A Practical Review of Mechanistic Interpretability for Transformer-Based Language Models

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https://github.com/Dakingrai/awesome-mechanistic-interpretability-lm-papers

Abstract

Mechanistic interpretability (MI) is an emerging sub-field of interpretability that seeks to understand a neural network model by reverse-engineering its internal computations. Recently, MI has garnered significant attention for interpreting transformer-based language models (LMs), resulting in many novel insights yet introducing new challenges. However, there has not been work that comprehensively reviews these insights and challenges, particularly as a guide for newcomers to this field. To fill this gap, we present a comprehensive survey outlining fundamental objects of study in MI, techniques that have been used for its investigation, approaches for evaluating MI results, and significant findings and applications stemming from the use of MI to understand LMs. In particular, we present a roadmap for beginners to navigate the field and leverage MI for their benefit. Finally, we also identify current gaps in the field and discuss potential future directions.

1 Introduction

In recent years, transformer-based language models (LMs) have achieved remarkable success in a wide range of tasks (Radford et al., 2019; Brown et al., 2020; Achiam et al., 2023; Touvron et al., 2023; Bubeck et al., 2023). Alongside these advancements, there are growing concerns over the safety, alignment, reliability, and robustness of their usage and development (Chang et al., 2024; Yao et al., 2024; Weidinger et al., 2022), especially as they are increasingly implemented in real-world applications. These concerns primarily stem from our limited understanding of these LMs and the difficulty in interpreting their behavior.

Recently, mechanistic interpretability (MI) has emerged as a promising technique that fills the gap in the research field of interpretability. This is a line of methods that interpret a model by reverse-engineering the underlying computation into human-understandable mechanisms (Olah et al., 2020; Elhage et al., 2021). It has shown promise in providing insights into the functions of LM components (e.g., neurons, attention heads), offering mechanistic explanations for various LM behaviors, and enabling users to leverage the explanations to enhance an LM's utilization (Wang et al., 2022a; Marks et al., 2024; Templeton et al., 2024). Despite the promise, however, there are concerns on the scalability and generalizability of MI and its helpfulness in addressing critical problems in AI safety (Räuker et al., 2023; Casper, 2023).

Observing these promises and challenges, we aim to provide a comprehensive review of MI in its applications to interpret transformer-based LMs. A *taxonomy* is present in Figure 1. There exist surveys on relevant topics, but they differ from ours in a number of key aspects. For example, while Räuker et al. (2023) discussed interpretability approaches broadly for all types of deep neural networks, we target an in-depth review of MI for transformer-based LMs. Similarly, Zhao et al. (2024) presented a broad survey of LM interpretability but did not focus on MI. Concurrent with our work, Ferrando et al. (2024) reviewed techniques developed for understanding the inner workings of transformer-based LMs but did not particularly focus on MI, and Bereska and Gavves (2024) emphasized MI advances for AI safety.

Our paper is organized as follows. We first present the background knowledge needed to understand this survey (Section 2). Then, we review the key developments in MI for LMs, including the fundamental objects of study, techniques, and evaluation (Sections 3-5). We then particularly present a *beginner's roadmap* in Section 6, which summarizes actionable items for newcomers to use MI for their benefits. This is then followed by an overview of findings and applications of MI in Section 7. Finally, we conclude the survey by discussing challenges and future work in this field.

