Towards Explainable and Interpretable Multimodal Large Language Models: A Comprehensive Survey

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Abstract—The rapid development of Artificial Intelligence (AI) has revolutionized numerous fields, with large language models (LLMs) and computer vision (CV) systems driving advancements in natural language understanding and visual processing, respectively. The convergence of these technologies has catalyzed the rise of multimodal AI, enabling richer, crossmodal understanding that spans text, vision, audio, and video modalities. Multimodal large language models (MLLMs), in particular, have emerged as a powerful framework, demonstrating impressive capabilities in tasks like image-text generation, visual question answering, and cross-modal retrieval. Despite these advancements, the complexity and scale of MLLMs introduce significant challenges in interpretability and explainability, essential for establishing transparency, trustworthiness, and reliability in high-stakes applications. This paper provides a comprehensive survey on the interpretability and explainability of MLLMs, proposing a novel framework that categorizes existing research across three perspectives: (I) Data, (II) Model, (III) Training & Inference. We systematically analyze interpretability from token-level to embedding-level representations, assess approaches related to both architecture analysis and design, and explore training and inference strategies that enhance transparency. By comparing various methodologies, we identify their strengths and limitations and propose future research directions to address unresolved challenges in multimodal explainability. This survey offers a foundational resource for advancing interpretability and transparency in MLLMs, guiding researchers and practitioners toward developing more accountable and robust multimodal AI systems.

Index Terms—Multimodal Large Language Models, Explainability, Interpretability, Survey.

I. INTRODUCTION

The rapid advancement of Artificial Intelligence (AI) has significantly transformed a wide array of fields. Recently one of the most influential advancements in AI is the development of large language models (LLMs), which exhibit remarkable language understanding and generating capabilities in a wide range of natural language tasks like text generation, translation, and conversational AI [1]. Similarly, advancements in computer vision (CV) have enabled systems to effectively process and interpret complex visual data, powering tasks like object detection, action recognition, and semantic segmentation with high precision [2]. More recently, the convergence of these technologies has spurred interest in multimodal

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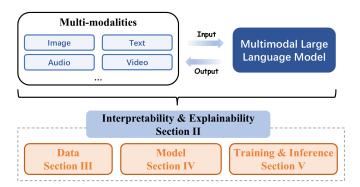


Fig. 1. The conceptual framework of this survey. MLLMs handle inputs and outputs that span multiple modalities, such as images, text, video, and audio. We explore interpretability and explainability along three major dimensions: the data, the model, and the training & inference.

AI, which seeks to integrate text, vision, audio, and video for a richer, more comprehensive understanding of multiple modalities [3, 4, 5, 6, 7, 8, 9, 10, 11]. Multimodal large language models (MLLMs) have experienced rapid advancements, driven by significant improvements in deep learning techniques [12, 13, 14, 15, 16, 17]. By integrating diverse data sources, MLLMs demonstrate advanced understanding, reasoning, and generative capabilities across a wide range of multimodal tasks, including image-text generation [18, 19, 20], visual question answering [21, 22, 23, 24, 25, 26, 27, 28], cross-modal retrieval [29, 30, 31], video understanding [32, 33, 34, 35, 36, 37, 38]. Consequently, MLLMs have found diverse applications across various domains [39, 40, 41], including natural language processing (NLP) [42, 43], CV [44, 45], video [15, 46, 47], autonomous driving [3, 48, 49], medicine [50, 51, 52], and robotics [53, 54, 55, 56, 57, 58]. However, as the complexity and scale of MLLMs grow, a critical challenge arises: deciphering the decision-making processes of MLLMs. [6, 59, 60].

The field of explainable artificial intelligence (XAI) has become pivotal in making the decision-making processes of complex AI systems more transparent and accessible [61, 62, 63]. Interpretability and explainability are defined as the ability to explain or to present in human-understandable terms [64, 65]. Although significant progress has been made

in unimodal explainability and interpretability, such as in convolutional neural networks (CNN) [66, 67] or transformers [68] for images and LLMs [69] for text, the multimodal domain presents unique challenges, such as the alignment and decomposition of different modalities. Moreover, the interpretability and explainability of MLLMs are essential for ensuring transparency and trustworthiness, especially in highstakes applications where artificial intelligence decisions have a significant human impact, which addresses how disparate data types are combined within a model and how their interplay affects outputs. Following recent research [64, 70, 71], in this paper, we define interpretability in MLLMs refers to the internal structures that are inherently understandable, allowing for straightforward comprehension of how inputs are transformed into outputs. Explainability in MLLMs, on the other hand, involves post-hoc techniques that provide external analyses of model behavior behind a model's decisions.

In this paper, we present a new insight for categorizing the interpretability and explainability of MLLMs by integrating perspectives from data, model, training and inference. As illustrated in Figure 1, we examine the interpretability and explainability of MLLMs from three perspectives: data (Section III), model (Section IV), training and inference (Section V). Following the data-driven explainability [72, 73, 74, 75] research, we examine the data perspective (Section III), exploring how both input and output data can be attributed to the model's decisions. We also analyze benchmarks and applications to evaluate the trustworthiness and reliability across various tasks, thereby ensuring the robustness and applicability in realworld scenarios [76, 77]. As for the model interpretability and explainability [78, 79, 80, 81, 82, 83, 84], from the model perspective (Section IV), we conduct an in-depth analysis at the token level, embedding level, neuron level, layer level, and architectural level. At the token level [85, 86, 87, 88, 89], we investigate the impact of individual tokens on model outputs and explore methodologies to enhance interpretability. At the embedding level [90], we assess how multimodal embeddings influence the performance and interpretability of MLLMs, providing a deeper understanding of the underlying representation mechanisms. For neuron-level [91, 92, 93], we analyze individual units and specialized groups of neurons to comprehend their contributions to overall model behavior. At the layer level [67, 78, 94], we investigate how different layers affect decision-making processes within the model. Regarding architecture, we differentiate between architecture-analysis and architecture-design [95, 96, 97, 98] approaches to interpretability, highlighting strategies that promote transparency and facilitate a better understanding of model operations. Furthermore, we explore training and inference strategies that enhance model transparency and explainability (Section V). In the training phase [79], we summarize how various training mechanisms and weight adjustments impact the interpretability of MLLMs. We discuss techniques aimed at improving alignment, reducing hallucinations, and promoting the acquisition of core knowledge and generalization capabilities in MLLMs. During inference, we investigate methods to mitigate issues such as hallucination without the need for retraining, including over-trust penalty mechanisms and chain-of-thought reasoning

techniques.

By integrating these perspectives [3, 99, 100], our survey offers a holistic understanding of the challenges and advancements in the interpretability and explainability of MLLMs. We believe this comprehensive analysis will serve as a valuable resource for researchers and practitioners dedicated to developing more transparent, reliable, and trustworthy multimodal models. The major contributions of this work are summarized as follows:

- We are the first to offer an in-depth and comprehensive review of existing research on the explainability and interpretability of MLLMs.
- We present a structured and comparative analysis of current methods for MLLMs explainability and interpretability, introducing a novel categorization that organizes these methods into data, model, training & inference perspectives.
- We highlight potential research directions that could advance the field, offering valuable guidance for researchers aiming to further develop explainability and interpretability approaches for MLLMs.

II. SURVEY LANDSCAPE

A. Survey Scope

Both multimodal models and XAI have achieved significant advancements in recent years, with a substantial body of research exploring methods for making these complex models more transparent and interpretable [72, 73, 74]. To narrow the scope of this survey to a manageable range, we focus on the explainability and interpretability of MLLMs. Interpretability of MLLMs refers to internal structures that are inherently understandable, allowing for straightforward insights into how inputs are processed and transformed into outputs [78, 79]. Interpretable MLLMs enable researchers and practitioners to gain deeper insights into these cross-modal dynamics, providing clarity on how each modality influences and shapes the model's decision-making processes [90]. Explainability involves using external techniques to clarify the reasons behind a model's decisions, which is essential in MLLMs for understanding the intricate interactions among multiple modalities [95]. This focus not only enhances our understanding of multimodal integration but also addresses the growing demand for transparency in complex AI systems [79].

In this survey, we concentrate on four main dimensions of explainability and interpretability within MLLMs: Data Explainability – How input data from different modalities is preprocessed, aligned, and represented to support interpretability across modalities, and how causal attribution methods are applied to outputs to enhance understanding of model decisions [72, 75]. Model Explainability – Techniques that elucidate the structure and functioning of the multimodal model itself, offering insights into how neurons, layers, and architectures contribute to interpretability [67, 78, 79, 80, 85, 86, 87, 90, 91, 95]. Training and Inference Explainability – Understanding how MLLMs' training and inference processes affect interpretability, which is vital for refining transparency during both the learning phase and real-world application.

	Explainable and Interpretable MLLMs					
Keywords	XAI, explainable AI, explanation, explainable,					
	explanatory, interpretable, intelligible, black-box,					
	white-box, explainability, interpretability, intelligibility,					
	text-to-image, image-to-text, diffusion, GAN, CLIP,					
	MLLMs, VLMs, VQA					

To maintain focus, we exclude single-modality explainability methods from the main scope of this survey, such as Transformer interpretability, CNN interpretability or LLMs interpretability, except for brief background information. Similarly, general approaches to explainability that do not address the unique challenges of multimodal interactions are outside the primary scope of this review. Instead, our emphasis remains on methods and models explicitly designed to interpret and explain the interactions between multiple modalities.

B. Survey Methodology

To provide a comprehensive overview of explainability and interpretability in MLLMs, we conducted an extensive review of research papers spanning the fields of machine learning, NLP, CV, and multimodal systems. We examined papers published over the past decade (2010-2024), focusing on the growing body of work that explores interpretability and explainability in these areas. Our methodology consisted of several key steps. First, we searched for papers using keywords such as "multimodal large models," "interpretability," and "explainability" in databases like Google Scholar, detailed is shown in Table I. To further ensure the completeness of our survey, we also reviewed reference lists of key papers and included early influential works that shaped this domain. After collecting the candidate papers, we followed a multistep filtering process. Titles were first reviewed to identify potentially relevant papers, followed by abstract screening to confirm relevance. In cases where the title and abstract were insufficient for a decision, we reviewed the full text. As is shown in Figure 2, the final selection covers a variety of interpretability and explainability techniques applied to MLLMs, including input-output analyses, model components, and training dynamics.

III. DATA

LLMs primarily focus on processing text inputs at the levels of words, phrases, or sentences [69]. Explainability in LLMs involves understanding how these models interpret input text data and generate interpretable text data [69]. In contrast, explainability in computer vision typically relies on models like CNNs [79] or Vision Transformers (ViTs) [100, 101] to analyze and interpret visual image data. MLLMs extend these capabilities by integrating visual, audio and language information, enabling the generation and understanding of multimodal data. In this section, we mainly explore the role of data in enhancing the interpretability of MLLMs. As is shown in Figure 2, we categorize these works into three groups:

 Input and Output (Section III-A): Focuses on methods to improve interpretability by analyzing how models process inputs and outputs, including techniques like perturbation, saliency maps, and causal inference.

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- Benchmarks (Section III-B): Highlights benchmarks, datasets, and metrics for evaluating interpretability and robustness in multimodal models.
- Applications (Section III-C): Explores interpretability techniques applied to domains beyond vision and language, such as audio, video, autonomous driving, and medicine.

