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# Explainability of Large Language Models: Opportunities and Challenges toward Generating Trustworthy Explanations

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## Abstract

Large language models have exhibited impressive performance across a broad range of downstream tasks in natural language processing. However, how a language model predicts the next token and generates content is not generally understandable by humans. Furthermore, these models often make errors in prediction and reasoning, known as hallucinations. These errors underscore the urgent need to better understand and interpret the intricate inner workings of language models and how they generate predictive outputs. Motivated by this gap, this paper investigates local explainability and mechanistic interpretability within Transformer-based large language models to foster trust in such models. In this regard, our paper aims to make three key contributions. First, we present a review of local explainability and mechanistic interpretability approaches and insights from relevant studies in the literature. Furthermore, we describe experimental studies on explainability and reasoning with large language models in two critical domains — healthcare and autonomous driving — and analyze the trust implications of such explanations for explanation receivers. Finally, we summarize current unaddressed issues in the evolving landscape of LLM explainability and outline the opportunities, critical challenges, and future directions toward generating human-aligned, trustworthy LLM explanations.

## 1 Introduction

Pretrained large language models (LLMs) have emerged as powerful tools for a range of complex natural language processing (NLP) applications in the field of artificial intelligence (AI). Primarily based on the Transformer architecture [1], recent LLMs, such as the family series from GPT [2, 3, 4], Vicuna [5], LLaMA [6, 7], Mistral [8], Claude [9, 10], Qwen [11, 12, 13], Gemini [14, 15], DeepSeek [16, 17, 18, 19], Grok [20, 21, 22] and Kimi [23, 24] have demonstrated impressive performance across many NLP tasks, and the list continues to expand. These models typically use a Transformer-based deep neural network as a base model and are augmented with an extended number of parameters, a larger volume of data, and an increased overall model size. Numerous empirical studies show that larger-size LLMs substantially outperform smaller models in terms of their emergent abilities, such

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as reasoning, instruction following, program execution, and general-purpose task-solving capabilities [2, 25, 26].

While LLMs' emergent abilities are impressive at first glance, there are several issues with these tools [27]. First, almost all state-of-the-art LLMs have a common problem of producing *hallucinations*, i.e., they produce convincing but falsified, factually incorrect content. Depending on the context, LLM-generated false statements can be detected easily; however, there are also cases where such statements may seem correct while actually not being evidence-grounded or confirmed without careful judgment [28, 29]. Furthermore, LLMs might have biases in their generated content while responding to a specific prompt, such as in politics, culture, race, and gender-based topics [30]. Finally, LLMs remain "black-box" models in general; people do not understand how the internal knowledge base and inner working mechanism enable these models to make their predictions. These problems hinder the applicability of such black-box AI models in safety-critical tasks and domains, and raise serious issues regarding their societal alignment and compliance with regulatory principles [31]. Consequently, there is an imminent need for a thorough investigation of interpretability and explainability in LLMs.

The topics of interpretability and explainability have been used interchangeably or as distinguished from each other in explainable artificial intelligence (XAI), depending on the use case and the nature of the tasks where they are considered [32, 33]. In the context of LLMs, those topics can be explored in two directions: Understanding these models 1) by their inner workings, i.e., mechanistic interpretability, and 2) based on the predictions they generate for particular tasks, i.e., local explainability (Figure 1). Our paper tries to elucidate both of these directions and specifically aims to underscore the implications of local and mechanistic explanations from the trust perspective for the targeted interaction partners. Given that interpretability and explainability in LLMs remain in their early stages of development, we begin by elucidating the foundational concepts within these tools and synthesizing the key insights and findings emerging from recent research within the LLM community. After analyzing the findings from the reviewed studies, we further summarize insights from empirical evidence in two safety-critical applications. Finally, building on our critical analysis and experimental results, we propose future directions for advancing the trustworthiness of LLM explanations.

## 1.1 Contributions

Focusing on LLM interpretability and explainability through the lenses of trustworthiness and human-centricity, our paper makes three key contributions:

- We review the local explainability and mechanistic interpretability techniques in the LLM literature, present insights from these studies, and reveal critical aspects of trustworthy LLM explanations;
- We draw insights from experiments in two safety-critical domains and show trust implications of LLM explanations for explanation receivers;
- We present unaddressed issues in the current approaches to LLM explainability and propose guidelines toward achieving eight fundamental goals of a trustworthy LLM with explanations.

## 1.2 Structure of the Paper

The paper is organized into the following sections. After the introduction, Section 2 presents background information on LLMs. Section 3 reviews related studies on LLM explainability and shows how our paper bridges the gap in the current literature. Section 4 presents a detailed review of local explainability and mechanistic interpretability approaches in LLMs. Critical aspects in presenting trustworthy LLM explanations and their assessment are covered in Sections 5 and 6, respectively. After that, Section 7 presents empirical insights from two safety-critical domains, and key findings from these studies in conjunction with the existing literature are presented in Section 8. Finally, Section 9 proposes potential future directions for advancing trustworthiness in LLM explanations, and Section 10 concludes the paper with an overall summary.

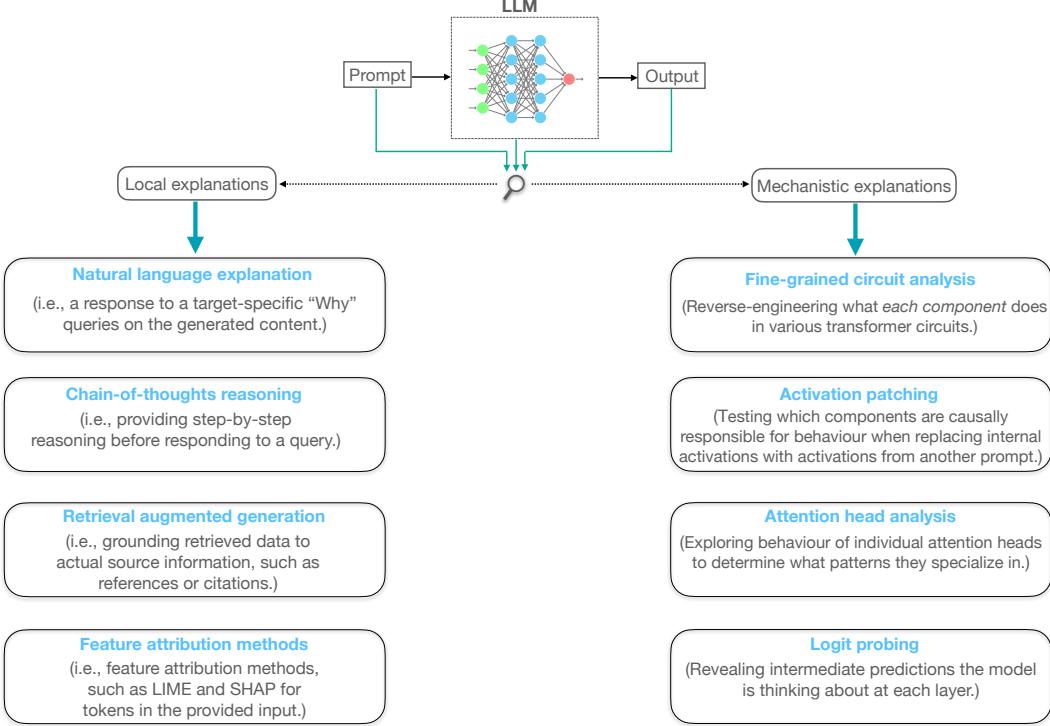


Figure 1: Local explainability and mechanistic interpretability approaches in LLMs.

## 2 Background of Language Models

### 2.1 The Rise of LLMs

The history of LLMs dates back to the early 1980s and all the way through 2025, with several evolutions based on their training mechanisms and capabilities. Unsurprisingly, all these models are based on the main theme of language modeling, i.e., predicting the probability of a word occurring given its surrounding context. Earlier statistical learning models [34, 35] were developed on a purely Markov assumption, i.e., the probability of a word occurrence is wholly dependent on the n-grams preceding it. However, these methods were not successful in predicting words accurately when the preceding context is large, which creates a huge computational burden of calculating an exponential number of transition probabilities. Subsequently, deep learning models that can learn distributed word representations more efficiently have been shown to exploit the back-propagation technique proposed by [36, 37]. Later, these methods were improved by posing them as a self-supervised classification task with a contrastive loss function and negative sampling; this improvement led to the development of language models such as Word2Vec [38] and FastText [39]. The resulting distributed representations primarily focus on how a word is connected to its neighboring words. Moreover, this method can help achieve high accuracy in several NLP domains when used to pre-train those models through various techniques, such as retrofitting [40], domain-specific embedding creation and mapping [41]. Subsequently, even more efficiency improvements emerged for task-specific context-aware embedding representation building. These include contextual word embedding methods, where a word's embedding vector becomes dynamic and changes based on its surrounding context, enabling the creation of an embedding representation for an entire sentence. In this research trajectory, the most popular methods were Google's Universal Sentence Embedding [42] and Allen AI's ELMO [43]. The basic architecture used here was based on the Bi-LSTM method to capture a word's context in both directions, or a simple MLP, first pre-trained in an unlabeled corpus and then fine-tuned on various mainstream NLP tasks.

The next revolution in the language modeling area emerged when Vaswani et al. [1] published their paper on the Self-Attention mechanism, which not only helped with learning an end-to-end high-performing model for language modeling, but also helped with identifying the salience of participating words for next word prediction or other downstream classification tasks. The first models using this

architecture were different variations of Google’s BERT [44] (such as ALBERT [45] and RoBERTa [46]), decoder-only or GPT models [47] (GPT-1,2, and 3), and models with a BERT-like encoder with a GPT-like Decoder, such as BART [48] from Meta. These models, with several enhancements in the costly Self-Attention weight calculation, revolutionized the applied NLP industry in most of the mainstream NLP tasks during the years 2018 to 2021, including Machine Translation, Summarization, and Text Classification. Still, the primary advantage of these BERT-based models emerged from the powerful hardware (GPU, TPUs) that were used to train these highly parameterized models. This included computing with millions of parameters and then fine-tuning with several downstream NLP tasks. Although these models demonstrated strong word prediction capabilities through bidirectional context and produced high-quality sentence embeddings for tasks such as text classification, they still lagged in generative ability—particularly in sustaining open-domain conversational exchanges with humans. This remained the case until the end of 2022, when OpenAI first released their conversational model, ChatGPT [49], based on GPT-3.5. Although ChatGPT used the same transformer architecture proposed by Google, it delivered significant improvement in the generative text domain because of its decoder-only training mechanism, which is primarily focused on optimizing the model for chat conversation continuation. So, these models not only used very large pre-training corpora but also text generation-specific fine-tuning that made them very efficient. Such Transformer-based families of models typically have billions of parameters (and are therefore called large language models or LLMs) and exhibit enhanced capabilities, or so-called emergent capabilities, through in-context learning [26].

Further improvements have been achieved by fine-tuning these models via reinforcement learning with human feedback (RLHF) [50], enabling them to learn from high-quality examples curated by human annotators. Recently, the key players in this family of models include proprietary GPT-4 [3], GPT-4 Omni [51], GPT-5 [4], Google’s Gemini [14], open-source LLaMA models from Meta [6, 7], and DeepSeek-R1 [19]. Due to the powerful in-context learning capabilities of these models and the reduction of hallucination via multi-modal fine-tuning, the LLM community has observed significant progress in the areas of prompt-based or zero-shot LLM models, especially in the areas of Retrieval Augmented Generation [52, 53] and Agentic Task Completion [54]. Although these are considerable advancements in the area of text generation compared to earlier language models, it remains unclear what enables these recent LLMs to acquire emergent capabilities, making it challenging to debug and understand the inner workings of these models. While techniques, such as the chain-of-thought (CoT), enable conversing with these models and aim to find out how they came up with particular reasoning, such methods are not always accurate, as it remains unclear whether the output of these models is faithful to the reasoning they provide to users [55, 56]. All these challenges and fundamental gaps underscore the need for more in-depth investigations into the true working mechanisms of LLMs.

## 2.2 The Transformer architecture

To understand how language models generate output from prompts, it is necessary to examine the internal elements and computational flow and pathways within these deep neural network models. The architecture used to build models with this generative ability for LLMs is called a *Transformer* [1]. This architecture processes sequential data, allowing an LLM to capture contextual relationships between all input elements simultaneously, enabling tasks such as natural language understanding and generation. Mathematically, the architecture has the following elements and computational pathways. Let’s denote a sequence of  $n$  items  $(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$  by  $\mathbf{X} \in \mathbb{R}^{n \times d}$ . Here,  $d$  is the embedding dimension representing each item. Self-attention aims to capture the interaction amongst all  $n$  items by encoding each item by using three learnable weight matrices to transform Queries ( $\mathbf{W}^Q \in \mathbb{R}^{d \times d_q}$ ), Keys ( $\mathbf{W}^K \in \mathbb{R}^{d \times d_k}$ ) and Values ( $\mathbf{W}^V \in \mathbb{R}^{d \times d_v}$ ), in which  $d_q = d_k$ . Here, the input sequence  $\mathbf{X}$  is first projected onto these weight matrices to obtain  $\mathbf{Q} = \mathbf{X}\mathbf{W}^Q$ ,  $\mathbf{K} = \mathbf{X}\mathbf{W}^K$  and  $\mathbf{V} = \mathbf{X}\mathbf{W}^V$ . The final output  $\mathbf{Z} \in \mathbb{R}^{n \times d_v}$  of the self-attention layer is then calculated as follows:

$$\mathbf{Z} = \text{softmax} \left( \frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d_q}} \right) \mathbf{V} \quad (1)$$

For a given item,  $\mathbf{x}_n$ , in the sequence, the role of self-attention is to calculate the dot product of the query with all keys, where the softmax operator is further used to get the attention scores. Each item,  $\mathbf{x}_n$ , eventually becomes the weighted sum of all items in the sequence  $\mathbf{X}$ , in which weights are given by the attention scores. Figure 2 shows the network architecture of the original attention-based Transformer.

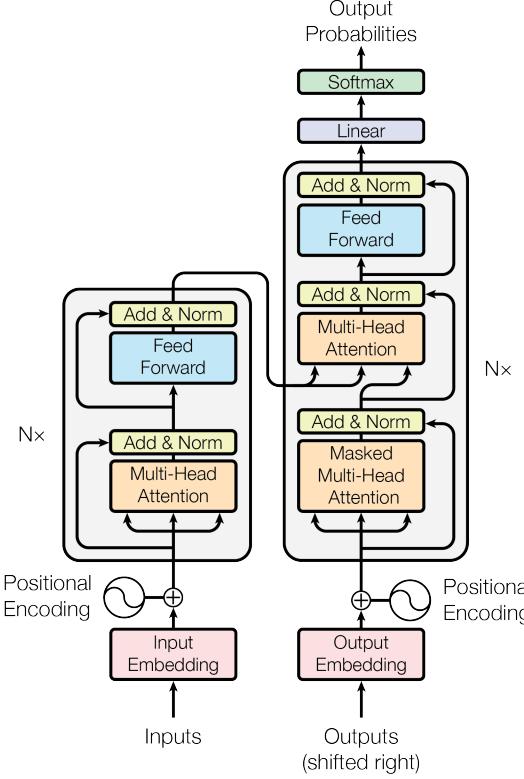


Figure 2: The architecture of Transformer. Source: [1].

### 3 Related Work

Several studies have recently explored the concepts of explainability and interpretability in the context of LLMs. Notably, Zhao et al.’s work [57] is the first detailed study on explainability for LLMs. The authors present techniques for local and global explanations coupled with model training. They categorize various methods based on conventional fine-tuning-based (i.e., feature attribution explanation, probing-based explanation, mechanistic interpretability, and concept-based explanation) and prompting-based paradigms (i.e., in-context learning, chain-of-thought prompting, and representation engineering).

Singh et al. [27] analyze the interpretation of LLMs in two ways: 1) interpreting an entire LLM model itself, including its output generation, and 2) using an LLM for producing individual explanations for each output. They propose, for a specific output of an LLM, that a *local explanation* can be explained via a combination of feature attribution (e.g., using SHAP [58]), natural language explanation, prediction decomposition (i.e., chain-of-thought-reasoning), and data grounding (i.e., retrieval augmented generation (RAG)). For the *global/mechanistic explanation* of an entire LLM model, they propose the use of attribution for LLM internals along with attention head summaries, coupled with some form of algorithmic understanding and data influence.

Luo and Specia [59] have further expanded the concepts proposed by Singh et al. [27]’s work by revealing the role of explanations in directly improving the LLM itself. In [59], the authors summarize local and global methods for LLM interpretability and also show that an LLM’s output can provide an opportunity to further enhance the LLM via model editing and other methods for enhancing a model’s capability. They posit that LLM outputs can be used to debug existing models and provide hints for refining and improving the model design.

Furthermore, Liu et al. [60] have evaluated LLMs from a causality perspective, with a focus on reasoning, fairness, safety, and multi-modality. The authors demonstrate that causal reasoning can enhance the reasoning capacity, fairness, and safety of LLMs, ultimately enabling these tools to generate explanations and elucidate how LLMs arrive at their conclusions.

Finally, some recent studies have reviewed general approaches to explaining LLM outcomes [61] and the computational pathways behind the inner workings of transformer-based LLMs [62, 63, 64, 65]

as scoping reviews.

