Uncertainty-Aware Attention Heads: Efficient Unsupervised Uncertainty Quantification for LLMs

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Abstract

Large language models (LLMs) exhibit impressive fluency, but often produce critical errors known as "hallucinations". Uncertainty quantification (UQ) methods are a promising tool for coping with this fundamental shortcoming. Yet, existing UQ methods face challenges such as high computational overhead or reliance on supervised learning. Here, we aim to bridge this gap. In particular, we propose RAUQ (Recurrent Attention-based Uncertainty Quantification), an unsupervised approach that leverages intrinsic attention patterns in transformers to detect hallucinations efficiently. By analyzing attention weights, we identified a peculiar pattern: drops in attention to preceding tokens are systematically observed during incorrect generations for certain "uncertainty-aware" heads. RAUO automatically selects such heads, recurrently aggregates their attention weights and token-level confidences, and computes sequence-level uncertainty scores in a single forward pass. Experiments across 4 LLMs and 12 question answering, summarization, and translation tasks demonstrate that RAUQ yields excellent results, outperforming state-of-the-art UQ methods using minimal computational overhead (<1% latency). Moreover, it requires no task-specific labels and no careful hyperparameter tuning, offering plug-and-play real-time hallucination detection in white-box LLMs.

1 Introduction

Large language models have become the de facto backbone of modern NLP systems; yet, the impressive fluency of their responses often conceals various inconsistencies known as "hallucinations" [24]. There are several ways to address hallucinations, such as post-hoc verification using external knowledge bases [33], incorporating retrieval-augmented generation to ground outputs in factual data [28], or filtering/altering responses based on the uncertainty of a model [27, 14]. The latter approach, based on uncertainty, is the focus of this work.

Uncertainty is a fundamental concept in machine learning, reflecting the fact that we usually lack complete information about the model's predictions or parameters [16, 23, 25]. High predictive uncertainty typically signals a greater likelihood of hallucinations in the model output. Unlike verification methods that rely on external knowledge sources to detect hallucinations, uncertainty quantification (UQ) leverages the model's internal capabilities, thereby mitigating issues related to the completeness of external sources and offering greater versatility. As shown in previous work, uncertainty scores can be used to detect hallucinations that arise due to limitations of LLM parametric knowledge or due to the ambiguity of requests in various generation tasks [32, 17, 2], including question-answering, machine translation, text summarization, and speech recognition.

UQ for classification and regression tasks is a well-established area spanning decades of research [54, 19, 48, 46, 43, 21]. At the same time, UQ for generative tasks has only recently emerged as an active topic and still features open challenges. A crucial difference over classification is that an LLM performs not a single, but multiple conditionally dependent predictions. While recent work has proposed several promising techniques for quantifying predictive uncertainty in generation, e.g. [27, 14, 10, 35, 31], prior methods have limitations. Namely, information–based scores such as maximum sequence probability (MSP) and token-level entropy are simple and fast, but often underperform on long-form generation tasks [52, 44]. Sampling-based scores offer stronger performance, but incur large computational overhead [27, 31, 42]. Supervised confidence regressors [1, 6], i.e., thin supplementary modules trained on supervised annotation, yield accurate scores, but require costly, task–specific annotation and often fail to generalize to out-of-distribution data or across tasks [44]. Thus, despite the recent surge of developments of UQ for LLMs, the research community still lacks an effective, versatile UQ method that (i) avoids the high computational costs associated with sampling-based approaches, and (ii) is robust across tasks and domains.

In this work, we aim to construct such a method. For this purpose, we peek into the attention weights of the transformer and identify patterns that are highly indicative of the presence of hallucinations. Self-attention matrices encode how strongly each newly generated token attends to its immediate context. We empirically observe a systematic drop in the attention weight to the preceding tokens in specific attention heads precisely at positions where the model later proves to be factually incorrect (Figure 1). Based on this finding, we argue that a small number of attention heads capture the behavior of transformer-based LLMs under uncertainty. We propose a method that automatically identifies such "uncertainty-aware" heads inside individual LLM layers and extracts the token-level signal from them. The method recurrently fuses this signal with token probabilities and confidence scores from previously generated tokens, capturing the conditional dependencies across generation steps. Finally, it aggregates token-level scores across the generated sequence and layers. The resulting sequence-level uncertainty score achieves state-of-the-art performance and demonstrates high robustness to the choice of its single hyperparameter. Moreover, since attention weights are readily available at inference time for white-box LLMs, the method requires no additional generation passes and adds almost no computational overhead to response latency.

Contributions:

- 1. **In-depth analysis** of attention-based patterns in LLMs associated with hallucinations, which uncovers what we term "uncertainty-aware" heads, i.e., attention heads whose signals notably correlate with hallucination occurrences.
- 2. **RAUQ** (Recurrent Attention-based Uncertainty Quantification) an unsupervised UQ method that turns raw attentions and LLM probabilities into reliable uncertainty scores while adding only <1% latency. RAUQ requires no task-specific labels or tuning of hyperparameters for a particular LLM, making it an easy plug-and-play for white-box LLMs.
- 3. **Thorough experimental evaluation** on four LLMs and 12 benchmarks, spanning summarization, translation, and question answering, showing that RAUQ achieves state-of-the-art results over 15 baselines. We also demonstrate the importance of each component within the method and illustrate that each individually could improve other UQ methods.

2 Related Work

Several recent studies have proposed attention-based UQ methods for detecting hallucinations in LLM-generated outputs.

Zhang et al. [53] use attention weights to propagate uncertainty across generation steps by capturing conditional dependencies, helping to mitigate overconfidence from prior hallucinations. However, attention plays a secondary role, with the method mainly relying on probability and entropy.

Yuksekgonul et al. [50] perform a mechanistic investigation of attention patterns linked to LLM factual errors and propose a supervised UQ method called SAT Probe. They associate hallucinations with weak attention to so-called "constrained" tokens in the prompt – key prompt elements that narrow down the scope of the answer. However, their experiments show that SAT Probe performs only on par with or slightly better than baselines. In a similar vein, Contextualized Sequence Likelihood [30] leverages attention to important tokens in the input context to reweight the contribution of token logits when computing weighted sequence likelihood. Lookback Lens [8] leverages attention maps to

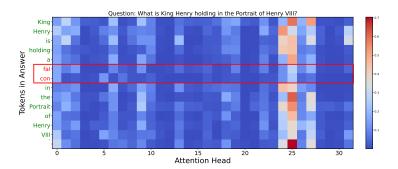


Figure 1: Attention weights in the 29th layer of Llama 3.1 8B from each generated token to its preceding token, given the prompt *What is King Henry holding in the Portrait of Henry VII?*. The y axis specifies the generated tokens, and the x axis specifies the attention heads. Warmer colors indicate higher attention values. The output contains the factually incorrect token falcon (the correct answer is gloves and dagger). Notably, the 25th attention head stands out by consistently assigning relatively high attention to the preceding token. However, for the hallucinated token falcon, this attention drops sharply – potentially serving as a signal for hallucination detection.

construct features for a supervised hallucination detector. The authors hypothesize that hallucinations correlate with less attention paid to the input context. They compute the ratio between cumulative attention weights to tokens in the answer and the prompt and train a linear classifier on top of these features. Attention-based features are also used in Trainable Attention-Based Dependency [44]. This method adds recurrence when computing uncertainty for subsequent tokens. It demonstrates strong results for in-domain tasks, outperforming Lookback Lens, but both methods lack generalization due to their supervised nature.