A. Input and Output

The robustness and explainability of MLLMs are critically dependent on how these models handle input data and produce outputs, as well as the transparency of their decision-making processes. Early works highlighted explainability in model input processing, zintgraf et al. [195] investigated the influence of specific regions within input images on model classification and revealed how different image regions contribute to predictions to make the decision-making processes of deep networks more interpretable. Park et al. [102] developed a multimodal explainability framework combining visual attention maps with textual justifications, enhancing model transparency across visual and textual inputs. Szegedy [196] showed that deep neural networks could be highly sensitive to small, almost imperceptible changes in input data.

Furthering the exploration of input explainability, methods such as TISE [197] and Extremal Perturbations [198] developed perturbation-based approaches to create saliency maps. These maps highlight critical areas in input images that significantly affect model predictions, thus providing interpretable explanations by revealing which input features are most influential in model decision-making. Complementing these methods, Kanehira [199] proposed a novel framework for generating visual explanations that combine linguistic and visual information. By maximizing the interaction between modalities, highlighting how complementary information from different modalities influences model decisions. More recently, Fel et al. [200] introduced a unified theoretical framework for concept-based explainability, formalizing concept extraction as a process of dictionary learning and concept importance estimation as an attribution method.

Beyond these methods, causal inference has emerged as a crucial approach for uncovering meaningful relationships in multimodal data. Morioka [201] introduced connectivity-contrastive learning (CCL), a framework for causal discovery in multimodal contexts. CCL disentangles mixed observations into independent latent components and identifies their causal structures, thus enhancing interpretability by providing insight into the underlying causal relationships in multimodal data. Within a similar context, CausalPIMA [104] presented a causal representation learning algorithm that integrates multimodal data and physics-based constraints. CausalPIMA employs a differentiable directed acyclic graph (DAG) learning structure with a variational autoencoder to discover essential causal relationships in an unsupervised manner, enabling interpretable

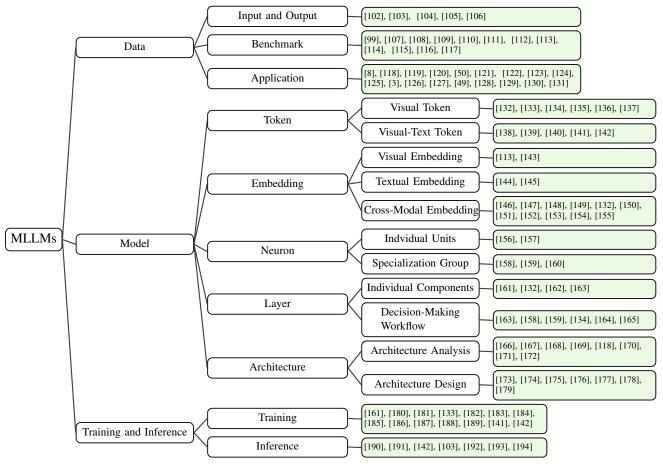


Fig. 2. We classify MLLM explainability into three main categories: Data, Model, and Training & Inference. This structure facilitates a comprehensive overview of the various techniques used to explain MLLMs, along with a discussion of the methods for evaluating these explanations across different paradigms.

causal patterns without predefined causal assumptions. Further advancing causal learning, Klaassen et al. [105] proposed a neural network architecture within the double machine learning (DML) framework, aimed at causal inference with unstructured data, such as text and images.

Recent works [202, 203, 204, 205] in diffusion models have provided new methods for interpretability, particularly through pixel-level attribution and information-theoretic approaches. DAAM [206] improved the interpretability of large-scale diffusion models by generating attribution maps that use cross-attention scores, offering insight into how specific words influence image regions. This method reveals complex syntactic and semantic relationships in image generation, such as feature entanglement between objects and descriptions. Liang et al. [106] proposed an efficient high-modality learning method that uses information-theoretic metrics to measure modality and interaction heterogeneity, improving multimodal model explainability in complex tasks. Building on this, Kong et al. [207] introduced an information-theoretic approach to enhance explainability in denoising diffusion models.

B. Benchmark

Recent advancements in MLLMs have provided transformative insights into processing and aligning visual and textual data [99, 107]. As these models become central to diverse

applications, understanding their decision-making is crucial for transparency, trust, and robustness. This paper explores benchmarks, evaluation frameworks, and interpretability methods to address challenges in alignment, robustness, and domain-specific explainability, emphasizing the importance of explainability in enhancing the reliability of MLLM datasets.

Alignment and Robustness. Efforts to improve transparency in visual-linguistic alignment have introduced new benchmarks and datasets. VISTA [108] aligned with human visual attention data, which compares internal heatmaps of vision-language models with human attention patterns to enhance model trustworthiness. Addressing robustness under distribution shifts, Cai et al. [109] developed BenchLMM, enabling models to detect image styles and explain errors under stylistic variations. Similarly, Mao et al. [208] introduced COCO-O, designed to evaluate the robustness of object detectors against natural distribution shifts, underscoring explainability's role in identifying vulnerabilities. Broadening this perspective, the Multimodal Uncertainty Benchmark (MUB) [110] assessed the vulnerability of MLLMs to explicit and implicit misleading instructions. Zhang et al. [111] further developed MultiTrust, a comprehensive evaluation framework spanning dimensions like truthfulness, safety, robustness, fairness, and privacy, revealing cross-modal explainability challenges.

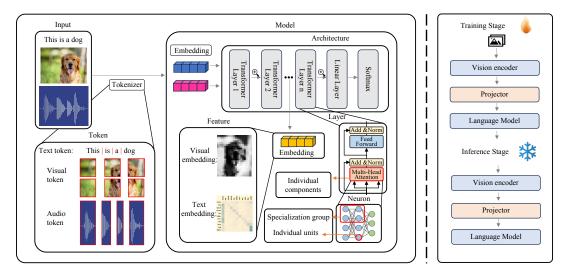


Fig. 3. Overview of our framework. The framework illustrates how input modalities like images, videos, or audio are tokenized into visual or textual tokens and then transformed into embeddings. The architecture includes individual neurons and neuron groups across layers, analyzed through architecture analysis and design. The workflow concludes with training and inference phases.

Image-Text Tasks. In image-text tasks, Madhyastha et al. [209] demonstrated the impact of explicit object information in identifying semantically incorrect captions, highlighting the importance of accurately encoding descriptive image features to enhance explainability. In language representation evaluation, Hewitt and Liang [210] introduced control tasks to verify whether linguistic probes genuinely capture underlying structures or merely memorize tasks, underscoring the need for selectivity in explainability assessments. In text-to-image generation, Hu et al. [112] proposed TIFA, an evaluation metric that uses visual question answering (VQA) to assess the faithfulness of generated images. By correlating model accuracy on generated question-answer pairs with human judgments, TIFA offers fine-grained assessments for explainability. Further exploring domain-specific explainability, Verma et al. [113] examined the impact of visual attributes on model behavior, while Tiong et al. [114] introduced six explainability factors to evaluate how vision-language models represent basic concepts.

Task-Specific Multimodal explainability. In the context of VQA, Alipour et al. [115] demonstrated that multimodal explanations enhance user accuracy, confidence, and understanding, especially when the model's response is inaccurate. Their introduction of active attention as a novel approach for examining causal effects highlights the role of transparency in building trust. For zero-shot learning, Liu et al. [116] developed the explainable zero-shot learning (XZSL) framework, which integrates visual and textual explanations into classification decisions via the Deep Multi-Modal Explanation (DME) model. Lastly, ScienceQA [117], a multimodal dataset, promotes explainability through chain-of-thought reasoning, enabling structured lectures and explanations to improve both question-answering performance and learning efficiency. Schwettmann et al. [211] introduced FIND, a benchmark suite for automated explainability, generating and validating descriptions of black-box functions to improve understanding

of neural network behavior.

C. Application

In recent years, the growing complexity of multimodal AI models has emphasized the need for explainability, which can provide insights into more applications across domains like medical, video processing, autonomous driving, audio processing, and music [12, 99, 107]. This survey reviews state-of-the-art explainability techniques for multimodal AI applications, highlighting advancements, challenges, and methodologies that address various needs for model transparency.

Agent Explainability. Xie et al. [8] explored a systematic review of large multimodal agents (LMAs), focusing on the essential components, categorization, collaborative frameworks, evaluation methodologies, and real-world applications while highlighting key advancements in multimodal explainability and proposing future research directions. Explainability agents are pivotal in analyzing model behaviors, automating feature interpretation, and identifying failure modes. MAIA [118] represented a multimodal automated explainability agent aimed at explaining vision-language models and deep networks. This agent uses neural models for feature interpretation and discovery of failure modes, enhancing the understanding of complex model behaviors in multimodal settings. Similarly, Cuadra et al. [119] introduced a multimodal LLMs agent to improve accessibility in digital form completion, especially for older adults and individuals with sensory impairments, thereby tailoring explainability to enhance usability and inclusivity in human-computer interaction.

Medical Explainability. Explainability in multimodal AI models is crucial in healthcare, where transparency can directly impact clinical decisions. UnitedNet [212] is an explainable multi-task deep neural network designed for biological data, which reveals relationships between gene expression and other modalities, supporting explainable biological data analysis. Rawls et al. [213] employed Causal Discovery Anal-

ysis (CDA) to model Alcohol Use Disorder (AUD) pathways, underscoring the influence of cognitive, social, and psychiatric factors on AUD severity. Furthermore, MCAN [51] bridged fMRI and EEG data using a Multimodal Causal Adversarial Network, facilitating dynamic brain network structure estimation and revealing abnormal activity patterns. Amara et al. [131] proposed a novel framework combining ontologies with MLLMs to enhance explainability in domain-specific tasks, using ontology-based guidance and evaluation to improve model alignment with domain concepts, particularly for plant disease classification. MedRegA [50] introduced a region-aware medical multimodal language model that aligns with clinical workflows by enabling region-specific identification and report generation across modalities, thereby enhancing explainability in clinical practice.

Video Explainability. The field of video analysis benefits from interpretable multimodal models that clarify decisions in complex visual-linguistic tasks. Kanehira et al. [121] proposed a counterfactual explanation method for video classification, enhancing interpretability by improving visual-linguistic compatibility and understanding. In VideoQA, Zang et al. [122] developed the Multimodal Causal Reasoning (MCR) framework, which separates causal and confounding features to improve robustness in answering video-related questions. Similarly, Flipped-VOA[123] addresses linguistic bias in LLMs by predicting reciprocal video, question, and answer pairs, enhancing VideoQA explainability. Holmes-VAD[124] tackles video anomaly detection by using a multimodal dataset with singleframe annotations, facilitating detailed anomaly explanations. TV-TREES [125] contributes an entailment tree generator for logical video-language understanding, allowing humaninterpretable proofs and achieving state-of-the-art performance in zero-shot scenarios on the TVQA benchmark.

Autonomous driving Explainability. In autonomous driving, explainability is essential for understanding complex decision-making processes and ensuring safety [3]. Hu et al. [126] proposed a probabilistic multimodal method for predicting vehicle behavior, addressing uncertainties and enhancing explainability. DriveGPT4 [127] processes video inputs to provide natural language explanations and low-level vehicle controls, improving understanding of autonomous driving systems. Reason2Drive [48] introduced a novel dataset with chain-based reasoning metrics, clarifying decision-making. Cog-GA [49] added cognitive mapping and dual-channel scene descriptions to support interpretable vision-language navigation, offering transparency in scene understanding and adaptive planning for autonomous driving.

