
	MMLU	0.3984	0.6571	0.0265
	ARC (Mercury)	0.5845	0.6731	0.0363
	ARC (Other)	0.6260	0.7011	0.0327
Llama 2 7B Chat	TriviaQA	0.5850	0.7819	0.0315
	WebQuestions	0.4343	0.7051	0.0213
	MMLU	0.4688	0.6701	0.0272
	ARC (Mercury)	0.6973	0.6375	0.0294
	ARC (Other)	0.7632	0.6719	0.0395
Llama 3 8B	TriviaQA	0.6582	0.7026	0.0366
	WebQuestions	0.4158	0.7034	0.0405
	MMLU	0.6055	0.7455	0.0171
	ARC (Mercury)	0.8496	0.6035	0.0459
	ARC (Other)	0.8423	0.5991	0.0313
Llama 3 8B Instruct	TriviaQA	0.6509	0.7037	0.0397
	WebQuestions	0.4460	0.7213	0.0530
	MMLU	0.6445	0.7201	0.0300
	ARC (Mercury)	0.8779	0.6014	0.0495
	ARC (Other)	0.8569	0.6658	0.0362
Llama 2 13B	TriviaQA	0.6680	0.6938	0.0324
	WebQuestions	0.4346	0.6948	0.0403
	MMLU	0.4958	0.7252	0.0284
	ARC (Mercury)	0.7290	0.5010	0.1029
	ARC (Other)	0.7764	0.6691	0.0239
Llama 2 13B Chat	TriviaQA	0.6377	0.7020	0.0414
	WebQuestions	0.4468	0.7202	0.0306
	MMLU	0.4902	0.6913	0.0208
	ARC (Mercury)	0.7134	0.6395	0.0475
	ARC (Other)	0.7637	0.5973	0.0192
Gemma 2 2B Instruct	TriviaQA	0.4180	0.7221	0.0136
	WebQuestions	0.2910	0.6501	0.0517
	MMLU	0.4617	0.6803	0.0344
	ARC (Mercury)	0.7876	0.6310	0.0228
	ARC (Other)	0.7705	0.6051	0.0612
Gemma 2 9B Instruct	TriviaQA	0.6392	0.7374	0.0306
	WebQuestions	0.3579	0.7264	0.0529
	ARC (Other)	0.9126	0.5786	0.0354