Finally, Sriramanan et al. [40] recently proposed the Attention Score method, where they compute a length-normalized sum of log attention weights to preceding tokens across the prompt and the answer. Lower scores signal the presence of hallucination.

Although recent studies show that attention weights offer valuable signals for detecting hallucinations in LLM outputs, existing methods suffer from various limitations that hinder their effectiveness. SAT Probe, Lookback Lens, and TAD are supervised and show limited generalization beyond their training domain. Zhang et al. [53] and Lin et al. [30] leverage attention only as a supplement to other scores. Sriramanan et al. [40] do not select proper attention heads before averaging, and allow the attention weights from prompt tokens to participate in the aggregation for the final score, which causes underperformance.

In this work, we aim to overcome the limitations of existing methods. To this end, we identify strong and generalizable attention-based patterns for LLM hallucination detection, isolate the key techniques required to effectively exploit these patterns, and develop a robust *unsupervised* UQ method that achieves state-of-the-art performance.

3 Identifying Hallucination-Associated Patterns in Attention Maps

We analyze the model's attention maps when an LLM generates correct vs. incorrect outputs. We start with an analysis of attention weights to the immediately preceding token, i.e. $a_{i,i-1}^{lh}$ – attention weight to the $\{i-1\}$ -th token during the generation of i-th token from the layer l and attention head h. Let N be the number of generated tokens in the answer, H the number of attention heads in each layer, and L be the number of layers in the LLM. For illustration, we use the Llama 3.1 8B model.

Difference between attention weights for hallucinated and non-hallucinated tokens. Figure 1 presents an example of the attention weights to preceding tokens $a_{i,i-1}^{lh}$ in one of the LLM layers for the input question from the TruthfulQA dataset: What is King Henry holding in the Portrait of Henry VII? Most of the generated tokens are aligned with the question. However, the token falcon represents a hallucination, i.e. it is factually incorrect (the answer should be glove and dagger).

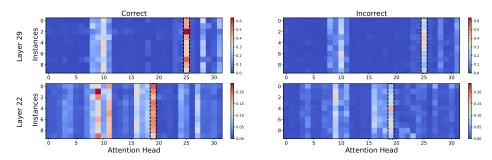


Figure 2: Average attention weights to the preceding token, aggregated over all answer tokens for questions from the TruthfulQA dataset using Llama 3.1 8B. The top 10 highest- and lowest-quality answers, as determined by a quality metric, are labeled as correct and incorrect, respectively. The black dashed box highlights the head with the highest average attention.

For most attention heads, the weights to previous tokens remain low across all generated tokens. In contrast, the 25th head exhibits a distinct pattern: it assigns relatively high attention to the preceding token for non-hallucinated (i.e., correct) tokens, but this attention drops significantly for the hallucinated token *falcon*.

This example demonstrates that attention weights from a small subset of attention heads can notably correlate with the factual correctness of generated tokens. While the choice of layer and head might vary, this case suggests that certain heads in specific layers are "uncertainty-aware", i.e., they are sensitive to generation accuracy and could help to identify hallucinations. More examples of the similar pattern for Llama and other LLMs are presented in Figures 6 to 9 in Appendix F.

Difference between average attention weights for incorrect and correct answers. We begin by selecting 10 correct and 10 incorrect answers generated by the LLM. To evaluate the correctness of each answer, we use AlignScore – a continuous metric that quantifies semantic similarity between the generated response and the gold-standard answer [51]. We sort all generations by their AlignScore, and designate the top 10 as correct answers and the bottom 10 as incorrect.

Then, we compute the average attention weight to the previous token across all tokens in the answer using the attention heads in the 29th and 22nd layers of the LLM, i.e. $\bar{a}^{lh} = \frac{1}{N-1} \sum_{i=2}^{N} a^{lh}_{i,i-1}$. Figure 2 presents the resulting values, where each row corresponds to a single selected answer, and each column indicates the average attention weight from a specific head.

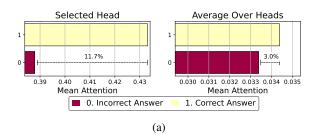
The attention maps in the figure demonstrate that certain heads consistently assign higher average attention when the LLM generates correct answers as compared to incorrect ones. Moreover, there is a notable correlation between the quality of the answer and average attention (see Figure 3b). This way, we empirically discovered a pattern for assessing the correctness of LLM generations.

Should we select uncertainty-aware heads, and how should we do it? We compute the average attention score \bar{a}^{lh} across tokens in two scenarios: (1) attention values are averaged across all heads in a layer, i.e. $\bar{a}^{l} = \sum_{h=1}^{H} \bar{a}^{lh}$; (2) attention values are extracted from a single head with the *highest* average attention across tokens, i.e. \bar{a}^{lh_l} , where $h_l = \arg\max_{h=1...H} \bar{a}^{lh}$. Figure 3a compares the resulting values for correct and incorrect answers.

When using only the selected attention head, we observe a clear difference in the values between correct and incorrect answers. However, averaging attention across all heads eliminates this difference. This once again highlights the importance of focusing on specific uncertainty-aware heads. These heads can be identified by selecting those with the highest average attention weights across all tokens.

Do we need to look further back at preceding tokens to better detect hallucinations? We analyze the attention weights to multiple preceding tokens. Here, we compute $a^{lh}_{i,i-k}$ – an attention weight to the $\{i-k\}$ -th token (k-th preceding token), $k=1,\ldots,6$. Figure 4 shows the difference between the average attention weights of the correct and incorrect answers.

We see that the attention weights differ substantially between correct and incorrect answers only for the two preceding tokens, with almost zero differences observed for earlier tokens. Notably, the difference is substantially larger for the first preceding token as compared to the second one.



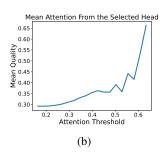


Figure 3: Attention weights to the preceding token averaged across all tokens in the generated responses of Llama 3.1 8B on the TruthfulQA dataset. a): Comparison between incorrect (AlignScore < 0.1) and correct (AlignScore > 0.9) answers. Attention values are presented for two scenarios: (left) from the selected head with the highest average attention; (right) averaged across all heads. b): The relationship between average response quality and the average attention weight in the selected head.

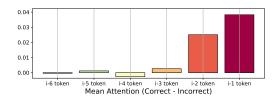


Figure 4: Difference between correct (AlignScore > 0.9) and incorrect answers (AlignScore < 0.1) in average attention weights to preceding tokens during the generation of answers for the questions from the TruthfulQA dataset using Llama 3.1 8B.