Audio Explainability. Audio processing models require interpretability to effectively recognize emotional and contextual cues. GBAN [128] employs a gated bidirectional alignment network to align speech and text modalities, enhancing both explainability and emotional recognition accuracy. Qwen-Audio [214] extended audio-language model capabilities with multi-turn dialogue support, improving explainability in audio-centered scenarios. Multimodal Attention Merging (MAM) [215] facilitated knowledge transfer from text and image models to audio models without additional fine-tuning, while Jalal et al. [216] use attention models in speech emotion

recognition to map vowel and word cues, revealing emotional patterns and improving the explainability of acoustic-based models. Zadeh et al. [129] presented the CMU-MOSEI dataset for multimodal sentiment and emotion recognition and introduced the Dynamic Fusion Graph (DFG), which enables detailed analysis of cross-modal interactions by visualizing the interactions between language, visual, and acoustic modalities.

Music Explainability. In music information retrieval, interpretability improves the analysis of complex audio features, enhancing transparency in music classification tasks. Won et al. [217] developed a self-attention-based model for music tagging, visualizing attention maps to capture dependencies between musical components. Lyberatos et al. [218] combined perceptual feature extraction with explainability techniques like SHAP to clarify ambiguous labels in music tagging. PECMAE[219] used a prototype-based model with a diffusion decoder for music classification, enabling explainability in genre and instrument detection. Concept-based methods by Foscarin et al. [220] provided the post-hoc explanations that relate high-level musical concepts to model predictions, facilitating musicological analysis. Finally, MUSICLIME [130] provided model-agnostic explanations in multimodal music models, showing how audio and lyrical features contribute to predictions for a well-rounded understanding of model decision-making.

IV. MODEL

This section delves into the mechanisms underpinning MLLMs, exploring how their internal representations are interpreted, components such as tokens, embedding, neurons, and layers are analyzed, and architecture is understood. As is shown in Figure 2, the discussion is structured as follows:

Token Interpretability (Section IV-A): examines interpretability at the token level, focusing on visual, textual, and visual-textual tokens.

- Visual Tokens (Section IV-A1): Explores their role in decision-making, focusing on methods like basis decomposition, attention mechanisms, and token redundancy reduction.
- Visual-textual Tokens (Section IV-A2): Explores visual-textual alignment, mitigating hallucination, and improving visual-language integration.

Feature Interpretability (Section IV-B): Focuses on coarse-grained analyses of multimodal embeddings and latent spaces.

- **Visual Embeddings** (Section IV-B1): Explores humanunderstandable visual embeddings, internal representations, and dynamic processes in generative models.
- Visual-Textual Embeddings (Section IV-B3): Discusses interpretable cross-modal embeddings and techniques for improving alignment and representational capacity.

Neuron Interpretability (Section IV-C): Investigates the interpretability of individual neurons in multimodal models.

• Individual Units (Section IV-C1): Explores the roles and semantic concepts of individual neurons in MLLMs.

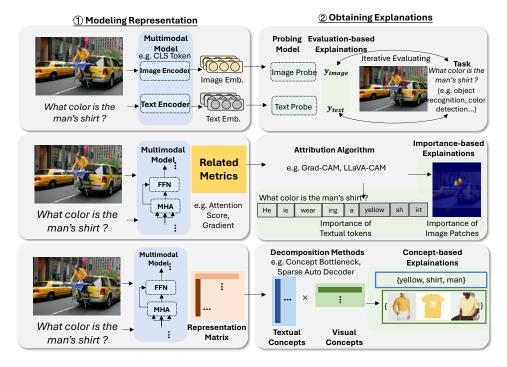


Fig. 4. Illustration of three key methodologies for embedding interpretability. Probing-based Interpretation: Evaluates representation quality by training a probing model; its performance reflects the utility of the representations for specific tasks. Attribution-based Interpretation: Assesses input contributions to model outputs using metrics like attention scores or gradients. Decomposition-based Interpretation: Analyzes representations by breaking them into meaningful features, often using sparse auto-encoders or similar tools.

Specialization Groups (Section IV-C2): Highlights neuron groups specialized in cross-modal or domain-specific tasks.

Layer Interpretability (Section IV-D): Analyzes the role of layers in neural networks and their decision-making processes.

- Individual Components (Section IV-B1): Examines the functions of attention heads, MLP layers, and other components.
- **Decision-Making Workflow** (Section IV-B1): Tracks representation transformations and information flow across layers.

Architecture Interpretability (Section IV-E): Explores model architecture as a whole to explain decision-making processes.

- Architecture Analysis (Section IV-E1): We present methods that analyze a model's characteristics or explainability. Most of these methods typically offer visual or textual explanations. We also use the type of explanation as a categorization criterion to organize these methods.
- Architecture Design (Section IV-E2): These methods primarily focus on designing specific modules or entire frameworks to enhance the inherent explainability of the model architecture. Typically, they do not provide explicit explanations. We categorize these methods based on their distinct characteristics.

A. Token

In this section, we focus on multimodal explainability at the token level, categorizing tokens into visual and visual-textual tokens. Visual tokens are primarily studied to understand their impact on model output and to reduce token redundancy, thereby improving model explainability. Visual-textual tokens, on the other hand, are analyzed to explore how their distribution affects model output, with the goal of compressing both visual and textual tokens to further enhance explainability. Visual Tokens (Section IV-A1): discusses the importance of visual tokens in the model's decision-making process and how methods like interpretable basis decomposition [228] and analysis of attention mechanisms in visual transformers enhance their interpretability. Additionally, it explores methods to improve model efficiency and interpretability by reducing token redundancy. Visual-Textual Tokens (Section IV-A2): explores the integration of visual and textual modalities, highlighting methods that enhance interpretability through visual-textual token alignment, mitigate undesirable behaviors like hallucination in multimodal models, and improve visuallanguage alignment.

1) Visual Token: The interpretability of visual tokens has become a crucial focus in the fields of computer vision and multimodal learning. Visual tokens refer to discrete units derived from an image, often representing specific regions or features, enabling models to handle high-dimensional visual information more efficiently. This review provides an in-depth overview of current research on visual tokens, emphasizing their role in enhancing model interpretability, performance, and computational efficiency.

Backgrounds. Initial studies aimed to clarify how these image tokens contribute to the model's predictions, with Zhou et al. [228] introducing a basis decomposition framework that

TABLE II

Overview of Embedding-Level Methods. The papers are categorized by perspective, models, interpretation methods, and tasks.

Perspective	Method	Models	Interpretation Method	Tasks				
Token Interpretability								
Wang et al. [136] Neo et al. [133] Visual Zhang et al. [134] Chen et al. [135] Yao et al. [137]		CLIP MLLMs MLLMs MLLMs MLLMs	Information Bottleneck Visual Token Localization Information Flow Analysis Pruning Irrelevant Visual Tokens Understanding Projector Module	Image Captioning Object Identification VQA, Image Captioning Image, Video Understanding VQA				
Visual-Textual	Gandelsman [132] Bi et al. [138] Zhao et al. [139] Li et al. [140] Dai et al. [141] Huang et al. [142] Wei and Zhang [221] Tang et al. [206]	CLIP MLLMs MLLMs MLLMs MLLMs MLLMs MLLMs Diffusion	Patch, Attention Decomposition Token Detection, Hard Negatives First-Token Logit Analysis Patch-Level Alignment Metric Token Alignment Penalizing Overconfidence Dynamic Token Penalization Pixel-Level Attribution Maps	Zero-Shot Image Segmentation Image-Text Matching Logit Analysis Cross-Modal Retrieval Hallucination Confidence Calibration Token Penalization Attention Visualization				
		Embed	ding-Level Interpretability					
Visual	Verma et al. [113] Shi et al. [143] Park et al. [222] Prasad et al. [223]	MLLMs MLLMs Diffusion Diffusion	Analyzing Visual Attributes Multiple Vision Encoders Visualizing Diffusion Process Tree of Diffusion	Attribute Analysis Encoder Analysis Diffusion Process Visualization Diffusion Interpretation				
Textual	Wolfe [224] Moayeri et al. [145]	CLIP CLIP	Contrastive Learning Embeddings Text-to-Concept Alignment	Embedding Analysis Concept Alignment				
Cross-Modal	Bhalla et al. [149] Frank et al. [150] Ramesh [155] Derby et al. [146] Chen et al. [147] Dominici et al. [148] Wang et al. [151] Parekh et al. [152] Lindström [225] Salin et al. [154] Crabbé et al. [226] Nguyen [165] Kwon et al. [227] Evirgen et al. [153]	CLIP CLIP CLIP MLLMs	Sparse Combinations of Concepts Exploring Structural Aspects Comparing Explainability Methods Sparse, Interpretable Vectors Grounded Representations Shared Concept Space Integrating Expert Knowledge Dictionary-Learning Framework Representation Probing Analyzing Fine-Tuning Effects SVD and Concept Encoding Multi-Task Learning Framework Asymmetric Reverse Process Explanation Methods	Concept Combination Structural Analysis Explainability Comparison Vector Interpretation Representation Learning Concept Space Analysis Knowledge Integration Concept Learning Probing Tasks Fine-Tuning Analysis Concept Encoding Multi-Task Learning Diffusion Process Analysis Model Explanation				

simplifies complex image representations into basic visual components, thereby elucidating the influence of individual tokens on model predictions. More recent advancements have centered on interpretability techniques specifically tailored to the unique self-attention structures in ViTs, with an emphasis on the interactions between image patches. For instance, Ma et al. [229] developed a method to visualize patch-wise interactions, highlighting how cross-patch correlations and attention distribution affect overall model performance. Extending these interpretability techniques, frameworks like ViT-NeT [230] and IA-ViT [231] introduced innovative visualization and training approaches. ViT-NeT utilizes a hierarchical tree structure with prototypes to organize and visualize attention layers, providing an insightful view of token interactions. Meanwhile, IA-ViT employs a joint training strategy for a feature extractor, predictor, and interpreter, ensuring that explanations remain consistent and faithful to the model's internal processes.

Token Efficiency and Redundancy. A significant line of research has examined the efficiency and redundancy of visual tokens within deep layers of vision-language models. DynamicViT [232] introduced a token sparsification method, dynamically pruning redundant tokens based on input, which enhances interpretability by focusing on the most informative

tokens. In multimodal settings, Zhang et al. [134] further investigated token redundancy in MLLMs, revealing that token contributions converge in the shallow layers and become redundant in the deeper layers, which has implications for model efficiency and interpretability. Building on token-level analysis, FastV [135] introduced a method to prune less relevant visual tokens in MLLMs, enhancing computational efficiency while preserving key interpretive insights. By concentrating on high-attention tokens, FastV highlights which visual elements the model prioritizes during decision-making, thereby clarifying the flow of visual information and enhancing the understanding of MLLMs. Additionally, vision token-specific analyses reveal further insights into semantic alignment between image and text in vision-language models. Gandelsman et al. [132] analyzed CLIP's image encoder by decomposing image representations into text-interpretable components, such as attention heads and image patches, uncovering specific roles for attention heads, including spatial localization and shape recognition. Similarly, Neo et al. [133] explored the interpretability of visual tokens in the LLaVA model, showing how object-specific information is gradually refined across layers for improved predictions. Yao et al. [137] focused on understanding the projector module in MLLMs, tracking how

semantic information flows from language tokens back to visual patches.

2) Visual-Textual Token: The integration of visual and textual modalities in machine learning has significantly advanced the interpretability of complex tasks such as activity recognition, visual question answering, and content moderation. Aligning visual elements with textual, multimodal interpretability methods provides a more comprehensive understanding of model behaviours and the decision-making process. This review discusses recent developments in this area, focusing on methodologies that enhance interpretability by leveraging visual-textual token alignment and related strategies.