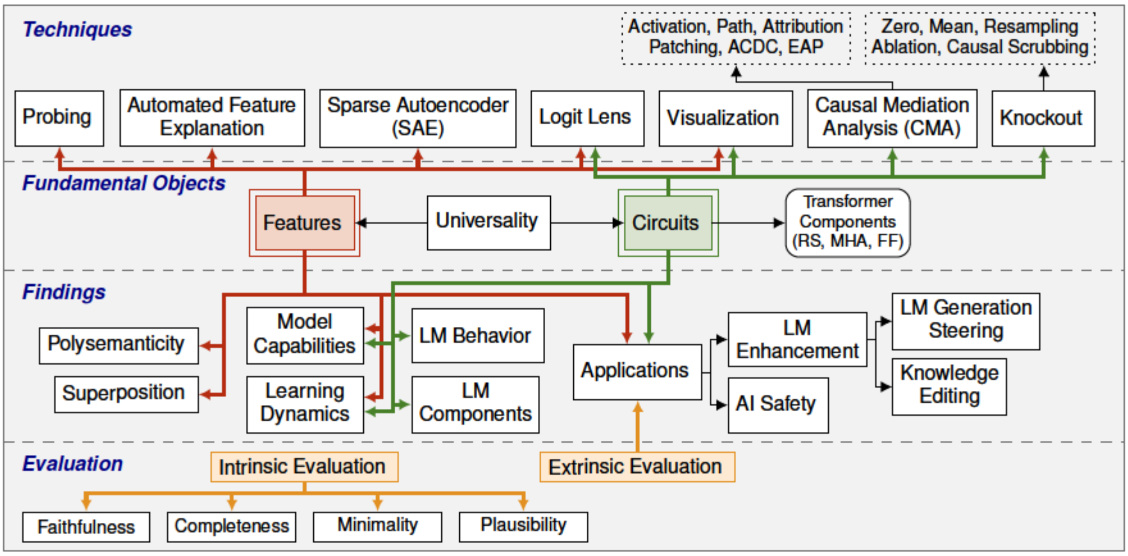


Figure 1: **Taxonomy** of the survey. Blocks are clickable to be directed to the corresponding sections.

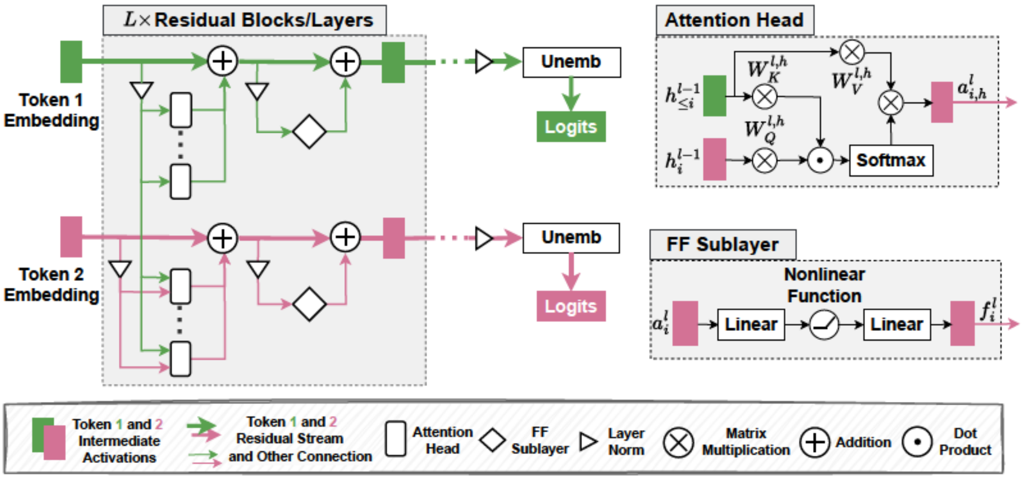


Figure 2: Architecture of transformer-based LMs.

2 Background: Transformer-based LM

A transformer-based LM (Vaswani et al., 2017) M takes input tokens $X = (x_1, ..., x_n)$ and outputs a vector in $\mathbb{R}^{|\mathcal{V}|}$, a probability distribution over the vocabulary $\mathcal{V}$, to predict the next token x_{n+1}. The model refines the representation of each token x_i layer by layer (Figure 2). In the first layer, h_i^0 is an embedding vector of x_i, resulting from a lookup operation in an embedding matrix $W_E \in \mathbb{R}^{|\mathcal{V}|\times d}$.[1] This representation is then updated layer-by-layer through the calculations of *multi-head attention (MHA)* and *feed-forward (FF)* sublayers in each layer, i.e.,

$$h_i^l = h_i^{l-1} + a_i^l + f_i^l, \tag{1}$$

where h_i^l denotes the representation of token x_i at layer l, a_i^l is the attention output from the MHA sublayer, and f_i^l is the output from the FF sublayer. The sequence of h_i^l across the layers is also referred to as the *residual stream* (RS) of transformer in literature (Elhage et al., 2021).

Briefly, the MHA sublayer with H attention heads is implemented via

$$a_i^l = \mathtt{concat}(a_{i,0}^l, .., a_{i,H}^l)W_O^l, \tag{2}$$

$$a_{i,h}^l = \mathtt{softmax}\left(\frac{(h_i^{l-1}W_Q^{l,h})(h_{\leq i}^{l-1}W_K^{l,h})^\top}{\sqrt{d_k}}\right) \cdot (h_{\leq i}^{l-1}W_V^{l,h}), \tag{3}$$

[1]For brevity, we omit components such as position embedding and layer normalization in transformer, as they will not affect our discussion of MI. Readers should refer to Vaswani et al. (2017) for a complete description.

where $a_{i,h}^l$ is the attention output from the h-th head, $W_Q^{l,h}, W_K^{l,h}, W_V^{l,h}$ are the query, key, and value (learned) projection matrices, respectively, and W_O^l projects the concatenated attention outputs from all heads to the model dimension d.