Table 2: Model performance metrics

E Full Results for Zero-Ablation

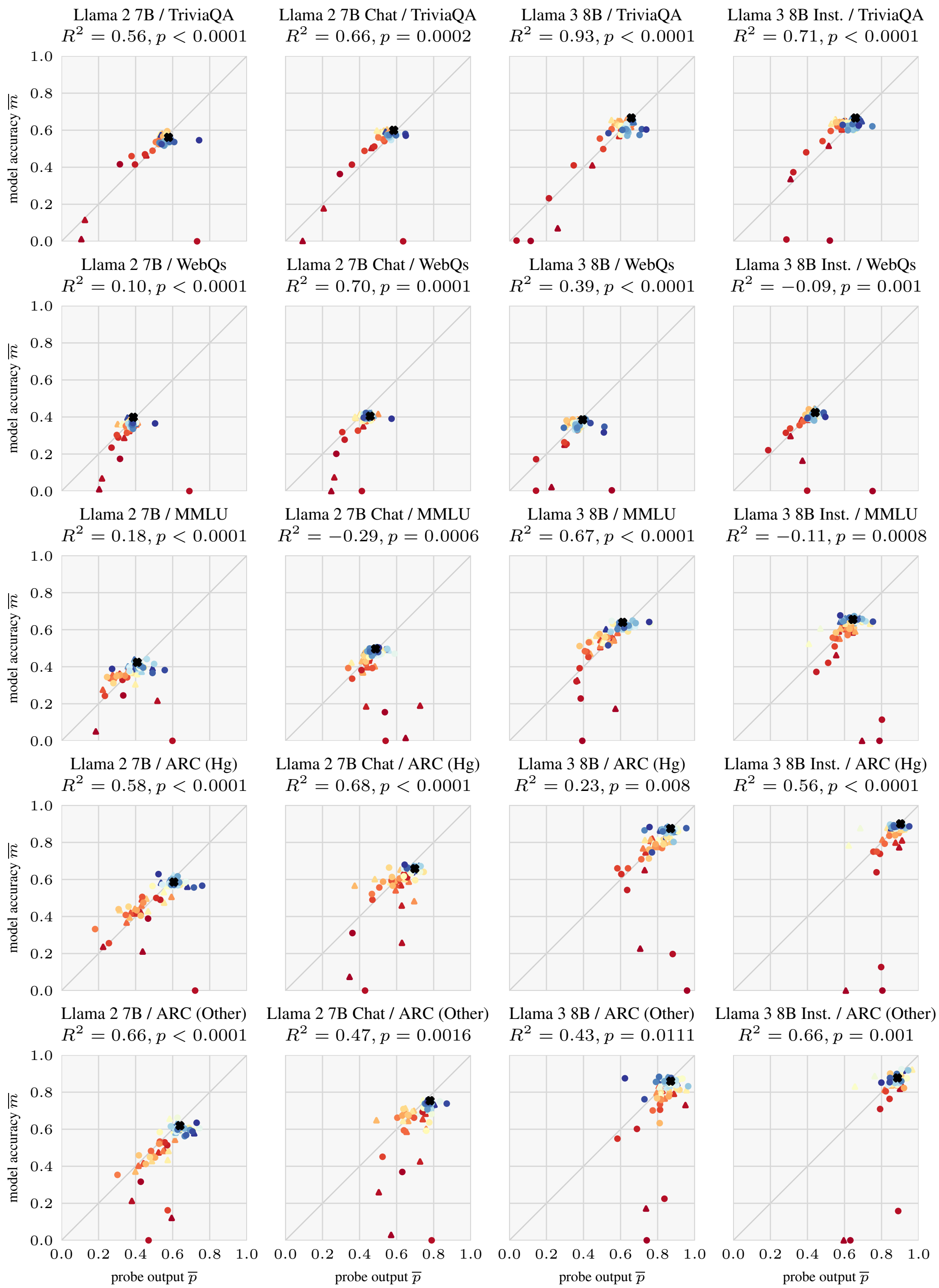

Figure 6: Results of zero-ablation for eight models and five datasets. Circle, triangle, and X markers represent MLP ablations, attention ablations, and clean runs respectively. Warmer colors represent earlier layers. Error bars for individual points are omitted for legibility, but std. err. < 0.032 in all cases (by the bounds on p and m).