While all these investigations provide valuable insights into explainability and interpretability of LLMs with a specific focus, the evolving landscape of research in understanding LLMs’ working mechanisms requires a deeper investigation to build trust in these tools. In this sense, our paper complements previous work with three significant new analyses. First, we examine the concepts of *tacit* and *explicit* knowledge, two distinct forms of knowledge that differ in how LLMs store, utilize, and generate information. Furthermore, explaining *fact*, *belief*, and *grey-zone information* with an LLM’s knowledge base is also a crucial topic requiring further analysis. Finally, the trustworthiness of LLM explanations with respect to explanation receivers, i.e., *explainees*, also needs rigorous exploration to ensure *explainees* understand and use such explanations in a meaningful and purposeful manner. Hence, our paper addresses these details as a complement to the current trends of explainability in LLMs, and presents opportunities and challenges toward presenting trustworthy LLM explanations.

## 4 Explainability within LLMs

This section revisits the expected properties of explainability and distinguishes local explainability and mechanistic interpretability concepts within LLMs.

### 4.1 LLMs meet XAI

Explainable artificial intelligence (XAI) has emerged as a potential solution to achieve transparent and trustworthy AI systems, particularly in safety-critical applications [33, 66, 67]. Historically, preliminary studies on XAI have leveraged explanations as a reasoning approach in expert systems or as symbolic representations for neural networks [68, 69, 70, 71]. But the rising dominance of deep learning and extensive use and deployment of deep neural network-based models have added further complexity, and increased the need for AI explanations. According to [33], explanations in modern AI systems should consider five essential perspectives: regulatory, scientific, industrial, developmental, and social perspectives. The regulatory compliance perspective primarily ensures the “right to explanation” from a legal perspective as first articulated by the General Data Protection Regulation (GDPR) of the European Union [72]. The key point with this recital is that an AI system must justify why it arrives at specific conclusions or decisions, particularly in critical domains and applications. Furthermore, XAI can help extract explicit useful information from black-box models trained on large datasets, where the extracted knowledge can lead to further scientific discovery within the field. In addition, as many industrial entities make customer satisfaction as a top priority in automated systems, AI explanations can have value in improving user trust by providing transparency in autonomous decision-making. Moreover, from the developmental viewpoint, explanations can help debug the black-box AI system, discover potential faults and flaws with existing systems, and incrementally improve both reliability and trust. Finally, from a societal perspective, one can better understand what an AI system aims for rather than focusing on what it has been trained for. These non-exhaustive points of view reveal that the value of explanations can be measured in various ways, depending on the needs and expectations of a targeted audience.

Having been recently applied in many domains and critical tasks [73, 74], all the above-mentioned explainability perspectives inherently find their alignment in LLMs. While emergent abilities of LLMs help enable them to reason, summarize, generalize, and make predictions across a variety of downstream tasks, model errors — primarily known as hallucinations — are serious issues with these models. In particular, for safety-critical applications and domains, hallucinations may drastically impact the outcome of tasks, resulting in serious trust, transparency, and accountability issues among the involved stakeholders [75, 76]. Consequently, explainability of LLMs, at least to a feasible extent, is a significant topic deserving careful exploration.

### 4.2 Local explainability of LLMs

Analogous to other learned models, LLM explanations for their predictive outputs can be classified as *local explanations* and *global explanations*. Local explanations refer to explanations provided in response to individual explicit outputs generated by LLM [57, 61]. More formally, we can define a formulation of LLM explainability as follows. Let us use the following notation:

- $f : \mathcal{X} \rightarrow \mathcal{Y}$  be a pretrained LLM, where  $\mathcal{X}$  is the input space (e.g., token sequences) and  $\mathcal{Y}$  is the output space (i.e., the token with the highest probability).
- $x \in \mathcal{X}$  be a specific input, i.e., a prompt.
- $f(x)$  is the model's output on input  $x$ .
- $h^{(l)} \in \mathbb{R}^{d_l}$  is the hidden representation at layer  $l \in \{1, \dots, L\}$ .
- $z^{(l)} \in \mathbb{R}^{d_l}$  is the pre-activation value (e.g., logits) at layer  $l$ .
- $T$  is the number of tokens in the prompt.

Based on this notation, a method  $\mathcal{E}_{\text{local}}$  provides a local explanation for an input–output pair  $(x, f(x))$  by constructing a simpler interpretable function  $g \in \mathcal{G}$  such that:

$$g \approx f \quad \text{in a neighborhood } \mathcal{N}_x \subset \mathcal{X} \text{ around } x$$

and

$$\mathcal{E}_{\text{local}}(x; f) := g$$

subject to the general objective, such as analogous to the one in LIME [77]:

$$\arg \min_{g \in \mathcal{G}} \mathcal{L}_{\text{fidelity}}(f, g; \mathcal{N}_x) + \lambda \cdot \Omega(g)$$

in which:

- $\mathcal{L}_{\text{fidelity}}$  measures the closeness of  $g$  to  $f$  in  $\mathcal{N}_x$ .
- $\Omega(g)$  penalizes complexity of the explanation function.
- $\lambda \geq 0$  is a regularization parameter.

Essentially, the local explainability method must provide an explanation for why the model generated a specific output in response to a user-entered prompt. At the highest level, local explanations can be distinguished as either natural language explanations, chain-of-thought reasoning, retrieval-augmented generation, feature attribution methods, or some combination of those methods [57]. We describe each of these approaches as follows:

(1) *Natural language explanations*: Given a user-provided prompt, the model generates an explanatory description for the prompt in natural language [27]. In this case, the LLM outputs both the predicted answer and an explanation, often structured with requests like “Explain your answer” in the prompt.

(2) *Chain-of-thought reasoning (CoT)*: This approach factors complex problems into a series of sequential steps or intermediate thoughts that sequentially lead to an answer for the provided prompt [80]. Rather than directly predicting an answer, the explanation process walks through intermediate reasoning steps that lead to the final decision, aiming to make its internal logic explicit for a specific input. This makes CoT a form of local explanation, as it focuses on clarifying a single predictive output rather than describe a model's behavior across all inputs. CoT is especially effective in producing explanations for complex reasoning tasks such as math word problems, commonsense reasoning, and multi-hop question answering. For instance, given a math question, the model might output: “We start with 10 apples, eat 3, then collect 5 more. So, in the end we have  $(10 - 3 + 5) = 12$  apples,” followed by the final answer. CoT explanations can be prompted with cues like “Think step by step,” or generated through few-shot prompting, or supervised training on datasets with annotated reasoning paths. Compared to other explanation methods, such as feature attributions, CoT can offer more understandable justifications for a model's behavior on individual examples. With that said, some recent investigations show that CoT may not always present faithful explanations for specific prompts despite seeming convincing in support of the output prediction [56, 89].

(3) *Retrieval-augmented generation (RAG)*: This is a technique that enhances the capabilities of an LLM by integrating relevant material from external knowledge bases (e.g., references, citations) into the generation process [52, 90]. The retrieval component of RAG focuses on retrieving relevant documents or data from an external knowledge base, as indicated in the user's query/prompt. Augmentation refers to the incorporation of context and additional details. These key points ultimately

Table 1: Selected representative studies on local explanation generation techniques for LLMs

Study	Goal of the study	LLM used	Key findings/takeaways
<i>Natural language explanation</i>			
Huang et al., [78], 2023	LLM’s ability to explain its predictions	ChatGPT	ChatGPT’s self-explanations differ from the compared metrics while being computationally less costly to produce.
Tanneru et al., [79], 2024	Introducing metrics to measure the uncertainty in LLM-generated explanations	InstructGPT, GPT-3.5, and GPT-4	Probing uncertainty correlates with explanation faithfulness, while verbalized confidence may be misleading.
<i>Chain-of-Thought reasoning</i>			
Wei et al., [80], 2022	Understanding the role of intermediate reasoning on the ability of LLMs to perform complex reasoning	GPT-3, LaMDA, PaLM, UL2 20B, Codex	Prompting LLMs with intermediate reasoning steps improves performance on complex tasks.
Lyu et al., [81], 2023	How to generate faithful reasoning for LLM predictions	Codex	Using symbolic reasoning chain and deterministic solver enhances faithfulness of chain-of-thought reasoning.
Turpin et al., [55], 2023	Critical examination of the faithfulness of LLM explanations when using CoT prompting	GPT-3.5 and Claude 1.0	CoT explanations can be misleading and may not always reflect the true reasoning behind predictions.
Arcuschin et al., [56], 2025	Investigating unfaithful CoTs on realistic prompts	GPT, Gemini, DeepSeek, LLaMA series (15 models)	Even frontier models like GPT-4o and Gemini 2.5 Pro may produce CoTs that sound logical but don’t match the actual decision process.
<i>Retrieval-augmented generation</i>			
Yuan et al., [82], 2024	Providing human-understandable justifications for driving decisions	Vicuna1.5-7B	RAG-Driver improves interpretability of autonomous driving systems by combining a multi-modal LLM with retrieval-augmented in-context learning.
Li et al., [83], 2025	Framework for personalized and explainable recommendations	LLaMA family	LLMs augmented with structured graph data move beyond generic recommendations to transparent, user-specific ones.
<i>Feature-attribution methods</i>			
Wu et al., [84], 2020	Analyzing linguistic knowledge embedded in BERT via perturbed masking	BERT	Perturbed Masking provides a faithful, parameter-free lens to reveal internal mechanisms of BERT.
Mohebbi et al., [85], 2021	How individual token representations within BERT contribute to probing tasks	BERT	BERT encodes meaningful knowledge in specific token representations.
Enguehard, [86], 2023	Refining Integrated Gradients (IG) for explainability	BERT, DistilBERT, RoBERTa	Sequential Integrated Gradients (SIG) provides a more accurate and intuitive explanation method.
Kokalj et al., [87], 2021	Adapting SHAP to transformer-based LLMs	BERT	TransSHAP bridges SHAP and transformers with a structure-aware explanation technique.
Wu and Ong, [88], 2021	How well attribution methods explain BERT’s decision-making in classification	BERT	Attribution methods generalize well across tasks with shared semantics.

enable the generation of a response that incorporates both the original query and the augmented information. The RAG process differs from purely generative methods, which rely solely on internal parameters; it grounds the explanation in potentially verifiable facts, which intuitively enhances trust and reduces hallucination.

(4) *Feature attribution-based explanations*: These explanations aim to quantify the contribution of each input feature (e.g., words, tokens) to a model’s generated prediction. This category includes perturbation-based methods, gradient-based methods, surrogate models, and decomposition-based methods [57].

- Perturbation-based methods modify input features and evaluate the output of the model against such modifications.
- Gradient-based methods reveal feature importance by leveraging the partial derivatives of the model’s output with respect to input features (but requires some precision in defining such partial derivatives).
- Surrogate feature attribution-based explanation methods, on the other hand, use simpler, interpretable models to approximate the behavior of complex LLMs and provide insights into how different features contribute to their predictions (i.e., LIME [77], SHAP [58]).
- Finally, decomposition-based methods explain the outputs of LLMs by breaking their reasoning into smaller, interpretable components, such as layer-based or individual neuron-based analysis.

Furthermore, attention-based explanations (e.g., heatmaps & visualization) and example-based explanations (counterfactual analysis [91] and human-adversarial examples [92]) can be considered as an analysis of local LLM predictions. Table 1 shows representative examples of local explanation generation methods in LLMs from the relevant studies.

Overall, from the broad spectrum, local explanation generation approaches follow three main paradigms by design [57]: the Explain-then-predict approach (e.g., CoT reasoning), the predict-then-explain (post-hoc explanation), and the joint predict-explain mechanisms (e.g., jointly training

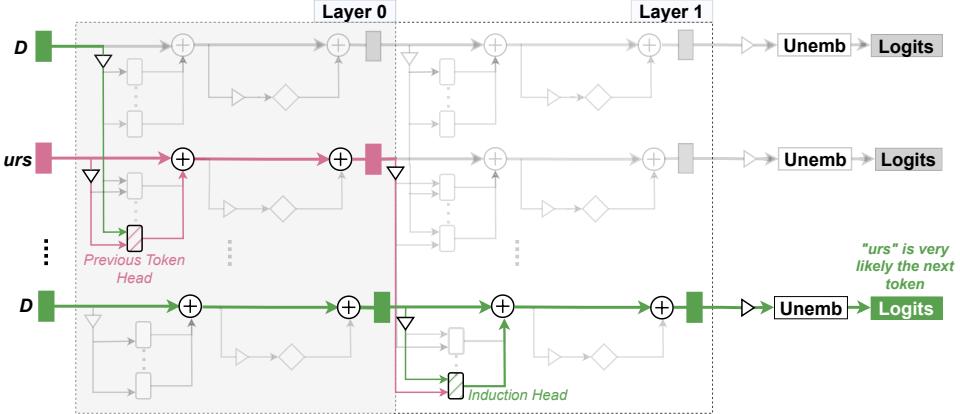


Figure 3: An example of an induction circuit provided by Rai et al. [63], based on Elhage et al.’s [93] findings, showing outputs of two attention heads as nodes, and link between them as edges, enabling the model to generalize from repeated patterns.

explanation and prediction heads). While the same LLM-generated explanations are favorable for the model’s predictions, there are a few approaches that incorporate another model to explain the behavior of a target LLM, as “LLM-as-a-Judge”, as such “judge” LLMs might have a better ability to provide cost-effective and consistent evaluation [94].

### 4.3 Mechanistic interpretability of LLMs

Global explanations, also sometimes referred to as “mechanistic explanations,” in the context of LLMs describe the model’s internal working mechanism by explaining the predictive behavior of the entire model [27, 95, 96]. In general, generating mechanistic explanations of LLMs is more challenging than generating local explanations. A significant part of the problem is that accurately conveying internal functions requires an embedded self-model, but existing LLMs do not possess such a representation. While local explanations focus on justifying a specific output, mechanistic interpretability deals with more complex tasks and aims to provide a holistic explanation of how LLM works in its entirety. Within the notation provided above, a mechanistic explanation  $\mathcal{E}_{\text{mech}}$  provides a mapping:

$$\mathcal{E}_{\text{mech}} : \{W^{(l)}, b^{(l)}, h^{(l)}\} \rightarrow \mathcal{S}$$

Here  $\mathcal{S}$  is a structured representation of functional roles of components, such as attention heads, neurons, and circuits. It is noteworthy to mention that these most common concepts are specific to the transformer architecture used to create most of the existing LLM internal representation models, and so do not easily convey any human-interpretable explanations. From the latter perspective, whether Transformer architectures are the only appropriate foundation model is currently a question of significant debate, and further research reveals the need for a broader spectrum of foundation architectures (e.g., [70, 97, 98]). Formally, mechanistic interpretability in Transformer seeks to identify functions  $\phi_k$  such that:

$$f(x) \approx F(\phi_1(x), \phi_2(x), \dots, \phi_K(x))$$

In which

- $\phi_k(x)$  represents a functional sub-component of the model.
- $F$  is a known or inferred composition function approximating  $f$ .

These functions are often discovered via probing or causal intervention methods (e.g., activation patching), such as:

$$\phi_k(x) := \psi(h_i^{(l)}(x)) \quad \text{for some } \psi : \mathbb{R} \rightarrow \{0, 1\}$$

A broader scope of mechanistic interpretability of LLMs generally falls into the umbrella of two key focus areas: *circuit* and *feature* analysis [63]. Features, which serve as the fundamental units of representation, are interpretable input-related attributes encoded in the language model’s activations [65]. They are “interpretable” because they have a natural interpretation in their application domain. For instance, when a user enters a prompt containing specific tokens, the language model can predict responses related to these features, which it has already learned during the pretraining stage. Therefore, decoding such features can be considered as one way of mechanistic interpretability in LLMs.

While feature-based analysis is one approach to LLM interpretability, understanding the entire LLM’s behaviour goes beyond the analysis of features and the interconnection of an LLM’s subgraphs. These interconnected components are responsible for guiding specific tasks, which are important to understand the entire model’s operating principles. Such subgraphs within an LLM are referred to as *circuits* and several types of circuits have recently been proposed and discovered through LLM interpretability research, such as induction circuits (generalizing from repeated patterns), copy circuits (copying tokens from earlier contexts), indirect object identification (IOI) circuits (resolving pronouns via syntactic structure), and logit attribution circuits (assigning influence on final token prediction to specific tokens in context).

Interpretability techniques within these focus areas include an analysis of a Transformer-based model’s internal elements and the way these elements form a network, such as attention head analysis, fine-grained circuit analysis, and the impact of various forms of training data distribution [27]. Meanwhile, a challenge arises from the interactions between neuron units, where each neuron can activate in response to a range of different concepts. For example, a neuron might activate for specific tokens in a language (e.g., Korean or academic citations), making it difficult to generalize or assign a single meaning to that neuron. This phenomenon has been called “polysemy” [99]. As a result, a neuron can capture a mixture of information, making it difficult for humans to interpret it in a meaningful and generalized way [96]. This behavior is often due to information mixing or superposition, where neurons do not represent a single, clear feature. Instead, features are represented by unique combinations of activations in multiple neurons.

Another relevant idea for understanding the behavior of LLMs is the use of a dictionary learning approach with sparse autoencoders. The authors in [95] focus on a single layer from a transformer model with a 512-neuron MLP layer, decomposing its activations into interpretable representations by training sparse auto-encoders on these activations. The findings indicate that sparse autoencoders can effectively uncover interpretable, relatively universal features from neural network activations, providing insights that are not visible at the neuron level alone. For example, sparse auto-encoders applied across different language models yield similar features, supporting the idea of shared, universal representations. Although considering only 512 neurons, the study shows that these neurons can represent thousands of distinct characteristics [95].

