Knowledge Boundary of Large Language Models: A Survey

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Abstract

Although large language models (LLMs) store vast amount of knowledge in their parameters, they still have limitations in the memorization and utilization of certain knowledge, leading to undesired behaviors such as generating untruthful and inaccurate responses. This highlights the critical need to understand the knowledge boundary of LLMs, a concept that remains inadequately defined in existing research. In this survey, we propose a comprehensive definition of the LLM knowledge boundary and introduce a formalized taxonomy categorizing knowledge into four distinct types. Using this foundation, we systematically review the field through three key lenses: the motivation for studying LLM knowledge boundaries, methods for identifying these boundaries, and strategies for mitigating the challenges they present. Finally, we discuss open challenges and potential research directions in this area. We aim for this survey to offer the community a comprehensive overview, facilitate access to key issues, and inspire further advancements in LLM knowledge research.

1 Introduction

Large language models (LLMs) store extensive knowledge within their parameters, enabling impressive performance across a wide range of tasks. However, LLMs have been criticized for significant issues related to the memorization and utilization of knowledge, such as generating responses that contain untruthful information (Ji et al., 2023), being misled by untruthful context (Wang et al., 2023a), or lacking precision to unclear queries (Zhang et al., 2024f). In light of this, recent studies have introduced the concept of LLM knowledge boundary (Yin et al., 2024), defining knowledge types based on the LLM's performance in knowledge question answering (QA). Understanding the knowledge boundary is crucial for ensuring the trustworthy deployment of LLMs.

We identify the major limitations in existing definitions of the LLM knowledge boundary. Firstly, the Know-Unknow Quadrant (Yin et al., 2023; Amayuelas et al., 2024) categorizes knowledge based on the LLM's possession and the LLM's awareness of such knowledge, but this definition is conceptual and lacks formalization. Besides, Yin et al. (2024) introduce a formalized definition separating the influence of the prompt from the LLM's mastery of the knowledge, yet they merely focus on the knowledge boundary of a specific LLM which lacks comprehensiveness. Additionally, some recent surveys (Li et al., 2024d; Wen et al., 2024b) also discuss certain topics related to the LLM knowledge boundary. However, Li et al. (2024d) lack a clear and formalized definition, and Wen et al. (2024b) merely focus on the abstention strategy for handling knowledge limitation. These limitations hinder a thorough and nuanced understanding of the LLM knowledge boundary.

To address these limitations, we propose a comprehensive and formalized definition of the knowledge boundary of LLMs. Our definition classifies knowledge from three dimensions: 1) whether the knowledge is known to human and expressible in textual QA form (***Universal Knowledge Boundary***), 2) whether it is abstractly embedded within the LLM's parameters (***Parametric Knowledge Boundary***), and 3) whether it is empirically validated on the LLM (***Outward Knowledge Boundary***). Based on these knowledge boundaries, we establish a formal four-type knowledge taxonomy to classify and define each knowledge type (§ 2).

Building on our proposed definition, we systematically review related research. Our survey is organized around three key research questions. First, we address ***RQ1: Why study knowledge boundaries?***, by detailing the LLMs' undesirable behaviors that stem from their unawareness of knowledge boundaries (§ 3). Next, we explore ***RQ2: How can knowledge boundaries be identified?***, highlighting

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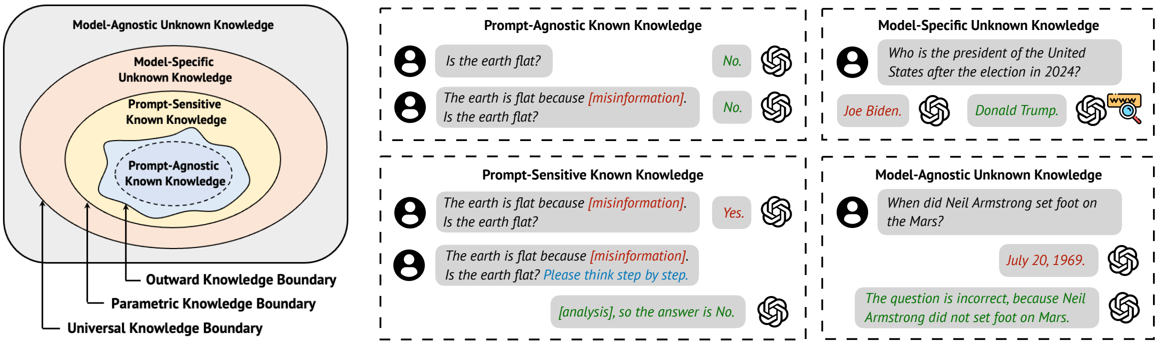

Is the earth flat? — No.

The earth is flat because [misinformation]. Is the earth flat? — No.

Who is the president of the United States after the election in 2024? — Joe Biden. — Donald Trump.

The earth is flat because [misinformation]. Is the earth flat? — Yes.

The earth is flat because [misinformation]. Is the earth flat? Please think step by step. — [analysis], so the answer is No.

When did Neil Armstrong set foot on the Mars? — July 20, 1969. — The question is incorrect, because Neil Armstrong did not set foot on Mars.

(a) Taxonomy of Knowledge Boundary

(b) Example Queries with Different Types of Knowledge

Figure 1: Illustration of the knowledge boundaries and knowledge taxonomy of LLM. The dashed circle in (a) represents the “truly” prompt-agnostic known knowledge k, which can be verified by any expression in Q_k. In practice, however, the prompt-agnostic nature of k can only be approximated using a limited subset $\hat{Q}_k \subseteq Q_k$. As a result, the outward knowledge boundary is depicted with an irregularly shaped line to reflect this approximation.

uncertainty, calibration and probing techniques to distinguish different knowledge types (§ 4). Furthermore, we investigate ***RQ3: How can issues caused by knowledge boundaries be mitigated?***, summarizing strategies to enhance the task performance and foster desired behaviors for each knowledge type (§ 5).

Finally, we discuss the open challenges and prospective directions for advancing the understanding of the LLM knowledge boundary. First, we advocate for more comprehensive benchmarks to assess knowledge boundaries across various types of knowledge limitations. Second, we emphasize the need for the generalization of knowledge boundary identification across domains and consider the potential utilization of LLM knowledge boundaries in future developments of LLMs. Lastly, we address unintended side effects of mitigation strategies, including over-refusal of knowledge within the boundaries and unnecessary costs incurred by implementing these strategies. The overview of this survey and related datasets are presented in Appendix A and B, respectively.

2 Definition of Knowledge Boundary

To mitigate the shortcomings of existing definitions, we provide a more complete and formalized definition of the knowledge boundary for LLMs. Formally, we denote $\mathcal{K}$ as the whole set of abstracted knowledge that is known to human, and k as a piece of knowledge that can be expressed by a set of input-output pairs $Q_k = \{(q_k^i, a_k^i)\}_i$. Let θ represent the parameters of a specific LLM. As shown in Figure 1, we define three types of knowledge boundaries for LLMs where one subsumes another:

- ***Outward Knowledge Boundary*** defines the observable knowledge boundary for a specific LLM. The knowledge verification is usually conducted on a limited available subset of expressions $\hat{Q}_k \subseteq Q_k$. Knowledge within this boundary refers to the knowledge that the LLM can generate correct outputs for the input for all instances in $\hat{Q}_k$.
- ***Parametric Knowledge Boundary*** defines the abstract knowledge boundary for a specific LLM. Knowledge within this boundary is possessed in the LLM parameters, which could be verified by at least one expression in Q_k.
- ***Universal Knowledge Boundary*** defines the whole set of knowledge known to human, which is verifiable by certain input-output pairs in Q_k.

Divided by the knowledge boundaries, four types of knowledge are defined as below. Figure 1 presents example queries with each type of knowledge.

- **Prompt-Agnostic Known Knowledge** (`PAK`) can be verified by all expressions in $\hat{Q}_k$ for the LLM θ regardless of the prompt, *i.e.,* the predicted output probability is larger than a threshold ϵ.

$$\mathcal{K}_{\mathsf{PAK}} = \{k \in \mathcal{K} | \forall (q_k^i, a_k^i) \in \hat{Q}_k, P_\theta(a_k^i | q_k^i) > \epsilon\} \quad (1)$$

- **Prompt-Sensitive Known Knowledge** (`PSK`) resides within the LLM's parameters but is sensitive to the form of the prompt. While certain expressions in $\hat{Q}_k$ may fail to verify this type of knowledge, appropriate expressions in Q_k can be found for successful verification.

$$\begin{aligned}\mathcal{K}_{\mathsf{PSK}} = \{k \in \mathcal{K} | (\exists (q_k^i, a_k^i) \in Q_k, P_\theta(a_k^i | q_k^i) > \epsilon) \\ \wedge (\exists (q_k^i, a_k^i) \in \hat{Q}_k, P_\theta(a_k^i | q_k^i) < \epsilon)\}\end{aligned} \quad (2)$$

- **Model-Specific Unknown Knowledge** (`MSU`) is not possessed in the specific LLM parameters θ, thus cannot be verified by any instance in Q_k for the LLM, but the knowledge itself is known to human, *i.e.,* Q_k is non-empty.

$$\mathcal{K}_{\mathsf{MSU}} = \{k \in \mathcal{K} | \forall (q_k^i, a_k^i) \in Q_k, P_\theta(a_k^i | q_k^i) < \epsilon\} \quad (3)$$

- **Model-Agnostic Unknown Knowledge** (MAU) is unknown to human (*i.e.*, Q_k is empty), thus unverifiable regardless of the model.

$$K_{\mathsf{MAU}} = \{k \in \mathcal{K} | Q_k = \emptyset\} \quad (4)$$

Summary & Ideas - Definition of Knowledge Boundary

- We provide a formalized definition for LLM knowledge boundaries, and define a four-type knowledge taxonomy accordingly.
- Our knowledge taxonomy can also be adapted to the Know-Unknow Quadrant (Yin et al., 2023; Amayuelas et al., 2024), where PAK and PSK can be viewed as a form of the known-knowns and the unknown-knowns respectively, while MSK and MAK jointly formulate the known-unknowns.

💡 We do not explicitly define the unknown-unknown, since it is largely underexplored in the study of LLM knowledge. Future research can further explore the unknown-unknowns for LLMs and humans.

3 Undesired Behaviours

We first address ***RQ1: Why study knowledge boundaries?*** Due to the unawareness of knowledge boundary, LLMs exhibit various undesired behaviors that compromise the reliability and utility of their outputs, including *factuality hallucinations*, *untruthful responses misled by the context*, and *truthful but undesired responses*, posing challenges for the successful applications of LLMs.

3.1 Factuality Hallucinations

Factuality hallucinations (Huang et al., 2023a) in LLMs occur when the model output diverges from real-world facts, which typically stem from the deficiency in the model's domain-specific knowledge, outdated knowledge encoded within the model, and overconfidence in addressing unknowns.

Deficiency of Domain-specific Knowledge LLMs, primarily trained on broad, publicly accessible datasets, often lack detailed knowledge in specialized domains, leading to inaccuracies in domain-specific queries. For example, ChatGPT often issues incorrect or imprecise biomedical advice (Pal et al., 2024), and misrepresents legal facts or arguments (Dahl et al., 2024). Similar issues arise in medical (Pal et al., 2023) and financial contexts (Kang and Liu, 2024), where LLMs exhibit hallucinations due to insufficient domain-specific knowledge.

Outdated Knowledge A significant limitation of LLMs is their reliance on outdated information, as their training data is bounded by temporal limitations. Without mechanisms to update their internal knowledge, LLMs struggle to adapt to new developments, often resorting to fabricating facts or using outdated responses (Onoe et al., 2022; Kasai et al., 2023). For instance, LLaMA2 (Touvron et al., 2023), despite its recent training cutoffs (e.g., 2022), tends to use data from earlier years (e.g., 2019) (Zhao et al., 2024a). Recent studies like Cheng et al. (2024a) highlight these temporal knowledge cutoffs, revealing the scope of outdated information in LLMs.

Overconfidence on Unknown Knowledge LLMs often show overconfidence when addressing topics beyond their knowledge, delivering assertive but incorrect responses. This tendency is partly due to the limited generalization of their reward systems which overfit familiar data and neglect less-known subjects, thus leading to amplifying overconfident outputs (Yan et al., 2024). LLMs also lack mechanisms to indicate uncertainty or acknowledge knowledge limits, which exacerbates the issue of overconfidence. Studies have shown that LLMs perform poorly on unfamiliar topics while maintaining high confidence (Agarwal et al., 2023; Deng et al., 2024).

3.2 Untruthful Responses Misled by Context

Even though LLMs possess the required knowledge, they often produce untruthful responses when misled by context, which occurs in two forms: *untruthful context*, where the context includes false or misleading information, and *irrelevant context*, where extraneous details divert the model from generating precise responses.

Untruthful Context Incorporating false information into the context significantly biases LLMs, severely impacting their performance (Chen et al., 2024a; Pan et al., 2023). Using in-context learning (ICL) allows for editing factual knowledge in LLMs, which may lead to varied factual outputs (Zheng et al., 2023a). When faced with untruthful views, LLMs often fail to stay true, being swayed by persuasive tactics despite initially correct responses (Wang et al., 2023a; Xu et al., 2024b).

Irrelevant Context Irrelevant context can dramatically affect LLMs, leading to off-topic or inaccurate responses. Irrelevant details in problem descriptions or retrieval systems drastically undermine model performance (Shi et al., 2023). When such information is semantically related to the context, it exacerbates this effect, causing LLMs to overlook crucial information and reduce response accuracy (Wu et al., 2024b).

3.3 Truthful but Undesired Responses

LLMs sometimes produce accurate yet improper responses when handling certain knowledge, leading to answers misaligned with user expectations.

Random Responses to Ambiguous Knowledge Ambiguous knowledge challenges LLMs' understanding, often leading them to guess responses due to their inability to recognize ambiguities (Liu et al., 2023; Zhang et al., 2024f). They typically provide arbitrary answers to unclear queries (Deng et al., 2023b), or generate a mix of low-probability correct answers and incorrect answers to semi-open-ended queries (Wen et al., 2024c).