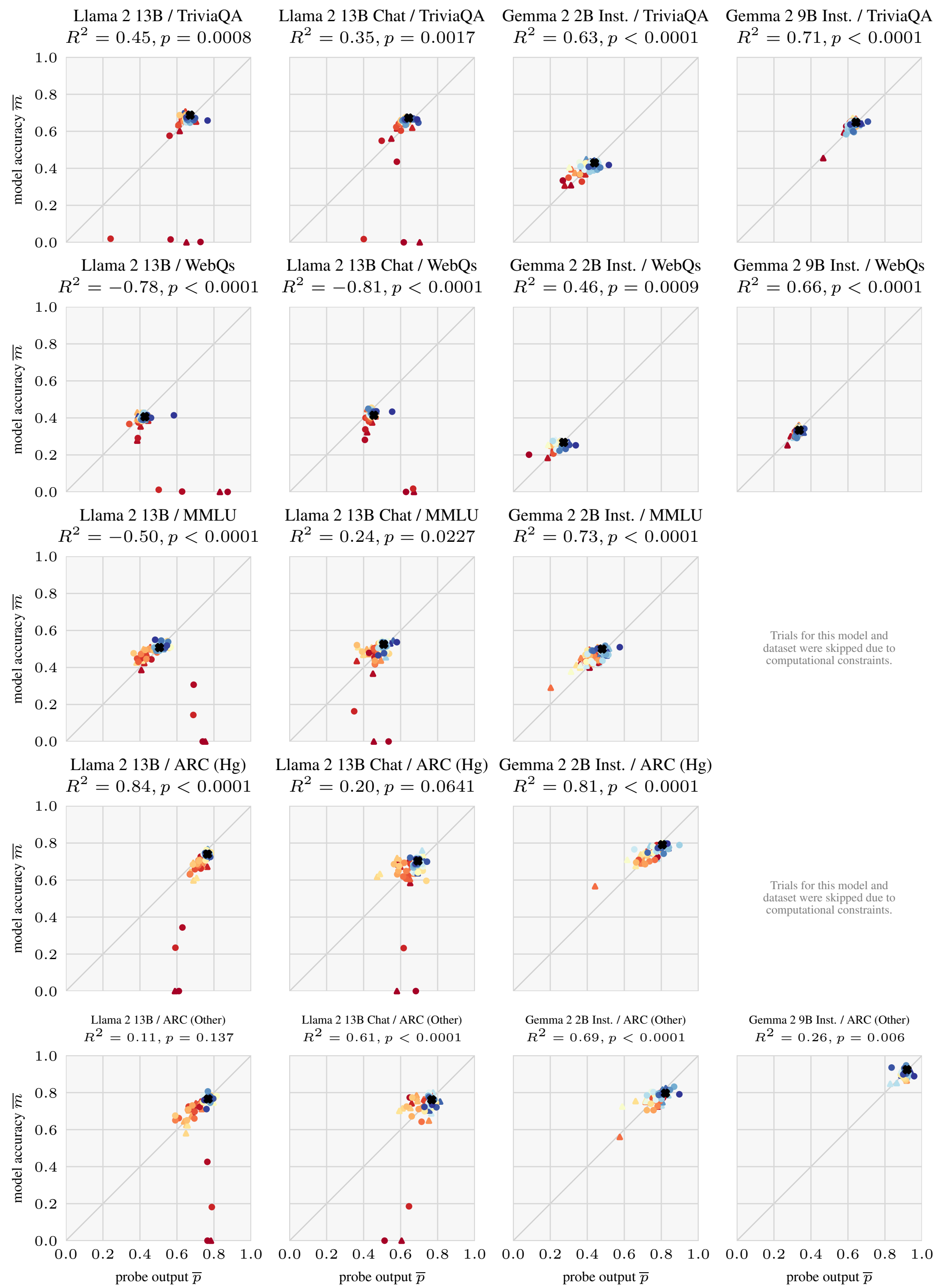

Figure 7: *(continued)* Results of zero-ablation for eight models and five datasets. Circle, triangle, and X markers represent MLP ablations, attention ablations, and clean runs respectively. Warmer colors represent earlier layers. Error bars for individual points are omitted for legibility, but std. err. < 0.032 in all cases (by the bounds on p and m).