Investigating the interpretability of MLLMs, VL-Match [138] emphasized interpretability through a generatordiscriminator structure. VL-Match operates by aligning tokens at a fine-grained level, utilizing negative sampling for instance-level alignment and ensuring token-level coherence between visual and textual representations. Zhao et al. [139] examined the logit distributions of initial tokens in MLLMs to reveal hidden knowledge within these models. Their findings indicate that analyzing these distributions can unveil inappropriate content generation, unanswerable questions, and other undesirable outputs, making the initial token analysis a useful tool for identifying and mitigating content generation issues. LexVLA [140] presented a patch-level interpretability metric that specifically evaluates the alignment between image patch features and category-specific text tokens, providing a fine-grained approach to interpretability by examining the coherence between visual patches and corresponding textual categories. Additionally, DAAM [206] proposed a novel method for interpreting large diffusion models like Stable Diffusion by generating pixel-level attribution maps using cross-attention scores, revealing how words in text prompts influence image generation, and analyzing syntactic and semantic phenomena affecting generation quality.

B. Embedding

Despite the extensive research on individual tokens, there has also been a focus on more coarse-grained analyses of multimodal embeddings and their latent spaces in MLLMs. Similarly, we categorize these studies into visual, textual, and cross-modal embeddings. Additionally, studies have examined how MLLMs understand linguistic knowledge and their ability to recognize text within images. As shown in figure 4, we illustrate three key methods: probing-based interpretation, attribution-based interpretation, and decomposition-based interpretation. More recently, some works have analyzed and improved the alignment and representational capacity of LLMs and MLLMs [89, 233, 234, 235, 236, 237]. The overview of embedding-level methods is summarized in Table II.

1) Visual Embedding: The interpretability of MLLMs has become a focal point for understanding how these models process and integrate visual information, a crucial aspect as these models scale in complexity and application scope. Foundational methods, such as layer-wise evaluation using linear classifiers [233], have been instrumental in clarifying the

progressive encoding of visual features across model layers, offering insights into the structural evolution of learned representations. Techniques like Integrated Gradients [238] provide a structured method for attributing model predictions to specific visual features, enhancing transparency by delineating the contribution of each feature to the output. Other interpretability approaches concentrate on mapping neural representations to human-understandable concepts. For instance, Network Dissection [239, 240] assigned semantic labels to individual units in convolutional networks, while Testing with Concept Activation Vectors (TCAV) [234] quantifies the impact of highlevel, user-defined concepts on predictions. In unsupervised settings, methods such as spatial masking [241] localized the influence of individual latent dimensions, capturing distinct, interpretable variations within visual data.

Expanding on interpretability challenges unique to MLLMs, recent research highlights the intricacies of textual and visual representation interactions. For instance, [113] discovered that domain-specific visual attributes within MLLMs are often represented within the LLMs rather than the cross-modal projection, underscoring the importance of understanding how LLMs encode visual information to improve interpretability. Moreover, shi et al. [143] examined the potential of incorporating multiple vision encoders within MLLMs, demonstrating that straightforward methods like concatenating visual tokens from diverse encoders can significantly boost both interpretability and model performance. Another area of interpretability research focuses on generative models, particularly diffusion models, where understanding dynamic processes is critical. Park et al. [222] visualized the diffusion process within generative models, showing how these models progressively build and refine semantic information by directing attention to relevant visual concepts and regions over successive time steps. Similarly, the Tree of Diffusion Life (TDL) Prasad et al. [223] visualized data evolution in diffusion models through an innovative embedding approach that preserves both semantic relationships and temporal dynamics, offering a more intuitive grasp of the generative process and rendering the complex evolution of model outputs interpretable over time.

2) Textual Embedding: In recent years, significant advances in understanding the internal structure of embeddings have greatly enhanced the interpretability of multimodal models. For instance, Hennigen et al. [242] propose a decomposable multivariate Gaussian probe for intrinsic analysis of text embeddings, uncovering that only a limited subset of neurons encodes core morphosyntactic features. This targeted approach improves interpretability by pinpointing how linguistic information is distributed across neural representations. Building on this, SVO-Probes [144] identified specific challenges in verb comprehension for multimodal image-language transformers, particularly in comparison to nouns, thus highlighting critical areas for refinement in model interpretability. Meanwhile, Wolfe et al. [224] demonstrate that CLIP embeddings achieve reduced anisotropy relative to those of GPT-2, enhancing semantic coherence and interoperability across word and sentence embeddings. In addition, Moayeri et al. [145] introduced an innovative "text-to-concept" alignment method that maps features from pre-trained models into CLIP's embedding

space, enabling more direct interpretation of model features through aligned text embeddings.

3) Cross-modal Embedding: To tackle the challenge of interpretability in MLLMs, researchers have developed various approaches that focus on creating cross-modal embeddings that align with human cognition. Joint Non-Negative Sparse Embedding (JNNSE) [146] introduced an early approach, generating sparse, interpretable vectors that capture multimodal semantic information by aligning with human behaviour and neuroimaging data. Building on this, STAIR [147] grounded image and text representations in human-understandable tokens, providing not only improved model explainability but also enhanced retrieval performance, which underscores the dual benefit of interpretability-focused embeddings. Expanding the interpretability of multimodal representations, SHARCS (Shared Concept Space) [148] unified interpretable concepts from diverse modalities into a shared space, thus creating a versatile framework for situations involving missing modalities and enhancing the general applicability of multimodal learning.

Further efforts to refine cross-modal embedding interpretability include SpLiCE [149], which transforms CLIP embeddings into sparse, interpretable combinations of humanfriendly concepts. By allowing concept-level analysis without explicit concept labels, SpLiCE preserves interpretability and downstream performance, enriching both qualitative and quantitative understanding of multimodal models. Additionally, Gandelsman et al. [132] and Frank et al. [150] have explored structural aspects of models like CLIP, revealing insights into information asymmetry and the role of specific attention heads in processing text and visual inputs. Lastly, FreeBind [151] introduced "space bonds" to integrate expert knowledge across multimodal spaces while maintaining unified interpretive coherence, and Parekh et al. [152] proposed a dictionary-learning framework that further elucidates multimodal concept extraction grounded in visual and textual representations. Together, these advancements reflect a continuous push towards more interpretable and balanced multimodal models.

Difussion Interpretability. Recent advancements in interpretability techniques for MLLMs have enabled more intuitive and controllable generative processes. The Asymmetric Reverse Process (Asyrp) [227] introduced a semantic latent space (h-space) in pretrained diffusion models, facilitating interpretable and precise image editing across different timesteps. Complementing these advances, Evirgen et al. [153] proposed novel explanation methods specifically for text-to-image systems, allowing users to better understand and utilize these models.

Probing explainability. Understanding how cross-modal embeddings encode and transfer information is essential for achieving deeper interpretability. Lindström et al. [225] provided valuable insights by examining visual-semantic embeddings and revealing how these embeddings capture complementary information from text and image modalities, particularly in tasks involving synonyms and polysemy. Salin et al. [154] further explored this area by employing probing tasks to analyze how fine-tuning affects the interpretability of Vision-Language model embeddings. Expanding on these

perspectives, Ramesh et al. [155] compared explainability frameworks—Label Attribution and Optimal Transport—to examine attention interactions in multimodal transformers like CLIP and ViLBERT, addressing the need for unified explainability across different models. Crabbé et al. [226] contributed to this field by using Singular Value Decomposition (SVD) and concept encoding to investigate privileged directions and polysemantic features within cross-modal embeddings, showing how these components encode complex information across multiple concepts.

Graph-Based Interpretability. Beyond embeddings, hierarchical and graph-based methods have been explored to enhance interpretability in multimodal models. LaPool [243] introduced an interpretable hierarchical graph pooling method that utilizes both node features and graph structure. This method significantly improves molecular representation in Graph Neural Networks (GNNs) and enhances interpretability in molecular tasks such as drug design, demonstrating the applicability of interpretable models in specialized domains.

C. Neuron

Neurons in pre-trained models have been a key focus for interpretability research, with studies in computer vision (CV) and natural language processing (NLP) analyzing their functions and semantic roles [91, 265]. In multimodal models, efforts extend to exploring neurons tied to specific concepts or domains. This section provides an overview of these studies, detailed shown in Table III, covering both detailed and broader analyses in multimodal and traditional domains.

1) Individual Units: It has been widely explored how to associate individual neurons in deep neural networks with specific concepts or functions.

Backgrounds. Upon the proposal of the transformer, Dai et al. [247] introduced the concept of "knowledge neurons" in transformer models, referring to neurons that activate when expressing factual information. Their work demonstrated that deactivating these knowledge neurons significantly impairs the accuracy of the corresponding facts stored within the transformer model. Meng et al. [249] further explored knowledge neurons in GPT, discovering that factual associations within GPT can be directly modified by locating and editing specific neurons in the MLP layers. This work provided deeper insights into how knowledge is structured within language models. Chen et al. [254] expanded on this research by analyzing knowledge neurons in multilingual large language models. They proposed a gradient-based detection method, AMIG, to identify neurons storing specific knowledge. Chen et al. categorized these knowledge neurons into two types: language-independent neurons and degenerate neurons, which were determined by whether the stored knowledge was shared across languages or specific to one language input. Qian et al. [93] identified that fairness and privacy-related neurons are coupled in LLMs. A simple and effective decoupled operation mitigated the fairness-privacy conflicts.

In the vision domain, Bau et al. [239] proposed the "network dissection" task, designed to identify and label the concepts captured by neurons in CNNs. Manually assigning

TABLE III

Overview of Neuron-Level Methods. The papers are sorted by year, and annotated with their authors, research perspectives, models, and interpretation forms/functions of neurons.

Perspective	Method	Venue	Models	Interpretation Form / Function
	Network Dissection [239] GAN Dissection[244]	CVPR'17 ICLR'18	CNN GAN	Concept Concept
Individual Units	Bau et al. [245] MILAN[246] Dai et al. [247] Goh et al. [156] CLIP-Dissect[248] ROME[249] HINT[250] Rosetta Neurons[251] Bills et al. [252] Cones[253] Chen et al. [254] Gao et al. [255] Gandelsman et al. [157] DEAN [93]	PANS'20 ICLR'22 ACL'21 Distill'21 ICLR'22 NeurIPS'22 CVPR'22 ICCV'23 Openaipublic'23 ICML'23 AAAI'23 arXiv'24 arXiv'24	GAN, CNN GAN, ViT, CNN BERT CLIP CNN GPT CNN CNN, CLIP, DINO GPT Diffusion m-BERT, m-GPT GPT-4 CLIP LLMS	Concept Natural Language Factual Knowledge Concept Concept Factual Knowledge Hierarchical Concept Concept Natural Language Concept Factual Knowledge Concept Concept Concept Concept Concept Concept Concept Concept
Specialization Group	NeMo [256] Schubert et al. [257] Curve Detectors[258] Zoom In [259] Mueller et al. [260] Schwettmann et al. [261] Pan et al. [158] Tianyi Tang[262] Kojima et al. [263] Gurnee et al. [264] MMNeuron [159] MINER[160]	Distill'20 Distill'20 Distill'20 CoNLL'22 ICCV'23 ACL'24 ACL'24 NAACL'24 TMLR'24 EMNLP'24 arXiv'24	CNN CNN CNN m-BERT, XGLM MLLMs MLLMs LLMs LLMs LLMs GPT MLLMs MLLMs MLLMs	Individual Samples High-Low Frequency Detection Curve Detection Meaningful Circuit Multilingual Multimodal Sensing Multimodal Sensing Multilingual Multilingual Multilingual Universal Pattern Vision Domain Sensing Modality Sensing

language-based labels to each neuron based on activation patterns provided a foundation for understanding the role of individual neurons, although the method was labor-intensive. Network dissection has also been applied to interpret neurons in GANs [244], with further refinements in subsequent studies by Bau et al. [245]. Furthermore, MILAN [246] introduced a mutual-information-guided linguistic annotation method that automates neuron annotation by maximizing pointwise mutual information between neuron activations and image regions, offering fine-grained, natural language descriptions of neurons. Oikarinen et al. [248] moved forward proposing an alternative for generating concept descriptions for individual visual neurons by comparing their activation vectors with a text matrix in CLIP. Wang et al. [250] extended the network dissection approach to construct bidirectional hierarchical connections between neurons and concepts, which they validated through weakly-supervised object localization. Dravid et al. [251] also explored "rosetta" neurons, referring to neurons that universally exist across different visual networks and capture similar features. More recently, Bills et al. [252] and Gao et al. [255] utilized sparse autoencoders to interpret neurons in LLMs, providing new perspectives on neuron functionality.