Summary. Our analysis uncovers attention patterns associated with the factuality of individual tokens and LLM responses in general. A key observation is that such systematic patterns emerge only for a small subset of specific attention heads. Effectively leveraging them requires first identifying the relevant uncertainty-aware attention heads. We also observe that the immediately preceding token provides the strongest signal, leading us to focus solely on it in our method design and subsequent experiments. Below, we leverage the insights from this mechanistic investigation to develop a new *unsupervised* UQ method for LLMs.

4 RAUO: Recurrent Attention-Based Uncertainty Quantification Method

Let x be the input sequence and $y = y_1 y_2 \dots y_N$ be its corresponding output sequence of length N.

Selecting an attention head in each layer. For an LLM with L layers and H attention heads per layer, we first select the most informative head. For each layer l, we select the head with the maximum average attention weights between consecutive tokens:

$$\mathbf{h}_{l}(\mathbf{y}) = \underset{h=1...H}{\arg\max} \ \frac{1}{N-1} \sum_{i=2}^{N} a_{i,i-1}^{lh}, \tag{1}$$

where $a_{i,i-1}^{lh}$ is the attention weight from token y_i to y_{i-1} computed by the h-th head in the layer l.

Token-level layer-wise recurrent confidence score. Following [53], we acknowledge that computing uncertainty at the generation step i requires propagating uncertainty from previous steps, due to the conditional dependencies in the probability distribution modeled by the LLM. Namely, even if previous tokens were generated with high uncertainty, a model may condition on them and be highly confident in a current token prediction. To take into account this issue, we introduce a formulation that recurrently incorporates uncertainty from previous steps. We recurrently compute the confidence score $\mathbf{c}_l(y_i)$ for the i-th token by leveraging the confidence of the previous token $\mathbf{c}_l(y_{i-1})$, the attention weight $a_{i,i-1}^{lh_l}$ from the selected head $\mathbf{h}_l = \mathbf{h}_l(\mathbf{y})$, and the conditional probability of the current token $P(y_i \mid y_{< i}, \mathbf{x})$ as follows:

$$\mathbf{c}_{l}(y_{i}) = \begin{cases} P(y_{i} \mid \mathbf{x}), & \text{if } i = 1, \\ \alpha \cdot P(y_{i} \mid y_{< i}, \mathbf{x}) + (1 - \alpha) \cdot a_{i, i-1}^{l \mathbf{h}_{l}} \cdot \mathbf{c}_{l}(y_{i-1}), & \text{if } i > 1, \end{cases}$$
(2)

Algorithm 1: RAUQ: Recurrent Attention-based Uncertainty Quantification method

where α is a hyperparameter that balances the contributions of each component. This recurrent formulation also helps to avoid an explosion in confidence scores with an increase in sequence length. We present an ablation study with the impact of varying the parameter α in Section 5.3 and show that a single value provides robust performance across various tasks and even models.

Sequence-level layer-wise uncertainty score. Sequence-level errors are typically either (1) *distributed* across all tokens, e.g. in the summarization task; or (2) *localized* in a single fact-related token, e.g. in the QA task. To take into account both cases in the sequence-level uncertainty score, we compute the mean logarithm of the confidence scores across all tokens in the reply (importantly, we do not aggregate scores for tokens in the prompt):

$$\mathbf{u}_l(\mathbf{y}) = -\frac{1}{N} \sum_{i=1}^{N} \log \mathbf{c}_l(y_i). \tag{3}$$

Final uncertainty score. Finally, to aggregate the layer-wise uncertainty scores in an unsupervised manner, we compute the maximum uncertainty score across the set of layers:

$$\mathbf{u}(\mathbf{y}) = \max_{l \in \mathcal{L}} \mathbf{u}_l(\mathbf{y}),\tag{4}$$

where \mathcal{L} denotes the set of the most informative layers. Following previous work [44], we select these layers from the middle of the model. An ablation study with various aggregation functions is presented in Section 5.3. The step-by-step description of RAUQ is presented in Algorithm 1.

5 Experiments

5.1 Experimental Setup

We conducted extensive experiments across three key generation tasks: question answering ("QA"), abstractive text summarization ("Summ"), and machine translation ("MT"). For each task, we evaluated RAUQ's ability to identify and filter out unreliable output through selective generation. We set $\alpha=0.0$ for the summarization task and $\alpha=0.2$ for all other tasks.

Datasets. For QA, we use seven datasets: TruthfulQA [29], SciQ [47] for scientific QA, MMLU [22], TriviaQA [26] for trivia questions, CoQA [36] for conversational QA, MedQUAD [4] for medical questions, and GSM8k [9] for mathematical reasoning. For summarization, we use three datasets with different summarization types: CNN/DailyMail [39] for news article summarization, SamSum [18] for dialogue summarization, and XSum [34] for summarizing into a single sentence. For the MT

UQ Method	L	ama-3.1 8	BB	Q	wen-2.5 7	В	G	emma-2 9	В	Fa	alcon-3 10		Mean
OQ Method	QA	Summ	MT	QA	Summ	MT	QA	Summ	MT	QA	Summ	MT	Mean
MSP	.347	.129	.397	.329	.350	.369	.361	.176	.381	.345	.174	.333	.307
Perplexity	.347	311	.380	.343	129	.406	.383	296	.405	.356	146	.439	.181
CCP	.285	.148	.340	.271	.246	.327	.329	.147	.320	.299	.066	.287	.255
Attention Score	.014	.053	.178	.038	.031	.142	.064	.120	.146	.054	091	.089	.070
Focus	.320	110	.361	.264	.087	.380	.416	085	.385	.313	007	.362	.224
Simple Focus	.342	.056	<u>.415</u>	.342	.252	.399	.396	.067	<u>.422</u>	.351	019	.385	.284
DegMat NLI Score entail.	.306	.199	.239	.356	.183	.275	.337	.150	.259	.352	.088	.222	.247
Ecc. NLI Score entail.	.274	.029	.284	.322	.039	.306	.298	018	.290	.327	.044	.281	.206
EVL NLI Score entail.	.293	.188	.217	.349	.181	.245	.332	.139	.252	.351	.140	.206	.241
Lexical Similarity Rouge-L	.250	.133	.324	.334	.141	.327	.306	.132	.342	.285	.033	.275	.240
EigenScore	.232	.082	.285	.298	.007	.302	.267	.119	.226	.247	.023	.236	.194
LŪQ	.287	.168	.214	.351	.047	.213	.344	.206	.259	.335	.142	.196	.230
Semantic Entropy	.254	.076	.315	.281	.292	.317	.291	.154	.337	.320	.083	.291	.251
SAR	.310	.238	.370	.351	.112	.393	.361	.159	.414	.334	.033	.337	.284
Semantic Density	.330	.043	.264	.352	.095	.291	.375	.055	.255	.358	.031	.280	.227
RAUQ (Ours)	.396	.375	.452	.358	.415	.438	.421	.471	.473	.392	.316	.465	.414

Table 1: Mean PRR↑ across tasks for the evaluated LLMs. Warmer color indicates better results.

task, we evaluate on two language pairs from WMT: German–English from WMT19 [3] and French–English from WMT14 [5]. Detailed statistics for all datasets are presented in Table 3 in Appendix A.