F Full Results for COAR

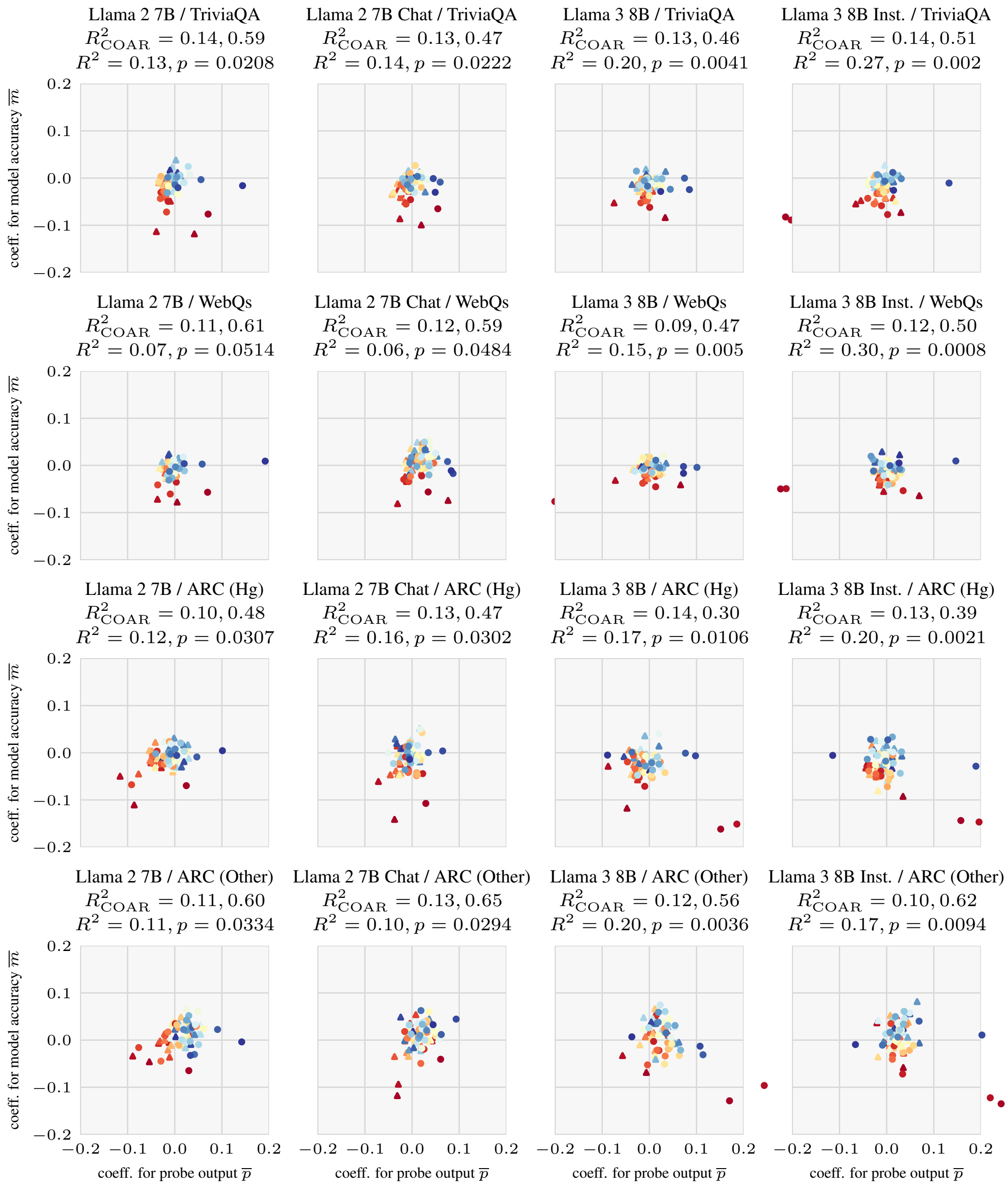

Figure 8: COAR coefficients for zero-ablation for eight models and four datasets. Circle and triangle markers represent MLP and attention ablations respectively. Warmer colors represent earlier layers. Error bars for individual points are omitted for legibility. The two values for R^2_{COAR} are the fraction of variance in m and p explained by the COAR prediction from the set of ablations.