Individual Neurons. In the multimodal domain, there has been notable work on concept neurons in multimodal networks. Goh et al. [156] introduced the concept of multimodal neurons in CLIP, which respond to concepts present in both real and textual images. Schwettmann et al. Gandelsman et al. [157] decomposed CLIP representations to analyze the indirect influence of individual neurons. By projecting decomposed embeddings into vocabulary space, they reveal the secondary semantic effects of neurons in CLIP. As for

multimodal generative AI, Liu et al. [253] introduced "Cones", a method to detect and edit concept neurons in diffusion models. By enabling selective activation or concatenation of concept neuron clusters, they managed to manipulate specific subjects in the generated images. Hintersdorf et al. [256] developed NEMO, a method to pinpoint and manage memorization neurons in cross-attention layers of diffusion models.

2) Specialization Group: While some researchers focus on analyzing the function of individual neurons, there is also a perspective that considers groups of neurons as collectively responsible for specific tasks.

Backgrounds. In visual networks, Cammarata et al. [258] discovered neurons specialized in detecting curves within images. Schubert et al. [257] extended these findings, identifying visual neurons responsible for detecting high- and lowfrequency features. Olah et al. [259] further confirmed that features and circuits similar to those in [257, 258] are universal across visual networks, providing insights into how these networks interpret images. There is also relevant research in language models. For example, Gurnee et al. [264] discussed universal neurons in GPT-2, noting that these neurons show consistent activation patterns across various model instances. These universal neurons are essential for adjusting prediction uncertainty and managing attention for specific tokens. Mueller et al. [260] used a causal-based method to examine neurons responsible for syntactic agreement across different languages, finding that these neurons show greater overlap in autoregressive models compared to masked language models. Tang et al. [262] introduced the concept of languagespecific neurons (LSNs) and demonstrated that activating or deactivating these LSNs can influence the output language

of multilingual large language models (XLLMs). Kojima et al. [263] found that LSNs are primarily located in the top and bottom layers of XLLMs and exhibit minimal overlap across languages.

Multimodal Neuron Groups. Research on multimodal models, however, often emphasizes neurons that bridge text and image features. [261] expanded this concept, detecting multimodal neurons even in the text-only language component of MLLMs. Similarly, Pan et al. [158] identified multimodal neurons in pre-trained transformers, assessing their sensitivity, specificity, and causal effects. Huo et al. [159] proposed the Domain Activation Probability Entropy (DAPE) score to identify domain-specific neurons and evaluated their impact on VQA tasks. Recently, Huang et al. [160] extend this concept to modality-specific neurons and propose an importance scorebased method to detect neurons specific to different modalities.

D. Layer

Classic deep neural networks, particularly transformer architectures, consist of stacked hidden layers connected by skip connections, such as decoder-based (e.g., GPT), encoder-based (e.g., BERT), or encoder-decoder models (e.g., T5 [266]). These layers can be further broken into components like MLP, multi-head attention (MHA), and layer normalization. This section Section IV-C reviews the literature on these layer-level elements from two perspectives: first, the function of specific layers (e.g., attention heads, MLP layers) and their contribution to model decisions; second, the overall decision-making process across layers, focusing on representation transformation. The methods summarized are presented in Table IV.

1) Individual Components: Numerous studies have attempted to interpret the roles of different layers in deep neural networks across domains such as CV, NLP, and multimodal applications.

Backgrounds. Mahendran et al. [267] explored the invertibility of hidden states in CNNs, showing that photographically accurate information about images is retained across several layers. Dosovitskiy et al. [268] inverted CNNs hidden states using an up-convolutional neural network, finding that colors and rough contours of input images could be reconstructed from activations in higher network layers, even from predicted class probabilities.

With the rise of transformers, several studies have examined the functions of attention heads and MLP layers within these models. Cordonnier et al. [269] argued that attention layers can effectively perform convolution and often learn to do so in practice. They also proved that a multi-head self-attention layer with a sufficient number of heads is at least as expressive as any convolutional layer. Sukhbaatar et al. [270] proposed augmenting the self-attention layer with a persistent memory vector, suggesting that these memory vectors could replace the transformer's MLP layers. Geva et al. [271] demonstrated that feed-forward layers in transformer-based language models act as key-value memories, with each key linked to textual patterns in training examples, while each value influences output vocabulary distributions. Michel et al. [272] conducted ablation studies on transformer attention heads, showing that

many heads could be removed during testing without substantial performance loss. Voita et al. [273] analyzed individual attention heads, finding that only a few critical heads have interpretable functions, such as attending to adjacent words and tracking specific syntactic relationships.

In NLP, the layers of pre-trained language models have been extensively analyzed. Clark et al. [274] examined BERT's attention heads, observing patterns such as attention to delimiter tokens, specific positional offsets, and broad sentencewide attention, often with similar behaviors among heads within the same layer. Kovaleva et al. [275] explored the information encoded by BERT's individual heads, revealing a limited set of attention patterns repeated across different heads. Htut et al. [276] investigated BERT and RoBERTa's ability to implicitly capture syntactic dependencies, finding some specialized attention heads for specific dependency types, although no generalist head was identified for holistic parsing. Ren et al. [94] analyzed the attention heads to explain LLMs' in-context learning.

Multimodal Components. Cao et al. [161] analyzed multimodal pre-training through probing tasks across various model architectures, identifying a subset of attention heads optimized for cross-modal interactions and effectively encoding linguistic knowledge. Gandelsman et al. [132] decomposed CLIP's image representation as a sum across individual image patches, layers, and attention heads, using CLIP's text representation to interpret these components. They found that each attention head's role could be characterized through text representations spanning its output space, concluding that MLPs in CLIP have minimal direct impact. Quantmeyer et al. [162] applied interpretability methods from language models, such as causal tracing, to multimodal models, isolating parts of CLIP's text encoder that handle negation and analyzing the roles of attention heads in this task. Si et al. [277] examined U-Net's contributions to the denoising process, revealing that its backbone primarily aids in denoising, while skip connections introduce high-frequency features into the decoder.

2) Decision-Making Workflow: Beyond analyzing the functions of different layers in neural networks, it is equally crucial to interpret the decision-making process of models across layers, from shallow to deep. This involves uncovering how pre-trained models perceive inputs and make decisions, providing deeper insights into their understanding and reasoning mechanisms.

Backgrounds. Understanding how learned representations transform within deep neural networks is another vital challenge in interpretability. Kowal et al. [278] proposed the "Visual Concept Connectome" (VCC) method, which identifies human-interpretable concepts and inter-layer connections in visual networks, quantifying the contributions of these concepts without needing labeled datasets. In NLP, Van Aken et al. [279] applied general and QA-specific probing tasks to reveal information stored in each representation layer, showing that transformations in BERT follow phases related to traditional pipeline tasks. Tenney et al. [280] discovered that BERT represents the steps of the traditional NLP pipeline in an interpretable, localized manner.

Workflow of Multimodal Models. Recent work has ex-

TABLE IV

Overview of Layer-Level Methods. The table summarizes key research contributions by perspectives (components or workflow), models, analysis topics, and application fields.

Perspective	Method	Venue	Models	Topics	Field
	Mahendran et al. [267]	CVPR'14	CNN	Convolutional Layer	CV
	Dosovitskiy et al. [268]	CVPR'15	CNN	Convolutional Layer	CV
	Cordonnier et al. [269]	ICLR'19	CNN, Transformer	Convolutional Layer, Self-Attention	CV
	Sukhbaatar et al. [270]	arXiv'19	Transformer	Self-Attention	NLP
	Geva et al. [271]	EMNLP'20	Transformer	FFN	NLP
	Michel et al. [272]	NeurIPS'19	Transformer	Multi-Head Attention	NLP
	Voita et al. [273]	ACL'19	Transformer	Multi-Head Self-Attention	NLP
Components	Clark et al. [274]	BlackboxNLP'19	BERT	Attention	NLP
	Kovaleva et al. [275]	EMNLP'19	BERT	Attention	NLP
	Htut et al. [276]	arXiv'19	BERT	Attention	NLP
	Ren et al. [94]	ACL'24	LLMs	Attention	NLP
	Cao et al. [161]	ECCV'20	Vilbert, Lxmert	Attention	MM
	Gandelsman et al. [132]	ICLR'23	CLIP	FFN, Attention	MM
	Quantmeyer et al. [162]	ALVR'24	CLIP	Attention	MM
	FreeU [277]	CVPR'23	Diffusion	U-Net	MM
	VCC [278]	CVPR'24	CNN	Inner Connection	CV
	Van Aken et al. [279]	CIKM'19	BERT	Representation Transformation	NLP
	Tenney et al. [280]	ACL'19	BERT	Pipeline	NLP
	Wolfe et al. [224]	ACL'22	GPT, CLIP	Representation Transformation	MM
Workflow	Xu et al. [163]	ICCV'23	Dual-stream VLM	Modality Alignment	MM
	Palit et al. [281]	ICCV'23	BLIP	Causal Relevance	MM
	MMNeuron [159]	EMNLP'24	MLLMs	Modality Alignment	MM
	Zhang et al. [134]	arXiv'24	MLLMs	Information Flow	MM
	Prasad et al. [282]	arXiv'23	Diffusion	U-Net	MM

plored the decision-making workflow of multimodal models. Xu et al. [163] combined convolutional and attention mechanisms with an adapter module, finding that placing this module in shallower layers enhanced the vision-language model performance more effectively than placing it in top layers. Wolfe et al. [224] observed that CLIP's sentence embeddings became progressively less self-similar across layers, indicating that contrastive pre-training objectives drive the formation of finegrained semantic sentence representations. Palit et al. [281] adopt a causal tracing tool for mechanistic interpretability in vision-language models, elucidating the causal role of representations in later layers during image-conditioned text generation, offering insights into the underlying mechanisms beyond simple input-output correlations. Huo et al. [159] proposed a three-stage hypothesis for how multimodal language models process visual embeddings, which they verified using the logit lens method. Zhang et al. [134] used LLaVA-CAM and attention scores to visualize information flow in reasoning processes across layers in MLLMs, finding that information converges in shallow layers and diverges in deep layers. Tao et al. [164] noted that intermediate layers of models encode more global semantic information, making them better suited for visual-language entailment tasks than top layers. Prasad et al. [282] evaluated time-step and U-Net component impacts on Stable Diffusion's final output, showing that lower layers primarily contribute to semantic alterations, while higher layers focus on denoising, especially after the initial generation phase. Nguyen et al. [165] propose a multi-task learning framework that leverages Dense Coattention layers to jointly learn hierarchical vision-language representations. By using task-specific decoders and attention map visualizations, their approach enhances interpretability

through explicit modeling of cross-modal interactions.