In another example, Rai et al. [63] present an example of an induction circuit in Figure 3, based on Elhage et al.’s [93] findings on a toy LLM. This circuit involves two attention heads - one called the previous token head and the other the induction head. These heads act as nodes, while the data flow between them, represented by input and output activations, forms the edges of the circuit. The purpose of the circuit is to recognize and continue repeated sequences in the input text (for example, turning “Mr D urs ley was thin and bold. Mr D” into “urs”). In this process, the previous token head captures that the string “urs” typically follows the token “D” in earlier parts of the text, and the induction head uses this information to boost the likelihood of predicting “urs” as the next token. Overall, important properties for reverse engineering a deep neural network are decomposability and linearity. Decomposability means that representations can be broken down into individual interpretable features, allowing each feature to be analyzed independently, making it easier for humans to understand. Linearity, on the other hand, means that each feature can be represented as a specific direction in the network’s internal space, typically relying on the concept of vector directions [100].

A deeper analysis of the related work reveals that understanding the entire LLM’s behavior requires a combination of component- and computation-based techniques within these models. Furthermore, another critical consideration is whether the same or similar LLM features and circuits appear in other LLMs [63]. This nuance raises a question about the *universality* of LLM interpretability, meaning to what degree similar LLM features and circuits are observed in different LLMs. Table 2 shows a scoping review of different studies on the mechanistic interpretability of LLMs. As seen, each study has focused on specific LLMs to discover their inner working principle. Within this context, a recent investigation by [101] shows that GPT-2 and LLaMA-2 encode bias differently, and their internal

Table 2: Empirical studies on mechanistic interpretability of LLMs, focusing on attention head analysis, fine-grained circuit analysis, logit probing, activation patching, as well as a combination of these methods

Study	Goal of the study	LLM used	Key findings/takeaways
Elhage et al., [93], 2021	Reverse engineering transformers with two or less layers and solely have attention blocks	GPT-3	Induction heads can help explain in-context learning in small models
Olsson et al., [102], 2022	Reverse engineering transformers with larger ( $>2$ ) attention blocks	GPT-2, GPT-3	“Induction heads might constitute the mechanism for the actual majority of all in-context learning in large transformer models.”
Wang et al., [103], 2023	Understanding LLMs via their circuits	GPT-2 small	Identification of attention heads compensating for the loss of function of other heads, and heads contributing negatively to the next token prediction.
Bills et al., [104], 2023	Understanding what patterns in text cause a neuron to activate	GPT-2, GPT-4	LLMs can be used to interpret and explain the behavior of individual neurons within LLMs.
Goldowsky-Dill et al., [105], 2023	Generalizing path patching to test hypotheses containing any number of paths from input to output	GPT-2	“Path patching is an expressive formalism for localization claims that is both principled and sufficiently efficient to run on real models”
Gurnee et al., [106], 2023	Understanding how high-level human-interpretable features are represented within the internal neuron activations of LLMs	EleutherAI’s Pythia suite	Sparse probing is an effective methodology to locate neurons contributing to interpretable structures.
Wu et al., [107], 2023	Efficient search for interpretable causal structure in large language models	Alpaca-7B	Boundless distributed alignment search solves a simple numerical reasoning problem in a human-interpretable manner.
Hase et al., [108], 2023	Understanding where to manipulate knowledge in language models	GPT-J	“Model edit success is essentially unrelated to where factual information is stored in models, as measured by Causal Tracing”.
Li et al., [109], 2023	Improving the truthfulness of language model outputs	LLaMA, Alpaca, Vicuna	Subset of attention heads plays a major role in the truthfulness of model outputs.
Hou et al., [110], 2023	Exploring mechanistic interpretability of language models for multi-step reasoning tasks	GPT-2, LLaMA	“We can often detect the information in the reasoning tree from the LM’s attention patterns.”
Conmy et al., [111], 2023	Finding the connections between the abstract neural network units that form a circuit.	GPT-2 small	Automatic circuit discovery algorithm conducts all the activation patching experiments essential to discover which circuit is responsible for the model’s behavior”.
Friedman et al., [112], 2023	Modifying Transformer that can be trained via gradient-based optimization and converted into a human-readable program	GPT-family	Transformer Programs can help trace information flows between model components and different positions.
Hanna et al., [113], 2023	Identifying circuits in an LLM model that performs mathematical tasks	GPT-2 Small	GPT-2 small’s final multi-layer perceptrons boost model’s mathematical reasoning ability.
Zhang and Nanda [114], 2024	Understanding impact of methodological details in activation patching	GPT-2 small, GPT-2 XL	Variations in metrics and methods in activation patching in language models might lead to different interpretability results.
Gould et al., [115], 2024	Discovering successor heads, a class of attention heads that lead detecting interpretable model features	GPT-2, Pythia, and LLaMA-2	“Successor heads exhibit a weak form of universality, arising in models across different architectures and scale.”
Lee et al., [116], 2024	Understanding how toxicity is represented and elicited in a pre-trained language model	GPT2-medium, LLaMA-2-7B	Subtracting specific vectors in MLP blocks from the residual stream can eliminate toxic outputs.
Jain et al., [117], 2024	Understanding effects of fine-tuning on procedurally defined tasks	GPT-3.5	Finetuning minimally changes a pretrained language model’s capabilities in procedurally defined tasks.
Ren et al., [118], 2024	Understanding in-context learning of LLMs	InternLM2-1.8B	“Specific attention heads encode syntactic dependencies and semantic relationships in natural languages”
Prakash et al., [119], 2024	Understanding impact of fine-tuning on the internal mechanisms implemented in language models.	LLaMA-7B, Vicuna 7-B, Goat-7B, FLoat-7B	Functionality of the base model’s circuit remains unchanged in fine-tuned models
Lan et al., [120], 2024	Comparing circuits for sequence continuation tasks on Arabic numerals, number words, and months	GPT-2 Small, LLaMA-2-7B	“Semantically related sequences rely on shared circuit subgraphs with analogous roles”.
Todd et al., [121], 2024	Understanding the role of function references in transformer-based language models	GPT-J, GPT-Neox, LLaMA-7B, 13B, 70B	Function vectors can be explicitly extracted from a small number of attention heads and represent the demonstrated task within a hidden state.

Continued on next page

Table 2: (Continued)

Study	Goal of the study	LLM used	Key findings/takeaways
Niu et al., [122], 2024	Analyzing the ability of language models to recall facts from a training corpus via knowledge neuron	BERT, GPT-2, LLaMA-2	“Knowledge neuron thesis does not adequately explain the process of factual expression.”
Singh et al., [123], 2024	Understanding emergence dynamics of induction heads in a controlled setting	GPT-2, GPT-3	“Induction heads operate additively, with multiple heads used to learn the ICL task more quickly.”
Ghandeharioun et al., [124], 2024	Using the language model itself to explain its internal representations in natural language	LLaMA-2 13B, Vicuna-13B, GPT-J 6B, Pythia-12B	Various kinds of information from LLM representations can be queried via Patchscopes in natural language.
Zhou et al., [125], 2024	Explaining LLM Safety through Intermediate Hidden States	LLaMA-2, LLaMA-3, Mistral, Vicuna, Falcon	LLMs tend to learn ethical concepts during the pretraining phase rather than alignment and can detect malicious or normal inputs in the early layers.
Ferrando and Voita [126], 2024	Interpreting LLM predictions by extracting the dominant part of the overall information flow	LLaMA-2	“Some model components can be specialized on specific domains such as coding or multilingual texts.”
He et al., [127], 2024	The emergence of in-context learning and skill composition in a collection of modular arithmetic tasks	GPT-style architectures	“The smallest model capable of out-of-distribution generalization requires two transformer blocks, while for deeper models, the out-of-distribution generalization phase is transient, necessitating early stopping.”

structures respond differently to interventions. Another study, which focuses on inference stages and robustness through layer-level interventions [128], has determined that various LLMs, such as GPT and Pythia, exhibit different levels of robustness and modularity, with implications for the general safety and optimization of LLMs. Such analyses and Table 2 give a reason for a more careful investigation of the interpretability concept in LLMs, as in fact, the way these neural dialogue models generate responses to prompts might be dependent on both the pretraining data and the construction mechanism of such models [129].

Overall, local explainability and mechanistic interpretability provide complementary pathways toward trustworthy LLMs: local explainability fosters trust at the *decision level*, whereas mechanistic interpretability could help deepen understanding and reliability of LLMs at the *system level*.

## 5 Critical Epistemic Properties of LLMs for Generating Trustworthy Explanations

### 5.1 LLM explanations for facts, beliefs, and the grey zone

Facts and beliefs are spread across a dichotomy in human reasoning: a similar dichotomy affects our ability to comprehend them in LLM explanations. A fact is something that can be confirmed as objectively true, either verified or proven through evidence, a documented source, observations, or experience, and is not influenced by personal feelings, subjective opinions, or interpretations [130]. For instance, the statement “*Akra is the capital city of Ghana.*” is a fact as this piece of information can easily be verified from government or official records. In another example from logic, “All men are mortal; Aristotle is a man; Therefore, Aristotle is mortal.” The implication is direct, and the evidence could not imply the opposite “Aristotle is immortal.” However, this is clear since all the facts can be confirmed. A belief, on the other hand, is an acceptance that something is true or exists, often without requiring definitive proof, and the presence of facts in a belief is hazy [131]. For instance, the statement “*Democracy is the best form of government.*” can be considered a belief as it reflects a subjective judgment influenced by cultural, ethical, or personal values. However, some might argue that an alternative government structure, such as technocracy, is a more preferred structure as the decision makers are experts in their field within such a government. So, beliefs often reflect personal perspectives. The formal literature on belief provides a more technical definition of belief as something consistent with a collection of supporting beliefs, even if not generally true (e.g., [132]). A final subtlety is that there is a grey zone where contradictions emerge, where there could be conflicting evidence against a presented statement. For example, while one might argue that “*Eating eggs every day improves human health,*” there are also conflicting scientific studies showing that higher regular intakes of eggs were linked to increased risks of cardiovascular disease and mortality [133]. These aspects are directly related to local LLM explanations, so that when an LLM presents explanatory information on its predictions, the target user must be aware of whether such pieces of information are a fact, a belief, or potentially on the borderline.

## 5.2 Tacit and explicit explanations by LLMs: Show vs tell

LLMs, as knowledge-based models, produce outputs with varying knowledge granularity depending on the prompt design. The knowledge these models retain could be *explicit*, i.e., as easily documentable and communicable, but also *tacit*, meaning such kind of knowledge arises from unspecified inference or is experiential and difficult to articulate. For example, when a novice asks *how to bike*, humans can't fully explain how to balance or steer to that person, as riding a bike is typically learned via experimenting through trial and error. This is an example of tacit knowledge. On the other hand, when one asks for *how to make a banana cake*, this question can be answered more easily as relevant measurements and steps for cooking a banana cake are written in a cookbook. This is an example of explicit knowledge. Tacit knowledge, popularized by Polanyi, refers specifically to the intuitive understanding behind an expert's judgment or skill and is rooted in personal experience that is difficult to verbalize or formalize [134, 135]. Such "intuitive" knowledge is based on personal insight and experience, which is subjective and cannot be easily expressed in symbols such as language, mathematical formulas, or charts and tables; it is distinguished from explicit knowledge that can be more easily expressed in words or other symbols.

Current LLMs utilize a representation model that learns patterns from textual data, using them as a basis for language generation and understanding. These models can encode "implicit rules" or cultural nuances from large amounts of data, but their processes and internal structures are often black boxes, as tacit knowledge is, by definition, subjective, barely textualized knowledge that makes up a large part of our common knowledge.

LLMs could have an evolving role in clarifying tacit explanations by acting as intermediaries between implicit knowledge and explicit understanding in several ways. First, LLMs can be used to transform implicit or context-dependent ideas into explicit language. For instance, if one enters a prompt like *how can I be a successful entrepreneur like a [Person]*, an LLM can infer underlying principles of successful entrepreneurship and articulate them as actionable advice, translating observed behavior into explicit steps. Furthermore, LLMs could analyze and translate context as cross-cultural and cross-domain mediators by uncovering why certain expressions, actions, or phrases might carry particular meanings in different cultures. For instance, LLMs may reveal the significance of communicative differences, such as silence, in Finnish versus Italian conversations [136]. Finally, an LLM can adjust its response to a prompt considering a user's comprehension of the provided response (e.g., explain [the concept] like I am five versus explain [the concept] to an expert.). Overall, from a broad spectrum, tacit and explicit explanations could be differentiated in the manifestation of the *show vs tell* dilemma: Tacit explanations *show* by explaining through actions or context while explicit explanations *tell* through words, rules, or data. Hence, LLMs can be considered *amplifiers of tacit understanding*, making implicit knowledge more intelligible and facilitating users' discussions on a topic, while also augmenting their creativity and intelligence.

## 6 Evaluating LLM Explanations

Understanding the accuracy, correctness, and faithfulness of LLM explanations is crucial for interaction partners to trust and responsibly use them. Hence, LLM explanations need careful evaluation to meet the human-centric requirements discussed above. In general, there are currently two dominant evaluation methods for LLM explanations: human evaluation and automatic evaluation [57, 73]. The following subsections describe these two evaluation approaches.

### 6.1 Human Evaluation

Human evaluation of LLM explanations refers to the manual assessment of the correctness and quality of LLM-generated explanations via human judgment. Depending on the nature of the task and the intelligibility of explanations, human participants can be people with diverse technical backgrounds and domain knowledge, from ordinary users to experts. Overall, human evaluation of LLM explanations has three primary factors: the number of evaluators, evaluators' expertise level in that specific task, and the criteria for explanations' evaluation [73, 57]. Given that people may have diverse functional and cognitive capabilities along with cultural and subjective preferences, their assessment of an explanation may be different. Consequently, having a sufficiently high number of people in judging LLM explanations may intuitively lead to more grounded and solid conclusions. Moreover, domain expertise may play a crucial role in assessing the quality of the explanation, and such studies should first identify people suitable for each specific explanation assessment. Finally,

You are a physician specialized in inflammatory bowel disease. A radiology report is provided below. Please 1. determine if the patient has Crohn's disease or not and 2. summarize the evidence using at most three sentences.

**Prompt** There is an abnormal appearance to the distal 18-20 cm of ileum with loss of folds and slight wall thickening containing fat. No adjacent inflammatory change. There is a second area approximately 10-15 CM proximal to this which measures 3-4 cm in length and has a similar appearance. The bowel loops proximal show no significant dilatation. No other obvious abnormalities in the GI tract. Liver and intrahepatic biliary tree unremarkable. Gallbladder has been removed. Spleen, pancreas, adrenal glands and kidneys are normal. No significant skeletal abnormality. Lung bases are clear

1. Yes, the findings support a diagnosis of Crohn's disease.

**Answer** 2. The abnormal appearance of the distal ileum with loss of folds, slight wall thickening, and fat deposition are characteristic of Crohn's disease, as is the presence of another similar lesion more proximally in the ileum. Absence of adjacent inflammatory change and lack of proximal bowel dilatation are consistent with chronicity rather than acute inflammation.

Figure 4: ChatGPT provides a diagnostic prediction and the corresponding evidence when provided with a radiology report on Crohn's disease. The prompt was tested on October 31st, 2024.

evaluation rubrics should include key factors in evaluating LLM explanations, as these metrics provide a framework for how to draw conclusions from the explanations. We present key factors for human-centric LLM evaluations in Subsection 8.3.

## 6.2 Automatic Evaluation

Automation evaluation of LLM explanations typically involves using established metrics and tools to evaluate the quality and correctness of LLM-generated explanations automatically. These approaches are primarily used to provide a basis for standardized assessment, and save time and avoid potential impacts of humans' subjective preferences [57, 73]. Depending on the task and requirements, various automatic evaluation tools can be used for LLM explanations [137]. However, at its essence, automatic evaluation approaches must present accurate and factually correct explanations [73]: these evaluation approaches are *accuracy* (e.g., Exact match, ROUGE score [138]), *faithfulness* [139], *calibrations* (e.g., classification accuracy, such as area under curve (AOC)), *fairness* (e.g., equalized odds difference), and *robustness* (e.g., attack success rate [140] and performance drop rate [141]). There have recently been attempts to develop methods for automating such evaluation approaches. For instance, G-Eval [142] has been proposed to evaluate natural language generation (NLG) outputs with GPT-4 for better human alignment. Furthermore, LLM-EVAL [143] assesses open-domain conversations with LLMs. In addition, REM [144] leverages the collective intelligence approach using numerous LLMs through a ranking mechanism to evaluate LLM outputs. Other notable automatic evaluation approaches include PandaLM [145], HELM [146], AGIEval [147], and PICO [148].

## 7 Empirical insights from critical applications

Having presented local and mechanistic explanations within LLMs, along with critical epistemic LLM properties and assessment methods for explanations, we now unify these concepts in experimental insights from two safety-critical applications. The following subsections present empirical studies from two domains - healthcare and autonomous driving - and describe implications of LLM explanations from the trust perspective for targeted interaction partners in these domains.

### 7.1 Insights from Healthcare

XAI has been widely adopted in the medical and healthcare domain to identify the most contributing input features for the decision-support function of predictive models (e.g., for both disease diagnosis and prognosis). The features identified as important then serve as explanations or evidence for the predictions. As a predictive model trained on a particular dataset might exploit some features biased towards that dataset, a model with high predictive performance in a particular test dataset might not necessarily perform well with new data (e.g., the medical data from a different hospital or province);

**Question**

A 24-year-old pregnant woman at 28 weeks gestation presents to the emergency department with complaints of fever with chills and pain in her knee and ankle joints for the past 2 days. She also complains of headaches and difficulty moving her neck. Further questioning reveals that she had a tick bite on her arm while gardening a few days ago. Pregnancy is progressing normally. On examination, an erythematous rash is seen on her right arm. Her obstetric examination is normal. Ultrasound of the fetus is reassuring with a normal heartbeat and no gross abnormalities. A specimen is collected to test for Lyme disease. What is the next best step for this patient?