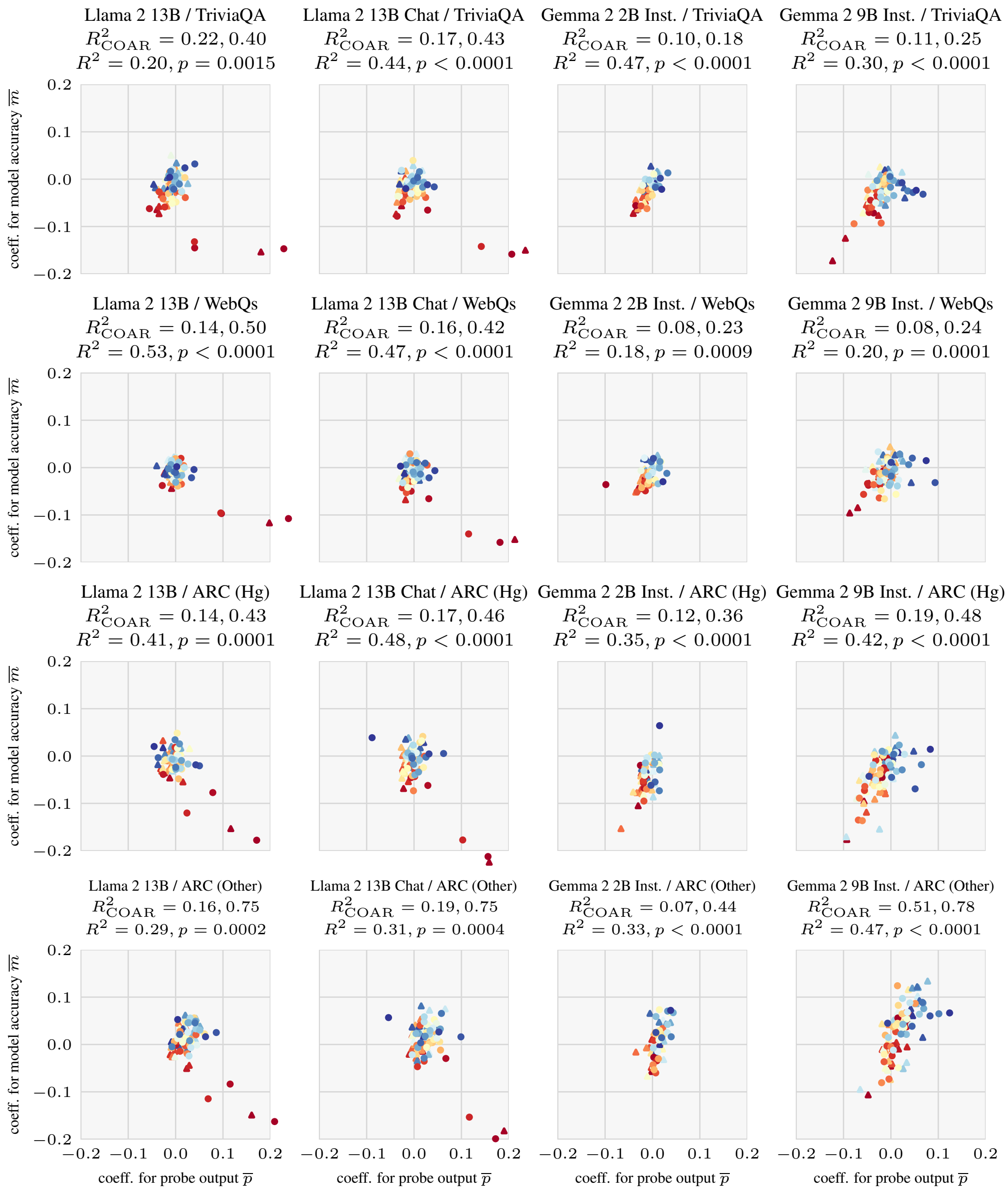

Figure 9: *(continued)* COAR coefficients for zero-ablation for eight models and four datasets. Circle and triangle markers represent MLP and attention ablations respectively. Warmer colors represent earlier layers. Error bars for individual points are omitted for legibility. The two values for R^2_{COAR} are the fraction of variance in m and p explained by the COAR prediction from the set of ablations.

G Computational Resources

This project has used approximately 1200 GPU-hours of computation time on an academic cluster, mainly on RTX8000 GPUs with 48 GB of memory, including approximately 600 GPU-hours for results used directly in this paper. Results for individual model/dataset combinations can be reproduced independently; for example, the code to produce the TriviaQA / Llama 3 8B Instruct results ran in approximately 20 GPU-hours.

H Ethics Statement

This paper intends to advance the areas of interpretability and uncertainty quantification for language models, with the primary aim of making language models more reliable and more trustworthy. We expect these research directions in general to reduce societal risks from machine learning (for example, by allowing for warning signals in situations where a model might be lying or making a dangerous mistake). Nevertheless, since reliability work also makes systems more useful, some caution is warranted: for example, users might be tempted to deploy the resultant more-reliable systems in higher-stakes contexts in which tail risks from failures are greater.

The humanoid and sciuroid robots in Fig. 1 were created using DALL-E 3.

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   Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

   Answer: [Yes]

   Justification: This paper proposes methods for studying uncertainty quantification in language models, and provides evidence for a "shared circuits" hypothesis across a range of models and tasks; we do not claim to address other settings (e.g., larger models or non-recall-based questions). Our introduction suggests some potential applications of our methods (e.g., the study of hallucinations) which we do not claim to pursue these in this paper.

2. **Limitations**

   Question: Does the paper discuss the limitations of the work performed by the authors?

   Answer: [Yes]

   Justification: We note the limited range of our experimental settings. We also acknowledge the major limitations of the mechanistic interpretability techniques we use (in particular, their tendency to produce noisy results which can be difficult to formalize) in Appendix B, and note that the hypotheses which we test formally are imperfect proxies for our shared circuits hypothesis.

3. **Theory Assumptions and Proofs**

   Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

   Answer: [NA]

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   Answer: [Yes]

   Justification: We present novel results based largely on existing mechanistic interpretability techniques, which we describe in sufficient detail to allow replication. We describe our probing setup in detail in Appendix 4.1. We also provide code for reproducing our work.

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7. **Experiment Statistical Significance**

   Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

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We describe the statistical tests used for our main results and note the details of our permutation sampling setup.

8. **Experiments Compute Resources**

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