Models. To show the generalization of the method across various models, we use several widely used open-weight LLMs: Llama-3.1 8B [11], Qwen-2.5 7B [49], Gemma-2 9B [38], and Falcon-3 10B [13]. Detailed descriptions of generation parameters are presented in Table 3 in Appendix A.

Uncertainty quantification baselines. We compare the proposed RAUQ method with 15 diverse UQ baselines. As a sanity check, we include simple unsupervised baselines such as Maximum Sequence Probability (MSP) and Perplexity [15]. Among state-of-the-art baselines for whitebox LLMs, we compare our method to Semantic Entropy [27], hallucination detection with stronger focus ("Focus") [53], Claim-Conditioned Probability ("CCP") [12], EigenScore [7], Shifting Attention to Relevance ("SAR") [10], Semantic Density [35], and Attention Score [40]. Additionally, we consider UQ methods for black-box LLMs, as they also demonstrate strong performance in recent works despite not having access to LLM logits or its hidden states. We use Lexical Similarity based on Rouge-L [15], Long-text Uncertainty Quantification ("LUQ") [52], and methods from [31] – Degree Matrix ("DegMat"), Eccentricity, and Sum of Eigenvalues of the graph Laplacian ("EVL").

Evaluation metrics. As the main evaluation metric, we use the standard Prediction Rejection Ratio (PRR) [32, 42]. PRR is calculated as the ratio of the area between the rejection curves of the UQ method and the random UQ baseline, and the same area between the ideal UQ method and the random UQ baseline. The rejection curve plots the average quality of remaining responses when we abstain from a fraction of the most uncertain predictions. We compute PRR over only the first 50% of the curve, as rejecting more than half of the instances is typically impractical. The metric is normalized so that a PRR of zero or below indicates performance at or below the level of random chance, while values approaching one reflect optimal performance. PRR is analogous to ROC-AUC or PR-AUC, but unlike them, it can be applied not only to discrete quality metrics (e.g. correct vs. incorrect answer) but also to continuous ones, such as those commonly used in summarization and MT. For different generation tasks, we use different response quality metrics: accuracy for MMLU and GSM8k; COMET [37] for MT; and AlignScore [51] for the rest. Additionally, we calculate ROC-AUC using discrete quality metrics obtained by thresholding the original continuous values.

5.2 Main Results

Table 1 presents the mean PRR for each task (QA, Summ, and MT) for each of the evaluated LLMs. To compute the mean PRR for each task, we average the PRR scores across all relevant datasets, for example, XSum, CNN, and SamSum for summarization. These aggregated PRR scores provide a robust measure of the performance of various methods for each task and model. Detailed results for each model and dataset are presented in Tables 11 to 14 in Appendix E. The results using the ROC-AUC metric are presented in Table 8 in Appendix D.1.

The results demonstrate that the proposed RAUQ method consistently outperforms previous state-of-the-art methods for the summarization and translation tasks by a substantial margin for all evaluated LLMs. For instance, for the summarization task using Gemma-2 9B, RAUQ largely outperforms the

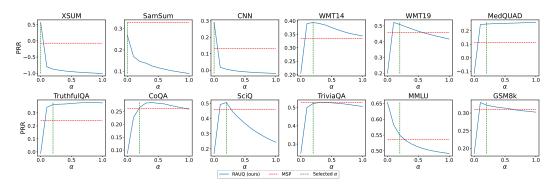


Figure 5: PRR \uparrow as a function of the hyperparameter α for Llama 3.1 8B. The vertical line marks the value of α used in our experiments.

second-best method (LUQ) by 0.265 of PRR. In contrast, other single-generation methods based on the attention weights, such as Focus and Attention Score, perform close to random chance.

For the QA task, RAUQ also achieves the best results across all models often with a substantial margin over the second best method. Notably, RAUQ improves over the second-best method (MSP) for Llama-3.1 8B by 0.049 in terms of PRR. However, for Qwen-2.5 7B in the QA task, computationally intensive DegMat comes close, trailing RAUQ by just 0.002 PRR. However, RAUQ consistently outperforms all other sampling-based baselines on average.

Overall, while methods such as MSP, Focus, or SAR might achieve top performance in specific settings, RAUQ demonstrates the most robust performance across all tasks and models, consistently ranking as the best method by average performance in a task.

Tables 9 and 10 in Appendix D.2 also provide a comparison with supervised UQ methods. While RAUQ slightly underperforms compared to supervised methods on their in-domain data, it greatly outperforms them on average in out-of-domain scenarios.

5.3 Hyperparameter Sensitivity and Ablation Studies

Impact of the hyperparameter α . The hyperparameter α from Equation (2) balances the contributions of attention, confidence from the previous token, and the conditional probability of the current token. When α is equal to 1, RAUQ becomes equivalent to perplexity. When α approaches 0, RAUQ relies solely on the attention weights from the selected head. Figure 5 presents the impact of α on the performance of the RAUQ method for Llama 8b v3.1. For the summarization, setting α equal to 0 consistently yields the best results. For all other tasks, except MMLU, the best possible performance is achieved with α between 0.2 and 0.5.

While dataset-specific fine-tuning of α can lead to further improvements, we do not perform such careful tuning in our main experiments (Table 1). Instead, we select α using a small out-of-domain subset for Llama 8b v3.1 and apply this value uniformly across all datasets and LLMs. Despite this, RAUQ achieves consistently strong performance across diverse tasks and LLMs, often achieving the top or near-top results. Strong performance with a fixed hyperparameter underscores the robustness of the proposed method.

Aggregation functions. Table 5 compares the performance of the RAUQ method using various aggregation functions of token-level confidence scores. We experiment with four aggregation strategies: mean, median, sum of logarithms (inspired by MSP), and mean of logarithms (inspired by perplexity). For the Summ tasks and certain QA datasets (SciQ, TriviaQA, and GSM8k), mean aggregation yields the best performance. For MMLU, the sum of logarithms substantially outperforms other aggregation strategies, while median performs best for XSum. However, the top two performing methods are those that apply length normalization. Among them, the mean of logarithms of token-level confidence scores used in RAUQ consistently delivers the strongest results across datasets.

Table 6 compares the performance of RAUQ using various aggregation functions of layer-wise uncertainty scores. We consider three aggregation strategies: mean, median, and maximum. Both maximum and median yield similarly strong performance, while the mean aggregation performs

UQ Method	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
Attention Score	.100	.017	.043	.176	.179	295	.081	028	142	.067	.209	.209	.051
Attention Score (Gen. Tokens)	.595	.269	.278	.196	.198	305	020	.064	.124	.130	.232	.192	.163
Attention Score (Gen. Tokens, Selected Head)	.547	.271	.300	.187	.200	113	025	.092	.161	.151	.414	.197	.198
RAUQ	.566	.269	.290	.394	.509	.241	.364	.265	.506	.522	.549	.323	.400

Table 2: PRR[↑] for Llama 3.1 8B across various modifications of the Attention Score method incorporating components from RAUQ. The best method is in **bold**, the second best is <u>underlined</u>.

slightly worse. Although the median slightly outperforms the maximum by an average margin of 0.003 PRR across tasks, this difference is negligible. Given that the maximum is a more intuitive choice – it effectively captures the peak uncertainty within a generation and achieves better results in 7 out of 12 tasks, we adopt it as the default layer-wise aggregation method in our experiments.