E. Architecture

In Section IV-C and Section IV-D, we examined interpretability at the fine-grained neuron and layer levels. However, some studies explore the interpretability of MLLMs at a more coarse-grained architecture level. We will provide a detailed definition of the architecture level and subsequently introduce and categorize these related works. Unlike previous methods that focus on the specific components of MLLMs, this subsection will treat the MLLMs model as a whole. We also aim to explore whether we can explain the decision-making process of MLLMs in this manner. We categorize these works into two groups:

- Architecture Analysis: (Section IV-E1) This approach
 is independent of any specific model structure or internal
 mechanism, such as attention operations in transformers
 or convolutional units in CNNs, enabling us to apply it
 for explanations of any MLLMs.
 - Feature Attribution: We introduce classic explanation methods that attribute importance scores to features, forming the basis for subsequent approaches.
 - Uni-modal Explanation: Here, we include methods that provide single-modality explanations (mostly for the image modality), offering a comprehensive global perspective.
 - Multi-modal Explanation: There are also methods that provide multi-modal explanations (e.g., combining image and text modalities), offering users a more comprehensive perspective.
 - Interactive Explanation: Methods that provide explanations based on human commands or preferences

are grouped here under the category of *interactive* explanation.

- Others: Architecture-level model analysis methods, which offer insights into model characteristics through model comparisons, are also included here for reference.
- Architecture Design: (Section IV-E2) These methods enhance model explainability by modifying the architecture with highly interpretable modules. Unlike architecture analysis, they do not generate explicit explanation outputs but focus on specific model types, leveraging unique structures or parameters to explore internal mechanisms and produce detailed insights.
 - Surrogate Model: A simpler model, such as a linear model or decision tree, is used to approximate the performance of a complex model.
 - Concept-based: This approach enables the model to learn human-understandable concepts, which are then used to generate predictions.
 - Causal-based: These methods incorporate concepts from causal learning into architecture design, such as causal reasoning or causal frameworks.
 - Others: We include here methods related to other modules in the architecture that cannot be categorized into the classes mentioned above.

We will then provide a detailed explanation of the methods within these categories.

1) Architecture Analysis: Unlike the analysis of neurons, layers, or modules mentioned earlier, this section introduces works that utilize the entire model architecture to provide explanations. As is shown in Figure 5, we categorize these methods based on an intuitive perspective—the type of explanation output: uni-modal explanations, multi-modal explanations, and interactive explanations. The methods summarized are presented in Table V.

Feature Attribution. These methods, primarily proposed in earlier years, were used as explanation techniques for CNNs or other models. Although they are not directly related to MLLMs, we include them here as background to provide readers with a more comprehensive understanding of the timeline in XAI development. We also hope these methods can inspire new explanation techniques for MLLMs.

[283, 284, 285] explained the decision-making process of models by assigning contribution values to sparse features. LIME [283] trained simple linear models in local subspaces of the input space, approximating the behavior of complex models in those regions. Experiments show that LIME is effective for both expert and non-expert users, enhancing interpretability across various tasks, such as model comparison, trust assessment, improving unreliable models, and gaining insights into predictions. DeepLIFT [284] propagated the contributions of each neuron in the network back to the input features to decompose the predicted output. It compares each neuron's activation value with its "reference activation value" to allocate contribution scores based on the differences. SHAP [285] unified six existing methods for explaining model predictions (including LIME and DeepLIFT) by introducing the concept

of "additive feature attribution," assigning contribution values to each feature to elucidate predictions for individual samples.

Uni-modal Explanation. Building on Class Activation Mapping (CAM) introduced in [286], several follow-up methods [287, 288, 289, 290], collectively known as the CAM Family, identify critical regions in input images and display them as class activation maps (heatmaps). CAM [286] originally demonstrated object localization in CNNs without bounding box annotations by highlighting important areas. Grad-CAM [287], a CAM variant, extends this to multiple CNNs architectures without modification. U-CAM [288] targets VQA tasks, generating visual attention maps through gradient-based estimates. Score-CAM [289] improved on CAM by using forward scores to compute activation weights, making it gradientindependent and effective in recognition and localization. Lastly, gScore-CAM [290] enhances CLIP interpretability, using gradient sampling groups to produce reliable attention maps while reducing complexity and avoiding distractions from text in images.

[291, 294] identify the most important image regions for the decision-making process by optimizing an objective function, typically aiming to minimize classification accuracy, and then use heatmaps or saliency maps to highlight significant areas of the image. I-GOS [294] determines the most important regions in an image by minimizing classification accuracy and employing integrated gradients instead of traditional gradients to calculate the descent direction. The paper [291] mentions two visualization techniques for CNNs: (1) using activation maximization to illustrate the category concepts captured by the CNN, and (2) calculating saliency maps for specific images and categories through backpropagated gradients. [292, 293, 297] are based on relevance propagation methods that define the correlation between features and classification outcomes and reverse this correlation back to the input image through various propagation strategies. [292, 297] discusses two strategies: (1) Taylor decomposition, which linearly approximates the classification function by performing a Taylor expansion around a neutral data point (one that does not belong to any category) to identify each pixel's contribution; (2) Layer-wise Relevance Propagation (LRP), which propagates the classification relevance from each layer to the previous one. [293] extends Deep Taylor Decomposition (DTD) to multilayer neural networks, generating heatmaps to assess the importance of individual pixels in classification.

Multi-modal Explanation. [166, 167, 168, 169, 295] offer multimodal interpretability, such as image and text explanations, providing more detailed and systematic insights compared to single-modal methods. [295] introduces a general transformer explanation framework capable of interpreting (i) self-attention architectures, (ii) hybrid self-attention and cross-attention models, and (iii) encoder-decoder attention designs. DIME [166] enhances fine-grained interpretability by decoupling information flows of different modalities, clarifying how each modality contributes to the model's decisions. CCM [167] improves answer explanations for VQA models with a collaborative correlation module that strengthens the link between answers and explanations and enhances the quality of visual and textual outputs. [168] integrates textual and visual

TABLE V

Overview of Architecture Analysis Methods. This table categorizes analysis methods into feature attribution, uni-modal, multi-modal, and interactive explanations, with details in Section IV-E1. It includes key highlights, architectures, tasks, and a comparison of explanation types and control signals.

	Method	Venue	Key Points	Explanation Type	Control Signal	Architecture	Task
Feature	LIME[283]	KDD'16	Local Space Decision Analysis			Any Model	Classification Regression
Attribution	DeepLIFT[284]	ICML'17	Reference Activation Importance Backpropagation	-	-	Vision Model	Classification
	SHAP[285]	NIPS'17	Unified Framework Additive Feature Attribution	-	-	Vision Model	Classification
Uni-modal	CAM[286]	CVPR'16	Class Activation Mapping Global Average Pooling	Saliency Map	-	Vision Model	Classification Localization
Explanation (CAM family)	Grad-CAM[287]	ICCV'17	Gradient-based Without Altering of Network	Saliency Map	-	Vision Model	Classification Image Captioning VQA
	U-CAM[288]	ICCV'19	Estimate Uncertainty	Saliency Map	-	Vision Model	VQA
	Score-CAM[289]	CVPR-W'20	Without Gradient	Saliency Map	-	Vision model	Image Recognition Localization
	gScore-CAM[290]	ACCV'22	Gradient-based	Saliency Map	-	CLIP	Object Detection
Uni-modal	Simonyan et al. [291]	ICLR-W'14	Activation Maximization Attribution	Saliency Map Synthetic Image	-	CNN	Classification
Explanation (Others)	Binder et al. [292]	ICANN'16	LRP Taylor Expansion	Saliency Map	-	Vision Model	Classification
	Montavon et al. [293]	PR'17	Deep Taylor Decomposition	Saliency Map	-	Vision Model	Classification
	I-GOS[294]	AAAI'20	Integrated Gradients Mask Optimization	Saliency Map	-	DNN	Classification
Multi-modal Explanation	Wu et al. [168]	ACL-W'19	Faithful Explanation	Segmentation Mask Text Explanation	-	VLM	VQA
	CCM[167]	WACV'20	Robust Explanation	Saliency Map Text Explanation	-	VLM	VQA
	Chefer et al. [295]	ICCV'21	Any Transformer Architecture Relevance Score	Saliency Map Text Relevancy	-	Transformer	Classification
	DIME[166]	AIES'22	Local Explanation Disentangling	Image Localization Text Distribution	-	MLP MDETR LXMERT	Classification Visual Reasoning
	VALE[169]	arXiv'24	SHAP + SAM + VLM	Segmentation Mask Text Explanation	-	Vision Model	Classification
Interactive Explanation	Olah et al. [296]	Distill'18	Multiple Interaction Modes	Saliency Map Synthetic Image Text Distribution	Select Pixel	GoogLeNet	Classification
	Diffusion Explainer[171]	arXiv'23	Interactive	Generated image	Prompt	Diffusion Model	Text to Image
	MAIA[118]	ICML'24	Use Tools Neuron-level Explanation	Image Localization Text Explanation	Prompt	VLM	Vision Tasks
	LVLM-Interpret[170]	CVPR-W'24	Interactive Attention Mechanisms	Saliency Map Text Distribution	Select Token	VLM	VQA

explanations in a VQA system, presenting answers in a humanlike style for better clarity and comprehension. VALE [169] combines SHAP for identifying influential image regions with SAM and pre-trained vision-language models (VLMs) to generate visual (e.g., heatmaps) and natural language explanations, offering a comprehensive view of the model's reasoning.

Interactive Explanation. The field of explainable AI has recently grappled with the question of whether the decision-making process of deep neural networks (DNNs) can be interpreted in terms of a set of sparse symbolic concepts. A body of work has explored different types of interactions between a DNN's input variables as a means of interpreting its inner workings. Sundararajan et al. [298], Janizek et al. [299], and Tsai et al. [300] have each proposed distinct approaches to modeling these input-level interactions. Building on this, Ren et al. [301] utilized the Harsanyi dividend to represent the AND-type interactions encoded by DNNs. Interestingly, their experimental findings suggest that DNNs tend to rely

on a sparse set of such interactions between input variables. Further advancing this line of inquiry, Li et al. [302] revealed that low-order interactions exhibit higher transferability across diverse input samples in discriminative neural networks. Complementing this, Ren et al. [303] formally derived the common conditions under which the sparsity of interactions can be guaranteed. Additionally, Ren et al. [304] introduced a method to learn optimal masked states of input variables based on their interactions, mitigating the bias introduced by sub-optimal masking in Shapley value-based interpretations. Taking a broader view, Chen et al. [305] extracted common interaction patterns shared across different neural network architectures, suggesting that such generalizable interactions may underpin the networks' inference mechanisms. Moreover, Cheng et al. [306] proposed an approach to extract interactions from a DNN's intermediate layers, shedding light on how these inference patterns are gradually learned and forgotten during the forward propagation process. GANSpace [307]

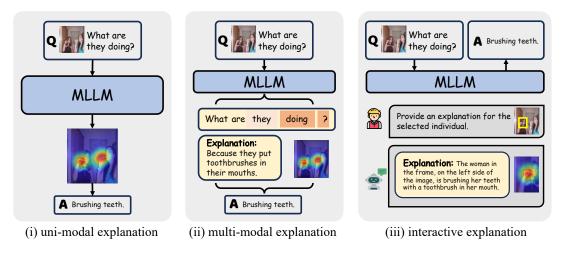


Fig. 5. Architecture Analysis. We classify architecture analysis methods into three types: uni-modal, multi-modal, and interactive explanations, based on explanation modalities and control signal acceptance.

employed principal component analysis (PCA) to uncover the key directions within the latent space. By selectively perturbing the layers along these primary axes, they achieved a high degree of explainability and control over the generated images.