Biased Responses to Controversial Knowledge Controversial knowledge involves subjective questions with varied answers depending on individual perspectives (Wang et al., 2024e; Amayuelas et al., 2024). These reveal biases in LLMs trained on skewed datasets, leading to partiality in responses. Such bias may cause unfair emphasis on certain viewpoints or stereotypical portrayals of demographics, exacerbating disparities (Singh et al., 2024; Naous et al., 2024).

Summary & Ideas - Undesired Behaviors

- Due to the unawareness of knowledge boundaries, LLMs often exhibit factuality hallucinations caused by outdated or insufficient domain knowledge and overconfidence on unknown knowledge, are susceptible to being misled by untruthful or irrelevant context, and produce random or biased responses that don't align with user expectations.

💡 Despite their strong relevance to the knowledge boundary of LLMs, existing studies fail to analyze or address these undesired behaviours through the lens of knowledge boundary, which can provide insights into their underlying causes and help develop strategies to mitigate their impact.

4 Identification of Knowledge Boundary

We then delve into ***RQ2: How to identify knowledge boundaries?*** We categorize the existing solutions into three types: *uncertainty estimation*, *confidence calibration*, and *internal state probing*.

4.1 Uncertainty Estimation

Uncertainty estimation (UE) aims to quantify the uncertainty of a model regading its predictions for a given input. High uncertainty indicates that the model is unlikely to produce correct predictions to the input, thus the input-related knowledge lies outside of certain knowledge boundaries of the model. UE has been widely studied on NLP models (Hu et al., 2023). In the era of LLMs, we highlight the following three groups of studies.

Uncertainty Decomposition The uncertainty of LLM can be decomposed into *epistemic uncertainty* and *aleatoric uncertainty* (Hou et al., 2024). *Epistemic uncertainty* refers to the model-specific uncertainty, quantifying the lack of model knowledge, which is related to our definition of ***Parametric Knowledge Boundary***. *Aleatoric uncertainty* refers to the data-level uncertainty, such as ambiguous prompts having multiple valid answers, referring to the gap between ***Outward Knowledge Boundary*** and ***Parametric Knowledge Boundary***. Quantifying these types of uncertainty can help to identify different approaches for mitigating the knowledge limitations (Section 5). Solutions to quantify the two types of uncertainty can be roughly classified into data-side and model-side approaches, where one type of uncertainty can be obtained by subtracting the other type from the total uncertainty. The data-side quantification include input-side clarification and perturbation (Hou et al., 2024; Ling et al., 2024; Gao et al., 2024), and output-side variation estimation (Yadkori et al., 2024; Aichberger et al., 2024). The model-side quantification include model parameter and configuration perturbation (Ling et al., 2024) and model internal states perturbation (Ahdritz et al., 2024).

However, many other current approaches of UE do not distinguish the two types of uncertainty and focus on the general identification of the ***Outward Knowledge Boundary***, detailed as below.

Token Probability-based Uncertainty Estimation Stemming from the traditional UE, the straightforward token probability-based UE computes the average token probability or the entropy of the LLM predictions as the uncertainty (Manakul et al., 2023; Huang et al., 2023b). Detailed designs involve considering different granularities of the predictions beyond token-level, such as sentence-level (Duan et al., 2023) and atomic fact-level (Fadeeva et al., 2024), weighted by the relevance of different components (Duan et al., 2023).

Semantic-based Uncertainty Estimation The token probability-based UE are unsuitable for proprietary LLMs, and might be insufficient in quantifying the semantic uncertainty of LLM predictions. Therefore, the semantic-based UE is proposed, roughly categorized into *consistency-based methods* and *verbalized methods*. The ***consistency-based methods*** view the inconsistency among multiple sampled predictions of the input as the uncertainty. The approaches to measure the semantic consistency of the sampled outputs include the semantic distance calculated by smaller models (Kuhn et al., 2023; Lin et al., 2024; Zhao et al., 2024c; Nikitin et al., 2024; Manakul et al., 2023), and the consistency in the LLM evaluation (Chen and Mueller, 2024; Manakul et al., 2023). The ***verbalized methods*** aim to enable LLMs to express their uncertainty directly as output tokens. Zhou et al. (2024) reveal that LLMs are reluctant to verbally express their uncertainty, possibly related to the lack of uncertainty expression in the training data. Lin et al. (2022a) and Chaudhry et al. (2024) adopt ICL and fine-tuning approaches to teach LLMs to generate uncertainty expressions.

4.2 Confidence Calibration

Calibration refers to the alignment between the estimated LLM confidence and the actual prediction correctness. This type of approach evaluates the confidence level of the LLM in a certain prediction. Low confidence suggests potential inaccurate prediction, indicating that the LLM may lack certain knowledge. We categorize existing methods into *prompt-based* and *fine-tuning* approaches.

4.2.1 Prompt-based Calibration

Prompting LLMs to elicit confidence This approach generally uses the prediction probability as a measure of the LLM confidence, estimated by the frequency of the prediction among multiple sampled predictions of the same input (Si et al., 2023; Wang et al., 2023b), or by the probability of the prediction being evaluated as correct by LLMs (Kadavath et al., 2022). Techniques to improve calibration include prompt ensemble (Jiang et al., 2023a), hybrid approach (Chen and Mueller, 2024), fidelity evaluation (Zhang et al., 2024d), and model ensemble (Shrivastava et al., 2024; Feng et al., 2024).

Prompting LLMs to express confidence This approach enables LLMs to directly generate the confidence as tokens in the prediction. Prompting RLHF-LLMs to express confidence can achieve better calibration than using token probability (Tian et al., 2023), and prompting LLMs to generating explanations can further be leveraged to enhance calibration (Zhao et al., 2024b; Li et al., 2024c). Combination with the former prompting approach can further improve performance (Xiong et al., 2024b).

4.2.2 Fine-tuning for Calibration

The fine-tuning methods involve self-updating the LLM parameters and tuning additional models for calibration. The self-update involves instruction tuning for confidence expression (Tao et al., 2024), and learning to adjust the output token probabilities (Liu et al., 2024d; Xie et al., 2024). Additional models can be trained for adjusting the LLM output probability towards calibration (Shen et al., 2024), or directly evaluating the correctness and estimating the confidence level of the LLM outputs (Mielke et al., 2022; Stengel-Eskin et al., 2024).

4.3 Internal State Probing

The internal states of LLM contain information related to the knowledge boundary. Linear probing on the internal states can be used to assess the factual accuracy of the LLM predictions (Li et al., 2024a; Azaria and Mitchell, 2023; Burns et al., 2023; Kossen et al., 2024), thus detecting the knowledge boundaries. The internal states involve attention heads (Li et al., 2024a), hidden layer activations (Azaria and Mitchell, 2023; Ji et al., 2024; Burns et al., 2023), neurons and tokens (Ji et al., 2024). Marks and Tegmark (2023) validate the rationality of the linear probes. Moreover, Liu et al. (2024b) and Marks and Tegmark (2023) study the the generalization ability of the probing method.

Summary & Ideas - Identification of Knowledge Boundary

- Most of the existing identification approaches target at the the outward knowledge boundary, while the uncertainty decomposition is also concerned about the parametric knowledge boundary.
- Uncertainty estimation and confidence calibration are effective for identifying the knowledge boundary via estimating prediction correctness.
- The internal states of LLMs contain information to the factuality of the prediction, which can be revealed via linear probing.

💡 Identification approaches should be designed for different knowledge boundaries, suiting different mitigation approaches.

5 Mitigation

Following the identification of knowledge boundaries, we discuss ***RQ3: How to mitigate the issues caused by the knowledge boundaries?*** This section is organized following our knowledge taxonomy.

5.1 Prompt-sensitive Known Knowledge

The undesired outputs for this type of knowledge stem from inappropriate user prompts that fail to activate the embedded knowledge within the LLM. Accordingly, mitigation strategies typically focus on crafting suitable prompts to better leverage the LLM's knowledge, thereby improving task performance. We introduce four types of approaches as summarized in Figure 2.

5.1.1 Prompt Optimization

Optimizing the prompt phrasing is essential for the LLM knowledge utilization and improved task performance. The prompt optimization can be categorized into two areas: ***instruction optimization*** and ***demonstration optimization***.

For instruction optimization, training-free methods include search-based techniques like Monte Carlo search (Zhou et al., 2023b; Li et al., 2023a; Yang et al., 2024c), tree search (Wang et al., 2024d),

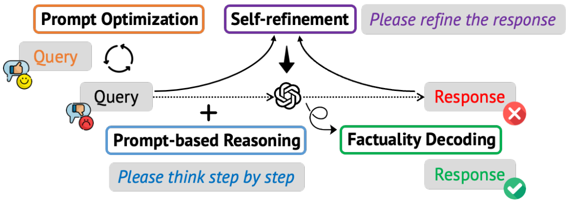

Figure 2: Summary of the mitigation techniques for prompt-sensitive known knowledge.

and searching on edit operations (Prasad et al., 2023), where the LLM is often involved as the prompt optimizer (Yang et al., 2024a; Pryzant et al., 2023; Long et al., 2024). The training-based methods typically rely on reinforcement learning to train additional modules for prompt optimization (Zhang et al., 2023a; Deng et al., 2022; Diao et al., 2023).

For demonstration optimization, the diversity and similarity of the demonstrations are crucial factors for optimization (Xu et al., 2024c). For example, the similar demonstrations are found by K-Nearest Neighbors (Liu et al., 2022a) and BM25 (Luo et al., 2023), and the diverse demonstrations are identified by support example selection (Li and Qiu, 2023) and diversity sampling (Mavromatis et al., 2023). Effective demonstrations can also be identified by training ranking models according to better LLM task performance (Li et al., 2023c; Rubin et al., 2022; Iter et al., 2023; Ye et al., 2023).

5.1.2 Prompt-based Reasoning

Prompt-based reasoning strategies are often adopted to improve the LLM knowledge utilization (Wei et al., 2022; Zhou et al., 2023a; Yao et al., 2023; Zheng et al., 2023b). For multi-step knowledge-based QA, the process generally involves individual steps such as question decomposition (Press et al., 2023), knowledge elicitation and inference (Wang et al., 2022; Jung et al., 2022; Liu et al., 2022b). External knowledge is often involved in this process to mitigate the knowledge gaps (Zhang et al., 2024c; Wu et al., 2024a; Zhao et al., 2023; Li et al., 2024e; Trivedi et al., 2023).

5.1.3 Self-refinement

The iterative self-refinement of the initial LLM prediction is also beneficial for knowledge utilization. The approaches can be broadly divided into *single-model refinement* and *multi-agent debate*. For single-model refinement, LLMs are prompted to refine the predictions under a designed evaluation and regeneration process (Madaan et al., 2024; Miao et al., 2024), or generate self-verification questions to check for prediction consistency (Manakul et al., 2023; Weng et al., 2023; Dhuliawala et al., 2024). While Huang et al. (2024) critique that LLMs struggle to achieve self-refinement without external feedback, Li et al. (2024b) show that self-estimated confidence may improve self-refinement. In multi-agent debate, the LLM plays different roles to assess and refine its predictions from multiple angles (Du et al., 2024; Fu et al., 2023).

5.1.4 Factuality Decoding

Different decoding strategies can also affect the LLM knowledge utilization, thus affecting the prediction factuality, which falls into two categories (Bi et al., 2024). The first category involves contrastive decoding against naive predictions with potential factual errors. The predictions for contrast come from smaller LLMs (Li et al., 2023b), lower layers of the LLM (Chuang et al., 2024; Chen et al., 2024b), tokens with lower predicted probabilities (Kai et al., 2024), or predictions with induced hallucination (Yang et al., 2024b; Zhang et al., 2023b). The second category leverages the truthful directions identified from LLM internal states (§ 4.3). By editing these internal representations during decoding, it steers the model towards truthful directions, thereby enhancing the factuality of predictions (Li et al., 2024a; Chen et al., 2024e; Qiu et al., 2024; Chen et al., 2024g; Zhang et al., 2024e).

Summary & Ideas - Mitigation of Prompt-sensitive Known Knowledge

- Improving the utilization of prompt-sensitivity known knowledge can be achieved from both the LLM input and output sides (*cf.* Figure 2).
- 💡 The utility of self-refinement is still an open research problem. It is a promising direction to leverage multiple LLM agents to enhance the knowledge utilization of LLMs for prediction refinement.
- 💡 Future research can focus on the possibility and rationality of reducing the prompt sensitivity towards effective LLM knowledge utilization.

5.2 Model-specific Unknown Knowledge

The mitigation of model-specific unknown knowledge focuses on bridging gaps in domain-specific or up-to-date knowledge that fall outside the models' training data. Figure 3 illustrates the mitigation strategies categorized into three key approaches.

5.2.1 External Knowledge Retrieval

External knowledge retrieval is typically used for retrieval-augmented generation (RAG), which dynamically incorporates external knowledge during inference, expanding the effective knowledge boundary of LLMs (Ren et al., 2023). Existing approaches can be divided into *pre-generation* and *on-demand* retrieval methods. ***Pre-generation*** methods (Gao et al., 2023; Shi et al., 2024; Yang et al., 2023a; Wang et al., 2023c) enhance the accuracy

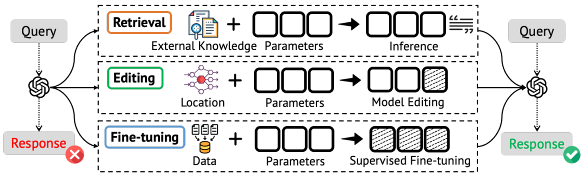

Figure 3: Summary of the mitigation techniques for model-specific unknown knowledge.

and relevance of responses by optimizing the retrieval process through methods such as refining user queries (Gao et al., 2023; Ma et al., 2023), leveraging reader performance signals (Shi et al., 2024), and incorporating intermediary components that better align the retrieved knowledge with the knowledge needs of LLM (Yang et al., 2023a; Ke et al., 2024; Wang et al., 2023c). ***On-demand*** techniques adaptively retrieve external knowledge during generation, based on the LLM's confidence on its responses (Jiang et al., 2023b), self-reflection results (Asai et al., 2024), or iterative retrieval (Shao et al., 2023). The goal is to refine the interaction between retrieved and parametric knowledge while mitigating factual gaps.