Recurrent uncertainty propagation functions. Table 7 presents the performance of the RAUQ method using various recurrent formulas for the calculation of token-level confidence scores. We consider five modifications of Equation (2): (1) removing attention weights, (2) removing recurrence, (3) replacing the confidence score of the previous token with its probability, (4) multiplying probabilities with attentions, and (5) the recurrent formula proposed in RAUQ.

The proposed formula achieves the best results on the majority of the datasets. Removing either recurrence or attention often leads to substantially worse performance. The results highlight the importance of each component in the proposed formula for achieving good results.

Extending our findings to the Attention Score method. To demonstrate the robustness and generalization of RAUQ components, we integrated them into the recently published Attention Score method [40], resulting in two modifications. We compare (1) the original official implementation of Attention Score; (2) Attention Score that uses only the attention weights of the generated tokens, excluding the prompt; (3) Attention Score that combines the previous feature and implements also the selection of the uncertainty-aware attention heads; (4) the full RAUQ method with recurrence.

Results in Table 2 show that excluding contributions from prompt tokens significantly boosts the average performance of Attention Score, yielding a 0.112 improvement in PRR. The highest improvement is achieved on the summarization tasks, where the modified Attention Score approaches the performance of RAUQ. Incorporating attention head selection further boosts the average performance by 0.035, with a large gain of 0.182 on MMLU. Nevertheless, our full method further incorporates token probabilities and recurrently aggregates uncertainty scores from previous generation steps, which provides a distinct advantage. Overall, these results suggest that our findings regarding attention heads and design choices in RAUQ are systematic and generalize to prior UQ methods as well.

5.4 Computational Efficiency

To demonstrate the computational efficiency of RAUQ, we conducted a comprehensive runtime comparison against other state-of-the-art UQ methods using Llama 8b v3.1. All experiments were performed on a single 80GB NVIDIA H100 GPU using single-batch inference, following the same setup as in Table 1. Table 4 in Appendix B reports the average runtime per instance for each UQ method, and quantifies their computational overhead relative to standard LLM inference without UQ.

State-of-the-art UQ methods such as DegMat [14], Semantic Entropy [27], and SAR [53] introduce huge computational overhead (400–800%) due to repeated sampling from the LLM. In contrast, the RAUQ method introduces less than 1% overhead since it does not require sampling or inference of an auxiliary model, making it a fast, lightweight, and plug-and-play solution for any white-box LLM.

6 Conclusion

We introduced RAUQ, an unsupervised, attention-based framework that converts the intrinsic signals already produced by every transformer layer into reliable sequence-level uncertainty scores with a single forward pass. A simple head-selection heuristic, a recurrent confidence propagation rule, and a length-normalized aggregation allow RAUQ to capture both local spikes and global drifts in confidence without external supervision or sampling. Extensive experiments on 12 datasets spanning QA, Summ, and MT, and on 4 open-weight LLMs show that RAUQ delivers state-of-the-art performance with only <1 % latency overhead, making it a practical off-the-shelf UQ technique.

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A Dataset and Generation Statistics

The detailed description of the used datasets and the generation parameters of LLMs is presented in Table 3. For all LLMs, we used the same generation hyperparameters, while for each dataset, we separately fixed the number of few-shot and maximum generation length.

Table 3: Statistics of the datasets and generation parameters of the used LLMs. For all datasets, we do not limit the maximum input length.

Task	Dataset	Number of test samples	N-shot	Generation length	Do sample	Temperature	Тор-р	Beams	Repetition Penalty
	TruthfulQA	817	5	128					
	SciQ	1000	0	20					
	MMLU	2000	5	3					
QA	TriviaQA	2000	5	20					
	CoQA	2000	all preceding questions	20	F 1	1.0			
	MedQUAD	1000	5	128	False	1.0	1.0	1	1
	GSM8k	1319	5	256					
	CNN/DailyMail	2000	0	128					
ATS	SamSum	819	0	128					
	XSum	2000	0	128					
NMT	WMT19 (DE-EN)	2000	0	107	l	1		l	1
INMI	WMT14 (FR-EN)	2000	0	107					

B Computational Efficiency

Table 4: Inference runtime of UQ methods measured on all test instances from all datasets with generations from Llama 8b v3.1. The best results are in **bold**.

UQ Method	Runtime per batch	Overhead
MSP	1.16 ± 0.45	-
DegMat NLI Score Entail. Lexical Similarity ROUGE-L Semantic Entropy SAR Semantic Density	$ \begin{array}{c} 6.40 \!\pm\! 1.76 \\ 6.11 \!\pm\! 1.75 \\ 6.40 \!\pm\! 1.76 \\ 10.71 \!\pm\! 3.21 \\ 6.27 \!\pm\! 1.76 \end{array} $	450% 425% 450% 820% 438%
RAUQ	1.17±0.45	0.3%

C Results of Ablation Studies

Table 5: PRR↑ for Llama 8b v3.1 model for various aggregation function of token-level confidence scores. The best method is in **bold**, the second best is <u>underlined</u>.

Token Aggregation	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
$-\frac{1}{N}\sum_{i=1}^{N} \mathbf{c}_{l}^{t}(t_{i})$.571	.322	.306	.359	.485	.140	.304	.259	.511	.534	.526	.339	.388
$-\text{median}_{i=1}^{N} \mathbf{c}_{l}^{t}(t_{i})$.615	.261	.099	.249	.340	<u>.154</u>	.317	.234	.430	.432	.635	.253	.335
$-\sum_{i=1}^{N} \log \mathbf{c}_{l}^{t}(t_{i})$.570	.270	.292	.224	.242	.107	.035	.114	.202	.300	.658	.213	.269
$-\frac{1}{N}\sum_{i=1}^{N} \log \mathbf{c}_{l}^{t}(t_{i})$.566	.269	.290	.394	.509	.249	.364	.265	.506	.522	.549	.323	.401

Table 6: PRR↑ for Llama 8b v3.1 model for various aggregation function of layer-wise uncertainty scores. The best method is in **bold**, the second best is <u>underlined</u>.