**Options**

A) Ibuprofen      B) Tetracycline      C) Amoxicillin      D) Gentamicin

**Physician**

Amoxicillin ✓

**Explanation:** Amoxicillin is a safe and effective treatment for Lyme disease in pregnancy. Ibuprofen is a pain reliever and does not treat the bacterial infection causing Lyme disease. Tetracycline antibiotic is not recommended during pregnancy; it can cross the placenta and affect fetal development, including causing discoloration of the baby's teeth and potential bone growth issues. Gentamicin, a potent antibiotic generally reserved for severe infections, is not typically used for treating Lyme disease.

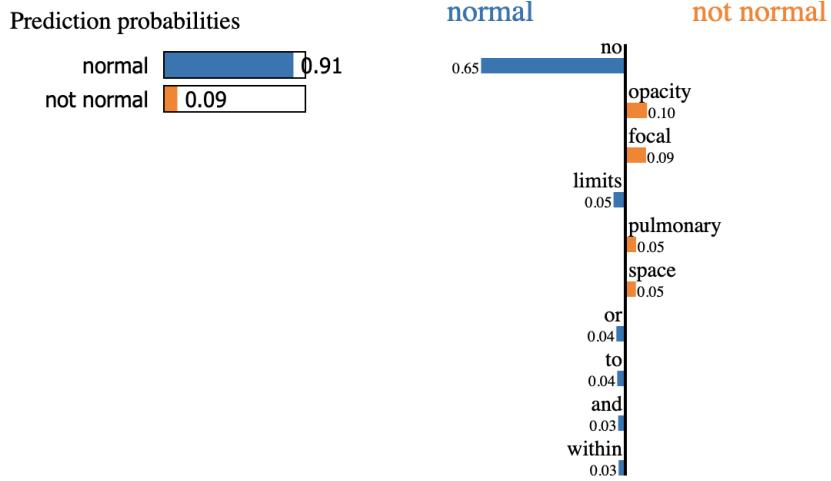
**GPT-3.5**

Tetracycline ✗

**Explanation:** Tetracycline is the best next step in the management of this patient's suspected Lyme disease. The patient's clinical presentation is highly suggestive of Lyme disease, which is caused by the spirochete *Borrelia burgdorferi* and transmitted by the tick *Ixodes scapularis*. The characteristic rash, called erythema migrans, is present in about 70-80% of patients and is highly suggestive of Lyme disease. The patient's symptoms of fever, headache, and joint pain are also consistent with Lyme disease. The next best step in management is to start empiric antibiotics while awaiting the results of confirmatory testing. Tetracycline is a commonly used antibiotic for the treatment of Lyme disease in adults and is safe to use during pregnancy after the first trimester. It has been shown to be effective in eradicating *B. burgdorferi* and preventing the progression of Lyme disease. Ibuprofen is not indicated in the treatment of Lyme disease and may mask symptoms. Ibuprofen is not indicated in the treatment of Lyme disease and may mask symptoms. Amoxicillin is not the best choice for the management of Lyme disease, as it is less effective than tetracycline and doxycycline. Gentamicin is not an effective treatment for Lyme disease.

Figure 5: An example of a serious hallucination of GPT 3.5 in clinical diagnosis on the Med-HALT benchmark. Source: [149].

It is essential to gain insights into what features are leading to the predictions, so that a human decision-maker can determine the trustworthiness of the predictions. For example, in the particular case of survival analysis in medicine [150, 151] - where the task is to predict the time for a particular event to occur given an individual (e.g., death for a cancer patient) from various modalities of data (e.g., medical imaging, textual reports and tabular data) - post-hoc XAI methods, such as SHAP and LIME are commonly employed to interpret how machine learning (ML) models make survival predictions for patients with cancer or those undergoing organ transplantation [152, 153, 154, 155, 156, 157]. In the study of applying XAI to diagnostic predictions [158, 159, 160, 161], the goal is to assist physicians and doctors with their diagnostic decisions by not only providing predictions using ML-based models but also evidence for the predictions. Particularly in life-critical domains like medicine, explanations must accurately reflect the reasons behind a predictive model's decision-making (i.e., the faithfulness of the explanations). We claim that the faithfulness of explanations lies in the explicitness of the control over the predictive models' decision-making. To demonstrate this idea and the differences in the faithfulness of the explanations provided by popular existing XAI methods, we discuss the following three examples: (1) asking an LLM to provide justifications to its own predictions, (2) using LIME [77] to provide feature-importance values for individual tokens in a post-hoc manner and (3) using rationale extraction that learns to extract subsets of features as explanations via a select-predict architecture [162, 163]. The corresponding examples on these topics are individually provided in Figures 4, 5, 6, and 7.



### Text with highlighted words

The heart, pulmonary XXXX and mediastinum are within normal limits. There is no pleural effusion or pneumothorax. There is no focal air space opacity to suggest a pneumonia.

Figure 6: Running LIME on classifying a medical note with BERT.

**Asking an LLM to justify itself** While asking an LLM to provide an answer for a given question, it is very intuitive to also ask the LLM to provide justifications due to its capability of generating human-readable texts, which is an example of natural language explanation or CoT reasoning described in Subsection 4.2. The resulting LLM-generated explanations might seem convincing to the users in some cases. As an example, in Figure 4, ChatGPT was able to identify some abnormality on the distal ileum, which was in support of the diagnostic prediction of Crohn’s disease. However, in another example shown in Figure 5, GPT 3.5 fails to make a correct prediction along with its underlying explanation, which is a serious case of a hallucination [149]. These two examples highlight the core problem with an LLM’s general working principle: a major drawback of any explanation provided by an LLM via auto-regressive next-token prediction, where the explanation is simply a collection of the most probable tokens and lacks explicit control over the inference process towards the answer. This means we can not guarantee that the explanation is truly the reason for the answer. Hence, given the design of current LLMs, we could conclude that the faithfulness of an LLM’s explanations can not be fulfilled by simply asking the LLM itself to explain. We previously noted that transformer-based foundation models do not have any capacity for self-representation; furthermore, another critical drawback of LLM-generated explanations is the parametric memory of LLMs for knowledge representation. This means that self-explanations generated by an LLM can hardly be verified without referring to external data sources.

**Post-hoc explanation via linear approximation** LIME, as well as SHAP, as post-hoc XAI tools, have gained the most attention and popularity due to their model-agnostic capability of providing feature importance scores as explanations. As shown in Figure 6, LIME suggested that the word “no” was the highest contributing feature for a BERT classifier to predict no abnormality. The identification of contributing features could provide some explanations for the decision-making of the predictive model. The mechanism of LIME is fairly simple. Given an input and a model (e.g., a medical report and a deep neural network, separately), to explain the model’s output on this input, LIME learns a linear model as a surrogate of the original model in the space created by perturbing the features of the input. Then, the coefficients of the linear model are viewed as the importance scores corresponding to the input features. Linear approximation, to a certain degree, gives insights on the behavior of the original model, but can not completely replace the original model (i.e., the approximation creates errors). For example, the perturbation in LIME is performed by randomly masking the features of the original input, which does not guarantee fair consideration of all subsets of features. In short, the explanations provided by a surrogate model may not truthfully explain the original model.

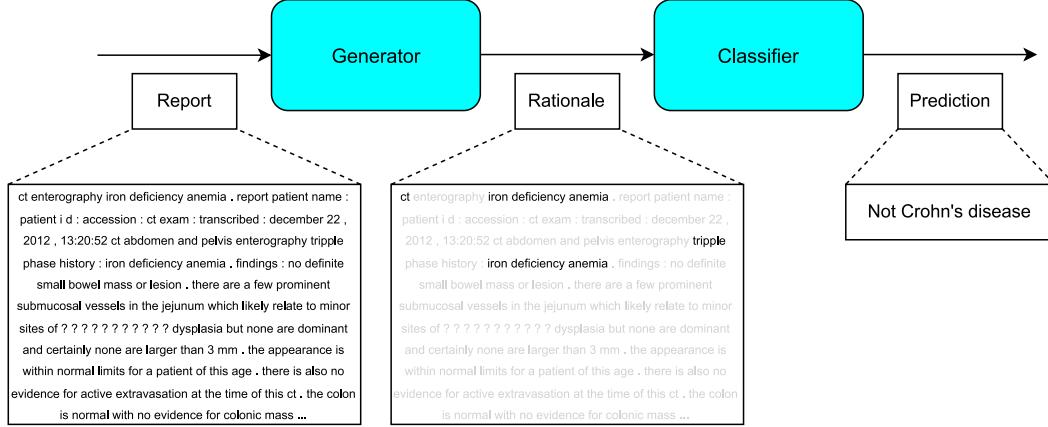


Figure 7: Rationale extraction selects a subset of features as a rationale for a diagnostic prediction on Crohn’s disease from a computed tomography enterography report, where the prediction is correct and the corresponding explanation justifies the prediction. The example is from [164].

**Rationale extraction that learns to explain** Rationale extraction aims to learn an intermediate representation for selecting the features of training inputs that are identified as critical for making predictions. The selected features are then used as the reason for a prediction. A rationale extraction architecture is typically composed of two neural networks, which are trained jointly. The first neural network (i.e., the generator) learns to select a subset of features from the original input, and the second neural network (i.e., the classifier) learns to make a prediction based on the selected subset of features. Rationale extraction is performed with only instance-level supervision (as in a classic supervised learning setting) to search for the most important features. For example, in Figure 7, only some words were extracted from the original radiology report by the generator to be used as input for the classifier to make a final prediction. This architecture controls a neural network’s decision-making by forcing the encoder to make a prediction solely based on the selected features, which guarantees that the selected features are truly the reason for the decision-making. These values indicate the contribution of individual features to the model’s decision. However, it is essential that these values accurately reflect the internal decision-making process of the model rather than being an approximation. So, while LLM-generated justifications can be intuitive and user-friendly, which brings great opportunities for providing more trustworthy AI-assisted medical diagnosis and prognosis, their faithfulness may vary. Further observations have highlighted that using CoT reasoning with LLMs is often mistakenly considered as real reasoning, can be misaligned with the models’ actual computation [89]. Hence, it is essential to ensure that these justifications are not merely plausible-sounding but are rooted in the actual reasoning process of the model. Thus, the faithfulness issue presents a fundamental challenge in applying LLM-based explanations in life-critical domains, such as medicine.

## 7.2 Insights from Autonomous Driving

Interactive explanations with human-machine interaction have recently been an area of interest for building trust in an autonomous vehicle (AV) [165, 166]. Understanding how an AV understands its operational surroundings and makes real-time decisions can help establish trust with on board passengers. The question-answering (QA) mechanism, particularly in terms of visual question answering (VQA) and video question answering (VideoQA), has been an area of interest for providing human-interpretable explanations for justifying AV actions in a variety of actual and simulated traffic scenes. In this sense, we experiment with a multimodal LLM model applied to an autonomous driving dataset and ask questions to the model to justify its answers as a follow-up. As the focus of this paper is explainability from a language aspect, we focus on analyzing model predictions from the latter perspective. We use the Video-LLM2 multi-modal LLM [167] for summarizing temporal driving scenes from the Berkeley DeepDrive Attention (BDD-A) dataset [168], a video dataset with dynamic traffic and critical situations. We carefully sample four driving scenes from the dataset and ask explanatory questions for each scenario shown in Figure 8. The goal is to determine whether the

model captures dynamic traffic environments with timing sensitivity and can explain its prediction of traffic scenes via intelligible, linguistic reasoning.

Figure 8 presents our experimental results. As seen, we first prompt the model to describe a scene and further ask causal, contrastive, and counterfactual questions. While the traditional approach for evaluating explanations has been to consider either descriptive or causal questions starting with the “What” and “Why” keywords, we instead argue that the model should also justify more challenging prompts — contrastive and counterfactual questions, as they are robustness test for models [169], to ensure that its emergent ability does not remain limited to simple tests. Traditionally, LLMs are constructed by fine-tuning labeled datasets of instructional prompts and corresponding outputs, and their generalization ability is usually tested within their built-in mechanism. However, we argue that a *local explanation* is *faithful* if the model also predicts correct answers in stress test prompts. In the selected scenes, once the model produces a response, we ask causal, counterfactual, and contrastive questions and observe that the model produces correct responses to these questions in Scenes 1,2 and 4. In Scene 3, the model produces an incorrect explanation at first and cannot rationalize a contrastive query as the follow-up of the first query. Based on these insights, we can summarize that a local LLM explanation in this example can be considered trustworthy if 1) it passes the causal reasoning test, 2) it can justify contrastive and causal questions correctly as a stress test, 3) it understands, distinguishes, and justify questions requiring fact or belief-based subjective answers accordingly, and 4) it avoids presenting falsified explanation in case it just cannot answer the question. The fourth property should be emphasized: depending on what data sources an LLM model is pretrained, it may not capture information beyond its knowledge base, and acknowledging its limitation by simply avoiding presenting a fictitious explanation is as significant as the first three properties. Hence, we argue that at least these four properties should be inherent requirements of trustworthy local LLM explanations.

## 8 Key findings and insights

### 8.1 LLM explanations have levels of granularity

Our analysis of the presented empirical studies and insights from the literature shows that intelligibility of explanations may change from user to user, depending on their technical knowledge and how they use such explanations. Consequently, we categorize LLM explanations with *three levels of granularity*:

- 1) *Coarse-grained explanations*: Explanations within these levels can be understood by everyone, such as general users and regulators, as they do not contain deep technical information and rather focus on being intelligible and understandable by everyone. For instance, referring to Scenario 1 in Figure 8, the causal explanation to the “Why?” question can be considered as an explanation with coarse granularity.
- 2) *Coarse-to-fine-grained explanations*: Such explanations are primarily targeted for domain experts. Coarse-to-fine-grained explanations describe a model’s predictions in which LLM first provides a coarse (high-level) overview of its reasoning — summarizing general patterns, modalities, or feature groups that drive a decision — and then progressively reveals fine-grained (detailed) evidence, such as specific features, regions, or textual tokens that substantiate the prediction. For instance, in the medical domain, LLM explanations for doctors are most effective when they follow the coarse-to-fine-grained structure, as clinical reasoning itself naturally progresses in that way: from general, first impressions to specific, grounded evidence. For instance, if an LLM predicts that a patient has community-acquired pneumonia, a model’s underlying explanation, such as “*The model identified a pneumonia-like pattern based on fever, cough symptoms, and chest X-ray abnormalities,*” provides preliminary reasoning on the outcome. As a deeper detail, “*Model’s attention map localizes to a 2 cm opacity in the right lower lobe on the chest X-ray, and to the textual phrase ‘new infiltrate’ in the provided radiology report.*” would be fine-grained reasoning to support such an outcome, as potential symptoms of community-acquired pneumonia [170]. Thus, such adaptive granularity, with the example from the medical field, could also support trust in specific domains far more effectively than either purely coarse or purely fine explanations alone.
- 3) *Fine-grained explanations*: These explanations are highly detailed and technical, often delving into the inner workings of an LLM model, such as individual weights and activations in neural networks. All explanations on the mechanistic interpretability of LLMs are good examples of fine-grained granularity. This level is generally targeted at LLM developers or experts who need to understand the

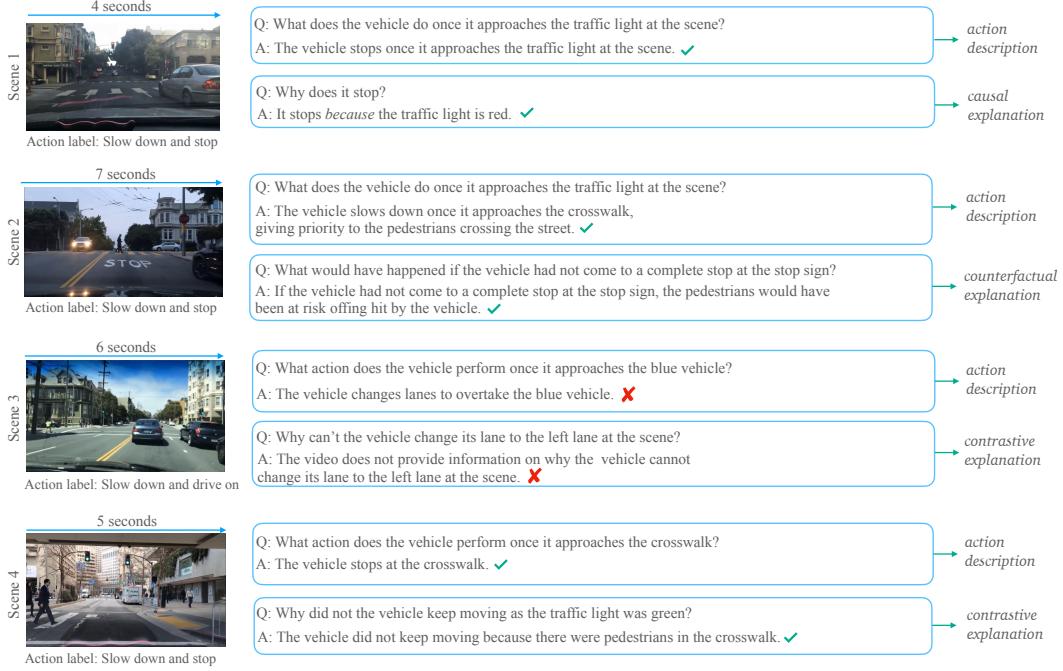


Figure 8: Scene understanding with the Video-LLaMA2 multimodal LLM: We first ask the model to explain action decisions/traffic scenes and further follow up with causal, contrastive, and counterfactual questions to stress test faithfulness of the previous responses.

model at a granular level to debug or improve it and understand the inner workings of the entire model.