5.2.2 Parametric Knowledge Editing

Researchers also develop knowledge editing methods for altering model behaviors to modify specific parameters within the LLM without extensive retraining. According to the memory mechanism, we categorize existing knowledge editing methods into three categories: *explicit memory space*, *implicit memory space*, and *no memory space*. As for *explicit memory space*, these approaches (Mitchell et al., 2022; Zheng et al., 2023a; Madaan et al., 2022; Song et al., 2024b; Zhong et al., 2023) use a memory pool to retrieve and apply edits via prompts. As for *implicit memory space*, these approaches activate the LLM's parametric memory space based on specific input triggers, such as codebook (Hartvigsen et al., 2023), neurons (Huang et al., 2023c; Dong et al., 2022), LoRA blocks (Yu et al., 2024), and FFN side memories (Wang et al., 2024c). Another group of methods does not adopt extra memory components. Instead, they adopt various techniques to directly edit the original model parameters, such as meta learning (Tan et al., 2024) and locate-then-edit (Meng et al., 2022, 2023).

5.2.3 Knowledge-enhanced Fine-tuning

Knowledge-enhanced fine-tuning internalizes new knowledge into models by leveraging structured or synthetic representations. This involves encoding knowledge as factual records, synthetic corpora, and domain-specific taxonomies. Techniques such as fact-based encoding (Mecklenburg et al., 2024), synthetic data creation (Joshi et al., 2024), and hierarchical organization (Liu et al., 2024c) ensure comprehensive domain coverage, while interleaved generation and context-aware structuring (Zhang et al., 2024b) aim to enhance the data quality.

Summary & Ideas - Mitigation of Model-specific Unknown Knowledge

- We review three mitigation strategies for supplementing model-specific unknown knowledge, categorized by the extent of modification to the LLM's parameters. (*cf.* Figure 3).

💡 Future research could explore adaptive frameworks that integrate external retrieval with internal model updates for continuous knowledge improvement with minimal disruption.

5.3 Model-agnostic Unknown Knowledge

In addressing model-agnostic unknown knowledge, two primary strategies, *refusal* and *asking clarification questions*, can be employed to ensure that LLMs respond appropriately.

5.3.1 Refusal

Faced with queries involving model-agnostic unknown knowledge, LLMs are expected to refuse to answer for preventing misinformation. There are two primary methods for learning to refuse: *prompt-based* and *alignment-based* approaches.

Prompt-based Approaches use designed prompts that help LLMs decide whether to refuse questions about unknown knowledge. The prompts are used to evaluate if a question involves unknown content to LLM (Wen et al., 2024a; Amayuelas et al., 2024; Agarwal et al., 2023), and to express the knowledge limitations (Chen et al., 2024c). Also, LLMs can be prompted to justify their decision to decline a question (Song et al., 2024a).

Alignment-based Approaches include supervised fine-tuning and reinforcement learning approaches. Supervised methods involve creating honesty alignment datasets, such as "I don't know" datasets, to teach LLMs to admit uncertainty in responses (Yang et al., 2023b; Cheng et al., 2024b; Zhang et al., 2024a). Reinforcement learning approaches generally constructs datasets that reflect user preferences, and use them to train LLMs through reward systems to discern when to refuse questions (Cheng et al., 2024b; Tomani et al., 2024; Xu et al., 2024a).

5.3.2 Asking Clarification Questions

When LLMs encounter questions involving model-agnostic unknown knowledge, asking clarification questions is an another common strategy. This method avoids direct uncertain responses and uses proactive dialogues to refine queries (Deng et al., 2023a; Aliannejadi et al., 2021; Guo et al., 2021; Leippert et al., 2024). This is supported by specific prompt frameworks, with schemes encouraging LLMs to analyze questions deeply before responding (Deng et al., 2023b; Chen et al., 2024f). Frameworks by Kuhn et al. (2022) and Mu et al. (2023) enable LLMs to request clarifications selectively or identify unclear requirements, enhancing response accuracy. Latest methods like contrastive self-training and reward model learning help improve the quality of LLMs' questions in dialogues (Chen et al., 2024d; Andukuri et al., 2024).

Summary & Ideas - Mitigation of Model-agnostic Unknown Knowledge

- Refusal and asking clarification questions are two most widely-studied strategies for mitigating model-agnostic unknown knowledge.
- 💡 Existing refusal strategies fail to differentiate between model-specific and model-agnostic unknown knowledge, leading to a degraded user experience when the query is, in fact, answerable.
- 💡 There are certain issues about unintended side effects when inappropriately adopting these strategies, such as over-refusal and unnecessary cost (§ 6).

6 Challenges and Prospects

In this section, we discuss several significant challenges and emerging prospects along with the exploration of knowledge boundaries in LLMs.

Benchmark for Knowledge Boundary Various knowledge-based QA datasets are key benchmarks for assessing LLMs' knowledge boundaries, as summarized in Appendix B. However, determining ground truth is challenging, as failures may stem from a lack of knowledge, poor prompts, or complicated reasoning. Additionally, failing to answer a single question does not necessarily indicate whether the LLM can handle related knowledge (Yin et al., 2024). There is a pressing need for more comprehensive benchmarks to effectively evaluate the knowledge boundaries of LLMs.

Generalization of Knowledge Boundary While knowledge boundary studies are often conducted in specific domains, understanding the general knowledge boundary in LLMs is vital. The internal state probing approach has been validated with a certain generalization ability (Liu et al., 2024b), but it is still an open challenge whether trained probes can generalize well across domains as a general knowledge boundary detector, fostering refusal and input clarification in open domains. Further theoretical analysis and studies are needed to identify the existence and utility of general knowledge boundaries.

Utilization of Knowledge Boundary Estimating and understanding LLMs' knowledge boundaries should not mark the end of the process. Instead, identifying these limitations can serve as a foundation for enhancing the model's performance in mitigating queries beyond their knowledge boundaries. For instance, the utilization of model uncertainty can reduce RAG costs and minimize the risk of introducing noise from external sources (Yao et al., 2024), or enhance the preference optimization by encouraging the LLM policy to differentiate reliable or unreliable feedback (Wang et al., 2024a).

Unintended Side Effects Although the mitigation strategies mentioned above aim to improve the performance of LLMs, they can also introduce a range of unintended side effects that may compromise the utility and effectiveness of the model. In the following, we detail several of these effects, highlighting the challenges and potential trade-offs.

- **Over-refusal** occurs when models excessively avoid responding, even to valid queries within their knowledge boundaries. Studies like Varshney et al. (2023) show that techniques like "self-check" can make LLMs overly cautious, reducing their utility. Zhu et al. (2024) further explores this issue, identifying static and dynamic conflicts in training as key contributors.
- **Unnecessary Cost** arises when LLMs use strategies (*e.g.*, clarifications, RAG, or self-correction) to manage queries beyond their knowledge boundaries. Although effective in avoiding undesired behaviors, these methods often consume additional time or effort, delaying responses. For instance, clarifications increase the round of interactions (Chen et al., 2024f), while RAG can introduce noise if LLMs already possess the necessary knowledge (Asai et al., 2024).

7 Conclusions

This survey presented a comprehensive overview of the knowledge boundary of LLMs, offering a formalized taxonomy and addressing key challenges in the field. By exploring undesirable behaviors, identification techniques, and mitigation strategies, we emphasized the critical role of understanding and managing these boundaries to improve the reliability and utility of LLMs. Despite significant progress, challenges persist, including lack of comprehensive benchmarks, achieving domain generalization, potential uses of knowledge boundaries, and addressing unintended side effects. We hope this survey inspires continued exploration and innovation toward more trustworthy and reliable LLMs.

Limitations

We identify several limitations of our work.

Formal Definition of Knowledge This survey does not give a formal definition of the knowledge k, which is a critical problem in the scope of NLP research on knowledge. In this survey, we define the abstracted concept of knowledge as k, which is represented by a set of textual expressions of input and output. This definition can facilitate practical NLP experiments and efficient validation. In fact, the formal definition of knowledge is still a debatable topic, calling for future exploration. For example, Fierro et al. (2024) try to bridge the philosophical definition to the knowledge of LLMs, though significant disagreements persist among various philosophical schools of thought.

(Un)Known to Human or Models Besides, in our definition, the known knowledge for LLM lies within the universal knowledge boundary, which is the knowledge known for human. We generally believe that LLMs do not possess knowledge beyond this boundary. However, there may be outliers that LLMs have knowledge that is unknown for human, which is not clearly studied in existing research. Wang et al. (2024b) hypothesize that LLMs may create new knowledge, but the creation may be unreliable, remaining an open question.

References

Vaibhav Adlakha, Shehzaad Dhuliawala, Kaheer Suleman, Harm de Vries, and Siva Reddy. 2022. TopiOCQA: Open-domain conversational question answering with topic switching. *Transactions of the Association for Computational Linguistics*, 10:468–483.

Ayushi Agarwal, Nisarg Patel, Neeraj Varshney, Mihir Parmar, Pavan Mallina, Aryan Bhavin Shah, Srihari Raju Sangaraju, Tirth Patel, Nihar Thakkar, and Chitta Baral. 2023. Can NLP models 'identify', 'distinguish', and 'justify' questions that don't have a definitive answer? In *TrustNLP Workshop at ACL 2023*.

Gustaf Ahdritz, Tian Qin, Nikhil Vyas, Boaz Barak, and Benjamin L. Edelman. 2024. Distinguishing the knowable from the unknowable with language models. In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net.

Lukas Aichberger, Kajetan Schweighofer, Mykyta Ielanskyi, and Sepp Hochreiter. 2024. How many opinions does your LLM have? improving uncertainty estimation in NLG. In *ICLR 2024 Workshop on Secure and Trustworthy Large Language Models*.

Mohammad Aliannejadi, Julia Kiseleva, Aleksandr Chuklin, Jeff Dalton, and Mikhail Burtsev. 2021. Building and evaluating open-domain dialogue corpora with clarifying questions. In *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing, EMNLP 2021, Virtual Event / Punta Cana, Dominican Republic, 7-11 November, 2021*, pages 4473–4484. Association for Computational Linguistics.

Alfonso Amayuelas, Kyle Wong, Liangming Pan, Wenhu Chen, and William Yang Wang. 2024. Knowledge of knowledge: Exploring known-unknowns uncertainty with large language models. In *Findings of the Association for Computational Linguistics, ACL 2024, Bangkok, Thailand and virtual meeting, August 11-16, 2024*, pages 6416–6432. Association for Computational Linguistics.

Chinmaya Andukuri, Jan-Philipp Fränken, Tobias Gerstenberg, and Noah D. Goodman. 2024. Star-gate: Teaching language models to ask clarifying questions. *CoRR*, abs/2403.19154.

Akari Asai, Zeqiu Wu, Yizhong Wang, Avirup Sil, and Hannaneh Hajishirzi. 2024. Self-rag: Learning to retrieve, generate, and critique through self-reflection. In *The Twelfth International Conference on Learning Representations, ICLR 2024, Vienna, Austria, May 7-11, 2024*. OpenReview.net.

Amos Azaria and Tom M. Mitchell. 2023. The internal state of an LLM knows when it's lying. In *Findings of the Association for Computational Linguistics: EMNLP 2023, Singapore, December 6-10, 2023*, pages 967–976. Association for Computational Linguistics.

Baolong Bi, Shenghua Liu, Yiwei Wang, Lingrui Mei, and Xueqi Cheng. 2024. Is factuality decoding a free lunch for llms? evaluation on knowledge editing benchmark. *CoRR*, abs/2404.00216.

Collin Burns, Haotian Ye, Dan Klein, and Jacob Steinhardt. 2023. Discovering latent knowledge in language models without supervision. In *The Eleventh International Conference on Learning Representations*.

Arslan Chaudhry, Sridhar Thiagarajan, and Dilan Gorur. 2024. Finetuning language models to emit linguistic expressions of uncertainty. *arXiv preprint arXiv:2409.12180*.

Canyu Chen, Baixiang Huang, Zekun Li, Zhaorun Chen, Shiyang Lai, Xiongxiao Xu, Jia-Chen Gu, Jindong Gu, Huaxiu Yao, Chaowei Xiao, Xifeng Yan, William Yang Wang, Philip Torr, Dawn Song, and Kai Shu. 2024a. Can editing llms inject harm? *Preprint*, arXiv:2407.20224.

Dingwei Chen, Feiteng Fang, Shiwen Ni, Feng Liang, Ruifeng Xu, Min Yang, and Chengming Li. 2024b. Lower layer matters: Alleviating hallucination via multi-layer fusion contrastive decoding with truthfulness refocused. *arXiv preprint arXiv:2408.08769*.

Jiuhai Chen and Jonas Mueller. 2024. Quantifying uncertainty in answers from any language model and enhancing their trustworthiness. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 5186–5200.

Lida Chen, Zujie Liang, Xintao Wang, Jiaqing Liang, Yanghua Xiao, Feng Wei, Jinglei Chen, Zhenghong Hao, Bing Han, and Wei Wang. 2024c. Teaching large language models to express knowledge boundary from their own signals. *CoRR*, abs/2406.10881.

Maximillian Chen, Ruoxi Sun, Sercan Ö. Arik, and Tomas Pfister. 2024d. Learning to clarify: Multi-turn conversations with action-based contrastive self-training. *ArXiv*, abs/2406.00222.

Shiqi Chen, Miao Xiong, Junteng Liu, Zhengxuan Wu, Teng Xiao, Siyang Gao, and Junxian He. 2024e. In-context sharpness as alerts: An inner representation perspective for hallucination mitigation. In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net.