Layer Aggregation	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
$\frac{1}{ \mathcal{L} } \sum_{l \in \mathcal{L}} \mathbf{u}_l(y)$.583	.273	.290	.389	.519	.154	.345	.274	.496	.535	.529	.337	.394
$median_{l \in \mathcal{L}} \mathbf{u}_l(y)$.606	.263	.286	.388	.526	.246	.351	.267	.502	.532	.532	.340	.403
$\max_{l \in \mathcal{L}} \mathbf{u}_l(y)$.566	.269	.290	.394	.509	.249	.364	.265	.506	.522	.549	.323	<u>.401</u>

Table 7: PRR \uparrow for Llama 8b v3.1 model for various function for recurrent calculation of confidence scores $\mathbf{c}_l(t_i)$ in Equation (2). The best method is in **bold**, the second best is <u>underlined</u>.

Recurrent Formula	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
$\alpha \cdot P(t_i \mid \mathbf{x}, t_{< i}) + (1 - \alpha) \cdot \mathbf{c}_l(t_{i-1})$.167	.172	.094	.238	.313	.274	.224	.267	.273	.514	.475	.279	.274
$\alpha \cdot P(t_i \mid \mathbf{x}, t_{\leq i}) + (1 - \alpha) \cdot a_{i,i-1}^{l \mathbf{h}_l}$.226	.161	.126	.332	.436	.209	.322	.257	.485	.517	.550	.305	.327
$\alpha \cdot P(t_i \mid \mathbf{x}, t_{< i}) + (1 - \alpha) \cdot a_{i,i-1}^{l'\mathbf{h}_l} \cdot P(t_{i-1} \mid \mathbf{x}, t_{< i-1})$	586	.246	.058	.370	.472	.237	.336	.279	.456	.517	.532	.318	.270
$P(t_i \mid \mathbf{x}, t_{\leq i}) \cdot a_{i,i-1}^{l \mathbf{h}_l}$	558	.246	.056	.226	.337	.150	.251	.161	.330	.330	.645	.255	.202
$\alpha \cdot P(t_i \mid \mathbf{x}, t_{< i}) + (1 - \alpha) \cdot a_{i,i-1}^{l \mathbf{h}_l} \cdot \mathbf{c}_l(t_{i-1})$.566	.269	.290	.394	.509	.249	.364	.265	.506	.522	.549	.323	.401

D Additional Experimental Results

D.1 Experiments Using the ROC-AUC Metric

The results evaluated using the ROC-AUC metric are presented in Table 8. For all generation quality metrics except accuracy, we compute scores by thresholding the original continuous values to obtain discrete versions of the quality metrics. The thresholds were empirically determined as follows: 0.3 for Summ, 0.5 for QA, and 0.85 for MT.

We observe similar trends to those with the PRR metric. RAUQ significantly outperforms all other methods for summarization and MT tasks. For QA, RAUQ is the best method for Llama-3.1 8B and Falcon-3 10B, while performing comparably to computationally intensive sampling-based approaches for other models. Overall, RAUQ achieves a 3.7% improvement over the second-best method (MSP) across all evaluated models.

Table 8: Mean ROC-AUC↑ across tasks for the evaluated LLMs. Warmer color indicates better results.

UO Method	L	ama-3.1 8			wen-2.5 7		G	emma-2 9			alcon-3 10		Mean
- Withou	QA	Summ	MT	QA	Summ	MT	QA	Summ	MT	QA	Summ	MT	Wican
MSP	.711	.528	.686	.700	.611	.685	.746	.547	.683	.721	.549	.688	.655
Perplexity	.701	.420	.690	.705	.477	.713	.735	.420	.699	.713	.477	.715	.622
CCP	.685	.525	.648	.668	.579	.658	.729	.536	.646	.703	.518	.657	.629
Attention Score	.497	.508	.553	.522	.507	.540	.519	.532	.543	.534	.482	.539	.523
Focus	.698	.475	.663	.642	.519	.682	.747	.463	.684	.699	.496	.672	.620
Simple Focus	<u>.718</u>	.524	<u>.694</u>	.703	.564	.700	.753	.530	.706	<u>.724</u>	.508	.691	.651
DegMat NLI Score entail.	.676	.549	.618	.691	.574	.637	.692	.558	.636	.700	.515	.620	.622
Ecc. NLI Score entail.	.659	.508	.630	.682	.523	.650	.678	.514	.642	.688	.509	.648	.611
EVL NLI Score entail.	.668	.547	.610	.688	.573	.630	.690	.557	.632	.703	.526	.612	.620
Lexical Similarity Rouge-L	.659	.534	.660	.687	.555	.677	.684	.548	.668	.673	.522	.646	.626
EigenScore	.643	.538	.629	.675	.508	.655	.658	.547	.614	.662	.526	.623	.607
LUQ	.667	.558	.618	.688	.532	.613	.690	.575	.629	.687	.542	.599	.616
Semantic Entropy	.661	.528	.658	.680	.595	.665	.683	.555	.661	.706	.530	.666	.632
SAR	.696	.556	.692	.708	.557	.710	.723	.551	.710	.712	.522	.670	.650
Semantic Density	.694	.517	.628	.705	.528	.635	.711	.521	.617	.721	.506	.624	.617
RAUQ	.724	.637	.713	.705	.636	.715	<u>.752</u>	.667	.718	.726	.585	.727	.692

D.2 Comparison with Supervised Methods

We compare our method against several state-of-the-art supervised methods that leverage hidden states or attention weights: Factoscope [20], SAPLMA [1], MIND [41], Sheeps [6], LookBack Lens [8], SATRMD+MSP [45], and TAD [44]. We evaluate these methods in two scenarios: in-domain, where the model is trained directly on the target task, and out-of-domain, where the model is trained on all datasets except one, which is held out for testing. Tables 9 and 10 show the performance of supervised methods in the in-domain and out-of-domain settings respectively.

The results show that in the in-domain experimental setup, supervised methods leveraging attention-based features, such as TAD and LookBackLens, outperform the RAUQ method. Methods that leverage hidden states, such as MIND and Sheeps, achieve performance comparable to RAUQ on average but underperform on summarization tasks. In contrast, in the out-of-domain experimental setup, RAUQ substantially outperforms on average all supervised methods, which experience a significant performance drop. Our method, however, maintains consistent performance due to its unsupervised nature.

Overall, RAUQ approaches the performance of most supervised methods in in-domain settings, underperforming only those based on attention, while requiring no access to the training dataset. In out-of-domain settings, RAUQ demonstrates a strong advantage, substantially outperforming all supervised approaches.

Table 9: Comparison with supervised methods by PRR \uparrow for the Llama 8b v3.1 model in the indomain setup across each dataset. The best method is in **bold**, the second best is <u>underlined</u>. Warmer color indicates better results.

UQ Method	XSum	SamSum	CNN	WMT19	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
Factoscope	250	.033	.086	.120	.064	.033	.313	.363	.585	.121	.147
SAPLMA	.259	.420	.082	.548	.252	002	.399	.399	.456	.358	.317
MIND	.482	.415	.187	.451	.373	.263	.499	.517	.727	.570	.448
Sheeps	240	.326	.260	.509	.370	.423	.552	.594	<u>.723</u>	.604	.412
LookBackLens	.665	<u>.535</u>	.284	.613	.471	.341	.542	.497	.718	.525	.519
SATRMD+MSP	.712	.399	.192	.475	.363	.333	.581	.561	.704	.528	.485
TAD	.631	.551	.301	<u>.588</u>	<u>.434</u>	.293	.537	.601	.695	.552	<u>.518</u>
RAUQ	.566	.269	<u>.290</u>	.509	.399	.265	.506	.522	.549	.323	.420

Table 10: Comparison with supervised methods by PRR \uparrow for the Llama 8b v3.1 model in the out-of-domain setup across each dataset. The best method is in **bold**, the second best is <u>underlined</u>. Warmer color indicates better results.