## 8.2 LLM explanations must pass stress tests

As stress tests are regularly used to evaluate the robustness and reliability of AI systems, LLM outputs should also be assessed with relevant checkpoints. As presented with the experiment in Figure 8, *counterfactual reasoning* is one form of stress test exploring alternative scenarios for causal reasoning. Furthermore, LLM explanations can also be evaluated against *benchmark datasets* dedicated to evaluating the robustness of various forms of explanations. A recent study shows that replacing keywords in questions results in the deterioration of the reasoning capabilities of seven well-known LLMs from OpenAI, Gemini, and LLaMA families [171]. For this purpose, this study presents the MMLU-SR benchmark enabling reasoning and understanding ability of LLM models by focusing on “Question Only,” “Answer Only,” and “Question and Answer” scenarios to ensure an LLM simply does not predict the next token but truly understands the concept and context in such predictions. Finally, it is important to test LLMs via specific *stress prompts* to evaluate the capability of such models in the real world, where stress cases are highly anticipated. StressPrompt, a novel benchmark by [172], shows that carefully crafted specific prompts can alter the internal states of LLM models, leading to incorrect responses in critical applications. Analogously, another recent benchmark, Humanity’s Last Exam [173], released in early 2025, shows that even the most advanced LLM models such as GPT-5 [4], Grok-2 [21], Grok 4 [22], GPT-4o [51], Gemini 2.5 [15], Claude 4.5 Sonnet [10], and DeepSeek-R1 [19] perform below or around 25% accuracy in predicting correct answers to 2,500 domain-specific difficult questions across various disciplines. Hence, the robustness of LLM explanations might be holistically assessed by the degree to which explanations remain consistent, faithful, and resistant to manipulation or noise across variations in input, context, or adversarial attacks, supported by the examples provided in Section 6.2 and [172]. Whether targeted explainees are laypeople, general domain users, or domain experts, truly understanding prompts/questions and predicting faithful and factually correct explanations for such queries is a paramount feature of a trustworthy LLM.

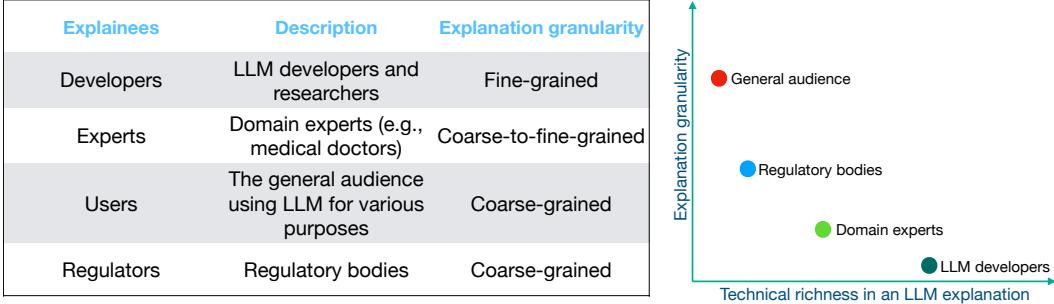


Figure 9: Granularity of LLM explanations with respect to the explainees

### 8.3 LLM explanations must align with fundamental principles of TrustLLM

A recently established benchmark by numerous institutions on trustworthy LLMs, named *TrustLLM*, identifies eight fundamental principles of such models [75]. According to TrustLLM, a language model must consider *safety*, *truthfulness*, *fairness*, *robustness*, *privacy*, *machine ethics*, *transparency*, and *accountability* in its underlying working mechanism. These concepts have been investigated in general XAI research [174, 175], so LLM explanations, in turn, must also align with these principles while being delivered to interaction partners. Below, we describe these nuances individually and in detail:

**Safety:** LLMs must ensure that their generated content does not harm a user in any way. The harmful prompt can be targeted at any user group or system in terms of jailbreak prompts, toxic queries, and the presentation of convincing but fictitious content in a safety-critical application. LLM explanations can help mitigate this undesirable behavior in a certain way. First, a *built-in defense mechanism* can trigger an LLM to avoid presenting information about harmful queries (e.g., *How can I make a <dangerous-item>?*). Furthermore, if a user queries about a safety-critical topic (e.g., *What medicine can I adopt for a <disease> and how many doses?*), a hallucination of an LLM in the response could have dire consequences if a user solely takes an action based on this response. To prevent such a case, an LLM can recommend a specific source or reference for a user's further look, as an explanation, which is a typical RAG approach. Recent acts and regulatory principles, such as the European Union's AI Act [176] and the Singapore Consensus on Global AI Safety Research Priorities [177], unanimously emphasize building safety guardrails on the LLM-generated content and underscore the substance of underlying explanations for what such models generate.

**Truthfulness:** [75] defines the term *truthfulness* as the *accurate representation of information, facts, and results*. As LLMs are pre-trained with massive information on the Internet, (unintentional) hallucinations with their abilities may be related to non-factual information, outdated data, or simply relying on language prior to generate falsified content. Furthermore, an incorrect LLM output may also be the result of training an LLM model with intentionally falsified information as well [178, 179]. [75] proposes that performing *sycophancy test* [180, 181, 182] in terms of persona and preference and testing them with adversarial queries are also crucial to validate the truthfulness of LLM outputs. In such cases, an LLM explanation can provide corrective measures, show incorrect details in the prompt, and present fact-based information by referring users to a specific source of information, as described in the previous section.

**Fairness:** Ensuring fairness in explanations has been one of the significant goals of XAI research, in general [174]. The concern with the fairness issue is that LLM outputs might be biased, such as being against or inclined toward specific demographic groups, genders, political figures, and so on [75]. So, LLM explanations must ensure the generated output does not contain discriminatory statements and present examples with equity when needed.

**Robustness:** We have covered the robustness perspective of LLM outputs with the experimental analysis above, but as a reiteration, we can conclude that LLM explanations should be robust against counterfactual analysis and stress prompts both in terms of informational content and in prompts requiring responses from a temporal analysis perspective.

**Privacy:** Primary concern with privacy in LLMs are data breaches in generated content and jailbreaking LLMs to spread confidential information [75, 183, 184, 185]. So, how can an LLM explanation help detect potential data breaches or leakage of confidential information? A simple solution can be to provide a reference or source information from which the content was generated. This way, the

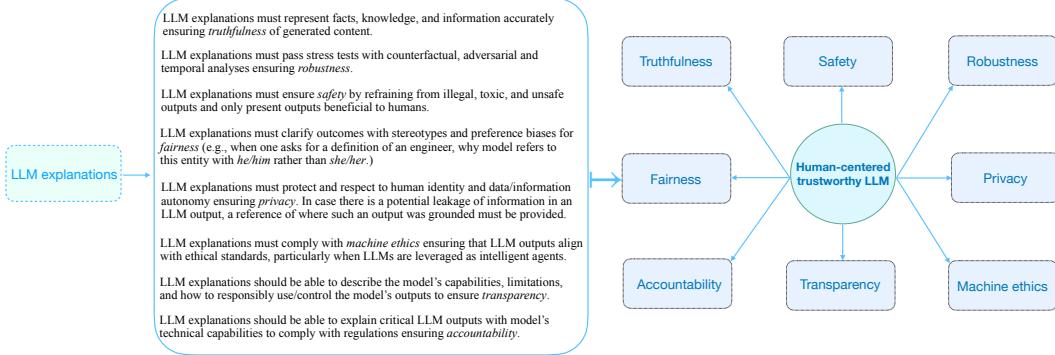


Figure 10: The eight principles of a human-centered trustworthy LLM and the role of LLM explanations in achieving these goals.

user could analyze the source information and judge whether LLM itself or the reference it was based on is a reason to spread privacy-concerning output.

**Machine Ethics:** The primary principles of machine ethics in AI research have been linked with Asimov's "three laws of robotics" [186]. These principles have evolved over the decades and have further been adjusted or augmented to some extent [187]. Applying these principles to trustworthy LLMs, [75] posits that machine ethics principles can be investigated in terms of *implicit ethics* (alignment with humans' general ethical standards), *explicit ethics* (an LLM's behavior in various ethical situations), and *emotional awareness* (an LLM's ability to identify its true mission, abilities, and understand humans' emotions). Linking these concepts to explanations, a model can, for example, provide causal reasoning on why it made a particular prediction, and if possible, describe potential implications of the generated content to enlighten users with the potential sensitivity of the presented information.

**Transparency:** Transparency of an LLM output generally refers to the ability to understand and explain how an LLM model generates its outputs and decisions [188]. At first glance, this is a considerably challenging topic because of the intricate structure of an LLM model and the massive data on which they are trained. Furthermore, LLM predictions or decisions have or require various degrees of transparency [75]; hence, the level of transparency should be explored with human factors consideration with respect to who requires explanation with granularity [189]. Although this is a general approach to transparent LLMs, the primary role of an explanation is to help various stakeholders achieve their desiderata with the LLM output presented to them [190].

**Accountability:** Finally, as LLMs are increasingly deployed across various domains and organizations for different purposes, the topic of accountability naturally arises as an actual problem with the usage of these models. Particularly, when an LLM makes a critical mistake, whether the organization that developed and deployed this model or a user that relied on the conclusion arrived at by such an LLM raises serious legal culpability issues (e.g., the example of an airline company's chatbot providing incorrect information on flight scheduling<sup>2</sup>). Consequently, AI acts on responsible AI development and deployment [176, 191] underscore accountability as a crucial feature of intelligent systems, underscoring "*a high-risk AI system should be capable of explaining its output with its technical capabilities*," and LLMs, as rapidly growing AI tools, must comply with these principles. Hence, LLM explanations may act as amplifiers to connect the dots between a model's internal operations and its external trustworthiness, making those unanimously adopted principles verifiable.

## 9 Future Directions

Although the growing interest in mechanistic interpretability and local explainability of LLMs has been successful to some extent, there remain significant directions that have been underexplored in the realm of generating trustworthy LLM explanations. In this regard, this section presents three directions for future exploration, necessitating collaborative work between LLM and XAI communities:

**Analyzing true logical reasoning in LLM explanations:** LLMs' remarkable content generation

<sup>2</sup><https://www.cbc.ca/news/canada/british-columbia/air-canada-chatbot-lawsuit-1.7116416>

ability on different downstream language tasks are impressive at the first glance. However, the key question is whether these models truly reason over the prompt. There have been few studies on understanding particular logical reasoning abilities of language models, such as via inductive reasoning [192], temporal logic [193], and deductive reasoning [194]; however, holistic evaluation of language models via various first-order and non-monotonic logic approaches still remains unexplored. *LogicBench* [195] has recently been introduced to test and ameliorate logical reasoning abilities of advanced LLMs to some extent. Experimental results show that even advanced models from the GPT-family series (e.g., GPT-4 [3]), Gemini-Pro [14], and LLaMA2 [7] do not perform well on LogicBench. Particularly, they fail in complex reasoning tasks and sometimes overlook contextual information crucial to support the arrived conclusion with correct reasoning. Furthermore, a recent study [196] shows that guiding LLMs through explicit logical reasoning steps via Planning Domain Definition Language (PDDL)-based representation, such as checking action applicability, modeling state transitions, and verifying plan validity, could potentially bridge the gap between LLMs' general reasoning and the logical precision needed for automated planning. Hence, further exploration of the true reasoning ability of LLMs is a significant future direction.

**Leveraging concept-bottleneck models for enhancing LLM interpretability:** The great majority of current LLMs produce output in a straightforward way based on the prompt, which does not specifically incorporate human-defined concepts into the reasoning process to arrive at the conclusions. *Concept bottleneck models*, as a potential solution, have recently been introduced to enhance the interpretability of end-to-end deep neural networks, where the model first predicts the human-defined *concepts*, and further uses only those predicted concepts in a *bottleneck layer* to make a final prediction [197, 198, 199] (e.g., referring to an example from [197]: “*If the model did not think there was a bone spur in the x-ray, would it still predict severe arthritis?*”). The topic has been investigated in several domains to present human-understandable explanatory information, such as in autonomous driving [200], clinical tasks [201], and various object classification tasks [198] with some empirical successes. However, concept bottleneck models have not been deeply investigated in the realm of LLMs and remain limited to few but promising studies [202]. By breaking down intricate data into comprehensible components, such models could allow researchers and practitioners to scrutinize and understand the reasoning behind LLMs' outputs. In particular, for safety-critical applications and tasks, integrating concept bottleneck models into the reasoning process can help domain-specific LLMs be more transparent, human-understandable, and trustworthy.

**Performance-interpretability trade-off: Could LLMs suffer from it?** Model performance vs interpretability has been an actual, ongoing, and debatable topic in XAI research over the last couple of years. The ungrounded belief is that complex ML models that are interpretable likely have low performance/accuracy [203]. However, this nuance remains as a general view as the evaluation of explanation can be task-specific and human-centric, and depending on the nature of the task, this trade-off could be correct or incorrect to some extent [174, 33, 203]. Thinking of LLMs as a deep neural network-based model, that trade-off also arises with respect to these models' working mechanisms. In a recent study, [204] has investigated the impact of incorporating interpretability constraints into LLMs, disclosing that while the interpretable model enhances human task efficiency and fosters appropriately calibrated confidence in their case, it also leads to a decline in the model's performance on an insurance liability classification task. Thus, as the topic is still in its infancy, the literature remains scarce on exploring potential interpretability-accuracy trade-offs in LLMs from a broader viewpoint and necessitates further exploration.

## 10 Conclusion

In this paper, we have presented a comprehensive analysis of interpretability and explainability in the context of LLMs. Delving into the local explainability and mechanistic interpretability of LLMs, our study sheds light on opportunities and challenges for generating human-centered and trustworthy explanations. In conjunction with the findings from related studies, our paper presents insights from safety-critical applications and shows key points and steps to achieve faithful explanations with human factors consideration. As general-purpose and domain-specific LLMs continue to proliferate across diverse applications, the need for trustworthy LLM explanations becomes increasingly critical. We believe that the proposed guidelines can help researchers and engaged target groups improve human alignment and faithfulness of LLMs and promote responsible use of these models in applied domains and tasks.

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## References

- [1] A Vaswani. Attention Is All You Need. *Advances in Neural Information Processing Systems*, 2017.
- [2] Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are few-shot learners. *Advances in Neural Information Processing Systems*, 33:1877–1901, 2020.
- [3] Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. GPT-4 Technical Report. *arXiv preprint arXiv:2303.08774*, 2023.
- [4] OpenAI. GPT-5 System Card, August 2025.
- [5] Wei-Lin Chiang, Zhuohan Li, Zi Lin, Ying Sheng, Zhanghao Wu, Hao Zhang, Lianmin Zheng, Siyuan Zhuang, Yonghao Zhuang, Joseph E. Gonzalez, Ion Stoica, and Eric P. Xing. Vicuna: An Open-Source Chatbot Impressing GPT-4 with 90%\* ChatGPT Quality, March 2023.
- [6] Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. LLaMA: Open and Efficient Foundation Language Models. *arXiv preprint arXiv:2302.13971*, 2023.
- [7] Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, et al. Llama 2: Open Foundation and Fine-Tuned Chat Models . *arXiv preprint arXiv:2307.09288*, 2023.
- [8] Albert Q Jiang, Alexandre Sablayrolles, Arthur Mensch, Chris Bamford, Devendra Singh Chaplot, Diego de las Casas, Florian Bressand, Gianna Lengyel, Guillaume Lample, Lucile Saulnier, et al. Mistral 7b. *arXiv preprint arXiv:2310.06825*, 2023.
- [9] Anthropic. Introducing Claude. <https://www.anthropic.com/news/introducing-claude>, 2023.
- [10] Anthropic. Introducing Claude Sonnet 4.5, September 2025.
- [11] Jinze Bai, Shuai Bai, Yunfei Chu, Zeyu Cui, Kai Dang, Xiaodong Deng, Yang Fan, Wenbin Ge, Yu Han, Fei Huang, et al. Qwen technical report. *arXiv preprint arXiv:2309.16609*, 2023.
- [12] Qwen Team. Qwen2 Technical Report. *arXiv preprint arXiv:2407.10671*, 2024.
- [13] An Yang, Anfeng Li, Baosong Yang, Beichen Zhang, Binyuan Hui, Bo Zheng, Bowen Yu, Chang Gao, Chengan Huang, Chenxu Lv, et al. Qwen3 Technical Report. *arXiv preprint arXiv:2505.09388*, 2025.
- [14] Rohan Anil, Sebastian Borgeaud, Yonghui Wu, Jean-Baptiste Alayrac, Jiahui Yu, Radu Soricut, Johan Schalkwyk, Andrew M Dai, Anja Hauth, et al. Gemini: A Family of Highly Capable Multimodal Models. *arXiv preprint arXiv:2312.11805*, 2023.
- [15] Gheorghe Comanici, Eric Bieber, Mike Schaeckermann, Ice Pasupat, Noveen Sachdeva, Inderjit Dhillon, Marcel Blistein, Ori Ram, Dan Zhang, Evan Rosen, et al. Gemini 2.5: Pushing the frontier with advanced reasoning, multimodality, long context, and next generation agentic capabilities. *arXiv preprint arXiv:2507.06261*, 2025.
- [16] Xiao Bi, Deli Chen, Guanting Chen, Shanhuang Chen, Damai Dai, Chengqi Deng, Honghui Ding, Kai Dong, Qiushi Du, Zhe Fu, et al. DeepSeek LLM: Scaling Open-Source Language Models with Longtermism. *arXiv preprint arXiv:2401.02954*, 2024.