The FF sublayer then performs two linear transformations over a_i^l with an element-wise non-linear function σ between them, i.e.,

$$f_i^l = W_v^l \sigma(W_k^l a_i^l + b_k^l) + b_v^l, \tag{4}$$

where W_v^l, W_k^l, b_k^l, and b_v^l are learned parameter matrices and biases. Finally, the RS of x_n at the final layer, h_n^L, is projected into a probability distribution over $\mathcal{V}$ by applying an *unembedding* matrix $W_U \in \mathbb{R}^{d \times |\mathcal{V}|}$ and a softmax operation.

3 Fundamental Objects of Study

MI is a bottom-up approach that interprets LMs by decomposing them into smaller components and more elementary computations. Following Olah et al. (2020), one of the earliest studies in MI, we categorize research of MI into three areas: the study of features, circuits, and their universality.

3.1 Features

A *feature* is a human-interpretable input property that is encoded in a model's activation.[2] For instance, a neuron or a set of neurons that consistently activates for French text can be interpreted as a "French text detector" feature (Gurnee et al., 2023).[3] MI aims to interpret LMs in terms of the independent features or components representing these features. To this end, Elhage et al. (2022b) proposed the *linear representation hypothesis*, which posits that neural networks have two properties – *linearity*, i.e. the network's activation space consists of meaningful (linear) vectors, each representing a feature, and *decomposability*, i.e., network activations can be decomposed and described in terms of these independent features. This hypothesis resonates with earlier research that also shows linearity in word embeddings (e.g. $\overrightarrow{man} - \overrightarrow{woman} \approx \overrightarrow{king} - \overrightarrow{queen}$) (Mikolov et al., 2013). In Section 7.1, we will review some identified features in LMs and how they are represented.

[2]We use "activations" and "representations" interchangeably to refer to the intermediate outputs of LM components.

[3]We refer to each element in the activation as a neuron, which implies that a neuron is a basis-aligned direction in the activation space (Marks et al., 2024).

3.2 Circuits

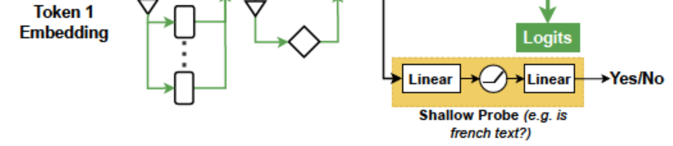
While the study of features helps us to understand what information is encoded in a model's activations, it does not inform us of how these features are extracted from the input and then processed to implement specific LM behaviors (e.g., reasoning). MI fills this gap by studying "circuits", which are meaningful computational pathways that connect features.

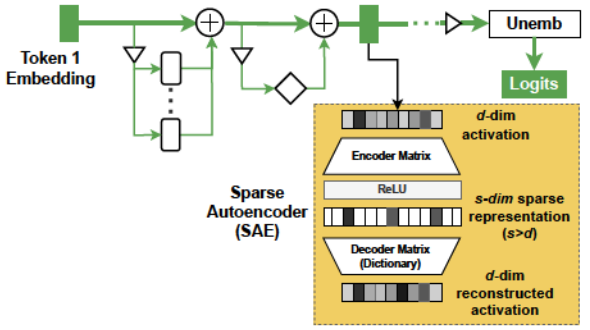
More formally, if we view an LM M as a computational graph with features as nodes and the weighted connections between them as edges, a circuit is a sub-graph of M responsible for implementing specific LM behaviors (Wang et al., 2022a). Additionally, although circuits were initially defined as connections between features (Olah et al., 2020), subsequent studies have generalized them as connections between the activation outputs of transformer components (Olsson et al., 2022; Wang et al., 2022a). Therefore, we include research on interpreting transformer components, both individually (e.g., interpreting RS in Eq 1 connecting the activations of MHA, FF, and the RS from earlier layers) and across multiple components (e.g., the induction circuit in Figure 3), as circuit study.

An example circuit discovered by Elhage et al. (2021) in a toy LM is shown in Figure 3. This is an induction circuit consisting of outputs of two attention heads (previous token head and induction head) as nodes and connection between them as edges of the circuit. The circuit implements the task of detecting and continuing repeated subsequences in the input (e.g., *Mr D urs ley was thin and bold. Mr D -> urs*), where the **previous token head** encodes the information *"urs" follows the "D" token* in the RS, which is then read by the **induction head** to promote *"urs"* as the next token prediction.