UQ Method	XSum	SamSum	CNN	WMT19	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
Factoscope	031	.078	003	.083	.036	.014	.084	017	.007	040	.021
SAPLMA	132	.161	.107	029	056	020	010	.224	000	.152	.040
MIND	041	.283	.085	.158	.281	.112	.166	.222	.352	.316	.193
Sheeps	.087	.220	019	.013	.410	.184	.365	.223	.535	.310	.233
LookBackLens	188	.062	019	018	.220	.116	.285	.178	.316	.189	.114
SATRMD+MSP	770	.269	.140	<u>.364</u>	.108	.142	.190	.170	.572	.307	.149
TAD	452	.063	007	.087	.224	.143	.251	<u>.394</u>	.432	.323	.146
RAUQ	.566	.269	.290	.509	<u>.399</u>	.265	.506	.522	.549	.323	.420

E Detailed Experimental Results

The detailed experimental results across each considered dataset are presented in Tables 11 to 14 for Llama-3.1 8b, Qwen-2.5 7b, Gemma-2 9b, and Falcon-3 10b models respectively.

Table 11: Detailed PRR↑ for the Llama 8b v3.1 model across each dataset. The best method is in **bold**, the second best is underlined. Warmer color indicates better results.

UQ Method	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
MSP	073	.328	.131	.335	.459	.091	.242	.262	.459	.527	.535	.310	.300
Perplexity	005	.090	020	.344	.416	.249	<u>.377</u>	.259	.244	.506	.492	.303	.188
CCP	026	.333	.137	.317	.363	.038	.080	.210	.351	.562	.446	.306	.260
Attention Score	.100	.017	.043	.176	.179	295	.081	028	142	.067	.209	.209	.051
Focus	575	.228	.018	.306	.416	.137	.380	.211	.422	.507	.305	.278	.219
Simple Focus	313	.366	.115	.358	<u>.472</u>	.074	.187	.281	<u>.486</u>	.545	.516	.302	.283
DegMat NLI Score entail.	.221	.239	.138	.193	.285	.146	.226	.316	.429	.583	.239	.203	.268
Ecc. NLI Score entail.	.026	.029	.032	.229	.340	.102	.145	.293	.380	.530	.231	.235	.214
EVL NLI Score entail.	.213	.218	.132	.183	.252	.137	.234	.314	.371	<u>.577</u>	.230	.188	.254
Lexical Similarity Rouge-L	.063	.202	.135	.246	.403	017	.110	.277	.378	.491	.242	.273	.233
EigenScore	092	.234	.105	.252	.318	010	.079	.263	.355	.462	.192	.283	.203
LÚQ	.037	.337	.130	.204	.224	.101	.235	.303	.394	.570	.249	.158	.245
Semantic Entropy	055	.200	.083	.252	.379	.093	.107	.232	.347	.479	.157	.366	.220
SAR	.236	.314	.165	.306	.435	.107	.181	.297	.439	.552	.275	.320	.302
Semantic Density	057	.067	.119	.233	.295	.175	.302	.380	.448	.571	.237	.197	.247
RAUQ	.566	.269	.290	.394	.509	<u>.241</u>	.364	.265	.506	.522	.549	.323	.400

Table 12: Detailed PRR↑ for the Qwen 7b v2.5 model across each dataset. The best method is in **bold**, the second best is <u>underlined</u>. Warmer color indicates better results.

UQ Method	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
MSP	.406	.466	.179	.286	.451	.030	101	.291	.551	<u>.610</u>	.654	.268	.341
Perplexity	614	.170	.055	.346	.466	.131	.156	.270	.385	.601	.400	.456	.235
CCP	.209	.379	.151	.266	.388	.015	089	.215	.468	.596	.412	.281	.274
Attention Score	201	.268	.027	.136	.149	.022	023	.007	105	.078	.157	.131	.054
Focus	200	.385	.076	.308	.452	.123	.137	.249	.462	.568	.037	.273	.239
Simple Focus	.169	<u>.461</u>	.125	.302	<u>.496</u>	.021	.037	.321	.536	.620	.550	.310	.329
DegMat NLI Score entail.	.221	.202	.126	.217	.332	.122	.293	.329	<u>.540</u>	.574	.235	.402	.299
Ecc. NLI Score entail.	126	.203	.040	.243	.368	.107	.151	.294	.535	.543	.237	.386	.249
EVL NLI Score entail.	.225	.198	.120	.196	.294	.122	.294	.329	.519	.571	.236	.372	.290
Lexical Similarity Rouge-L	.022	.305	.095	.284	.370	.075	.141	.297	.507	.531	.274	.511	.284
EigenScore	063	.036	.047	.231	.374	.018	003	.281	.510	.500	.243	.537	.226
LŪQ	108	.158	.092	.161	.265	.096	.340	.337	.449	.580	.321	.331	.252
Semantic Entropy	.512	.249	.115	.268	.366	.073	.058	.265	.491	.536	.165	.380	.290
SAR	077	.261	.150	.340	.445	.088	.196	.318	.526	.585	.288	.459	.298
Semantic Density	.051	.164	.070	.225	.358	.095	.285	.386	.514	.603	.203	.381	.278
RAUQ	.663	.424	<u>.159</u>	.344	.533	.123	020	.252	.499	.608	.584	.458	.385

Table 13: Detailed PRR↑ for the Gemma 9b v2 model across each dataset. The best method is in **bold**, the second best is underlined. Warmer color indicates better results.

UQ Method	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
MSP	.002	.494	.031	.279	.484	.004	.152	.310	.501	.649	.599	.310	.318
Perplexity	949	.115	055	.362	.449	.397	.240	.314	.234	.660	.578	.256	.217
CCP	044	.468	.016	.270	.369	.028	.092	.277	.385	.633	.550	.339	.282
Attention Score	.202	.114	.045	.131	.161	150	.083	016	112	.075	.300	.268	.092
Focus	444	.203	013	.305	.465	.514	.230	.289	.434	.619	.563	.265	.286
Simple Focus	287	.425	.064	.324	<u>.521</u>	.170	.238	.335	.523	<u>.656</u>	.570	.280	.318
DegMat NLI Score entail.	.174	.200	.076	.206	.312	.167	.141	.312	.422	.619	.401	.293	.277
Ecc. NLI Score entail.	077	.025	000	.237	.343	.037	.132	.299	.419	.569	.399	.228	.218
EVL NLI Score entail.	.157	.189	.069	.202	.302	.176	.159	.304	.389	.615	.398	.284	.270
Lexical Similarity Rouge-L	.076	.193	.126	.279	.404	035	.113	.319	.395	.585	.418	.346	.268
EigenScore	.085	.135	.138	.204	.249	024	.132	.270	.359	.519	.371	.241	.223
LŪQ	.240	.303	.074	.242	.276	.222	.250	.301	.342	.618	.440	.237	.295
Semantic Entropy	.173	.196	.094	.273	.401	.083	.026	.265	.355	.551	.427	.328	.264
SAR	.091	.271	.116	.373	.455	.203	.166	.323	.362	.626	.493	.355	.320
Semantic Density	.078	014	.099	.196	.313	.272	.357	.401	.463	.654	.295	.183	.275
RAUQ	.831	.453	.129	.391	.554	.331	.257	.331	.481	.633	.628	.283	.442

Table 14: Detailed PRR \uparrow for the Falcon 10b v3 model across each dataset. The best method is in **bold**, the second best is <u>underlined</u>. Warmer color indicates better results.