Yue Chen, Chen Huang, Yang Deng, Wenqiang Lei, Dingnan Jin, Jia Liu, and Tat-Seng Chua. 2024f. Style: Improving domain transferability of asking clarification questions in large language model powered conversational agents. In *Annual Meeting of the Association for Computational Linguistics*.

Zhiyu Chen, Wenhu Chen, Charese Smiley, Sameena Shah, Iana Borova, Dylan Langdon, Reema N Moussa, Matthew I. Beane, Ting-Hao 'Kenneth' Huang, Bryan R. Routledge, and William Yang Wang. 2021. Finqa: A dataset of numerical reasoning over financial data. *ArXiv*, abs/2109.00122.

Zhongzhi Chen, Xingwu Sun, Xianfeng Jiao, Fengzong Lian, Zhanhui Kang, Di Wang, and Chengzhong Xu. 2024g. Truth forest: Toward multi-scale truthfulness in large language models through intervention without tuning. In *Thirty-Eighth AAAI Conference on Artificial Intelligence, AAAI 2024*, pages 20967–20974. AAAI Press.

Jeffrey Cheng, Marc Marone, Orion Weller, Dawn Lawrie, Daniel Khashabi, and Benjamin Van Durme. 2024a. Dated data: Tracing knowledge cutoffs in large language models. *ArXiv*, abs/2403.12958.

Qinyuan Cheng, Tianxiang Sun, Xiangyang Liu, Wenwei Zhang, Zhangyue Yin, Shimin Li, Linyang Li, Zhengfu He, Kai Chen, and Xipeng Qiu. 2024b. Can AI assistants know what they don't know? In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net.

Yung-Sung Chuang, Yujia Xie, Hongyin Luo, Yoon Kim, James R. Glass, and Pengcheng He. 2024. Dola: Decoding by contrasting layers improves factuality in large language models. In *The Twelfth International Conference on Learning Representations*.

Matthew Dahl, Varun Magesh, Mirac Suzgun, and Daniel E Ho. 2024. Large Legal Fictions: Profiling Legal Hallucinations in Large Language Models. *Journal of Legal Analysis*, 16(1):64–93.

Mingkai Deng, Jianyu Wang, Cheng-Ping Hsieh, Yihan Wang, Han Guo, Tianmin Shu, Meng Song, Eric Xing, and Zhiting Hu. 2022. Rlprompt: Optimizing discrete text prompts with reinforcement learning. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing*, pages 3369–3391.

Yang Deng, Wenqiang Lei, Wai Lam, and Tat-Seng Chua. 2023a. A survey on proactive dialogue systems: Problems, methods, and prospects. In *Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence, IJCAI 2023*, pages 6583–6591.

Yang Deng, Lizi Liao, Liang Chen, Hongru Wang, Wenqiang Lei, and Tat-Seng Chua. 2023b. Prompting and evaluating large language models for proactive dialogues: Clarification, target-guided, and non-collaboration. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 10602–10621.

Yang Deng, Yong Zhao, Moxin Li, See-Kiong Ng, and Tat-Seng Chua. 2024. Don't just say "i don't know"! self-aligning large language models for responding to unknown questions with explanations. In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing, EMNLP 2024, Miami, FL, USA, November 12-16, 2024*, pages 13652–13673. Association for Computational Linguistics.

Shehzaad Dhuliawala, Mojtaba Komeili, Jing Xu, Roberta Raileanu, Xian Li, Asli Celikyilmaz, and Jason Weston. 2024. Chain-of-verification reduces hallucination in large language models. In *Findings of the Association for Computational Linguistics, ACL 2024, Bangkok, Thailand and virtual meeting, August 11-16, 2024*, pages 3563–3578. Association for Computational Linguistics.

Shizhe Diao, Zhichao Huang, Ruijia Xu, Xuechun Li, LIN Yong, Xiao Zhou, and Tong Zhang. 2023. Black-box prompt learning for pre-trained language models. *Transactions on Machine Learning Research*.

Qingxiu Dong, Damai Dai, Yifan Song, Jingjing Xu, Zhifang Sui, and Lei Li. 2022. Calibrating factual knowledge in pretrained language models. In *Findings of the Association for Computational Linguistics: EMNLP 2022, Abu Dhabi, United Arab Emirates, December 7-11, 2022*, pages 5937–5947. Association for Computational Linguistics.

Qingxiu Dong, Jingjing Xu, Lingpeng Kong, Zhifang Sui, and Lei Li. 2024. Statistical knowledge assessment for large language models. *Advances in Neural Information Processing Systems*, 36.

Yilun Du, Shuang Li, Antonio Torralba, Joshua B. Tenenbaum, and Igor Mordatch. 2024. Improving factuality and reasoning in language models through multiagent debate. In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net.

Jinhao Duan, Hao Cheng, Shiqi Wang, Chenan Wang, Alex Zavalny, Renjing Xu, Bhavya Kailkhura, and Kaidi Xu. 2023. Shifting attention to relevance: Towards the uncertainty estimation of large language models. *CoRR*, abs/2307.01379.

Yanai Elazar, Nora Kassner, Shauli Ravfogel, Abhilasha Ravichander, Eduard Hovy, Hinrich Schütze, and Yoav Goldberg. 2021. Measuring and improving consistency in pretrained language models. *Transactions of the Association for Computational Linguistics*, 9:1012–1031.

Ekaterina Fadeeva, Aleksandr Rubashevskii, Artem Shelmanov, Sergey Petrakov, Haonan Li, Hamdy Mubarak, Evgenii Tsymbalov, Gleb Kuzmin, Alexander Panchenko, Timothy Baldwin, Preslav Nakov, and Maxim Panov. 2024. Fact-checking the output of large language models via token-level uncertainty quantification. In *Findings of the Association for Computational Linguistics, ACL 2024, Bangkok, Thailand and virtual meeting, August 11-16, 2024*, pages 9367–9385. Association for Computational Linguistics.

Zhiwei Fei, Xiaoyu Shen, Dawei Zhu, Fengzhe Zhou, Zhuo Han, Alan Huang, Songyang Zhang, Kai Chen, Zhixin Yin, Zongwen Shen, Jidong Ge, and Vincent Ng. 2024. Lawbench: Benchmarking legal knowledge of large language models. In *Conference on Empirical Methods in Natural Language Processing*.

Shangbin Feng, Weijia Shi, Yike Wang, Wenxuan Ding, Vidhisha Balachandran, and Yulia Tsvetkov. 2024. Don't hallucinate, abstain: Identifying LLM knowledge gaps via multi-LLM collaboration. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 14664–14690, Bangkok, Thailand. Association for Computational Linguistics.

Constanza Fierro, Ruchira Dhar, Filippos Stamatiou, Nicolas Garneau, and Anders Søgaard. 2024. Defining knowledge: Bridging epistemology and large language models. In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing, EMNLP 2024, Miami, FL, USA, November 12-16, 2024*, pages 16096–16111. Association for Computational Linguistics.

Yao Fu, Hao Peng, Tushar Khot, and Mirella Lapata. 2023. Improving language model negotiation with self-play and in-context learning from ai feedback. *arXiv preprint arXiv:2305.10142*.

Luyu Gao, Xueguang Ma, Jimmy Lin, and Jamie Callan. 2023. Precise zero-shot dense retrieval without relevance labels. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 1762–1777, Toronto, Canada. Association for Computational Linguistics.

Xiang Gao, Jiaxin Zhang, Lalla Mouatadid, and Kamalika Das. 2024. Spuq: Perturbation-based uncertainty quantification for large language models. In *Proceedings of the 18th Conference of the European Chapter of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 2336–2346.

Meiqi Guo, Mingda Zhang, Siva Reddy, and Malihe Alikhani. 2021. Abg-coqa: Clarifying ambiguity in conversational question answering. In *3rd Conference on Automated Knowledge Base Construction, AKBC 2021, Virtual, October 4-8, 2021*.

Tom Hartvigsen, Swami Sankaranarayanan, Hamid Palangi, Yoon Kim, and Marzyeh Ghassemi. 2023. Aging with GRACE: lifelong model editing with discrete key-value adaptors. In *Advances in Neural Information Processing Systems 36: Annual Conference on Neural Information Processing Systems 2023, NeurIPS 2023*.

Xanh Ho, Anh-Khoa Duong Nguyen, Saku Sugawara, and Akiko Aizawa. 2020. Constructing a multi-hop qa dataset for comprehensive evaluation of reasoning steps. In *Proceedings of the 28th International Conference on Computational Linguistics*, pages 6609–6625.

Bairu Hou, Yujian Liu, Kaizhi Qian, Jacob Andreas, Shiyu Chang, and Yang Zhang. 2024. Decomposing uncertainty for large language models through input clarification ensembling. In *Forty-first International Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. OpenReview.net.

Mengting Hu, Zhen Zhang, Shiwan Zhao, Minlie Huang, and Bingzhe Wu. 2023. Uncertainty in natural language processing: Sources, quantification, and applications. *arXiv preprint arXiv:2306.04459*.

Jie Huang, Xinyun Chen, Swaroop Mishra, Huaixiu Steven Zheng, Adams Wei Yu, Xinying Song, and Denny Zhou. 2024. Large language models cannot self-correct reasoning yet. In *The Twelfth International Conference on Learning Representations*.

Lei Huang, Weijiang Yu, Weitao Ma, Weihong Zhong, Zhangyin Feng, Haotian Wang, Qianglong Chen, Weihua Peng, Xiaocheng Feng, Bing Qin, and Ting Liu. 2023a. A survey on hallucination in large language models: Principles, taxonomy, challenges, and open questions. *ArXiv*, abs/2311.05232.

Yuheng Huang, Jiayang Song, Zhijie Wang, Shengming Zhao, Huaming Chen, Felix Juefei-Xu, and Lei Ma. 2023b. Look before you leap: An exploratory study of uncertainty measurement for large language models. *arXiv preprint arXiv:2307.10236*.

Zeyu Huang, Yikang Shen, Xiaofeng Zhang, Jie Zhou, Wenge Rong, and Zhang Xiong. 2023c. Transformer-patcher: One mistake worth one neuron. In *The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023*. OpenReview.net.

Dan Iter, Reid Pryzant, Ruochen Xu, Shuohang Wang, Yang Liu, Yichong Xu, and Chenguang Zhu. 2023. In-context demonstration selection with cross entropy difference. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 1150–1162.

Ziwei Ji, Delong Chen, Etsuko Ishii, Samuel Cahyawijaya, Yejin Bang, Bryan Wilie, and Pascale Fung. 2024. LLM internal states reveal hallucination risk faced with a query. In *Proceedings of the 7th BlackboxNLP Workshop: Analyzing and Interpreting Neural Networks for NLP*, pages 88–104, Miami, Florida, US. Association for Computational Linguistics.

Ziwei Ji, Nayeon Lee, Rita Frieske, Tiezheng Yu, Dan Su, Yan Xu, Etsuko Ishii, Yejin Bang, Andrea Madotto, and Pascale Fung. 2023. Survey of hallucination in natural language generation. *ACM Comput. Surv.*, 55(12):248:1–248:38.

Mingjian Jiang, Yangjun Ruan, Sicong Huang, Saifei Liao, Silviu Pitis, Roger Baker Grosse, and Jimmy Ba. 2023a. Calibrating language models via augmented prompt ensembles. *ICML 2023 Workshop DeployableGenerativeAI*.

Zhengbao Jiang, Frank Xu, Luyu Gao, Zhiqing Sun, Qian Liu, Jane Dwivedi-Yu, Yiming Yang, Jamie Callan, and Graham Neubig. 2023b. Active retrieval augmented generation. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 7969–7992, Singapore. Association for Computational Linguistics.

Qiao Jin, Bhuwan Dhingra, Zhengping Liu, William W. Cohen, and Xinghua Lu. 2019. Pubmedqa: A dataset for biomedical research question answering. In *Conference on Empirical Methods in Natural Language Processing*.

Mandar Joshi, Eunsol Choi, Daniel S Weld, and Luke Zettlemoyer. 2017. Triviaqa: A large scale distantly supervised challenge dataset for reading comprehension. *arXiv preprint arXiv:1705.03551*.

Raviraj Joshi, Kanishk Singla, Anusha Kamath, Raunak Kalani, Rakesh Paul, Utkarsh Vaidya, Sanjay Singh Chauhan, Niranjan Wartikar, and Eileen Long. 2024. Adapting multilingual llms to low-resource languages using continued pre-training and synthetic corpus. *ArXiv*, abs/2410.14815.

Jaehun Jung, Lianhui Qin, Sean Welleck, Faeze Brahman, Chandra Bhagavatula, Ronan Le Bras, and Yejin Choi. 2022. Maieutic prompting: Logically consistent reasoning with recursive explanations. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing*, pages 1266–1279.

Saurav Kadavath, Tom Conerly, Amanda Askell, Tom Henighan, Dawn Drain, Ethan Perez, Nicholas Schiefer, Zac Hatfield-Dodds, Nova DasSarma, Eli Tran-Johnson, et al. 2022. Language models (mostly) know what they know. *arXiv preprint arXiv:2207.05221*.

Jushi Kai, Tianhang Zhang, Hai Hu, and Zhouhan Lin. 2024. SH2: self-highlighted hesitation helps you decode more truthfully. In *Findings of the Association for Computational Linguistics: EMNLP 2024, Miami, Florida, USA, November 12-16, 2024*, pages 4514–4530. Association for Computational Linguistics.

Haoqiang Kang and Xiao-Yang Liu. 2024. Deficiency of large language models in finance: An empirical examination of hallucination. In *I Can't Believe It's Not Better Workshop: Failure Modes in the Age of Foundation Models*.

Jungo Kasai, Keisuke Sakaguchi, Yoichi Takahashi, Ronan Le Bras, Akari Asai, Xinyan Yu, Dragomir Radev, Noah A. Smith, Yejin Choi, and Kentaro Inui. 2023. Realtime QA: what's the answer right now? In *Advances in Neural Information Processing Systems 36: Annual Conference on Neural Information Processing Systems 2023, NeurIPS 2023*.