3.3 Universality

For any feature or circuit that we have identified in an LM in one task, the critical question arises: Do they similarly exist in other LMs or in other tasks? The investigation into this question has then given rise to the notion of *universality*, i.e., the extent to which similar features and circuits are formed across different LMs and tasks (Olah et al., 2020; Gurnee et al., 2024). The implications of universal features and circuits can be significant. For instance, many studies (Olsson et al., 2022; Elhage et al., 2022a,b) on features and circuits were





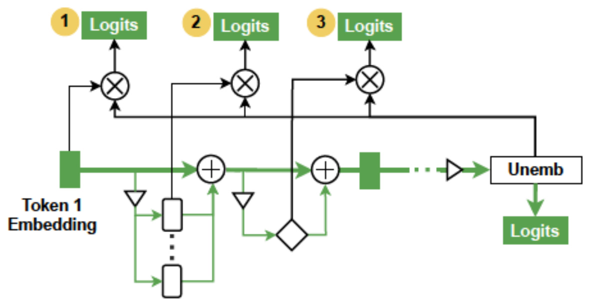


Figure 4: Logit lens implementation at (1) RS, (2) attention head, and (3) FF sublayer.

performed with only toy or small LMs. If these features and circuits are universal, the insights from these studies can be transferred to other unexamined LMs and potentially state-of-the-art large LMs (LLMs). However, if they are not universal, then a significant amount of independent effort will be required to interpret each LM.

4 Techniques

Next, we review the techniques that have been developed to study the fundamental objects described in Section 3 and to perform MI analysis on LMs.

4.1 Logit Lens

The *logit lens* (Figure 4) was first introduced by nostalgebraist (2020), which provides insights on how LMs refine their prediction across layers. This approach has been applied to interpret *activations* in both feature (Geva et al., 2021) and circuit discovery (Lieberum et al., 2023; Wang et al., 2022a). Specifically, the activation h_i^l in each layer l can be projected to the vocabulary space by multiplying it with the unembedding matrix W_U, yielding the logits over the vocabulary $\mathcal{V}$. In doing so, tokens with the highest logits can be used to infer what information is encoded in h_i^l.

The logit lens can also be used to interpret the *weights* of transformer components. For example, Geva et al. (2022) used it to understand the role of the FF sublayer in the LM's prediction by projecting the columns of W_v^l parameter matrix to the vocabulary space. Dar et al. (2023) applied the technique to project query-key ($W_Q^{l,h} W_K^{l,h}$) and value-output ($W_V^{l,h} W_O^l$) interaction parameter matrices to vocabulary space to study how attention heads transfer and mix information from source tokens to the target token.

However, vocabulary space projection may yield seemingly nonsensical results for some models. For instance, the top-1 projected token for BLOOM (Scao et al., 2022) in many intermediate layers is often the input token (Belrose et al., 2023). The authors posited that this may be caused by the discrepancy between the intermediate layers and the last layer (where W_U was trained to apply to). To address it, Belrose et al. (2023); Din et al. (2023); Pal et al. (2023) transformed the intermediate activations to align with the representation space of the final layer.

4.2 Probing

The probing technique (Figure 5) is used extensively in (and also before) MI to investigate whether specific information, such as the part-of-speech linguistic property, is encoded in given intermediate activations (a single neuron or set of neurons) (Conneau et al., 2018; Tenney et al., 2019a,b).

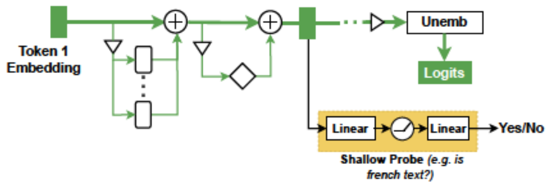


Figure 5: Probing on RS to detect whether it encodes a "French text" feature.

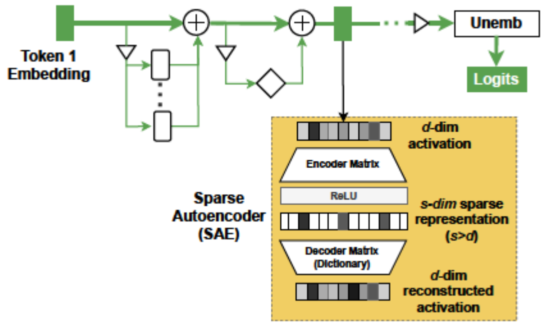


Figure 6: Sparse Autoencoder (SAE) applied to activation on RS.

To do so, it trains a shallow (or linear) classifier, known as a *probe*, to predict whether a feature is present in that activations (Gurnee et al., 2023; Dalvi et al., 2019; Durrani et al., 2020; Antverg and Belinkov, 2021). However, it is important to note that the results of probing analyses only indicate a correlation, not a causal relation, between the feature and activations.