The Harsanyi interaction theory [308] offers a compelling perspective on the representational capabilities of neural networks, providing insights into their behavior and learning processes. This can be detailed as follows. Wang et al. [309] established and mathematically verified an inverse relationship between the adversarial transferability of deep neural networks (DNNs) and the interactions present within adversarial perturbations. Ren et al. [310] highlighted that adversarial attacks predominantly target higher-order interactions rather than lower-order ones. Similarly, Zhou et al. [311] demonstrated that lower-order interactions exhibit superior generalization properties compared to their higher-order counterparts. Liu et al. [312] provided an explanation for the observation that DNNs are more adept at learning lower-order interactions than higher-order ones. Deng et al. [313] identified a surprising bottleneck: neural networks often fail to encode middle-order bivariate interactions effectively. Ren et al. [314] showed that Bayesian neural networks (BNNs) are less likely than standard neural networks to capture complex Harsanyi interactions. Additionally, Ren et al. [315] and Zhang et al. [316] uncovered a two-phase learning dynamic in neural networks' interaction acquisition, a phenomenon consistently observed across various architectures and tasks. Finally, Deng et al. [317] unified a range of classical attribution methods by proving that their underlying mechanisms could be reformulated as distinct ways of redistributing interaction effects among input variables.

Some explainability methods support interactive explanations, offering flexible, fine-grained analyses based on user preferences, such as focusing on specific image areas or neurons in MLLMs. These systems integrate various modalities, like text, images, and charts, to create comprehensive explanation frameworks. Their flexibility and depth provide users with broader insights, aiding informed decision-making in complex scenarios. [118, 170, 296] proposed the use of

comprehensive explanation systems or agents to provide multimodal insights into model behavior. [118, 296] combined multiple explainability tools to enhance the understanding of complex neural networks. Specifically, [296] unified various explainability techniques into a coherent syntax and created richer, more effective user interfaces. These interfaces, especially in visual tasks, help users better grasp the internal workings of neural networks. [118] introduced MAIA, which integrates and automates a series of explainability tools. MAIA addresses two key challenges: (1) reducing sensitivity to spurious features and (2) automatically detecting potentially misclassified inputs, offering deeper insights into complex neural models. LVLM-Interpret [170] focused on identifying the critical image patches influencing model outputs. It proposes a novel interactive application that enhances the explainability of these patches, helping users understand the internal mechanics of LVLMs. Together, these works emphasize the importance of combining multiple explainability tools and user interaction to achieve more comprehensive and accessible model explanations. Diffusion Explainer [171] is an interactive visualization tool for diffusion, designed to explain how stable diffusion transforms text prompts into images. By comparing the image generation results of different text prompts, users can identify how changes in keywords impact the generated images.

Others. Additionally, some studies analyze model properties from an architectural perspective. Tran et al.[318] compared recurrent (RNN) and non-recurrent (Transformer) structures in modeling hierarchical information, showing that recurrent structures are advantageous for capturing hierarchy and offering insights for interpretability research. Yang et al.[172] and Ramesh et al.[155] focus on analyzing MLLMs: Yang et al.[172] propose the "Law of Vision Representation," revealing a strong link between cross-modal alignment, vision consistency, and model performance, while Ramesh et al. [155] examined various interpretability methods (e.g., attention weights, gradient-based approaches), evaluating their strengths and limitations across multimodal tasks and providing recommendations for improvement.

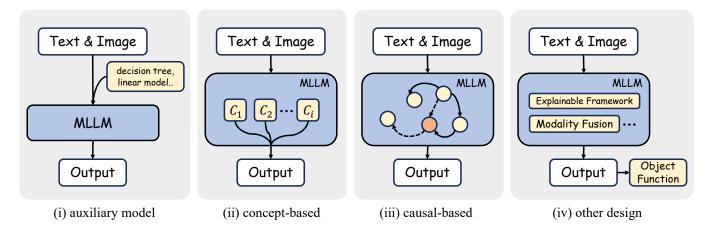


Fig. 6. Architecture Design. This category focuses on modifying modules to improve explainability without generating explicit explanations. Methods include auxiliary models, concept-based, causal-based, and other approaches.

2) Architecture Design: As is shown in Figure 6, this class of methods focuses on designing specific modules within the model's architecture to enhance its inherent interpretability. Many approaches leverage simple yet interpretable surrogate models, such as decision trees or linear models, integrating them into the architecture to improve explainability. Some methods first predict human-understandable concepts and then use these concepts to generate predictions, making the results easier to interpret. Additionally, numerous works build architectures based on causal frameworks to embed explainability. Methods that do not fit into the above categories are grouped under the other designs category. The methods summarized are presented in Table VI.

Surrogate Model. A common approach is to use a Surrogate Model to serve as a stand-in for complex models during the explanation or decision-making process. The chosen surrogate model can be a decision tree or a simple linear model. These simpler models offer greater transparency in their decision-making processes and can effectively approximate the behavior of complex models, thereby retaining a degree of the high accuracy characteristic of deep neural networks. This method enhances the interpretability of the model, allowing users to better understand its decision mechanisms. Liu et al.[320] and Wan et al.[173] propose using decision trees to approximate the behavior of complex models, effectively balancing interpretability and high accuracy by leveraging the strengths of both neural networks and decision trees. Liu et al.[320] transfer the knowledge of deep neural networks to decision trees through knowledge distillation. NBDT by Wan et al.[173] employs differentiable decision sequences and an alternative loss function to replace the final linear layer of the neural network, encouraging the model to learn higherlevel concepts and reducing reliance on uncertain decisions. Wong et al. [321] utilize elastic net regularization to train a sparse linear decision layer on the deep features of pre-trained deep networks, allowing for model behavior debugging by examining less important features and their linear coefficients.

Concept-based. Koh et al.[322] and Yüksekgönül et al.[323] enhanced interpretability by enabling models to predict human-understandable concepts. CBM [322] employs

interpretable concepts to predict final outputs, applicable to any network architecture, by simply adjusting the number of neurons in a given layer to match the number of concepts while constraining the layer's output with a loss function. However, CBM has two main drawbacks: (1) it requires dense concept annotations and (2) it may reduce the model's accuracy. PCBM [323] improves upon CBM by (1) allowing concept transfer from other datasets or through multimodal models without needing dense annotations, and (2) incorporating SVM to introduce interpretability while maintaining model performance, addressing both of CBM's limitations. LaBo [174], a languageguided concept bottleneck model (CBM) approach, uses GPT-3 to automatically generate interpretable bottleneck concepts aligned with visual data through CLIP, achieving performance comparable to or better than black box models, especially in low-data settings, while maintaining interpretability.

Causal-based. Some works have introduced causal learning to enhance model interpretability: Li et al. [325] proposes a causality-based debiasing framework that guides the design and selection of debiasing prompts using causal insights from the training corpus and LLMs inference. [175, 176, 324, 326] present methods for multimodal tasks, with Chen et al. [324] addressing the challenges of extensive data annotation and limited causal reasoning in video QA by introducing the LLCP framework, which analyzes the spatial-temporal dynamics of objects in events. TRACE [175] presented a causal event modeling framework that represents videos as event sequences, leveraging prior temporal information, video inputs, and textual instructions to predict current events. MGCE [176] utilized multimodal causal embedding learning networks to enhance the learning of high-quality causal embeddings at both structural and feature levels. Liu et al. [326] presented a unified causal model specifically designed for multimodal data, showcasing the advantages of multimodal contrastive representation learning in identifying latent coupled variables.

Others. Before the emergence of MLLMs, several works focused on injecting interpretability into module design: Cognitive Attention Network (CAN) [319] was introduced to address the Visual Commonsense Reasoning (VCR) task. CAN comprises two key modules: (1) Image-text fusion module:

TABLE VI

Overview of Architecture Design Methods. This table categorizes design methods into surrogate, concept-based, causal-based, and others (details in Section IV-E2). It includes publication venues, highlights, architectures, tasks, and √indicators for causal or concept learning.

Method	Venue	Key Points	Causal	Concept	Auxiliary Model	Architecture	Task
CAN[319]	ICANN'21	Modality Fusion Module Inference Module	-	-	_	Vision Model	VCR
IA-ViT[231]	arXiv'23	Attention Training Objective	-	=	-	ViT-based	Classification
MultiModN[177]	NeurIPS'23	Module Separation	-	=	-	MM	Classification Regression
VL-MoE[178]	arXiv'23	МоЕ	_	-	-	VLM	Classification Natural Language Inference VQA Image-Text Retrieval
Liu et al. [320]	ICDM-W'18	Knowledge Distillation	-	✓	Decision Tree	Vision Model	Classification
Wong et al. [321]	ICML'21	Elastic Net Sparse Decision Layer	_	✓	Linear Layer	Vision Model	Classification
NBDT[173]	ICLR'21	Sequential, Discrete Decisions	-	✓	Decision Tree	Vision Model	Classification
CBM[322]	ICML'20	Bottleneck	-	✓	-	Vision Model	Classification
PCBM[323]	ICLR'23	Post-hoc Concept Transfer	_	✓	SVM	Vision Model	Classification
LaBo[174]	CVPR'23	LLMs Generated Concepts CBM-based	-	✓	LLMs	Vision Model	Classification
TRACE[175]	arXiv'24	Causal Event Modeling	✓	_	-	Video LLMs	VTG
LLCP[324]	ICLR'24	Latent Causal Process	✓	-	-	MM	VideoQA
MGCE[176]	TKDE'24	Causal Graph	✓	-	-	MM	Recommendation
Li et al. [325]	arXiv'24	Debiasing Framework	✓	-	-	LLMs	Debiasing
Liu et al. [326]	arXiv'24	Disentangled Representations	✓	-	_	MM	Classification

This module integrates information from both images and text, enhancing the model's ability to process multimodal inputs. (2) Inference module: It encodes commonsense relationships among the image, query, and response, enabling the model to reason beyond mere object recognition by understanding relationships between elements using commonsense knowledge. Many works also apply this idea to multimodal models. IA-ViT [231] designed a Vision Transformer with enhanced interpretability by analyzing image patches, improving explainability across various visual tasks. MultiModN [177] utilized a modular and sequential fusion architecture, enabling clear tracking of each modality's contribution and enhancing both interpretability and robustness against biases from missing data. VL-MoE [178] utilized sparsely-gated Mixtureof-Experts (MoE) to improve efficiency and interpretability in vision-language tasks by dynamically scaling the model based on input modality, offering insights into handling tradeoffs between model complexity and performance. IMKGA-SM [179] enhanced interpretability in multimodal knowledge graph link prediction by employing a sequence modeling approach with fine-grained multimodal fusion and perceptual interaction-based reward mechanisms, achieving efficient and interpretable reasoning in complex multimodal settings.