UQ Method	XSum	SamSum	CNN	WMT14	WMT19	MedQUAD	TruthfulQA	CoQA	SciQ	TriviaQA	MMLU	GSM8k	Mean
MSP	058	.400	.182	.269	.396	004	001	.300	.459	<u>.674</u>	.621	.364	.300
Perplexity	910	.330	.141	.355	.524	.266	.209	.276	.158	.660	.617	.307	.244
CCP	141	.246	.094	.249	.325	041	002	.259	.349	.653	.533	.339	.239
Attention Score	380	.098	.010	.113	.064	037	024	034	073	.109	.226	.210	.024
Focus	387	.224	.141	.262	.463	.123	.208	.218	.304	.656	.486	.195	.241
Simple Focus	510	.307	.146	.313	.457	.005	.160	.325	.388	.680	.603	.294	.264
DegMat NLI Score entail.	.046	.238	020	.140	.304	.115	.203	.326	.391	.617	.418	.391	.264
Ecc. NLI Score entail.	092	.243	020	.203	.360	.097	.066	.298	.432	.593	.437	.368	.249
EVL NLI Score entail.	.214	.220	015	.131	.281	.111	.204	.319	.436	.618	.403	.366	.274
Lexical Similarity Rouge-L	240	.272	.068	.211	.339	.035	.087	.306	.238	.595	.454	.281	.221
EigenScore	078	.056	.091	.177	.294	067	.104	.283	.336	.542	.357	.173	.189
LÚQ	.206	.172	.048	.126	.265	.127	.237	.307	.270	.622	.423	.358	.263
Semantic Entropy	048	.152	.146	.222	.361	.026	.102	.301	.379	.587	.462	.381	.256
SAR	277	.282	.096	.256	.419	.070	.180	.308	.253	.650	.514	.364	.259
Semantic Density	244	.269	.067	.208	.352	.075	.272	.350	.524	.620	.352	.314	.263
RAUQ	.541	.277	.131	.376	.553	.224	.110	.292	<u>.474</u>	.674	.626	.344	.385

F Additional Examples

We provide more examples of attention maps, similar to the Figure 1, in Figures 6 to 9. These examples show that the similar patterns exist for several text instances.

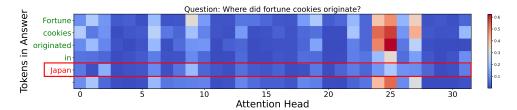


Figure 6: Attention weights in the 30th layer of Llama 3.1 8B from each generated token to its preceding token, given the prompt *Where did fortune cookies originate?*. The y axis specifies the generated tokens, and the x axis specifies the attention heads. Warmer colors indicate higher attention values. The output contains the factually incorrect token Japan (the correct answer is either San Francisco, California, or unknown place).

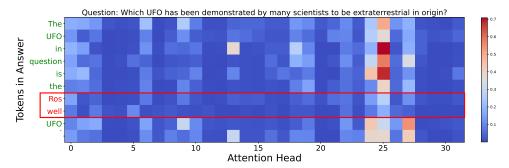


Figure 7: Attention weights in the 30th layer of Llama 3.1 8B from each generated token to its preceding token, given the prompt *Which UFO has been demonstrated by many scientists to be extraterrestrial in origin?*. The *y* axis specifies the generated tokens, and the *x* axis specifies the attention heads. Warmer colors indicate higher attention values. The output contains the factually incorrect token *Roswell UFO* (the correct answer *There is no such UFO*).

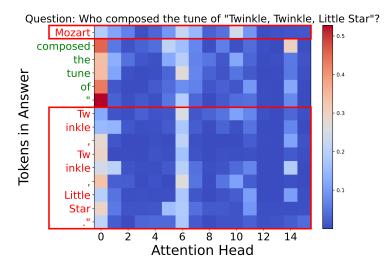


Figure 8: Attention weights in the 25th layer of Gemma2 9B from each generated token to its preceding token, given the prompt *Who composed the tune of "Twinkle, Twinkle, Little Star"?*. The y axis specifies the generated tokens, and the x axis specifies the attention heads. Warmer colors indicate higher attention values. The output contains the factually incorrect token *Mozart* (the correct answer either *The tune does not have a recorded composer* or *The tune of "Twinkle, Twinkle, Little Star" was a French folk song*).

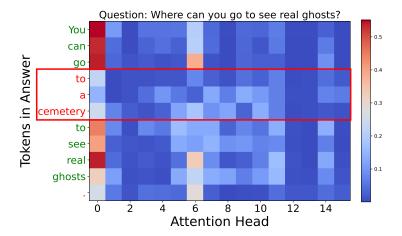


Figure 9: Attention weights in the 25th layer of Gemma2 9B from each generated token to its preceding token, given the prompt *Where can you go to see real ghosts?*. The y axis specifies the generated tokens, and the x axis specifies the attention heads. Warmer colors indicate higher attention values. The output contains the factually incorrect token to a cemetery (the correct answer *There aren't any places where you can see real ghosts*).

G Limitations

Our approach is unsupervised and involves only a single hyperparameter. While we demonstrate that a predefined value yields robust performance across various tasks, fine-tuning this parameter for specific datasets could lead to further improvements, which would require a validation set. Additionally, our method relies on access to the attention weights of LLMs and is therefore applicable only to white-box models. Further investigation could explore whether this technique can be effectively applied to black-box LLMs when combined with a supplementary white-box LLM.

H Broader Impact

In this work, we propose RAUQ, a plug-and-play method for real-time hallucination detection in white-box LLMs that requires no task-specific labels or multiple samples. RAUQ is efficient, easy to integrate, and demonstrates significant performance improvements over baseline methods in our experiments. We believe that our work is a meaningful step toward more trustworthy and responsible use of LLMs, particularly in safety-critical domains such as healthcare and legal documentation. In our experiments, we considered open-source LLMs and datasets not aimed at harmful content. Furthermore, our approach poses no negative social impact, as it does not rely on sensitive data, user annotations, or other elements that might raise ethical concerns.