4.3 Sparse Autoencoder (SAE)

SAEs (Figure 6) serve as an unsupervised technique for discovering features from activations, especially those that demonstrate *superposition*, a phenomenon in LMs where their d-dimensional representation encodes more than d features (Elhage et al., 2022b; Sharkey et al., 2023; Cunningham et al., 2023; Bricken et al., 2023; Yun et al., 2021). In contrast to dimensionality reduction techniques (e.g., Principal Component Analysis), SAEs seek to embed the activation vectors into a much higher-dimensional space, but with strong sparsity. Specifically, an encoder maps the d-dimensional input into an s-dimensional vector ($s > d$), which the decoder then maps back to the d-dimension. The encoder and decoder are jointly trained for input reconstruction and sparsity of the s-dimensional representation. This s-dimensional representation, owing to its sparsity, makes the discovery of independent (or *monosemantic*) features more easily.

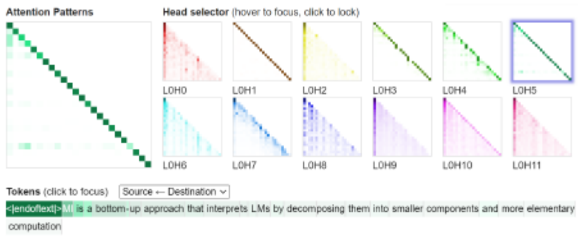


Figure 7: Attention visualization, created using Cooney and Nanda (2023).

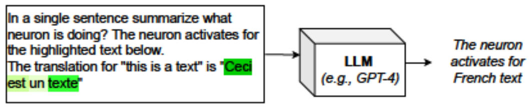


Figure 8: Automated feature explanation, where the highlighted text represents the activation strength for a neuron. An LLM can then be used to generate a textual explanation of the neuron.

4.4 Visualization

Visualization (Figure 7) is employed across various stages of an MI investigation, from generating initial hypotheses to refining them, conducting qualitative analyses, and validating results. For instance, attention patterns are often visualized to understand attention heads (Lieberum et al., 2023; Olsson et al., 2022); a neuron activation across the input text is visualized to identify its functionality (Elhage et al., 2022a; Bricken et al., 2023). While visualization can be highly useful, it requires human effort to interpret results and carries the risks of overgeneralization. Thus, any claims need to be substantiated with further experimentation and analysis.

4.5 Automated Feature Explanation

For feature discovery, human effort is required to annotate neurons with interpretable feature labels based on their activation patterns (Elhage et al., 2022a; Conmy et al., 2024) or the projected tokens when using logits lens (Geva et al., 2022). To reduce human labor, Bills et al. (2023) proposed using LLMs to generate feature labels automatically (Figure 8). Additionally, they also introduced a quantitative automatic explanation score to measure the quality of these explanations, using LLMs to simulate activations based on the automatically generated labels and comparing them with the ground-truth activations.

4.6 Knockout / Ablation

Knockout or *ablation* (Figure 9) is primarily used to identify components in a circuit that are impor-

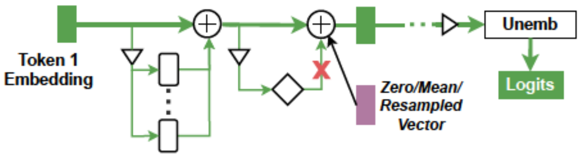


Figure 9: An example of ablation, where the output activation from an FF sublayer is replaced with a zero/mean/resampled vector.

tant to a certain LM behavior. It removes specific components and analyzes the change in the LM behavior, where a significant change suggests importance. There are three main ablation methods: (1) **zero**: replacing the output of the component with a zero vector (Olsson et al., 2022); (2) **mean**: replacing the output with the mean value of randomly sampled inputs from the same input distribution (Wang et al., 2022a); (3) **resampling**: replacing the output with that of another random input (Chan et al., 2022).

Chan et al. (2022) introduced **causal scrubbing** which employs resampling ablation for hypothesis verification. Rather than a direct ablation, they formalize a hypothesis as (G, I, c), where G is the model's computational graph, I is an interpretation graph reflecting the hypothesis, and c is a function that maps between nodes of I to G. Resampling ablation is then performed on G to validate I. The model's behavior should be preserved when one ablates activations in G with random samples that follow the same hypothesis.

4.7 Causal Mediation Analysis (CMA)

Causal mediation analysis (CMA) is popular for circuit discovery, including two main patching approaches (Figure 10).