Zixuan Ke, Weize Kong, Cheng Li, Mingyang Zhang, Qiaozhu Mei, and Michael Bendersky. 2024. Bridging the preference gap between retrievers and LLMs. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 10438–10451, Bangkok, Thailand. Association for Computational Linguistics.

Jannik Kossen, Jiatong Han, Muhammed Razzak, Lisa Schut, Shreshth Malik, and Yarin Gal. 2024. Semantic entropy probes: Robust and cheap hallucination detection in llms. *arXiv preprint arXiv:2406.15927*.

Lorenz Kuhn, Yarin Gal, and Sebastian Farquhar. 2022. Clam: Selective clarification for ambiguous questions with large language models. *arXiv preprint arXiv:2212.07769*.

Lorenz Kuhn, Yarin Gal, and Sebastian Farquhar. 2023. Semantic uncertainty: Linguistic invariances for uncertainty estimation in natural language generation. In *The Eleventh International Conference on Learning Representations*.

Tom Kwiatkowski, Jennimaria Palomaki, Olivia Redfield, Michael Collins, Ankur Parikh, Chris Alberti, Danielle Epstein, Illia Polosukhin, Jacob Devlin, Kenton Lee, et al. 2019. Natural questions: a benchmark for question answering research. *Transactions of the Association for Computational Linguistics*, 7:453–466.

Alina Leippert, Tatiana Anikina, Bernd Kiefer, and Josef Genabith. 2024. To clarify or not to clarify: A comparative analysis of clarification classification with fine-tuning, prompt tuning, and prompt engineering. *Proceedings of the 2024 Conference of the North*

American Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 4: Student Research Workshop).

Kenneth Li, Oam Patel, Fernanda Viégas, Hanspeter Pfister, and Martin Wattenberg. 2024a. Inference-time intervention: Eliciting truthful answers from a language model. *Advances in Neural Information Processing Systems*, 36.

Loka Li, Guangyi Chen, Yusheng Su, Zhenhao Chen, Yixuan Zhang, Eric Xing, and Kun Zhang. 2024b. Confidence matters: Revisiting intrinsic self-correction capabilities of large language models. *arXiv preprint arXiv:2402.12563*.

Moxin Li, Wenjie Wang, Fuli Feng, Yixin Cao, Jizhi Zhang, and Tat-Seng Chua. 2023a. Robust prompt optimization for large language models against distribution shifts. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 1539–1554.

Moxin Li, Wenjie Wang, Fuli Feng, Fengbin Zhu, Qifan Wang, and Tat-Seng Chua. 2024c. Think twice before trusting: Self-detection for large language models through comprehensive answer reflection. In *Findings of the Association for Computational Linguistics: EMNLP 2024, Miami, Florida, USA, November 12-16, 2024*, pages 11858–11875. Association for Computational Linguistics.

Siheng Li, Cheng Yang, Taiqiang Wu, Chufan Shi, Yuji Zhang, Xinyu Zhu, Zesen Cheng, Deng Cai, Mo Yu, Lemao Liu, Jie Zhou, Yujiu Yang, Ngai Wong, Xixin Wu, and Wai Lam. 2024d. A survey on the honesty of large language models. *arXiv preprint arXiv:2409.18786*.

Xiang Lisa Li, Ari Holtzman, Daniel Fried, Percy Liang, Jason Eisner, Tatsunori B Hashimoto, Luke Zettlemoyer, and Mike Lewis. 2023b. Contrastive decoding: Open-ended text generation as optimization. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 12286–12312.

Xiaonan Li, Kai Lv, Hang Yan, Tianyang Lin, Wei Zhu, Yuan Ni, Guotong Xie, Xiaoling Wang, and Xipeng Qiu. 2023c. Unified demonstration retriever for in-context learning. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 4644–4668.

Xiaonan Li and Xipeng Qiu. 2023. Finding support examples for in-context learning. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 6219–6235.

Xingxuan Li, Ruochen Zhao, Yew Ken Chia, Bosheng Ding, Shafiq Joty, Soujanya Poria, and Lidong Bing. 2024e. Chain-of-knowledge: Grounding large language models via dynamic knowledge adapting over heterogeneous sources. In *The Twelfth International Conference on Learning Representations*.

Stephanie Lin, Jacob Hilton, and Owain Evans. 2022a. Teaching models to express their uncertainty in words. *Trans. Mach. Learn. Res.*, 2022.

Stephanie Lin, Jacob Hilton, and Owain Evans. 2022b. Truthfulqa: Measuring how models mimic human falsehoods. In *Proceedings of the 60th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 3214–3252.

Zhen Lin, Shubhendu Trivedi, and Jimeng Sun. 2024. Generating with confidence: Uncertainty quantification for black-box large language models. *Transactions on Machine Learning Research*.

Chen Ling, Xujiang Zhao, Xuchao Zhang, Wei Cheng, Yanchi Liu, Yiyou Sun, Mika Oishi, Takao Osaki, Katsushi Matsuda, Jie Ji, et al. 2024. Uncertainty quantification for in-context learning of large language models. In *Proceedings of the 2024 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 1: Long Papers)*, pages 3357–3370.

Alisa Liu, Zhaofeng Wu, Julian Michael, Alane Suhr, Peter West, Alexander Koller, Swabha Swayamdipta, Noah A. Smith, and Yejin Choi. 2023. We're afraid language models aren't modeling ambiguity. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing, EMNLP 2023, Singapore, December 6-10, 2023*, pages 790–807. Association for Computational Linguistics.

Genglin Liu, Xingyao Wang, Lifan Yuan, Yangyi Chen, and Hao Peng. 2024a. Examining llms' uncertainty expression towards questions outside parametric knowledge. *Preprint*, arXiv:2311.09731.

Jiachang Liu, Dinghan Shen, Yizhe Zhang, William B Dolan, Lawrence Carin, and Weizhu Chen. 2022a. What makes good in-context examples for gpt-3? In *Proceedings of Deep Learning Inside Out (DeeLIO 2022): The 3rd Workshop on Knowledge Extraction and Integration for Deep Learning Architectures*, pages 100–114.

Jiacheng Liu, Alisa Liu, Ximing Lu, Sean Welleck, Peter West, Ronan Le Bras, Yejin Choi, and Hannaneh Hajishirzi. 2022b. Generated knowledge prompting for commonsense reasoning. In *Proceedings of the 60th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 3154–3169.

Junteng Liu, Shiqi Chen, Yu Cheng, and Junxian He. 2024b. On the universal truthfulness hyperplane inside llms. In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing, EMNLP 2024, Miami, FL, USA, November 12-16, 2024*, pages 18199–18224. Association for Computational Linguistics.

Kai Liu, Ze Chen, Zhihang Fu, Rongxin Jiang, Fan Zhou, Yao-Shen Chen, Yue Wu, and Jieping Ye. 2024c. Structure-aware domain knowledge injection for large language models.

Xin Liu, Muhammad Khalifa, and Lu Wang. 2024d. Litcab: Lightweight language model calibration over short-and long-form responses. In *The Twelfth International Conference on Learning Representations*.

Do Xuan Long, Yiran Zhao, Hannah Brown, Yuxi Xie, James Xu Zhao, Nancy F. Chen, Kenji Kawaguchi, Michael Shieh, and Junxian He. 2024. Prompt optimization via adversarial in-context learning. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2024, Bangkok, Thailand, August 11-16, 2024*, pages 7308–7327. Association for Computational Linguistics.

Man Luo, Xin Xu, Zhuyun Dai, Panupong Pasupat, Mehran Kazemi, Chitta Baral, Vaiva Imbrasaite, and Vincent Y Zhao. 2023. Dr.ICL: Demonstration-retrieved in-context learning. In *R0-FoMo:Robustness of Few-shot and Zero-shot Learning in Large Foundation Models*.

Xinbei Ma, Yeyun Gong, Pengcheng He, Hai Zhao, and Nan Duan. 2023. Query rewriting in retrieval-augmented large language models. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 5303–5315, Singapore. Association for Computational Linguistics.

Aman Madaan, Niket Tandon, Peter Clark, and Yiming Yang. 2022. Memory-assisted prompt editing to improve GPT-3 after deployment. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing, EMNLP 2022, Abu Dhabi, United Arab Emirates, December 7-11, 2022*, pages 2833–2861. Association for Computational Linguistics.

Aman Madaan, Niket Tandon, Prakhar Gupta, Skyler Hallinan, Luyu Gao, Sarah Wiegreffe, Uri Alon, Nouha Dziri, Shrimai Prabhumoye, Yiming Yang, et al. 2024. Self-refine: Iterative refinement with self-feedback. *Advances in Neural Information Processing Systems*, 36.

Alex Mallen, Akari Asai, Victor Zhong, Rajarshi Das, Daniel Khashabi, and Hannaneh Hajishirzi. 2022. When not to trust language models: Investigating effectiveness of parametric and non-parametric memories. *arXiv preprint arXiv:2212.10511*.

Potsawee Manakul, Adian Liusie, and Mark Gales. 2023. Selfcheckgpt: Zero-resource black-box hallucination detection for generative large language models. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 9004–9017.

Samuel Marks and Max Tegmark. 2023. The geometry of truth: Emergent linear structure in large language model representations of true/false datasets. *arXiv preprint arXiv:2310.06824*.

Costas Mavromatis, Balasubramaniam Srinivasan, Zhengyuan Shen, Jiani Zhang, Huzefa Rangwala, Christos Faloutsos, and George Karypis. 2023. Which examples to annotate for in-context learning? towards effective and efficient selection. *arXiv preprint arXiv:2310.20046*.

Nick Mecklenburg, Yiyou Lin, Xiaoxiao Li, Daniel Holstein, Leonardo Nunes, Sara Malvar, Bruno Leonardo Barros Silva, Ranveer Chandra, Vijay Aski, Pavan Kumar Reddy Yannam, Tolga Aktas, and Todd Hendry. 2024. Injecting new knowledge into large language models via supervised fine-tuning. *ArXiv*, abs/2404.00213.

Kevin Meng, David Bau, Alex Andonian, and Yonatan Belinkov. 2022. Locating and editing factual associations in GPT. In *Advances in Neural Information Processing Systems 35: Annual Conference on Neural Information Processing Systems 2022, NeurIPS 2022*.

Kevin Meng, Arnab Sen Sharma, Alex J. Andonian, Yonatan Belinkov, and David Bau. 2023. Mass-editing memory in a transformer. In *The Eleventh International Conference on Learning Representations, ICLR 2023*.

Ning Miao, Yee Whye Teh, and Tom Rainforth. 2024. Selfcheck: Using LLMs to zero-shot check their own step-by-step reasoning. In *The Twelfth International Conference on Learning Representations*.

Sabrina J Mielke, Arthur Szlam, Emily Dinan, and Y-Lan Boureau. 2022. Reducing conversational agents' overconfidence through linguistic calibration. *Transactions of the Association for Computational Linguistics*, 10:857–872.

Eric Mitchell, Charles Lin, Antoine Bosselut, Christopher D. Manning, and Chelsea Finn. 2022. Memory-based model editing at scale. In *International Conference on Machine Learning, ICML 2022*, volume 162 of *Proceedings of Machine Learning Research*, pages 15817–15831.

Fangwen Mu, Lin Shi, Song Wang, Zhuohao Yu, Binquan Zhang, ChenXue Wang, Shichao Liu, and Qing Wang. 2023. Clarifygpt: Empowering llm-based code generation with intention clarification. *ArXiv*, abs/2310.10996.

Tarek Naous, Michael J. Ryan, Alan Ritter, and Wei Xu. 2024. Having beer after prayer? measuring cultural bias in large language models. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2024, Bangkok, Thailand, August 11-16, 2024*, pages 16366–16393. Association for Computational Linguistics.

Alexander Nikitin, Jannik Kossen, Yarin Gal, and Pekka Marttinen. 2024. Kernel language entropy: Fine-grained uncertainty quantification for llms from semantic similarities. *arXiv preprint arXiv:2405.20003*.

Yasumasa Onoe, Michael J. Q. Zhang, Eunsol Choi, and Greg Durrett. 2022. Entity cloze by date: What lms know about unseen entities. In *Findings of the Association for Computational Linguistics: NAACL 2022, Seattle, WA, United States, July 10-15, 2022*, pages 693–702. Association for Computational Linguistics.

Ankit Pal, Logesh Kumar Umapathi, and Malaikannan Sankarasubbu. 2023. Med-halt: Medical domain hallucination test for large language models. In *Proceedings of the 27th Conference on Computational Natural Language Learning, CoNLL 2023, Singapore, December 6-7, 2023*, pages 314–334. Association for Computational Linguistics.

Soumen Pal, Manojit Bhattacharya, Sang-Soo Lee, and Chiranjib Chakraborty. 2024. A domain-specific next-generation large language model (llm) or chatgpt is required for biomedical engineering and research. *Annals of biomedical engineering*, 52(3):451–454.

Yikang Pan, Liangming Pan, Wenhu Chen, Preslav Nakov, Min-Yen Kan, and William Yang Wang. 2023. On the risk of misinformation pollution with large language models. In *Findings of the Association for Computational Linguistics: EMNLP 2023, Singapore, December 6-10, 2023*, pages 1389–1403. Association for Computational Linguistics.

Archiki Prasad, Peter Hase, Xiang Zhou, and Mohit Bansal. 2023. Grips: Gradient-free, edit-based instruction search for prompting large language models. In *Proceedings of the 17th Conference of the European Chapter of the Association for Computational Linguistics*, pages 3845–3864.

Ofir Press, Muru Zhang, Sewon Min, Ludwig Schmidt, Noah A Smith, and Mike Lewis. 2023. Measuring and narrowing the compositionality gap in language models. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 5687–5711.

Reid Pryzant, Dan Iter, Jerry Li, Yin Lee, Chenguang Zhu, and Michael Zeng. 2023. Automatic prompt optimization with "gradient descent" and beam search. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 7957–7968.