- [17] Aixin Liu, Bei Feng, Bin Wang, Bingxuan Wang, Bo Liu, Chenggang Zhao, Chengqi Deng, Chong Ruan, Damai Dai, Daya Guo, et al. Deepseek-v2: A strong, economical, and efficient mixture-of-experts language model. *arXiv preprint arXiv:2405.04434*, 2024.
- [18] Aixin Liu, Bei Feng, Bing Xue, Bingxuan Wang, Bochao Wu, Chengda Lu, Chenggang Zhao, Chengqi Deng, Chenyu Zhang, Chong Ruan, et al. Deepseek-v3 technical report. *arXiv preprint arXiv:2412.19437*, 2024.
- [19] Daya Guo, Dejian Yang, Haowei Zhang, Junxiao Song, Ruoyu Zhang, Runxin Xu, Qihao Zhu, Shirong Ma, Peiyi Wang, Xiao Bi, et al. DeepSeek-R1: Incentivizing Reasoning Capability in LLMs via Reinforcement Learning . *arXiv preprint arXiv:2501.12948*, 2025.
- [20] xAI. Open Release of Grok-1. <https://x.ai/news/grok-os>, 2024.
- [21] xAI. Grok-2 beta release. <https://x.ai/news/grok-2>, 2024.
- [22] xAI. Grok 4. <https://x.ai/news/grok-4>, 2025.
- [23] Kimi Team, Angang Du, Bofei Gao, Bowei Xing, Changjiu Jiang, Cheng Chen, Cheng Li, Chenjun Xiao, Chenzhuang Du, Chonghua Liao, et al. Kimi k1.5: Scaling Reinforcement Learning with LLMs. *arXiv preprint arXiv:2501.12599*, 2025.
- [24] Kimi Team, Yifan Bai, Yiping Bao, Guanduo Chen, Jiahao Chen, Ningxin Chen, Ruijue Chen, Yanru Chen, Yuankun Chen, Yutian Chen, et al. Kimi k2: Open agentic intelligence. *arXiv preprint arXiv:2507.20534*, 2025.
- [25] Danny Driess, Fei Xia, Mehdi SM Sajjadi, Corey Lynch, Aakanksha Chowdhery, Brian Ichter, Ayzaan Wahid, Jonathan Tompson, Quan Vuong, Tianhe Yu, et al. PaLM-E: An Embodied Multimodal Language Model. In *International Conference on Machine Learning*, pages 8469–8488. PMLR, 2023.
- [26] Jason Wei, Yi Tay, Rishi Bommasani, Colin Raffel, Barret Zoph, Sebastian Borgeaud, Dani Yogatama, Maarten Bosma, Denny Zhou, Donald Metzler, et al. Emergent Abilities of Large Language Models. *Transactions on Machine Learning Research*, 2022.
- [27] Chandan Singh, Jeevana Priya Inala, Michel Galley, Rich Caruana, and Jianfeng Gao. Rethinking Interpretability in the Era of Large Language Models. *arXiv preprint arXiv:2402.01761*, 2024.
- [28] Lei Huang, Weijiang Yu, Weitao Ma, Weihong Zhong, Zhangyin Feng, Haotian Wang, Qian-glong Chen, Weihua Peng, Xiaocheng Feng, Bing Qin, et al. A Survey on Hallucination in Large Language Models: Principles, Taxonomy, Challenges, and Open Questions. *ACM Transactions on Information Systems*, 43(2):1–55, 2025.
- [29] Yiyou Sun, Yu Gai, Lijie Chen, Abhilasha Ravichander, Yejin Choi, and Dawn Song. Why and How LLMs Hallucinate: Connecting the Dots with Subsequence Associations. *arXiv preprint arXiv:2504.12691*, 2025.
- [30] Patrick Haller, Ansar Ayneddinov, and Alan Akbik. OpinionGPT: Modelling Explicit Biases in Instruction-Tuned LLMs. *arXiv preprint arXiv:2309.03876*, 2023.
- [31] Iason Gabriel. Artificial Intelligence, Values, and Alignment. *Minds and Machines*, 30(3):411–437, 2020.
- [32] Mi-Young Kim, Shahin Atakishiyev, Housam Khalifa Bashier Babiker, Nawshad Farruque, Randy Goebel, Osmar R Zaïane, Mohammad-Hossein Motallebi, Juliano Rabelo, Talat Syed, Hengshuai Yao, et al. A Multi-Component Framework for the Analysis and Design of Explainable Artificial Intelligence. *Machine Learning and Knowledge Extraction*, 3(4):900–921, 2021.
- [33] Waddah Saeed and Christian Omlin. Explainable AI (XAI): A systematic meta-survey of current challenges and future opportunities. *Knowledge-Based Systems*, 263:110273, 2023.

- [34] Peter F Brown, Vincent J Della Pietra, Peter V Desouza, Jennifer C Lai, and Robert L Mercer. Class-based n-gram models of natural language. *Computational linguistics*, 18(4):467–480, 1992.
- [35] Hermann Ney, Ute Essen, and Reinhard Kneser. On structuring probabilistic dependences in stochastic language modelling. *Computer Speech & Language*, 8(1):1–38, 1994.
- [36] David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. Learning representations by back-propagating errors. *Nature*, 323(6088):533–536, 1986.
- [37] Yoshua Bengio, Réjean Ducharme, and Pascal Vincent. A Neural Probabilistic Language Model . *Advances in Neural Information Processing Systems*, 13, 2000.
- [38] Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg S Corrado, and Jeff Dean. Distributed representations of words and phrases and their compositionality. *Advances in Neural Information Processing Systems*, 26, 2013.
- [39] Piotr Bojanowski, Edouard Grave, Armand Joulin, and Tomas Mikolov. Enriching word vectors with subword information. *Transactions of the Association for Computational Linguistics*, 5:135–146, 2017.
- [40] Manaal Faruqui, Jesse Dodge, Sujay K Jauhar, Chris Dyer, Eduard Hovy, and Noah A Smith. Retrofitting word vectors to semantic lexicons. *arXiv preprint arXiv:1411.4166*, 2014.
- [41] Nawshad Farrueque, Osmar Zaiane, and Randy Goebel. Augmenting semantic representation of depressive language: From forums to microblogs. In *Joint European conference on machine learning and knowledge discovery in databases*, pages 359–375. Springer, 2019.
- [42] Daniel Cer, Yinfei Yang, Sheng-yi Kong, Nan Hua, Nicole Limtiaco, Rhomni St John, Noah Constant, Mario Guajardo-Cespedes, Steve Yuan, Chris Tar, et al. Universal sentence encoder for english. In *Proceedings of the 2018 conference on empirical methods in natural language processing: system demonstrations*, pages 169–174, 2018.
- [43] Matthew E. Peters, Mark Neumann, Mohit Iyyer, Matt Gardner, Christopher Clark, Kenton Lee, and Luke Zettlemoyer. Deep contextualized word representations. *CoRR*, abs/1802.05365, 2018.
- [44] Jacob Devlin Ming-Wei Chang Kenton and Lee Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of naacl-HLT*, volume 1, page 2. Minneapolis, Minnesota, 2019.
- [45] Zhenzhong Lan, Mingda Chen, Sebastian Goodman, Kevin Gimpel, Piyush Sharma, and Radu Soricut. ALBERT: A Lite BERT for Self-supervised Learning of Language Representations. In *International Conference on Learning Representations*, 2020.
- [46] Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. RoBERTa: A Robustly Optimized BERT Pretraining Approach. *arXiv preprint arXiv:1907.11692*, 2019.
- [47] Tianyu Wu, Shizhu He, Jingping Liu, Siqi Sun, Kang Liu, Qing-Long Han, and Yang Tang. A brief overview of chatgpt: The history, status quo and potential future development. *IEEE/CAA Journal of Automatica Sinica*, 10(5):1122–1136, 2023.
- [48] Mike Lewis, Yinhan Liu, Naman Goyal, Marjan Ghazvininejad, Abdelrahman Mohamed, Omer Levy, Veselin Stoyanov, and Luke Zettlemoyer. BART: Denoising Sequence-to-Sequence Pre-training for Natural Language Generation, Translation, and Comprehension. In *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*, pages 7871–7880, 2020.
- [49] OpenAI. Introducing ChatGPT, 2022.
- [50] Shreyas Chaudhari, Pranjal Aggarwal, Vishvak Murahari, Tanmay Rajpurohit, Ashwin Kalyan, Karthik Narasimhan, Ameet Deshpande, and Bruno Castro da Silva. RLHF Deciphered: A Critical Analysis of Reinforcement Learning from Human Feedback for LLMs. *ACM Computing Surveys*, 58(2):1–37, 2025.

- [51] Aaron Hurst, Adam Lerer, Adam P Goucher, Adam Perelman, Aditya Ramesh, Aidan Clark, AJ Ostrow, Akila Welihinda, Alan Hayes, Alec Radford, et al. GPT-4o System Card. *arXiv preprint arXiv:2410.21276*, 2024.
- [52] Patrick Lewis, Ethan Perez, Aleksandra Piktus, Fabio Petroni, Vladimir Karpukhin, Namnan Goyal, Heinrich Küttler, Mike Lewis, Wen-tau Yih, Tim Rocktäschel, et al. Retrieval-Augmented Generation for Knowledge-Intensive NLP Tasks. *Advances in Neural Information Processing Systems*, 33:9459–9474, 2020.
- [53] Jiawei Chen, Hongyu Lin, Xianpei Han, and Le Sun. Benchmarking Large Language Models in Retrieval-Augmented Generation. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 38, pages 17754–17762, 2024.
- [54] Aditi Singh, Abul Ehtesham, Saket Kumar, and Tala Talaei Khoei. Enhancing ai systems with agentic workflows patterns in large language model. In *2024 IEEE World AI IoT Congress (AIoT)*, pages 527–532. IEEE, 2024.
- [55] Miles Turpin, Julian Michael, Ethan Perez, and Samuel Bowman. Language Models Don’t Always Say What They Think: Unfaithful Explanations in Chain-of-Thought Prompting. *Advances in Neural Information Processing Systems*, 36:74952–74965, 2023.
- [56] Iván Arcuschin, Jett Janiak, Robert Krzyzanowski, Senthooran Rajamanoharan, Neel Nanda, and Arthur Conmy. Chain-of-thought reasoning in the wild is not always faithful. *arXiv preprint arXiv:2503.08679*, 2025.
- [57] Haiyan Zhao, Hanjie Chen, Fan Yang, Ninghao Liu, Huiqi Deng, Hengyi Cai, Shuaiqiang Wang, Dawei Yin, and Mengnan Du. Explainability for Large Language Models: A Survey. *ACM Transactions on Intelligent Systems and Technology*, 15(2):1–38, 2024.
- [58] Scott M Lundberg and Su-In Lee. A Unified Approach to Interpreting Model Predictions . *Advances in Neural Information Processing Systems*, 30, 2017.
- [59] Haoyan Luo and Lucia Specia. From Understanding to Utilization: A Survey on Explainability for Large Language Models. *arXiv preprint arXiv:2401.12874*, 2024.
- [60] Xiaoyu Liu, Paiheng Xu, Junda Wu, Jiaxin Yuan, Yifan Yang, Yuhang Zhou, Fuxiao Liu, Tianrui Guan, Haoliang Wang, Tong Yu, et al. Large Language Models and Causal Inference in Collaboration: A Comprehensive Survey. *arXiv preprint arXiv:2403.09606*, 2024.
- [61] Egor N Volkov and Alexey N Averkin. Local Explanations for Large Language Models: a Brief Review of Methods. In *2024 XXVII International Conference on Soft Computing and Measurements (SCM)*, pages 189–192. IEEE, 2024.
- [62] Javier Ferrando, Gabriele Sarti, Arianna Bisazza, and Marta R Costa-Jussà. A Primer on the Inner Workings of Transformer-based Language Models. *arXiv preprint arXiv:2405.00208*, 2024.
- [63] Daking Rai, Yilun Zhou, Shi Feng, Abulhair Saparov, and Ziyu Yao. A Practical Review of Mechanistic Interpretability for Transformer-Based Language Models. *arXiv preprint arXiv:2407.02646*, 2024.
- [64] Lee Sharkey, Bilal Chughtai, Joshua Batson, Jack Lindsey, Jeff Wu, Lucius Bushnaq, Nicholas Goldowsky-Dill, Stefan Heimersheim, Alejandro Ortega, Joseph Bloom, et al. Open Problems in Mechanistic Interpretability . *arXiv preprint arXiv:2501.16496*, 2025.
- [65] Sandeep Reddy Gantla. Exploring Mechanistic Interpretability in Large Language Models: Challenges, Approaches, and Insights. In *2025 International Conference on Data Science, Agents & Artificial Intelligence (ICDSAAI)*, pages 1–8. IEEE, 2025.
- [66] Md Imran Hossain, Ghada Zamzmi, Peter R Mouton, Md Sirajus Salekin, Yu Sun, and Dmitry Goldgof. Explainable AI for Medical Data: Current Methods, Limitations, and Future Directions. *ACM Computing Surveys*, 57(6):1–46, 2025.

- [67] Shahin Atakishiyev, Mohammad Salameh, Hengshuai Yao, and Randy Goebel. Explainable Artificial Intelligence for Autonomous Driving: A Comprehensive Overview and Field Guide for Future Research Directions. *IEEE Access*, 12:101603–101625, 2024.
- [68] Randy Goebel, Ajay Chander, Katharina Holzinger, Freddy Lecue, Zeynep Akata, Simone Stumpf, Peter Kieseberg, and Andreas Holzinger. Explainable AI: the new 42? In *International Cross-Domain Conference for Machine Learning and Knowledge Extraction*, pages 295–303. Springer, 2018.
- [69] Roberto Confalonieri, Ludovik Coba, Benedikt Wagner, and Tarek R Besold. A historical perspective of explainable Artificial Intelligence. *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery*, 11(1):e1391, 2021.
- [70] Artur S. d’Avila Garcez and Luís C. Lamb. Neurosymbolic AI: the 3rd wave. *Artificial Intelligence Review*, 56(11):12387–12406, 2023.
- [71] Bruce G Buchanan and Edward H Shortliffe. *Rule based expert systems: the mycin experiments of the stanford heuristic programming project (the Addison-Wesley series in artificial intelligence)*. Addison-Wesley Longman Publishing Co., Inc., 1984.
- [72] Protection Regulation. Regulation (EU) 2016/679 of the European Parliament and of the Council. *Regulation (EU)*, 679(2016):10–13, 2016.
- [73] Yupeng Chang, Xu Wang, Jindong Wang, Yuan Wu, Linyi Yang, Kaijie Zhu, Hao Chen, Xiaoyuan Yi, Cunxiang Wang, Yidong Wang, et al. A Survey on Evaluation of Large Language Models. *ACM Transactions on Intelligent Systems and Technology*, 15(3):1–45, 2024.
- [74] Mohaimenul Azam Khan Raiaan, Md Saddam Hossain Mukta, Kaniz Fatema, Nur Mohammad Fahad, Sadman Sakib, Most Marufatul Jannat Mim, Jubaer Ahmad, Mohammed Eunus Ali, and Sami Azam. A Review on Large Language Models: Architectures, Applications, Taxonomies, Open Issues and Challenges. *IEEE Access*, 2024.
- [75] Yue Huang, Lichao Sun, Haoran Wang, Siyuan Wu, Qihui Zhang, Yuan Li, Chujie Gao, Yixin Huang, Wenhan Lyu, Yixuan Zhang, et al. Position: TrustLLM: Trustworthiness in Large Language Models. In *International Conference on Machine Learning*, pages 20166–20270, 2024.
- [76] Haiyang Wang, Yihao Li, Yue Wang, Pan Liu, and Pengxiao Li. Navigating the Risks: A Review of Safety Issues in Large Language Models. In *2024 IEEE 24th International Conference on Software Quality, Reliability, and Security Companion (QRS-C)*, pages 74–83. IEEE, 2024.
- [77] Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. "Why Should I Trust You?": Explaining the Predictions of Any Classifier. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 1135–1144, 2016.
- [78] Shiyuan Huang, Siddarth Mamidanna, Shreedhar Jangam, Yilun Zhou, and Leilani H Gilpin. Can Large Language Models Explain Themselves? A Study of LLM-Generated Self-Explanations. *arXiv preprint arXiv:2310.11207*, 2023.
- [79] Sree Harsha Tanneru, Chirag Agarwal, and Himabindu Lakkaraju. Quantifying uncertainty in natural language explanations of large language models. In *International Conference on Artificial Intelligence and Statistics*, pages 1072–1080. PMLR, 2024.
- [80] Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Fei Xia, Ed Chi, Quoc V Le, Denny Zhou, et al. Chain-of-Thought Prompting Elicits Reasoning in Large Language Models. *Advances in Neural Information Processing Systems*, 35:24824–24837, 2022.
- [81] Qing Lyu, Shreya Havaldar, Adam Stein, Li Zhang, Delip Rao, Eric Wong, Marianna Apidianaki, and Chris Callison-Burch. Faithful Chain-of-Thought Reasoning. In *The 13th International Joint Conference on Natural Language Processing and the 3rd Conference of the Asia-Pacific Chapter of the Association for Computational Linguistics (IJCNLP-AACL 2023)*, 2023.