Activation patching localizes important *components* in a circuit (Vig et al., 2020; Meng et al., 2022), which performs three rounds of model inference. First, the *clean run* uses a prompt that demonstrates the LM capability in investigation. Then, the *corrupt run* uses the same prompt, but with a few important tokens corrupted with noise such that the LM fails to demonstrate the capability.[4] Finally, the *patch run* uses all activation values of the corrupt run, except those of the localized component, which uses the clean run values. The recovery of the lost capability indicates that the patched component is important.

[4]Alternatively, counterfactual prompts can be used as the corruption procedure (Wang et al., 2022a).

Path patching localizes important *connections* between components (Wang et al., 2022a; Goldowsky-Dill et al., 2023). To assess whether the connection between two components, C_1 and C_2, is significant, path patching applies activation patching to the output of C_1 but only along paths serve as the input to C_2. If a change in behavior is observed, then the connection between the two components is considered important.

Circuit discovery via patching is often computationally inefficient, as one has to iteratively patch each component or connection in an LM to measure its importance. To address it, Conmy et al. (2024) proposed ACDC (Automatic Circuit DisCovery) to automate the iterative localization process. Nanda et al. (2022); Kramár et al. (2024) proposed **attribution patching** to approximate activation patching, which requires only two forward passes and one backward pass for measuring all model components. Syed et al. (2023) further extended it to edge attribution patching (EAP), which outperforms ACDC in circuit discovery.

5 Evaluation

Existing work has performed two types of evaluation, i.e., *intrinsic evaluation* that seeks to establish the quality of the explanations on their own, without the context of any particular application, and *extrinsic evaluation*, which measures the quality of the interpretation by applying the obtained insights to a relevant downstream task. This section will focus on the former, whereas the latter was driven by the applications which we will present in Section 7.6.

Faithfulness Faithfulness measures the degree to which an MI interpretation accurately reflects the actual decision-making process underlying a model's behavior under study (Jacovi and Goldberg, 2020). For feature discovery, Elhage et al. (2022a) and Bricken et al. (2023) recruited human annotators to rate the interpretation of a feature based on its activations over texts, and Bills et al. (2023) automated it with GPT-4. For circuit discovery, localization is evaluated by comparing the full model vs. the partial model with the localized circuit alone (Olsson et al., 2022; Wang et al., 2022a; Marks et al., 2024), while the explanation of circuit components is often validated by knocking out the component and manually examining its effect.

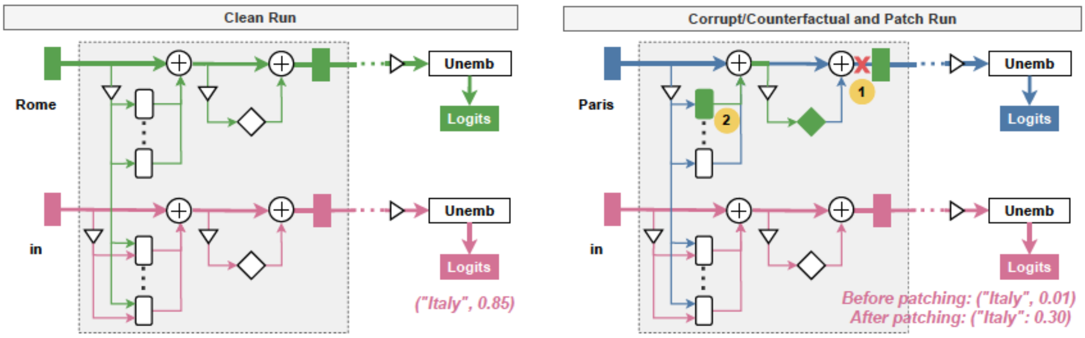


Figure 10: (1) Activation Patching, where in the counterfactual run, an intermediate RS activation is patched (i.e. replaced) by the corresponding activation from the clean run. (2) Path Patching, where all intermediate activations between the green highlighted attention head and FF sublayer are patched by the corresponding activations from the clean run.

Completeness and Minimality Besides faithfulness, completeness and minimality are also desirable (Wang et al., 2022a). For example, when studying the model's ability to recognize French text, an explanation algorithm may identify a group of neurons N or a circuit C. A complete explanation would mean that no other neurons outside of N are responsible (e.g., highly activated), or no other circuits besides C implement this functionality. It can be measured by ablation-based techniques (Wang et al., 2022a; Marks et al., 2024). Specifically, if the model behavior remains unchanged after removing the neuron or circuit, then the explanation is incomplete. On the other hand, minimality measures whether all parts of the explanation (e.g., N or C) are necessary, often by ablating parts of the explanation and computing the change in model behavior (Wang et al., 2022a).

Plausibility Jacovi and Goldberg (2020) defined plausibility as "how convincing the interpretation is to humans". In MI, for example, attributing a model behavior to polysemantic neurons may be less plausible as compared to monosemantic ones (Bricken et al., 2023; Marks et al., 2024), as humans may have trouble understanding the former during the evaluation.