Yifu Qiu, Zheng Zhao, Yftah Ziser, Anna Korhonen, Edoardo M Ponti, and Shay B Cohen. 2024. Spectral editing of activations for large language model alignment. *arXiv preprint arXiv:2405.09719*.

Ruiyang Ren, Yuhao Wang, Yingqi Qu, Wayne Xin Zhao, Jing Liu, Hao Tian, Hua Wu, Ji-Rong Wen, and Haifeng Wang. 2023. Investigating the factual knowledge boundary of large language models with retrieval augmentation. *arXiv preprint arXiv:2307.11019*.

Ohad Rubin, Jonathan Herzig, and Jonathan Berant. 2022. Learning to retrieve prompts for in-context learning. In *Proceedings of the 2022 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pages 2655–2671.

Abulhair Saparov and He He. 2023. Language models are greedy reasoners: A systematic formal analysis of chain-of-thought. In *The Eleventh International Conference on Learning Representations*.

Zhihong Shao, Yeyun Gong, Yelong Shen, Minlie Huang, Nan Duan, and Weizhu Chen. 2023. Enhancing retrieval-augmented large language models with iterative retrieval-generation synergy. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 9248–9274, Singapore. Association for Computational Linguistics.

Maohao Shen, Subhro Das, Kristjan Greenewald, Prasanna Sattigeri, Gregory Wornell, and Soumya Ghosh. 2024. Thermometer: Towards universal calibration for large language models. *arXiv preprint arXiv:2403.08819*.

Freda Shi, Xinyun Chen, Kanishka Misra, Nathan Scales, David Dohan, Ed H Chi, Nathanael Schärli, and Denny Zhou. 2023. Large language models can be easily distracted by irrelevant context. In *International Conference on Machine Learning*, pages 31210–31227. PMLR.

Weijia Shi, Sewon Min, Michihiro Yasunaga, Minjoon Seo, Richard James, Mike Lewis, Luke Zettlemoyer, and Wen-tau Yih. 2024. REPLUG: Retrieval-augmented black-box language models. In *Proceedings of the 2024 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 1: Long Papers)*, pages 8371–8384, Mexico City, Mexico. Association for Computational Linguistics.

Vaishnavi Shrivastava, Percy Liang, and Ananya Kumar. 2024. Llamas know what GPTs don't show: Surrogate models for selective classification.

Chenglei Si, Zhe Gan, Zhengyuan Yang, Shuohang Wang, Jianfeng Wang, Jordan Lee Boyd-Graber, and Lijuan Wang. 2023. Prompting GPT-3 to be reliable. In *The Eleventh International Conference on Learning Representations*.

Smriti Singh, Shuvam Keshari, Vinija Jain, and Aman Chadha. 2024. Born with a silver spoon? investigating socioeconomic bias in large language models. *ArXiv*, abs/2403.14633.

Maojia Song, Shang Hong Sim, Rishabh Bhardwaj, Hai Leong Chieu, Navonil Majumder, and Soujanya Poria. 2024a. Measuring and enhancing trustworthiness of llms in rag through grounded attributions and learning to refuse. *ArXiv*, abs/2409.11242.

Xiaoshuai Song, Zhengyang Wang, Keqing He, Guanting Dong, Yutao Mou, Jinxu Zhao, and Weiran Xu. 2024b. Knowledge editing on black-box large language models. *CoRR*, abs/2402.08631.

Elias Stengel-Eskin, Peter Hase, and Mohit Bansal. 2024. Lacie: Listener-aware finetuning for confidence calibration in large language models. *arXiv preprint arXiv:2405.21028*.

Chenmien Tan, Ge Zhang, and Jie Fu. 2024. Massive editing for large language models via meta learning. In *The Twelfth International Conference on Learning Representations, ICLR 2024, Vienna, Austria, May 7-11, 2024*. OpenReview.net.

Shuchang Tao, Liuyi Yao, Hanxing Ding, Yuexiang Xie, Qi Cao, Fei Sun, Jinyang Gao, Huawei Shen, and Bolin Ding. 2024. When to trust LLMs: Aligning confidence with response quality. In *Findings of the Association for Computational Linguistics ACL 2024*, pages 5984–5996, Bangkok, Thailand and virtual meeting. Association for Computational Linguistics.

Katherine Tian, Eric Mitchell, Allan Zhou, Archit Sharma, Rafael Rafailov, Huaxiu Yao, Chelsea Finn, and Christopher D Manning. 2023. Just ask for calibration: Strategies for eliciting calibrated confidence scores from language models fine-tuned with human feedback. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 5433–5442.

Christian Tomani, Kamalika Chaudhuri, I. Evtimov, Daniel Cremers, and Mark Ibrahim. 2024. Uncertainty-based abstention in llms improves safety and reduces hallucinations. *ArXiv*, abs/2404.10960.

Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, Dan Bikel, Lukas Blecher, Cristian Canton-Ferrer, Moya Chen, Guillem Cucurull, David Esiobu, Jude Fernandes, Jeremy Fu, Wenyin Fu, Brian Fuller, Cynthia Gao, Vedanuj Goswami, Naman Goyal, Anthony Hartshorn, Saghar Hosseini, Rui Hou, Hakan Inan, Marcin Kardas, Viktor Kerkez, Madian Khabsa, Isabel Kloumann, Artem Korenev, Punit Singh Koura, Marie-Anne Lachaux, Thibaut Lavril, Jenya Lee, Diana Liskovich, Yinghai Lu, Yuning Mao, Xavier Martinet, Todor Mihaylov, Pushkar Mishra, Igor Molybog, Yixin Nie, Andrew Poulton, Jeremy Reizenstein, Rashi Rungta, Kalyan Saladi, Alan Schelten, Ruan Silva, Eric Michael Smith, Ranjan Subramanian, Xiaoqing Ellen Tan, Binh Tang, Ross Taylor, Adina Williams, Jian Xiang Kuan, Puxin Xu, Zheng Yan, Iliyan Zarov, Yuchen Zhang, Angela Fan, Melanie Kambadur, Sharan Narang, Aurélien Rodriguez, Robert Stojnic, Sergey Edunov, and Thomas Scialom. 2023. Llama 2: Open foundation and fine-tuned chat models. *CoRR*, abs/2307.09288.

Harsh Trivedi, Niranjan Balasubramanian, Tushar Khot, and Ashish Sabharwal. 2022. MuSiQue: Multi-hop questions via single-hop question composition. *Transactions of the Association for Computational Linguistics*, 10:539–554.

Harsh Trivedi, Niranjan Balasubramanian, Tushar Khot, and Ashish Sabharwal. 2023. Interleaving retrieval with chain-of-thought reasoning for knowledge-intensive multi-step questions. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 10014–10037.

Neeraj Varshney, Pavel Dolin, Agastya Seth, and Chitta Baral. 2023. The art of defending: A systematic evaluation and analysis of llm defense strategies on safety and over-defensiveness. *ArXiv*, abs/2401.00287.

Tu Vu, Mohit Iyyer, Xuezhi Wang, Noah Constant, Jerry Wei, Jason Wei, Chris Tar, Yun-Hsuan Sung, Denny Zhou, Quoc Le, and Thang Luong. 2023. Freshllms: Refreshing large language models with search engine augmentation. In *Annual Meeting of the Association for Computational Linguistics*.

Boshi Wang, Xiang Deng, and Huan Sun. 2022. Iteratively prompt pre-trained language models for chain of thought. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing*, pages 2714–2730.

Boshi Wang, Xiang Yue, and Huan Sun. 2023a. Can chatgpt defend its belief in truth? evaluating LLM reasoning via debate. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 11865–11881.

Jianing Wang, Yang Zhou, Xiaocheng Zhang, Mengjiao Bao, and Peng Yan. 2024a. Self-evolutionary large language models through uncertainty-enhanced preference optimization. *arXiv preprint arXiv:2409.11212*.

Mengru Wang, Yunzhi Yao, Ziwen Xu, Shuofei Qiao, Shumin Deng, Peng Wang, Xiang Chen, Jia-Chen Gu, Yong Jiang, Pengjun Xie, Fei Huang, Huajun Chen, and Ningyu Zhang. 2024b. Knowledge mechanisms in large language models: A survey and perspective. In *Findings of the Association for Computational Linguistics: EMNLP 2024, Miami, Florida, USA, November 12-16, 2024*, pages 7097–7135. Association for Computational Linguistics.

Peng Wang, Zexi Li, Ningyu Zhang, Ziwen Xu, Yunzhi Yao, Yong Jiang, Pengjun Xie, Fei Huang, and Huajun Chen. 2024c. WISE: rethinking the knowledge memory for lifelong model editing of large language models. *CoRR*, abs/2405.14768.

Xinyuan Wang, Chenxi Li, Zhen Wang, Fan Bai, Haotian Luo, Jiayou Zhang, Nebojsa Jojic, Eric Xing, and Zhiting Hu. 2024d. Promptagent: Strategic planning with language models enables expert-level prompt optimization. In *The Twelfth International Conference on Learning Representations*.

Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc V Le, Ed H. Chi, Sharan Narang, Aakanksha Chowdhery, and Denny Zhou. 2023b. Self-consistency improves chain of thought reasoning in language models. In *The Eleventh International Conference on Learning Representations*.

Zhen Wang, Peide Zhu, and Jie Yang. 2024e. Controversialqa: Exploring controversy in question answering. In *Proceedings of the 2024 Joint International Conference on Computational Linguistics, Language Resources and Evaluation, LREC/COLING 2024, 20-25 May, 2024, Torino, Italy*, pages 3962–3966. ELRA and ICCL.

Zhiruo Wang, Jun Araki, Zhengbao Jiang, Md Rizwan Parvez, and Graham Neubig. 2023c. Learning to filter context for retrieval-augmented generation. *arXiv preprint arXiv:2311.08377*.

Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Fei Xia, Ed Chi, Quoc V Le, Denny Zhou, et al. 2022. Chain-of-thought prompting elicits reasoning in large language models. *Advances in neural information processing systems*, 35:24824–24837.

Bingbing Wen, Bill Howe, and Lucy Lu Wang. 2024a. Characterizing LLM abstention behavior in science QA with context perturbations. In *Findings of the Association for Computational Linguistics: EMNLP 2024, Miami, Florida, USA, November 12-16, 2024*, pages 3437–3450. Association for Computational Linguistics.

Bingbing Wen, Jihan Yao, Shangbin Feng, Chenjun Xu, Yulia Tsvetkov, Bill Howe, and Lucy Lu Wang. 2024b. Know your limits: A survey of abstention in large language models. *arXiv preprint arXiv:2407.18418*.

Zhihua Wen, Zhiliang Tian, Zexin Jian, Zhen Huang, Pei Ke, Yifu Gao, Minlie Huang, and Dongsheng Li. 2024c. Perception of knowledge boundary for large language models through semi-open-ended question answering. *CoRR*, abs/2405.14383.

Yixuan Weng, Minjun Zhu, Fei Xia, Bin Li, Shizhu He, Shengping Liu, Bin Sun, Kang Liu, and Jun Zhao. 2023. Large language models are better reasoners with self-verification. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 2550–2575.

Jian Wu, Linyi Yang, Yuliang Ji, Wenhao Huang, Börje F Karlsson, and Manabu Okumura. 2024a. Gendec: A robust generative question-decomposition method for multi-hop reasoning. *arXiv preprint arXiv:2402.11166*.

Siye Wu, Jian Xie, Jiangjie Chen, Tinghui Zhu, Kai Zhang, and Yanghua Xiao. 2024b. How easily do irrelevant inputs skew the responses of large language models? *ArXiv*, abs/2404.03302.

Johnathan Xie, Annie S Chen, Yoonho Lee, Eric Mitchell, and Chelsea Finn. 2024. Calibrating language models with adaptive temperature scaling. In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing*, pages 18128–18138, Miami, Florida, USA. Association for Computational Linguistics.

Guangzhi Xiong, Qiao Jin, Zhiyong Lu, and Aidong Zhang. 2024a. Benchmarking retrieval-augmented generation for medicine. *ArXiv*, abs/2402.13178.

Miao Xiong, Zhiyuan Hu, Xinyang Lu, YIFEI LI, Jie Fu, Junxian He, and Bryan Hooi. 2024b. Can LLMs express their uncertainty? an empirical evaluation of confidence elicitation in LLMs. In *The Twelfth International Conference on Learning Representations*.

Hongshen Xu, Zichen Zhu, Da Ma, Situo Zhang, Shuai Fan, Lu Chen, and Kai Yu. 2024a. Rejection improves reliability: Training llms to refuse unknown questions using rl from knowledge feedback. *ArXiv*, abs/2403.18349.

Rongwu Xu, Brian S. Lin, Shujian Yang, Tianqi Zhang, Weiyan Shi, Tianwei Zhang, Zhixuan Fang, Wei Xu, and Han Qiu. 2024b. The earth is flat because...: Investigating llms' belief towards misinformation via persuasive conversation. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2024*, pages 16259–16303.

Xin Xu, Yue Liu, Panupong Pasupat, Mehran Kazemi, et al. 2024c. In-context learning with retrieved demonstrations for language models: A survey. *arXiv preprint arXiv:2401.11624*.

Yasin Abbasi Yadkori, Ilja Kuzborskij, András György, and Csaba Szepesvári. 2024. To believe or not to believe your llm. *arXiv preprint arXiv:2406.02543*.

Yuzi Yan, Xingzhou Lou, Jialian Li, Yiping Zhang, Jian Xie, Chao Yu, Yu Wang, Dong Yan, and Yuan Shen. 2024. Reward-robust rlhf in llms. *arXiv preprint arXiv:2409.15360*.

Chengrun Yang, Xuezhi Wang, Yifeng Lu, Hanxiao Liu, Quoc V Le, Denny Zhou, and Xinyun Chen. 2024a. Large language models as optimizers. In *The Twelfth International Conference on Learning Representations*.