- [82] Jianhao Yuan, Shuyang Sun, Daniel Omeiza, Bo Zhao, Paul Newman, Lars Kunze, and Matthew Gadd. RAG-Driver: Generalisable Driving Explanations with Retrieval-Augmented In-Context Learning in Multi-Modal Large Language Model. *Robotics: Science and Systems*, 2024.
- [83] Yuhan Li, Xinni Zhang, Linhao Luo, Heng Chang, Yuxiang Ren, Irwin King, and Jia Li. G-Refer: Graph Retrieval-Augmented Large Language Model for Explainable Recommendation. In *Proceedings of the ACM on Web Conference 2025*, pages 240–251, 2025.
- [84] Zhiyong Wu, Yun Chen, Ben Kao, and Qun Liu. Perturbed Masking: Parameter-free Probing for Analyzing and Interpreting BERT. In *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*, pages 4166–4176, 2020.
- [85] Hosein Mohebbi, Ali Modarressi, and Mohammad Taher Pilehvar. Exploring the role of BERT token representations to explain sentence probing results. In *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing*, pages 792–806, Online and Punta Cana, Dominican Republic, 2021. Association for Computational Linguistics.
- [86] Joseph Enguehard. Sequential Integrated Gradients: a simple but effective method for explaining language models. *ACL Findings*, 2023.
- [87] Enja Kokalj, Blaž Škrlj, Nada Lavrač, Senja Pollak, and Marko Robnik-Šikonja. BERT meets Shapley: Extending SHAP Explanations to Transformer-based Classifiers. In *Proceedings of the EACL hackashop on news media content analysis and automated report generation*, pages 16–21, 2021.
- [88] Zhengxuan Wu and Desmond C Ong. On explaining your explanations of bert: An empirical study with sequence classification. *arXiv preprint arXiv:2101.00196*, 2021.
- [89] Fazl Barez, Tung-Yu Wu, Iván Arcuschin, Michael Lan, Vincent Wang, Noah Siegel, Nicolas Collignon, Clement Neo, Isabelle Lee, Alasdair Paren, Adel Bibi, Robert Trager, Damiano Fornasiere, John Yan, Yanai Elazar, and Yoshua Bengio. Chain-of-Thought Is Not Explainability, 2025.
- [90] Yunfan Gao, Yun Xiong, Xinyu Gao, Kangxiang Jia, Jinliu Pan, Yuxi Bi, Yi Dai, Jiawei Sun, and Haofen Wang. Retrieval-Augmented Generation for Large Language Models: A Survey. *arXiv preprint arXiv:2312.10997*, 2023.
- [91] Furui Cheng, Vilém Zouhar, Robin Shing Moon Chan, Daniel Fürst, Hendrik Strobelt, and Mennatallah El-Assady. Interactive Analysis of LLMs using Meaningful Counterfactuals. *arXiv preprint arXiv:2405.00708*, 2024.
- [92] Anselm Paulus, Arman Zharmagambetov, Chuan Guo, Brandon Amos, and Yuandong Tian. Ad-vPrompter: Fast Adaptive Adversarial Prompting for LLMs. *arXiv preprint arXiv:2404.16873*, 2024.
- [93] Nelson Elhage, Neel Nanda, Catherine Olsson, Tom Henighan, Nicholas Joseph, Ben Mann, Amanda Askell, Yuntao Bai, Anna Chen, Tom Conerly, Nova DasSarma, Dawn Drain, Deep Ganguli, Zac Hatfield-Dodds, Danny Hernandez, Andy Jones, Jackson Kernion, Liane Lovitt, Kamal Ndousse, Dario Amodei, Tom Brown, Jack Clark, Jared Kaplan, Sam McCandlish, and Chris Olah. A mathematical framework for transformer circuits. *Transformer Circuits Thread*, 2021. <https://transformer-circuits.pub/2021/framework/index.html>.
- [94] Jiawei Gu, Xuhui Jiang, Zhichao Shi, Hexiang Tan, Xuehao Zhai, Chengjin Xu, Wei Li, Yinghan Shen, Shengjie Ma, Honghao Liu, et al. A Survey on LLM-as-a-Judge. *arXiv preprint arXiv:2411.15594*, 2024.
- [95] Trenton Bricken, Adly Templeton, Joshua Batson, Brian Chen, Adam Jermyn, Tom Conerly, Nick Turner, Cem Anil, Carson Denison, Amanda Askell, Robert Lasenby, Yifan Wu, Shauna Kravec, Nicholas Schiefer, Tim Maxwell, Nicholas Joseph, Zac Hatfield-Dodds, Alex Tamkin, Karina Nguyen, Brayden McLean, Josiah E Burke, Tristan Hume, Shan Carter, Tom Henighan, and Christopher Olah. Towards Monosematicity: Decomposing Language Models With Dictionary Learning. *Transformer Circuits Thread*, 2023. <https://transformer-circuits.pub/2023/monosemantic-features/index.html>.

- [96] Adly Templeton, Tom Conerly, Jonathan Marcus, Jack Lindsey, Trenton Bricken, Brian Chen, Adam Pearce, Craig Citro, Emmanuel Ameisen, Andy Jones, Hoagy Cunningham, Nicholas L Turner, Callum McDougall, Monte MacDiarmid, C. Daniel Freeman, Theodore R. Sumers, Edward Rees, Joshua Batson, Adam Jermyn, Shan Carter, Chris Olah, and Tom Henighan. Scaling Monosemanticity: Extracting Interpretable Features from Claude 3 Sonnet. *Transformer Circuits Thread*, 2024.
- [97] Wenguan Wang, Yi Yang, and Fei Wu. Towards Data-And Knowledge-Driven AI: A Survey on Neuro-Symbolic Computing. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2024.
- [98] Giuseppe Marra, Sebastijan Dumančić, Robin Manhaeve, and Luc De Raedt. From statistical relational to neurosymbolic artificial intelligence: A survey. *Artificial Intelligence*, 328:104062, 2024.
- [99] Adam Scherlis, Kshitij Sachan, Adam S Jermyn, Joe Benton, and Buck Shlegeris. Polysemy and Capacity in Neural Networks . *arXiv preprint arXiv:2210.01892*, 2022.
- [100] Nelson Elhage, Tristan Hume, Catherine Olsson, Nicholas Schiefer, Tom Henighan, Shauna Kravec, Zac Hatfield-Dodds, Robert Lasenby, Dawn Drain, Carol Chen, et al. Toy models of superposition. *arXiv preprint arXiv:2209.10652*, 2022.
- [101] Bhavik Chandna, Zubair Bashir, and Procheta Sen. Dissecting Bias in LLMs: A Mechanistic Interpretability Perspective. *arXiv preprint arXiv:2506.05166*, 2025.
- [102] Catherine Olsson, Nelson Elhage, Neel Nanda, Nicholas Joseph, Nova DasSarma, Tom Henighan, Ben Mann, Amanda Askell, Yuntao Bai, Anna Chen, Tom Conerly, Dawn Drain, Deep Ganguli, Zac Hatfield-Dodds, Danny Hernandez, Scott Johnston, Andy Jones, Jackson Kernion, Liane Lovitt, Kamal Ndousse, Dario Amodei, Tom Brown, Jack Clark, Jared Kaplan, Sam McCandlish, and Chris Olah. In-context learning and induction heads. *Transformer Circuits Thread*, 2022. <https://transformer-circuits.pub/2022/in-context-learning-and-induction-heads/index.html>.
- [103] Kevin Ro Wang, Alexandre Variengien, Arthur Conmy, Buck Shlegeris, and Jacob Steinhardt. Interpretability in the wild: a circuit for indirect object identification in GPT-2 small. In *The Eleventh International Conference on Learning Representations*, 2023.
- [104] Steven Bills, Nick Cammarata, Dan Mossing, Henk Tillman, Leo Gao, Gabriel Goh, Ilya Sutskever, Jan Leike, Jeff Wu, and William Saunders. Language models can explain neurons in language models. <https://openaipublic.blob.core.windows.net/neuron-explainer/paper/index.html>, 2023.
- [105] Nicholas Goldowsky-Dill, Chris MacLeod, Lucas Sato, and Aryaman Arora. Localizing model behavior with path patching. *arXiv preprint arXiv:2304.05969*, 2023.
- [106] Wes Gurnee, Neel Nanda, Matthew Pauly, Katherine Harvey, Dmitrii Troitskii, and Dimitris Bertsimas. Finding neurons in a haystack: Case studies with sparse probing. *Transactions on Machine Learning Research*, 2023.
- [107] Zhengxuan Wu, Atticus Geiger, Thomas Icard, Christopher Potts, and Noah Goodman. Interpretability at scale: Identifying causal mechanisms in alpaca. *Advances in Neural Information Processing Systems*, 36, 2024.
- [108] Peter Hase, Mohit Bansal, Been Kim, and Asma Ghandeharioun. Does Localization Inform Editing? Surprising Differences in Causality-Based Localization vs. Knowledge Editing in Language Models. *Advances in Neural Information Processing Systems*, 36, 2024.
- [109] Kenneth Li, Oam Patel, Fernanda Viégas, Hanspeter Pfister, and Martin Wattenberg. Inference-Time Intervention: Eliciting Truthful Answers from a Language Model. *Advances in Neural Information Processing Systems*, 36, 2024.

- [110] Yifan Hou, Jiaoda Li, Yu Fei, Alessandro Stolfo, Wangchunshu Zhou, Guangtao Zeng, Antoine Bosselut, and Mrinmaya Sachan. Towards a mechanistic interpretation of multi-step reasoning capabilities of language models. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 4902–4919, 2023.
- [111] Arthur Conmy, Augustine Mavor-Parker, Aengus Lynch, Stefan Heimersheim, and Adrià Garriga-Alonso. Towards automated circuit discovery for mechanistic interpretability. *Advances in Neural Information Processing Systems*, 36:16318–16352, 2023.
- [112] Dan Friedman, Alexander Wettig, and Danqi Chen. Learning transformer programs. *Advances in Neural Information Processing Systems*, 36, 2024.
- [113] Michael Hanna, Ollie Liu, and Alexandre Variengien. How does gpt-2 compute greater-than?: Interpreting mathematical abilities in a pre-trained language model. *Advances in Neural Information Processing Systems*, 36, 2024.
- [114] Fred Zhang and Neel Nanda. Towards best practices of activation patching in language models: Metrics and methods. *International Conference on Learning Representations*, 2024.
- [115] Rhys Gould, Euan Ong, George Ogden, and Arthur Conmy. Successor heads: Recurring, interpretable attention heads in the wild. *International Conference on Learning Representations*, 2024.
- [116] Andrew Lee, Xiaoyan Bai, Itamar Pres, Martin Wattenberg, Jonathan K. Kummerfeld, and Rada Mihalcea. A mechanistic understanding of alignment algorithms: A case study on DPO and toxicity. In *Proceedings of the 41st International Conference on Machine Learning, Proceedings of Machine Learning Research*, pages 26361–26378. PMLR, 2024.
- [117] Samyak Jain, Robert Kirk, Ekdeep Singh Lubana, Robert P. Dick, Hidenori Tanaka, Tim Rocktäschel, Edward Grefenstette, and David Krueger. Mechanistically analyzing the effects of fine-tuning on procedurally defined tasks. In *International Conference on Learning Representations*, 2024.
- [118] Jie Ren, Qipeng Guo, Hang Yan, Dongrui Liu, Quanshi Zhang, Xipeng Qiu, and Duhua Lin. Identifying semantic induction heads to understand in-context learning. In *Findings of the Association for Computational Linguistics: ACL 2024*, pages 6916–6932, 2024.
- [119] Nikhil Prakash, Tamar Rott Shaham, Tal Haklay, Yonatan Belinkov, and David Bau. Fine-tuning enhances existing mechanisms: A case study on entity tracking. In *International Conference on Learning Representations*, 2024.
- [120] Michael Lan, Philip Torr, and Fazl Barez. Towards interpretable sequence continuation: Analyzing shared circuits in large language models. In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing*, pages 12576–12601, 2024.
- [121] Eric Todd, Millicent Li, Arnab Sen Sharma, Aaron Mueller, Byron C Wallace, and David Bau. Function vectors in large language models. In *International Conference on Learning Representations*, 2024.
- [122] Jingcheng Niu, Andrew Liu, Zining Zhu, and Gerald Penn. What does the knowledge neuron thesis have to do with knowledge? In *International Conference on Learning Representations*, 2024.
- [123] Aaditya K Singh, Ted Moskovitz, Felix Hill, Stephanie C.Y. Chan, and Andrew M Saxe. What needs to go right for an induction head? A mechanistic study of in-context learning circuits and their formation. In *Proceedings of the 41st International Conference on Machine Learning, Proceedings of Machine Learning Research*, pages 45637–45662. PMLR, 2024.
- [124] Asma Ghandeharioun, Avi Caciularu, Adam Pearce, Lucas Dixon, and Mor Geva. Patchscopes: A Unifying Framework for Inspecting Hidden Representations of Language Models. In *International Conference on Machine Learning*, 2024.

- [125] Zhenhong Zhou, Haiyang Yu, Xinghua Zhang, Rongwu Xu, Fei Huang, and Yongbin Li. How Alignment and Jailbreak Work: Explain LLM Safety through Intermediate Hidden States. In *Findings of the Association for Computational Linguistics: EMNLP 2024*, pages 2461–2488, 2024.
- [126] Javier Ferrando and Elena Voita. Information Flow Routes: Automatically Interpreting Language Models at Scale. In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing*, pages 17432–17445, 2024.
- [127] Tianyu He, Darshil Doshi, Aritra Das, and Andrey Gromov. Learning to grok: Emergence of in-context learning and skill composition in modular arithmetic tasks. *Advances in Neural Information Processing Systems*, 37:13244–13273, 2024.
- [128] Vedang K Lad. *Mechanistic Interpretability for Progress Towards Quantitative AI Safety*. PhD thesis, Massachusetts Institute of Technology, 2024.
- [129] Nouha Dziri, Sivan Milton, Mo Yu, Osmar R Zaiane, and Siva Reddy. On the Origin of Hallucinations in Conversational Models: Is it the Datasets or the Models? In *Proceedings of the 2022 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pages 5271–5285, 2022.
- [130] David Malet Armstrong. *Belief, Truth and Knowledge*. Cambridge University Press, 1973.
- [131] Henry Habberley Price. *Belief*. Routledge, 2002.
- [132] Carlos E. Alchourrón, Peter Gärdenfors, and David Makinson. On the logic of theory change: Partial meet contraction and revision functions. *Journal of Symbolic Logic*, 50(2):510–530, 1985.
- [133] Pan Zhuang, Fei Wu, Lei Mao, Fanghuan Zhu, Yiju Zhang, Xiaoqian Chen, Jingjing Jiao, and Yu Zhang. Egg and cholesterol consumption and mortality from cardiovascular and different causes in the United States: a population-based cohort study. *PLoS Medicine*, 2021.
- [134] Michael Polanyi. Personal knowledge : Towards a post-critical philosophy. *Chicago: University of Chicago Press*, 1958.
- [135] Michael Polanyi. The Tacit Dimension. In *Knowledge in organisations*, pages 135–146. Routledge, 2009.
- [136] Ilaria Gabbatore, Katja Dindar, Veera Pirinen, Hannu Vähänikkilä, Laura Mämmelä, Aija Kotila, Francesca M Bosco, Eeva Leinonen, and Soile Loukusa. Silent Finns and talkative Italians? An investigation of communicative differences and similarities as perceived by parents in typically developing children. *First Language*, 43(3):313–335, 2023.
- [137] Taojun Hu and Xiao-Hua Zhou. Unveiling LLM Evaluation Focused on Metrics: Challenges and Solutions. *arXiv preprint arXiv:2404.09135*, 2024.
- [138] Chin-Yew Lin. ROUGE: A Package for Automatic Evaluation of Summaries. In *Text summarization branches out*, pages 74–81, 2004.
- [139] Katie Matton, Robert Ness, John Guttag, and Emre Kiciman. Walk the Talk? Measuring the Faithfulness of Large Language Model Explanations. In *The Thirteenth International Conference on Learning Representations*, 2025.
- [140] Boxin Wang, Chejian Xu, Shuohang Wang, Zhe Gan, Yu Cheng, Jianfeng Gao, Ahmed Hassan Awadallah, and Bo Li. Adversarial GLUE: A Multi-Task Benchmark for Robustness Evaluation of Language Models. In *Thirty-fifth Conference on Neural Information Processing Systems Datasets and Benchmarks Track (Round 2)*, 2021.
- [141] Kaijie Zhu, Jindong Wang, Jiaheng Zhou, Zichen Wang, Hao Chen, Yidong Wang, Linyi Yang, Wei Ye, Yue Zhang, Neil Gong, et al. Promptrobust: Towards evaluating the robustness of large language models on adversarial prompts. In *Proceedings of the 1st ACM Workshop on Large AI Systems and Models with Privacy and Safety Analysis*, pages 57–68, 2023.