V. TRAINING AND INFERENCE

We examine training strategies, mechanisms, and inference methods to enhance and analyze the explainability of

MLLMs. Training strategies are pivotal for improving model explainability by influencing weight distributions and uncovering feature interactions within the model. Optimizing these strategies lays a solid foundation for future research on explainable AI. In training, pre-training methods reveal how attention mechanisms and cross-modal alignment enhance understanding. During inference, techniques such as Chain-of-Thought (CoT) reasoning and in-context learning (ICL) provide structured, interpretable outputs. CoT facilitates step-by-step explanations to minimize hallucinations, while multi-modal ICL highlights key representation dynamics, enabling robust, real-time explainability. Together, these approaches enhance the transparency and reliability of MLLMs, fostering their adoption in real-world applications.

A. Training

Pre-trained Explainability. The explainability of pre-trained VLMs is foundational to building robust, transparent AI systems, especially as they are deployed in real-world scenarios requiring explainability. Early research by Value [161] explored how attention mechanisms, through tasks like Visual Coreference Resolution and Visual Relation Detection, contribute to cross-modal and modality-specific alignment, shedding light on the critical role of self-attention patterns in model explainability. Building on this, Salin et al. [154] analyzed pre-trained and fine-tuned VLM representations, revealing inherent biases—particularly concerning object positioning and

size—thereby underscoring the need for frameworks that can identify and address these biases for equitable AI applications. Further advancing these explainability efforts, Concept Discovery and Learning (CDL) [180] introduced methods to identify and rank visual concepts based on multimodal data, enhancing models' capacity for interpretable object recognition and broadening their usability in tasks demanding contextual understanding. Yun et al. [327] investigated how pretrained models learn basic concepts such as colors and shapes and introduce Compositional Concept Mapping (CompMap) to evaluate explainability in predicting composite concepts. LIMA [328] demonstrated that foundational knowledge and generalization capabilities are established during pre-training, with targeted fine-tuning improving explainability by refining, rather than overhauling, core knowledge. To further address the challenges of large-scale training, DistTrain [181] enhanced explainability and efficiency in multimodal LLMs training by tackling model and data heterogeneity, optimizing resource allocation, and minimizing computational inefficiencies across large-scale clusters. Neo et al. [133] expanded this line of inquiry by examining internal visual processing within VLMs, providing insights into their interpretive mechanisms and further clarifying how these models understand and represent visual information.

Alignment Interpretability. Effective alignment of visionlanguage representations is essential for reducing issues like hallucinations and enhancing the reliability of multimodal models. Factually Augmented RLHF [182] addressed this by incorporating factual data into the training process, minimizing hallucinations, and generating more accurate, interpretable outputs. The ViGoR framework [183] enhanced interpretability by using fine-grained reward modeling to improve visual grounding, supported by both human and automated evaluations for better accuracy in multimodal tasks. RLHF has emerged as an effective method for aligning MLLMs with human expectations, thereby improving interpretability. The LLaVA-RLHF model [182] illustrated this approach by combining human feedback with factual augmentation to reduce hallucinations and enhance model transparency. Expanding on this methodology, RLHF-V [184] integrated Dense Direct Preference Optimization (DDPO) to refine policy models further, effectively mitigating hallucinations and boosting robustness in complex multimodal scenarios. Addressing hallucinations is essential for achieving reliable interpretability. HA-DPO [187] reduced hallucinations by creating style-consistent hallucination sample pairs and focusing on preference learning, allowing models to prioritize factual accuracy and thereby enhancing the interpretability of outputs. Similarly, Silkie [329] utilized Reinforcement Learning from AI Feedback (RLAIF), drawing on preferences distilled from stronger MLLMs to reinforce faithful and interpretable outputs. RLAIF-V [188] also emphasized trustworthiness by aligning MLLMs with open-source feedback and iteratively improving feedback quality through deconfounded response generation. POVID [189] innovatively incorporated AI-generated dispreferred data to introduce plausible hallucinations, fostering a nuanced preference optimization framework without human intervention.

Gradient Interpretability. Gradient-based methods offer a significant approach to enhancing the interpretability of multimodal models by focusing on how models attribute importance to different modalities. SMOOTHGRAD [330] refined gradient-based sensitivity maps by averaging noise-perturbed versions to sharpen the visualization of pixel importance, which is particularly effective in image classification tasks. Building on this, Multimodal Routing [185] enhanced interpretability by dynamically adjusting weights between input modalities and output predictions, enabling both local and global insight into modality-prediction relationships. IFI [186] further improved interpretability in transformer-based models by refining feature selection for video and sensor data fusion, which enhances model performance in specific applications such as risk detection and video classification.

Hallucination Explainability. Recent advancements also focus on reducing undesirable behaviours such as hallucination in multimodal models. Dai et al. [141] introduced a model that mitigates hallucination by utilizing smaller, patch-based features and a novel object-masked language modeling loss. These design choices not only enhance interpretability by reducing model misalignment with reality but also contribute to improved performance, offering a balance between accuracy and clarity in model outputs. Furthermore, OPERA [142] addressed overconfidence issues by analyzing token interactions by introducing a penalty for excessive trust in summary tokens, effectively reducing hallucinations during decoding and leading to more accurate and reliable interpretations. Complementing this, DOPRA [221] dynamically penalizes excessive token accumulation and employs a backtracking reallocation strategy to align generated content more closely with image data without relying on external resources.

B. Inference

Recent works [190, 331, 332] have explored the phenomenon of hallucination in LLMs, a pressing issue that affects the reliability of models used in multimodal applications. Hallucination refers to instances where models generate information that appears plausible but is actually incorrect or unsupported by input data. Such issues are particularly complex in MLLMs due to the integration of information from both text and visual modalities.

COT Explainability. CoT reasoning has emerged as a powerful technique for enhancing interpretability in reasoning tasks, especially within multimodal models. Multimodal-CoT [192] contributes to this area by integrating text and visual information, generating coherent rationales that improve inference accuracy and reduce hallucination. Further advancements in CoT reasoning have been made by models that explicitly decouple reasoning steps. Studies like [193, 194, 333] introduce manual separation of CoT reasoning steps, facilitating more nuanced multimodal interactions and enhancing model interpretability. In addition, Visual CoT [334] presents a unique dataset and multi-turn processing pipeline, focusing dynamically on key visual areas to support interpretable reasoning steps in VQA tasks. More sophisticated CoT frameworks integrate external knowledge structures. For instance,

KAM-CoT [335] leveraged knowledge graphs within CoT reasoning across multiple modalities, dynamically emphasizing critical information to foster transparency in inference. M³CoT [336] benchmark addresses challenges across multiple domains and multi-step reasoning scenarios, delivering a robust evaluation framework for understanding complex reasoning. Visual Chain-of-Thought (VCOT) [337] further advances interpretability by generating multimodal synthetic infillings that provide human-interpretable insights, effectively bridging logical gaps in sequential reasoning tasks and improving performance. Tree-augmented Vision-Language (3VL) [338] model, enhancing interpretability and compositional reasoning in vision-language models through a hierarchical tree structure for text representation, along with Anchor and Differential Relevance (DiRe) tools that clarify model behavior by visualizing successes and failures in compositional understanding

ICL Explainability. In-context learning (ICL) capabilities in LLMs offer a unique approach for real-time, contextually relevant responses without the need for retraining [339]. However, challenges remain in achieving uniform interpretability across all model components. For example, [340] explored only specific attention heads and feed-forward networks that contribute significantly to performance. Addressing explainability in multimodal ICL, [341] introduced a multimodal contrastive ICL framework to enhance explainability by employing contrastive learning techniques to reveal key representational dynamics.

Hallucination Explainability. To address this challenge, a detailed survey [191] invsigated hallucination in MLLMs, reviewing its root causes, current evaluation benchmarks, and available mitigation strategies. To tackle hallucination during inference without requiring additional data or retraining, OPERA [142] introduced an over-trust penalty mechanism and enhanced both interpretability and performance, providing a promising approach for reducing hallucination in MLLMs. Visual Contrastive Decoding (VCD) [103] employed a training-free technique that compares output distributions generated from original versus distorted visual inputs. By emphasizing discrepancies in output consistency, VCD effectively reduced object hallucinations, thereby improving the reliability and explainability of MLLMs outputs.

VI. FUTURE DIRECTION

A. Dataset and More Modalities

Future work in multimodal explainability should focus on improving input-output data representation and benchmarking. For input data, standardized preprocessing and annotation pipelines are needed to ensure consistency across modalities like text, images, video, and audio while preserving essential modality-specific features. For outputs, frameworks should generate multimodal explanations, such as natural language rationales with visual or temporal highlights, aligned with human understanding. On benchmarks, future efforts should create task-specific datasets and evaluation protocols that assess explainability across fidelity, comprehensibility, and bias detection, while reflecting real-world complexities, including diverse domains and multilingual datasets.

B. Multimodal Embeddings

Future work on token-level and embedding-level interpretability in multimodal models should aim to bridge fine-grained interpretability with overall system transparency. At the token level, research should focus on tracing and attributing predictions to specific input tokens across modalities, exploring dynamic token importance mechanisms, and aligning attributions with human reasoning. At the feature level, efforts should enhance the interpretability of intermediate representations, such as visual embeddings and latent textual features, by uncovering meaningful patterns and correlations. Integrating token- and feature-level insights into unified frameworks could provide a comprehensive understanding of how models process multimodal information.

C. Components of MLLMs

Future research in multimodal neuron analysis should focus on modality alignment mechanisms and efficient model editing. While multimodal neurons can perceive concepts across modalities, the mechanisms behind this remain unclear. Further studies should investigate alignment processes through neuron analysis and develop methods for fine-grained, efficient neuron editing. Extending this analysis to circuits could reveal interconnections between units, offering deeper insights into model behavior. For layer-level interpretability, future work should explore the roles of components and workflows in cross-modal decision-making. This includes understanding how various encoders (e.g., vision, audio, point cloud) and projectors align non-text inputs with LLMs' text space. Additionally, research should clarify how post-projection embeddings are processed, identify layers handling cross-modal inputs, and analyze their impact on LLM inference capabilities.

D. Model Archtectures

Future work on architecture-level multimodal interpretability should focus on enhancing the transparency of multimodal models by investigating the specific roles of different architectural components in processing cross-modal information. This includes exploring how various encoders, such as vision, audio, and point cloud encoders, interact with one another and align their outputs within the text space of LLMs. It is essential to understand the flow of information from raw modality inputs to their integrated representations and to uncover how these components contribute to the final decision-making process. Additionally, examining the functionality of post-projection embeddings and identifying which layers are responsible for processing multimodal inputs will be critical in revealing the underlying mechanisms of cross-modal inference. Such insights could pave the way for more interpretable architectures that facilitate trust and understanding while improving the reliability of multimodal models in real-world applications.

E. Training Dynamics and Inferencing

Future work in multimodal explainability should focus on unified frameworks that integrate interpretability into training and inference. During training, models should prioritize transparency and alignment with human understanding while maintaining scalability. Inference should provide real-time, task-adaptive explanations to enhance trust and clarity. Robust benchmarks for evaluating interpretability at both stages will be essential, enabling the development of transparent, reliable, and high-performing multimodal systems for real-world applications.

VII. CONCLUSION

This survey systematically explores the interpretability and explainability of MLLMs, emphasizing the importance of transparency in their decision-making. We categorized interpretability methods into three main areas—data, model, and training and inference—offering a structured framework to organize research and guide future studies. While significant progress has been made, challenges remain in explainability and interpretability methods and ensuring broad applicability. Future efforts should address these gaps to build a unified understanding of MLLMs, fostering innovations that make multimodal systems more reliable and trustworthy.

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