Dingkang Yang, Dongling Xiao, Jinjie Wei, Mingcheng Li, Zhaoyu Chen, Ke Li, and Lihua Zhang. 2024b. Improving factuality in large language models via decoding-time hallucinatory and truthful comparators. *arXiv preprint arXiv:2408.12325*.

Haoyan Yang, Zhitao Li, Yong Zhang, Jianzong Wang, Ning Cheng, Ming Li, and Jing Xiao. 2023a. PRCA: Fitting black-box large language models for retrieval question answering via pluggable reward-driven contextual adapter. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 5364–5375, Singapore. Association for Computational Linguistics.

Muchen Yang, Moxin Li, Yongle Li, Zijun Chen, Chongming Gao, Junqi Zhang, Yangyang Li, and Fuli Feng. 2024c. Dual-phase accelerated prompt optimization. In *Findings of the Association for Computational Linguistics: EMNLP 2024*, pages 12163–12173, Miami, Florida, USA. Association for Computational Linguistics.

Yuqing Yang, Ethan Chern, Xipeng Qiu, Graham Neubig, and Pengfei Liu. 2023b. Alignment for honesty. *ArXiv*, abs/2312.07000.

Zhilin Yang, Peng Qi, Saizheng Zhang, Yoshua Bengio, William W. Cohen, Ruslan Salakhutdinov, and Christopher D. Manning. 2018. Hotpotqa: A dataset for diverse, explainable multi-hop question answering. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing, Brussels, Belgium, October 31 - November 4, 2018*, pages 2369–2380. Association for Computational Linguistics.

Shunyu Yao, Dian Yu, Jeffrey Zhao, Izhak Shafran, Tom Griffiths, Yuan Cao, and Karthik Narasimhan. 2023. Tree of thoughts: Deliberate problem solving with large language models. In *Advances in Neural Information Processing Systems 36: Annual Conference on Neural Information Processing Systems 2023, NeurIPS 2023, New Orleans, LA, USA, December 10 - 16, 2023*.

Zijun Yao, Weijian Qi, Liangming Pan, Shulin Cao, Linmei Hu, Weichuan Liu, Lei Hou, and Juanzi Li. 2024. Seakr: Self-aware knowledge retrieval for adaptive retrieval augmented generation. *arXiv preprint arXiv:2406.19215*.

Jiacheng Ye, Zhiyong Wu, Jiangtao Feng, Tao Yu, and Lingpeng Kong. 2023. Compositional exemplars for in-context learning. In *International Conference on Machine Learning*, pages 39818–39833. PMLR.

Xunjian Yin, Xu Zhang, Jie Ruan, and Xiaojun Wan. 2024. Benchmarking knowledge boundary for large language models: A different perspective on model evaluation. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2024, Bangkok, Thailand, August 11-16, 2024*, pages 2270–2286. Association for Computational Linguistics.

Zhangyue Yin, Qiushi Sun, Qipeng Guo, Jiawen Wu, Xipeng Qiu, and Xuanjing Huang. 2023. Do large language models know what they don't know? In *Findings of the Association for Computational Linguistics: ACL 2023, Toronto, Canada, July 9-14, 2023*, pages 8653–8665. Association for Computational Linguistics.

Lang Yu, Qin Chen, Jie Zhou, and Liang He. 2024. MELO: enhancing model editing with neuron-indexed dynamic lora. In *Thirty-Eighth AAAI Conference on Artificial Intelligence, AAAI 2024*, pages 19449–19457. AAAI Press.

Hanning Zhang, Shizhe Diao, Yong Lin, Yi R. Fung, Qing Lian, Xingyao Wang, Yangyi Chen, Heng Ji, and Tong Zhang. 2024a. R-tuning: Instructing large language models to say 'i don't know'. In *Proceedings of the 2024 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 1: Long Papers), NAACL 2024*, pages 7113–7139.

Jiaxin Zhang, Wendi Cui, Yiran Huang, Kamalika Das, and Kumar Sricharan. 2024b. Synthetic knowledge ingestion: Towards knowledge refinement and injection for enhancing large language models. In *Conference on Empirical Methods in Natural Language Processing*.

Kun Zhang, Jiali Zeng, Fandong Meng, Yuanzhuo Wang, Shiqi Sun, Long Bai, Huawei Shen, and Jie Zhou. 2024c. Tree-of-reasoning question decomposition for complex question answering with large language models. In *Thirty-Eighth AAAI Conference on Artificial Intelligence, AAAI 2024*, pages 19560–19568. AAAI Press.

Mozhi Zhang, Mianqiu Huang, Rundong Shi, Linsen Guo, Chong Peng, Peng Yan, Yaqian Zhou, and Xipeng Qiu. 2024d. Calibrating the confidence of large language models by eliciting fidelity. In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing, EMNLP 2024, Miami, FL, USA, November 12-16, 2024*, pages 2959–2979. Association for Computational Linguistics.

Shaolei Zhang, Tian Yu, and Yang Feng. 2024e. Truthx: Alleviating hallucinations by editing large language models in truthful space. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2024, Bangkok, Thailand, August 11-16, 2024*, pages 8908–8949. Association for Computational Linguistics.

Tianjun Zhang, Xuezhi Wang, Denny Zhou, Dale Schuurmans, and Joseph E. Gonzalez. 2023a. TEMPERA: Test-time prompt editing via reinforcement learning. In *The Eleventh International Conference on Learning Representations*.

Tong Zhang, Peixin Qin, Yang Deng, Chen Huang, Wenqiang Lei, Junhong Liu, Dingnan Jin, Hongru Liang, and Tat-Seng Chua. 2024f. CLAMBER: A benchmark of identifying and clarifying ambiguous information needs in large language models. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2024*, pages 10746–10766.

Yue Zhang, Leyang Cui, Wei Bi, and Shuming Shi. 2023b. Alleviating hallucinations of large language models through induced hallucinations. *CoRR*, abs/2312.15710.

Bowen Zhao, Zander Brumbaugh, Yizhong Wang, Hannaneh Hajishirzi, and Noah A. Smith. 2024a. Set the clock: Temporal alignment of pretrained language models. In *Findings of the Association for Computational Linguistics, ACL 2024, Bangkok, Thailand and virtual meeting, August 11-16, 2024*, pages 15015–15040. Association for Computational Linguistics.

Ruochen Zhao, Xingxuan Li, Shafiq Joty, Chengwei Qin, and Lidong Bing. 2023. Verify-and-edit: A knowledge-enhanced chain-of-thought framework. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2023, Toronto, Canada, July 9-14, 2023*, pages 5823–5840. Association for Computational Linguistics.

Xinran Zhao, Hongming Zhang, Xiaoman Pan, Wenlin Yao, Dong Yu, Tongshuang Wu, and Jianshu Chen.

2024b. Fact-and-reflection (FaR) improves confidence calibration of large language models. In *Findings of the Association for Computational Linguistics ACL 2024*, pages 8702–8718, Bangkok, Thailand and virtual meeting. Association for Computational Linguistics.

Yukun Zhao, Lingyong Yan, Weiwei Sun, Guoliang Xing, Chong Meng, Shuaiqiang Wang, Zhicong Cheng, Zhaochun Ren, and Dawei Yin. 2024c. Knowing what llms DO NOT know: A simple yet effective self-detection method. In *Proceedings of the 2024 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 1: Long Papers), NAACL 2024, Mexico City, Mexico, June 16-21, 2024*, pages 7051–7063. Association for Computational Linguistics.

Ce Zheng, Lei Li, Qingxiu Dong, Yuxuan Fan, Zhiyong Wu, Jingjing Xu, and Baobao Chang. 2023a. Can we edit factual knowledge by in-context learning? In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing, EMNLP 2023, Singapore, December 6-10, 2023*, pages 4862–4876. Association for Computational Linguistics.

Chuanyang Zheng, Zhengying Liu, Enze Xie, Zhenguo Li, and Yu Li. 2023b. Progressive-hint prompting improves reasoning in large language models. *CoRR*, abs/2304.09797.

Haoxiang Zhong, Chaojun Xiao, Cunchao Tu, T. Zhang, Zhiyuan Liu, and Maosong Sun. 2019. Jec-qa: A legal-domain question answering dataset. *ArXiv*, abs/1911.12011.

Zexuan Zhong, Zhengxuan Wu, Christopher D. Manning, Christopher Potts, and Danqi Chen. 2023. Mquake: Assessing knowledge editing in language models via multi-hop questions. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing, EMNLP 2023, Singapore, December 6-10, 2023*, pages 15686–15702. Association for Computational Linguistics.

Denny Zhou, Nathanael Schärli, Le Hou, Jason Wei, Nathan Scales, Xuezhi Wang, Dale Schuurmans, Claire Cui, Olivier Bousquet, Quoc V. Le, and Ed H. Chi. 2023a. Least-to-most prompting enables complex reasoning in large language models. In *The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023*. OpenReview.net.

Kaitlyn Zhou, Jena D. Hwang, Xiang Ren, and Maarten Sap. 2024. Relying on the unreliable: The impact of language models' reluctance to express uncertainty. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), ACL 2024, Bangkok, Thailand, August 11-16, 2024*, pages 3623–3643. Association for Computational Linguistics.

Yongchao Zhou, Andrei Ioan Muresanu, Ziwen Han, Keiran Paster, Silviu Pitis, Harris Chan, and Jimmy Ba. 2023b. Large language models are human-level prompt engineers. In *The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023*. OpenReview.net.

Fengbin Zhu, Wenqiang Lei, Youcheng Huang, Chao Wang, Shuo Zhang, Jiancheng Lv, Fuli Feng, and Tat seng Chua. 2021. Tat-qa: A question answering benchmark on a hybrid of tabular and textual content in finance. *ArXiv*, abs/2105.07624.

Runchuan Zhu, Zhipeng Ma, Jiang Wu, Junyuan Gao, Jiaqi Wang, Dahua Lin, and Conghui He. 2024. Utilize the flow before stepping into the same river twice: Certainty represented knowledge flow for refusal-aware instruction tuning. *CoRR*, abs/2410.06913.

A Overview

We begin by introducing the definition of knowledge boundary, outlining three types of knowledge boundaries and a four-type knowledge taxonomy. Following this, we describe the typical undesired behaviors that arise from knowledge limitations, emphasizing the importance of addressing such issues. These challenges highlight the critical need for methods that can detect when LLMs operate beyond their knowledge capabilities. To this end, we present three distinct identification techniques that help delineate where knowledge gaps exist. Once these gaps are identified, various mitigation strategies can be employed to address the issues caused by the knowledge boundaries. Finally, we explored several significant challenges and emerging prospects in understanding and managing knowledge boundaries in LLMs. Figure 4 illustrates a comprehensive framework for managing the knowledge boundaries of LLMs, focusing on three key components: Undesired Behaviors, Identification of Knowledge Boundaries, and Mitigation Strategies.

B Dataset

In the pursuit of advancing LLM capabilities and understanding their boundaries in knowledge processing, various datasets have been meticulously designed and utilized. The following sections categorize these datasets into three distinct groups based on the type of knowledge they aim to verify: Prompt-Sensitive Known Knowledge, Model-Specific Unknown Knowledge, and Model-Agnostic Unknown Knowledge. A summary of these datasets can be viewed in Table 1.

Datasets for Prompt-Sensitive Known Knowledge This type of datasets mainly aim to assess

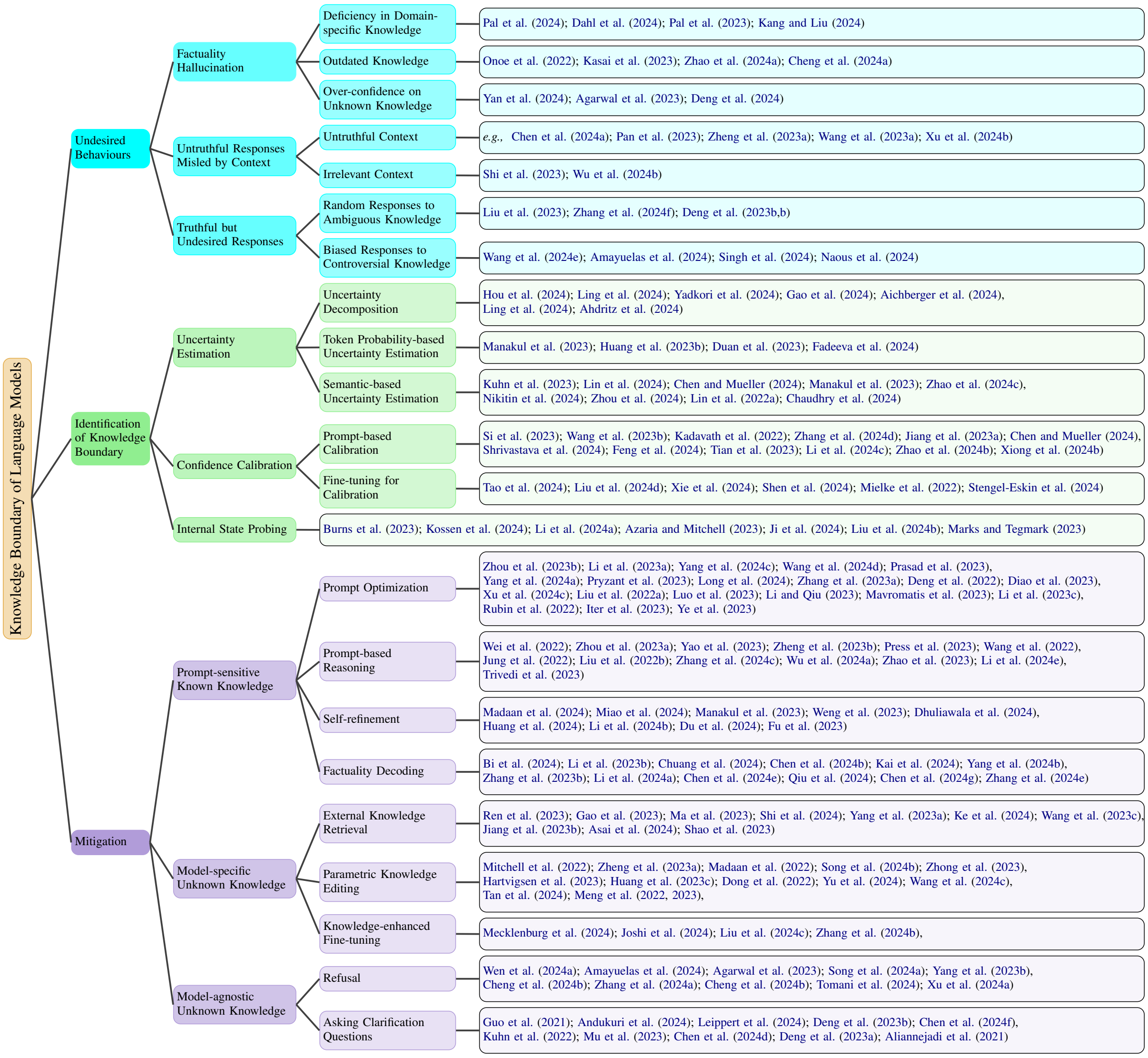

Figure 4: The main content flow and categorization of this survey.