6 A Beginner's Roadmap to MI

A key motivation for this survey is to provide a friendly guide for researchers and developers interested in MI to quickly pick up the field. To this end, we provide a *beginner's roadmap* in Figure 11.

6.1 Feature Study

The study of features can be broadly divided into two categories, i.e., *targeted feature discovery*, which aims to determine if a pre-defined feature (e.g., a "French text" feature) is encoded in the activations of LMs, and *open-ended feature discovery*, which aims to discover all interpretable features in the activations of LMs.

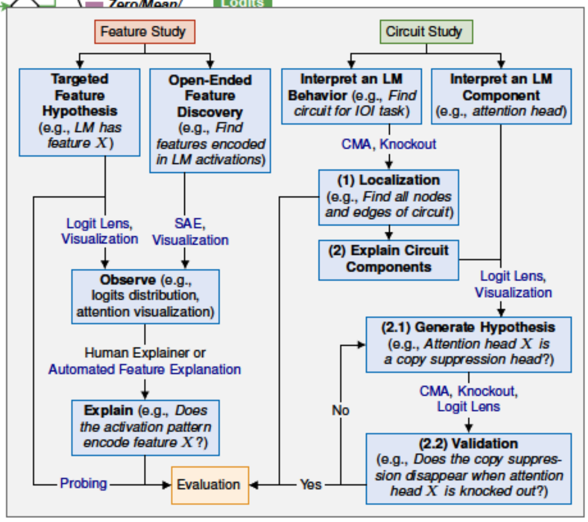


Figure 11: A **Beginner's Roadmap** showing the workflow and common techniques for conducting a feature or circuit study. Both types of studies start with formulating a research question, followed by various steps (enclosed within the blue rectangle) to answer it. Techniques employed to execute each step are indicated along the incoming edge.

Probing, logit lens, and visualization are common techniques used for targeted feature discovery. For probing, a labeled dataset indicating the presence or absence of the target feature is required to train the probe. If the trained probe achieves high accuracy on a held-out test set, it can be inferred that the activation encodes the target feature. On the other hand, the logit lens or visualization requires a human explainer to interpret the logit lens projection or the visualization of the highlighted text. Alternatively, LLMs (e.g., GPT-4) can also be employed to automatically interpret the logit lens projection or highlighted text to confirm if the feature is encoded in the activations. Open-ended feature discovery is typically conducted via SAEs and visualization. Interpretation results of these approaches are then passed to human explainers or LLMs (if going with automatic feature explanation) for annotating them with interpretable feature labels, similar to the annotation process in targeted feature discovery.

Finally, the faithfulness of both categories can be measured by humans based on how interpretable the discovered features are (e.g., "on a scale of 0–3, rate your confidence in this interpretation" as executed by Bricken et al. (2023)) and using automatic explanation scores proposed by Bills et al. (2023).

6.2 Circuit Study

Similarly, the study of circuits can be broadly divided into two categories, i.e., *interpret an LM behavior (e.g., IOI)* and *interpret an LM component (e.g., attention head)*.

The first category involves finding a circuit that is responsible for the LM behavior. To do so, we start with *(1) localization* i.e. identifying all the important components and the edges connecting them via CMA and knockout. Subsequently, the second step is to *(2) explain each component and its connection* one by one. The functional interpretation of each component or edge can be further divided into two sub-steps — *(2.1) Generating a hypothesis:* The behavior of the component under study is analyzed under relevant input using various visualization techniques (e.g., attention visualization) and logit lens vocabulary projection. A human can then generate a plausible hypothesis based on the analysis (e.g., attention head X is hypothesized to function as a copy suppression head, when it was observed to decrease the logit of the token it attends to). *(2.2) Validating the hypothesis:* The hypothesis can be validated using techniques such as knockout, CMA, and logit lens. For instance, if the hypothesis suggests that attention head X is a copy suppression head, then knocking out attention head X should remove the suppression effect. If the hypothesis is validated, the model component is considered interpreted; otherwise, further analysis and new hypotheses are needed. Finally, the discovered circuit, with or without the second-step explanation, can be evaluated in terms of faithfulness, completeness, and minimality (Section 5).

The second category of the circuit study, i.e., interpreting an LM component, follows similar steps but starts with the second step of the first category, given that the target component to interpret has been provided.