- [142] Yang Liu, Dan Iter, Yichong Xu, Shuohang Wang, Ruochen Xu, and Chenguang Zhu. G-Eval: NLG Evaluation using GPT-4 with Better Human Alignment. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 2511–2522, 2023.
- [143] Yen-Ting Lin Yun-Nung Chen. Llm-eval: Unified multi-dimensional automatic evaluation for open-domain conversations with large language models. In *The 5th Workshop on NLP for Conversational AI*, page 47, 2023.
- [144] Jintao Yang, Yushan Tan, Wenpeng Hu, Zonghao Yang, Xian Zhou, Zhunchen Luo, and Wei Luo. REM: A Ranking-Based Automatic Evaluation Method for LLMs. In *International Conference on Artificial Neural Networks*, pages 371–385. Springer, 2024.
- [145] Yidong Wang, Zhuohao Yu, Wenjin Yao, Zhengran Zeng, Linyi Yang, Cunxiang Wang, Hao Chen, Chaoya Jiang, Rui Xie, Jindong Wang, Xing Xie, Wei Ye, Shikun Zhang, and Yue Zhang. PandaLM: An Automatic Evaluation Benchmark for LLM Instruction Tuning Optimization. In *The Twelfth International Conference on Learning Representations*, 2024.
- [146] Percy Liang, Rishi Bommasani, Tony Lee, Dimitris Tsipras, Dilara Soylu, Michihiro Yasunaga, Yian Zhang, Deepak Narayanan, Yuhuai Wu, Ananya Kumar, Benjamin Newman, Binhang Yuan, Bobby Yan, Ce Zhang, Christian Alexander Cosgrove, Christopher D Manning, Christopher Re, Diana Acosta-Navas, Drew Arad Hudson, Eric Zelikman, Esin Durmus, Faisal Ladhak, Frieda Rong, Hongyu Ren, Huaxiu Yao, Jue WANG, Keshav Santhanam, Laurel Orr, Lucia Zheng, Mert Yuksekgonul, Mirac Suzgun, Nathan Kim, Neel Guha, Niladri S. Chatterji, Omar Khattab, Peter Henderson, Qian Huang, Ryan Andrew Chi, Sang Michael Xie, Shibani Santurkar, Surya Ganguli, Tatsunori Hashimoto, Thomas Icard, Tianyi Zhang, Vishrav Chaudhary, William Wang, Xuechen Li, Yifan Mai, Yuhui Zhang, and Yuta Koreeda. Holistic evaluation of language models. *Transactions on Machine Learning Research*, 2023.
- [147] Wanjun Zhong, Ruixiang Cui, Yiduo Guo, Yaobo Liang, Shuai Lu, Yanlin Wang, Amin Saied, Weizhu Chen, and Nan Duan. AGIEval: A Human-Centric Benchmark for Evaluating Foundation Models. In *Findings of the Association for Computational Linguistics: NAACL 2024*, pages 2299–2314, 2024.
- [148] Kun-Peng Ning, Shuo Yang, Yuyang Liu, Jia-Yu Yao, Zhenhui Liu, Yonghong Tian, Yibing Song, and Li Yuan. PiCO: Peer Review in LLMs based on Consistency Optimization. In *The Thirteenth International Conference on Learning Representations*, 2025.
- [149] Ankit Pal, Logesh Kumar Umapathi, and Malaikannan Sankarasubbu. Med-HALT: Medical Domain Hallucination Test for Large Language Models. In *Proceedings of the 27th Conference on Computational Natural Language Learning (CoNLL)*, pages 314–334, 2023.
- [150] Antonio Viganò, Marlene Dorgan, Jeanette Buckingham, Eduardo Bruera, and Maria E Suarez-Almazor. Survival prediction in terminal cancer patients: a systematic review of the medical literature. *Palliative Medicine*, 14(5):363–374, 2000. PMID: 11064783.
- [151] Dong Wook Kim, Sanghoon Lee, Sunmo Kwon, Woong Nam, In-Ho Cha, and Hyung Jun Kim. Deep learning-based survival prediction of oral cancer patients. *Scientific Reports*, 9(1):6994, 2019.
- [152] Maxim S. Kovalev, Lev V. Utkin, and Ernest M. Kasimov. Survlime: A method for explaining machine learning survival models. *Knowledge-Based Systems*, 203:106164, 2020.
- [153] Arturo Moncada-Torres, Marissa C van Maaren, Mathijs P Hendriks, Sabine Siesling, and Gijs Geleijnse. Explainable machine learning can outperform cox regression predictions and provide insights in breast cancer survival. *Sci. Rep.*, 11(1):6968, March 2021.
- [154] Lucile Ter-Minassian, Sahra Ghalebikesabi, Karla Diaz-Ordaz, and Chris Holmes. Explainable ai for survival analysis: a median-shap approach, 2024.
- [155] Mateusz Krzyziński, Mikołaj Spytek, Hubert Baniecki, and Przemysław Biecek. Survshap(t): Time-dependent explanations of machine learning survival models. *Knowledge-Based Systems*, 262:110234, 2023.

- [156] Sameer Sundrani and James Lu. Computing the hazard ratios associated with explanatory variables using machine learning models of survival data. *JCO Clinical Cancer Informatics*, (5):364–378, 2021. PMID: 33797958.
- [157] Xianjing Liu, Tobias E Sangers, Tamar Nijsten, Manfred Kayser, Luba M Pardo, Eppo B Wolvius, Gennady V Roshchupkin, and Marlies Wakkee. Predicting skin cancer risk from facial images with an explainable artificial intelligence (XAI) based approach: a proof-of-concept study. *EClinicalMedicine*, 71(102550):102550, May 2024.
- [158] Yiming Zhang, Ying Weng, and Jonathan Lund. Applications of explainable artificial intelligence in diagnosis and surgery. *Diagnostics*, 12(2), 2022.
- [159] Jiayi Dai. Rationale Extraction and Crohn’s Disease Detection from Computed Tomography Enterography Reports. Master’s thesis, University of Alberta, 2023.
- [160] Pedro A. Moreno-Sánchez. Data-driven early diagnosis of chronic kidney disease: Development and evaluation of an explainable ai model. *IEEE Access*, 11:38359–38369, 2023.
- [161] Houwu Gong, Miye Wang, Hanxue Zhang, Md Fazla Elahe, and Min Jin. An explainable ai approach for the rapid diagnosis of covid-19 using ensemble learning algorithms. *Frontiers in Public Health*, 10, 2022.
- [162] Tao Lei, Regina Barzilay, and Tommi Jaakkola. Rationalizing neural predictions. In Jian Su, Kevin Duh, and Xavier Carreras, editors, *Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing*, pages 107–117, Austin, Texas, November 2016. Association for Computational Linguistics.
- [163] Jiayi Dai, Mi-Young Kim, and Randy Goebel. Interactive rationale extraction for text classification. In *Workshop on Trustworthy and Socially Responsible Machine Learning, NeurIPS*, 2022.
- [164] Jiayi Dai, Mi-Young Kim, Reed T. Sutton, J. Ross Mitchell, Randolph Goebel, and Daniel C. Baumgart. Comparative analysis of natural language processing methodologies for classifying computed tomography enterography reports in Crohn’s disease patients. *npj Digital Medicine*, 8(1), 2025.
- [165] Ana-Maria Marcu, Long Chen, Jan Hünermann, Alice Karnsund, Benoit Hanotte, Prajwal Chidananda, Saurabh Nair, Vijay Badrinarayanan, Alex Kendall, Jamie Shotton, et al. LingoQA: Visual Question Answering for Autonomous Driving. In *European Conference on Computer Vision*, pages 252–269. Springer, 2024.
- [166] Shahin Atakishiyev, Mohammad Salameh, and Randy Goebel. Incorporating Explanations into Human-Machine Interfaces for Trust and Situation Awareness in Autonomous Vehicles. In *2024 IEEE Intelligent Vehicles Symposium (IV)*, pages 2948–2955, 2024.
- [167] Zesen Cheng, Sicong Leng, Hang Zhang, Yifei Xin, Xin Li, Guanzheng Chen, Yongxin Zhu, Wenqi Zhang, Ziyang Luo, Deli Zhao, et al. VideoLLaMA 2: Advancing Spatial-Temporal Modeling and Audio Understanding in Video-LLMs. *arXiv preprint arXiv:2406.07476*, 2024.
- [168] Ye Xia, Danqing Zhang, Jinkyu Kim, Ken Nakayama, Karl Zipser, and David Whitney. Predicting Driver Attention in Critical Situations. In *Computer Vision–ACCV 2018: 14th Asian Conference on Computer Vision, Perth, Australia, December 2–6, 2018, Revised Selected Papers, Part V 14*, pages 658–674. Springer, 2019.
- [169] Ilia Stepin, Jose M Alonso, Alejandro Catala, and Martín Pereira-Fariña. A Survey of Contrastive and Counterfactual Explanation Generation Methods for Explainable Artificial Intelligence. *IEEE Access*, 9:11974–12001, 2021.
- [170] Elena Prina, Otavio T Ranzani, and Antoni Torres. Community-acquired pneumonia. *The Lancet*, 386(9998):1097–1108, 2015.
- [171] Wentian Wang, Sarthak Jain, Paul Kantor, Jacob Feldman, Lazaros Gallos, and Hao Wang. MMLU-SR: A benchmark for stress-testing reasoning capability of large language models. In *Proceedings of the 2nd GenBench Workshop on Generalisation (Benchmarking) in NLP*, pages 69–85, Miami, Florida, USA, 2024. Association for Computational Linguistics.

- [172] Guobin Shen, Dongcheng Zhao, Aorigele Bao, Xiang He, Yiting Dong, and Yi Zeng. StressPrompt: Does Stress Impact Large Language Models and Human Performance Similarly? In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 39, pages 711–719, 2025.
- [173] Long Phan, Alice Gatti, Ziwen Han, Nathaniel Li, Josephina Hu, Hugh Zhang, Sean Shi, Michael Choi, Anish Agrawal, Arnav Chopra, et al. Humanity’s Last Exam. *arXiv preprint arXiv:2501.14249*, 2025.
- [174] Alejandro Barredo Arrieta, Natalia Díaz-Rodríguez, Javier Del Ser, Adrien Bennetot, Siham Tabik, Alberto Barbado, Salvador García, Sergio Gil-López, Daniel Molina, Richard Benjamins, et al. Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI. *Information Fusion*, 58:82–115, 2020.
- [175] Luca Longo, Mario Brcic, Federico Cabitza, Jaesik Choi, Roberto Confalonieri, Javier Del Ser, Riccardo Guidotti, Yoichi Hayashi, Francisco Herrera, Andreas Holzinger, et al. Explainable artificial intelligence (xai) 2.0: A manifesto of open challenges and interdisciplinary research directions. *Information Fusion*, 106:102301, 2024.
- [176] European Parliament and Council of the European Union. Artificial Intelligence Act: European Parliament legislative resolution of 13 March 2024 on the proposal for a regulation of the European Parliament and of the Council on laying down harmonised rules on Artificial Intelligence (Artificial Intelligence Act) and amending certain Union Legislative Acts (COM(2021)0206 – C9-0146/2021 – 2021/0106(COD)). [https://artificialintelligenceact.eu/wp-content/uploads/2024/04/TA-9-2024-0138\\_EN.pdf](https://artificialintelligenceact.eu/wp-content/uploads/2024/04/TA-9-2024-0138_EN.pdf), March 2024.
- [177] Yoshua Bengio, Tegan Maharaj, Luke Ong, Stuart Russell, Dawn Song, Max Tegmark, Lan Xue, Ya-Qin Zhang, Stephen Casper, Wan Sie Lee, et al. The Singapore Consensus on Global AI Safety Research Priorities. *arXiv preprint arXiv:2506.20702*, 2025.
- [178] Yikang Pan, Liangming Pan, Wenhui Chen, Preslav Nakov, Min-Yen Kan, and William Wang. On the Risk of Misinformation Pollution with Large Language Models. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 1389–1403, 2023.
- [179] Jiawei Zhou, Yixuan Zhang, Qianni Luo, Andrea G Parker, and Munmun De Choudhury. Synthetic Lies: Understanding AI-Generated Misinformation and Evaluating Algorithmic and Human Solutions. In *Proceedings of the 2023 CHI Conference on Human Factors in Computing Systems*, pages 1–20, 2023.
- [180] Aaron Fanous, Jacob Goldberg, Ank A Agarwal, Joanna Lin, Anson Zhou, Roxana Daneshjou, and Sanmi Koyejo. SycEval: Evaluating LLM Sycophancy. *arXiv preprint arXiv:2502.08177*, 2025.
- [181] Lars Malmqvist. Sycophancy in Large Language Models: Causes and Mitigations. In *Intelligent Computing-Proceedings of the Computing Conference*, pages 61–74. Springer, 2025.
- [182] Haoxi Li, Xueyang Tang, Jie ZHANG, Song Guo, Sikai Bai, Peiran Dong, and Yue Yu. Causally Motivated Sycophancy Mitigation for Large Language Models. In *The Thirteenth International Conference on Learning Representations*, 2025.
- [183] Jie Huang, Hanyin Shao, and Kevin Chen-Chuan Chang. Are large pre-trained language models leaking your personal information? In *Findings of the Association for Computational Linguistics: EMNLP 2022*, pages 2038–2047, 2022.
- [184] Tianyu Han, Sven Nebelung, Firas Khader, Tianci Wang, Gustav Müller-Franzes, Christiane Kuhl, Sebastian Förtsch, Jens Kleesiek, Christoph Haarburger, Keno K Bressem, et al. Medical large language models are susceptible to targeted misinformation attacks. *NPJ digital medicine*, 7(1):288, 2024.
- [185] Siwon Kim, Sangdoo Yun, Hwaran Lee, Martin Gubri, Sungroh Yoon, and Seong Joon Oh. PropILE: Probing Privacy Leakage in Large Language Models. *Advances in Neural Information Processing Systems*, 36, 2024.

- [186] Isaac Asimov. Runaround. I, robot. *New York: Doubleday*, 1950.
- [187] James H Moor. The Nature, Importance, and Difficulty of Machine Ethics. *IEEE Intelligent Systems*, 21(4):18–21, 2006.
- [188] Q Vera Liao and Jennifer Wortman Vaughan. AI Transparency in the Age of LLMs: A Human-Centered Research Roadmap. *Harvard Data Science Review*, (Special Issue 5), 2024.
- [189] Kristian Gonzalez Barman, Nathan Wood, and Paweł Pawłowski. Beyond transparency and explainability: on the need for adequate and contextualized user guidelines for LLM use. *Ethics and Information Technology*, 26(3):47, 2024.
- [190] Markus Langer, Daniel Oster, Timo Speith, Holger Hermanns, Lena Kästner, Eva Schmidt, Andreas Sesing, and Kevin Baum. What do we want from Explainable Artificial Intelligence (XAI)?—A stakeholder perspective on XAI and a conceptual model guiding interdisciplinary XAI research. *Artificial Intelligence*, 296:103473, 2021.
- [191] Carlo Casonato and Giulia Olivato. AI Regulation in Europe: Exploring the Artificial Intelligence Act. In *Digital Environments and Human Relations*, pages 87–111. Springer, 2024.
- [192] Koustuv Sinha, Shagun Sodhani, Jin Dong, Joelle Pineau, and William L Hamilton. CLUTRR: A Diagnostic Benchmark for Inductive Reasoning from Text. In *Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP)*, pages 4506–4515, 2019.
- [193] Christopher Hahn, Frederik Schmitt, Jens U. Kreber, Markus Norman Rabe, and Bernd Finkbeiner. Teaching Temporal Logics to Neural Networks. In *International Conference on Learning Representations*, 2021.
- [194] Peter Clark, Oyvind Tafjord, and Kyle Richardson. Transformers as soft reasoners over language. In *Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence*, 2020.
- [195] Mihir Parmar, Nisarg Patel, Neeraj Varshney, Mutsumi Nakamura, Man Luo, Santosh Mashetty, Arindam Mitra, and Chitta Baral. LogicBench: Towards Systematic Evaluation of Logical Reasoning Ability of Large Language Models. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 13679–13707, 2024.
- [196] Pulkit Verma, Ngoc La, Anthony Favier, Swaroop Mishra, and Julie A Shah. Teaching LLMs to Plan: Logical Chain-of-Thought Instruction Tuning for Symbolic Planning. *arXiv preprint arXiv:2509.13351*, 2025.
- [197] Pang Wei Koh, Thao Nguyen, Yew Siang Tang, Stephen Mussmann, Emma Pierson, Been Kim, and Percy Liang. Concept Bottleneck Models. In *International Conference on Machine Learning*, pages 5338–5348. PMLR, 2020.
- [198] Mert Yuksekgonul, Maggie Wang, and James Zou. Post-hoc concept bottleneck models. In *The Eleventh International Conference on Learning Representations*, 2023.
- [199] Konstantinos Panousis, Dino Ienco, and Diego Marcos. Coarse-to-Fine Concept Bottleneck Models. *Advances in Neural Information Processing Systems*, 37:105171–105199, 2025.
- [200] Eoin M Kenny, Akshay Dharmavaram, Sang Uk Lee, Tung Phan-Minh, Shreyas Rajesh, Yunqing Hu, Laura Major, Momchil S Tomov, and Julie A Shah. Explainable deep learning improves human mental models of self-driving cars. *arXiv preprint arXiv:2411.18714*, 2024.
- [201] Winnie Pang, Xueyi Ke, Satoshi Tsutsui, and Bihan Wen. Integrating Clinical Knowledge into Concept Bottleneck Models. In *International Conference on Medical Image Computing and Computer-Assisted Intervention*, pages 243–253. Springer, 2024.
- [202] Chung-En Sun, Tuomas Oikarinen, Berk Ustun, and Tsui-Wei Weng. Concept Bottleneck Large Language Models. In *The Thirteenth International Conference on Learning Representations*, 2025.

- [203] Cynthia Rudin. Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nature Machine Intelligence*, 1(5):206–215, 2019.
- [204] Eoin M Kenny and Julie A Shah. Regulation of Language Models With Interpretability Will Likely Result In A Performance Trade-Off. *arXiv preprint arXiv:2412.12169*, 2024.