Knowledge Category	Dataset	Reference	Size	Description
Prompt-Sensitive Known Knowledge	ProntoQA	Saparov and He (2023)	9.7k	A question-answering dataset which generates examples with chains-of-thought that describe the reasoning required to answer the questions correctly.
	2WikiMultiHopQA	Ho et al. (2020)	192,606	A multi-hop QA benchmark combining structured and unstructured data.
	MuSiQue	Trivedi et al. (2022)	25k	A multi-hop QA benchmark with 2-4 hop questions.
	HotpotQA	Yang et al. (2018)	113k	A multi-hop QA dataset requiring reasoning over two Wikipedia paragraphs, with supporting facts provided for explainability and evaluation.
	TruthfulQA	Lin et al. (2022b)	817	A benchmark across 38 categories, designed to evaluate whether language models generate truthful answers, particularly in cases prone to false beliefs.
	PARAREL	Elazar et al. (2021)	328	A dataset of English cloze-style query paraphrases for 38 relations, designed to evaluate the consistency of PLMs in handling factual knowledge across meaning-preserving input variations.
	KAssess	Dong et al. (2024)	139k	A comprehensive assessment suite with 994,123 entities and 600 relations, designed to evaluate the factual knowledge of LLMs by estimating their ability to generate correct answers across diverse prompts compared to random chance.
	FARM	Xu et al. (2024b)	1,952	A dataset of factual questions paired with systematically generated persuasive misinformation, designed to evaluate the susceptibility of LLMs to belief manipulation through multi-turn persuasive conversations.
	Misinfo-QA	Pan et al. (2023)	3,034	A dataset designed to study the impact of misinformation on open-domain question answering (ODQA) systems by injecting synthetic misinformation passages to evaluate how QA models respond under such conditions.
Model-Specific Unknown Knowledge	Natural Questions	Kwiatkowski et al. (2019)	7,842	A large-scale dataset of real anonymized Google queries, annotated with long and short answers from Wikipedia or marked null if no answer is present.
	TopiOCQA	Adlakha et al. (2022)	3,920	An open-domain conversational dataset with information-seeking conversations featuring topic switches.
	PopQA	Mallen et al. (2022)	14k	Long-tail relation triples from WikiData are converted into QA pairs; no explicit unanswerable questions but questions are about long-tail entities.
	TriviaQA	Joshi et al. (2017)	950k	A realistic text-based question answering dataset which includes question-answer pairs from documents collected from Wikipedia and the web.
	RealtimeQA	Kasai et al. (2023)	4,356	A dynamic open-domain question-answering dataset that evaluates models based on real-time, time-sensitive questions sourced weekly from news articles.
	FreshQA	Vu et al. (2023)	600	A dynamic QA benchmark designed to evaluate LLMs on fast-changing world knowledge and debunking false premises.
	PubMedQA	Jin et al. (2019)	273.5k	A biomedical research question-answering dataset, which features questions derived from research article titles in PubMed, requiring complex reasoning and interpretation of quantitative biomedical content.
	MIRAGE	Xiong et al. (2024a)	7,663	A benchmark dataset for medical question answering, focusing on retrieving information from medical literature to answer multiple-choice medical questions, with an emphasis on zero-shot reasoning and systematic evaluation of retrieval performance.
	TAT-QA	Zhu et al. (2021)	16,552	A question-answering dataset for the financial domain, combining tabular and textual content from real financial reports.
	FinQA	Chen et al. (2021)	8,281	A question-answering dataset for the financial domain, with questions and answers crafted by financial experts, involving complex numerical reasoning over tables and text from financial reports.
	JEC-QA	Zhong et al. (2019)	26,365	A legal-domain question-answering dataset with questions sourced from the National Judicial Examination of China, covering legal concept understanding and case analysis.
	LawBench	Fei et al. (2024)	20,000	A legal reasoning evaluation benchmark designed for the Chinese legal environment, covering tasks such as legal knowledge memorization, document proofreading, case analysis, charge prediction, and legal consultation.
Model-Agnostic Unknown Knowledge	KUQ	Amayuelas et al. (2024)	6,884	A dataset designed to explore uncertainty in question-answering by focusing on questions without definitive answers.
	UnknownBench	Liu et al. (2024a)	13,319	A benchmark consisting of answerable and unanswerable questions, designed to evaluate LLMs' ability to express uncertainty and handle knowledge gaps while maintaining honesty and helpfulness.
	SelfAware	Yin et al. (2023)	2,337	A dataset containing unanswerable questions across five categories, designed to evaluate LLMs' self-knowledge by detecting uncertainty and their ability to identify limitations in their knowledge.
	QnotA	Agarwal et al. (2023)	400	A dataset featuring questions without definitive answers across five categories, paired with corresponding answerable alternatives.
	KUQP	Deng et al. (2024)	320	A dataset of known and unknown question pairs, designed to evaluate language models' ability to handle unanswerable, ambiguous, or incorrect queries.

Table 1: Representative datasets for studying the knowledge boundary of language models.

the prompt-sensitive known knowledge of LLMs, requiring specific prompting strategies and decoding strategies for the LLM to fully recall and utilize such knowledge.

The first type of datasets focuses on ***multi-step reasoning***, such as multi-step knowledge-based question answering datasets (*e.g.*, 2WikiMultiHopQA (Ho et al., 2020), MuSiQue (Trivedi et al., 2022), and HotpotQA (Yang et al., 2018)) and logical reasoning datasets like ProntoQA (Saparov and He, 2023). These tasks require the LLM to achieve a step-by-step reasoning process or benefit from prompting strategies that focus on question decomposition and explicit knowledge recall.

The second type is ***fact-based question answering*** datasets that evaluate the LLM's factuality, *e.g.,* TruthfulQA (Lin et al., 2022b). In these datasets, the decoding strategy can influence how accurately knowledge is expressed (Li et al., 2024a).

The third type of datasets explicitly study the influence of ***varied prompt phrasing*** in LLM knowledge, including PARAREL (Elazar et al., 2021) and KAssess (Dong et al., 2024).

The fourth type involves datasets with ***misleading contexts***. Wang et al. (2023a) curate queries with misleading user opinion to test LLM's ability to defend its response. FARM (Xu et al., 2024b) contains persuasive misinformation in the dialog context to evaluate LLM's belief change. MisinfoQA (Pan et al., 2023) includes model-generated misinformation to perturb open-domain QA.

Dataset for Model-Specific Unknown Knowledge This type of datasets can be used for assessing the model-specific unknown knowledge of LLMs, which challenges LLMs by probing their ability to handle highly specialized and temporally-sensitive information, testing their adaptive knowledge boundaries. These datasets are specifically designed to evaluate knowledge that lies outside the parametric scope of LLMs, requiring external knowledge retrieval or new knowledge injection to generate accurate responses.

Open-domain question answering datasets form an important category. These datasets evaluate the ability of language models to answer questions across a broad range of domains, leveraging both retrieval and parametric knowledge. Representative examples include Natural Questions (Kwiatkowski et al., 2019), TopiOCQA (Adlakha et al. 2022), PopQA (Mallen et al. 2022), and TriviaQA-unfiltered (Joshi et al. 2017). These datasets often focus on queries that require world knowledge or niche details, testing the model's capacity to combine retrieval and internalized knowledge effectively. Meanwhile, various domain-specific QA datasets can be adopted to evaluate the model-specific unknown knowledge for each specialized applications, such as medical domain (*e.g.*, PubMedQA (Jin et al., 2019) and MIRAGE (Xiong et al., 2024a)), finance domain (*e.g.*, TAT-QA (Zhu et al., 2021) and FinQA (Chen et al., 2021)) , and legal domain (*e.g.*, JEC-QA (Zhong et al., 2019) and LawBench (Fei et al., 2024)).

Another crucial subdomain focuses on time-sensitive datasets that test a model's ability to generalize to out-of-distribution data. Datasets such as RealtimeQA (Kasai et al. 2023) and FreshQA(Vu et al. 2023) require language models to stay current with global events and provide accurate, up-to-date responses. These datasets evaluate the model's capacity to adapt to evolving information and address queries that rely on recent developments.

This diverse set of datasets for studying model-sensitive unknown knowledge systematically evaluates the gaps in parametric knowledge of language models, testing their ability to retrieve, adapt, and reason with external information under various constraints.

Dataset for Model-Agnostic Unknown Knowledge As for the model-agnostic unknown knowledge, datasets such as Known-Unknown Questions (KUQ) (Amayuelas et al., 2024) and UnknownBench (Liu et al., 2024a) are specifically crafted to probe questions that remain unresolved or are based on uncertain future developments and incorrect assumptions. These datasets encapsulate complex scenarios including counterfactuals and ambiguities, which emphasize the current boundaries of our knowledge and the unpredictable nature of future inquiries.

Further pushing these boundaries, the SelfAware dataset (Yin et al., 2023) explores questions that defy scientific consensus, are subjective, or philosophical, often requiring responses that extend beyond factual representation and into personal belief or theoretical speculation. Similarly, resources like QnotA (Agarwal et al., 2023) and Known-Unknown Question Pairs (KUQP) (Deng et al., 2024) challenge models with incomplete or erroneous information and speculative predictions about the future. These datasets collectively serve to test LLM's capability in navigating the complexities of human inquiry where the answers are unknown.

C Details in Mitigation Approaches

C.1 Prompt-Sensitive Known Knowledge

Prompt Optimization. For instruction optimization, APE (Zhou et al., 2023b) leverages LLMs to automatically generate and perform Monte Carlo search for the instructions, and evaluate the zero-shot performance of the candidate instructions. ORPO (Yang et al., 2024a) utilizes natural language as optimization instructions for LLMs to iteratively optimize the prompts. For demonstration optimization, KATE (Liu et al., 2022a) retrieve the K nearest in-context examples by the semantic similarity to the test example, measured by the embedding from an encoder model.

Prompt-based Reasoning. Tree-of-thoughts (Yao et al., 2023) improves the linear chain-of-thoughts reasoning into tree structure, each node representing a piece of thoughts, and branches represents alternative thoughts. It allows LLMs to perform various forms of reasoning steps. Progressive-hint-prompting (Zheng et al., 2023b) appends the LLM-generated answers to the prompt as hints to iteratively arrive at the correct answers.

Self-refinement. Self-refine (Madaan et al., 2024) prompts LLMs to generate feedback on its previous answer for iterative answer refinement. Self-verification (Weng et al., 2023) transforms the generated answer into abductive reasoning questions to examine the consistency with the given context.

Factuality Decoding. DoLA (Chuang et al., 2024) contrasts the logits obtained from the later layers with that obtained from the earlier layers to reduce generating factual errors. ITI (Li et al., 2024a) changes the direction of the activations towards a factuality-improving direction obtained via probing to enhance factuality during inference.

C.2 Model-specific Unknown Knowledge

External Knowledge Retrieval For pre-generation methods, HyDE (Gao et al., 2023) enhance retrieval by rewriting or expanding the user's input to obtain more comprehensive and accurate relevant information required by the model. This approach focuses on adapting the query to improve retrieval performance. For on-demand methods, FLARE (Jiang et al., 2023b) evaluates the confidence levels in the model's generated content and actively retrieves pertinent documents to regenerate low-confidence segments, enhancing factual accuracy.

Parametric Knowledge Editing PostEdit (Song et al., 2024b) edits the outputs of black-box LLMs while preserving data privacy and maintaining the original text style through fine-grained modifications. MELO (Yu et al., 2024) dynamically activates LoRA blocks using a neuron-indexed vector database, enabling efficient and precise updates to LLMs with minimal computational cost.

Knowledge-enhanced Fine-tuning Joshi et al. (2024) enhances low-resource language adaptation by constructing a synthetic Hindi corpus through English text translation, transliteration, and noise filtering, followed by training on the curated dataset. StructTuning (Liu et al., 2024c) constructs structured domain knowledge by automatically extracting knowledge taxonomies from corpora, linking text segments to specific knowledge points for efficient model fine-tuning.

C.3 Model-agnostic Unknown Knowledge

Refusal Amayuelas et al. (2024) guides LLMs to recognize "known-unknown" questions and express uncertainty in high-uncertainty scenarios, enabling them to refrain from answering questions lacking definitive answers. R-tuning (Zhang et al., 2024a) identifies the gap between the knowledge contained in the dataset and the knowledge encapsulated in the pre-trained parameters, thereby constructing a refusal-aware dataset and training the model based on it.

Asking Clarification Questions Deng et al. (2023b) constructed a proactive prompting scheme for dialogue between users and LLMs, requiring LLMs to carefully analyze and think through the question before posing clarification questions. ACT (Chen et al., 2024d) guides the model to optimize dialogue strategies through contrastive learning in multi-turn conversations, especially when facing ambiguous user requests, enabling it to automatically recognize and ask clarification questions instead of guessing user intent or providing incorrect answers.