7 Findings and Applications

7.1 Findings on Features

Monosemantics vs. Polysemantics Earlier work studied neurons as a natural candidate for encoding features, leading to the discovery of "sentiment neurons" (Radford et al., 2017), "knowledge neurons" (Dai et al., 2022), "Base64 neurons" (Elhage et al., 2022a), "skill neurons" (Wang et al., 2022b), "positional neurons" (Voita et al., 2023), etc. However, many of these studies found that neurons within LMs are not *monosemantic*, i.e. they do not activate only for a single feature. In contrast, they are *polysemantic*, i.e. they activate in response to multiple unrelated features (Elhage et al., 2022a; Gurnee et al., 2023; Elhage et al., 2022b). For instance, a single neuron could activate for both French texts and texts encoded in Base64. Due to its polysemantic nature, mapping a neuron to a specific feature becomes challenging.

Superposition The discovery of polysemantic neurons has led to the hypothesis of *superposition*, i.e., a model can represent a greater number of independent features than the number of available neurons. Specifically, features represented in superposition are encoded in activations by a linear combination of multiple neurons, rather than by a single neuron, at the cost of some interference with each other. This hypothesis has been verified by Elhage et al. (2022b), where the authors showed that when features are sparse, the model tends to encode features in activation space using superposition. To extract features from such representations, SAEs have become a widely adopted approach (Bricken et al., 2023; Sharkey et al., 2023; Riggs, 2023; Cunningham et al., 2023), as discussed in Section 4.3. Early studies on SAEs have shown promising results, with the extracted features from SAEs appearing more interpretable than those from neurons, according to both human analysis and automatic explanation scores (Bricken et al., 2023).

7.2 Findings on Circuits

Interpreting LM Behaviors Specific circuits have been identified for various LM behaviors such as in-context learning (Olsson et al., 2022), indirect object identification (IOI) (Wang et al., 2022a), greater-than operations (Conmy et al., 2024), Python docstring formatting (Heimersheim and Janiak, 2023), modular addition (Nanda et al., 2023a; Zhong et al., 2024), and more (Lieberum et al., 2023; Marks et al., 2024). These circuits are defined at varying levels of granularity, where nodes in the computation graph are defined as the outputs of MHA and FF sublayers (Olsson et al., 2022; Wang et al., 2022a) or as SAE features (Marks et al., 2024; Cunningham et al., 2023). In addition, Merullo et al. and Quirke et al. (2024) showed that the same components (e.g., induction heads) are reused by different circuits (e.g., IOI and induction circuits) to implement different tasks. Finally, to demonstrate the scalability of current techniques for identifying circuits in LLMs, Lieberum et al. (2023) identified the circuit used for the multiple-choice question-answering task on the 70B Chinchilla LLM (Hoffmann et al., 2022)

Interpreting Transformer Components The study of circuits has also yielded insights into the functionalities of transformer components.

The RS can be viewed as a one-way communication channel that transfers information from earlier to later layers. Furthermore, Elhage et al. (2021) hypothesized that MHA and FF in different layers write their output in different subspaces of the RS, which prevents interference of information. In addition, nostalgebraist (2020) proposed to view the RS as an LM's current "guess" for the output, which is iteratively refined layer-by-layer..

The MHA sublayers are responsible for moving information between tokens, which enables information from other tokens (i.e., context) to be incorporated into each token's representation. Elhage et al. (2021) showed that each attention head in a layer operates independently and can be interpreted independently. Several MI studies have shown that these attention heads seem to have specialized roles. For instance, "negative heads" discovered in GPT2-small by McDougall et al. (2023) are responsible for reducing the logit values of the tokens that have already appeared in the context. Other notably identified attention heads include previous token heads (Wang et al., 2022a), duplicate token heads (Wang et al., 2022a), copying heads (Elhage et al., 2021), induction heads (Olsson et al., 2022), and successor heads (Gould et al., 2023).

The FF sublayers are attributed for the majority of feature extraction (Gurnee et al., 2023), storing and recalling pre-trained knowledge (Meng et al., 2022) and arithmetic computation (Stolfo et al., 2023a). More generally, Geva et al. (2021) viewed FF sublayers as key-value stores where the outputs of the first layer (W_k^l) of the FF sublayer serves as keys that activate values (stored knowledge) within the weight matrices of the second layer (W_v^l). Furthermore, they demonstrated that earlier FF layers typically process shallow (syntactic or grammatical) input patterns, while later layers focus more on semantic patterns (e.g., text related to TV shows).

7.3 Findings on Universality

Studies on universality have yielded mixed results. Early circuit analyses identified components such as induction heads (Olsson et al., 2022), successor heads (Gould et al., 2023), and duplication heads (Wang et al., 2022a) across multiple LMs. Similarly, Merullo et al. found that different circuits implementing different tasks (IOI and colored objects task) reuse the same components (e.g., induction head), demonstrating universality across tasks. However, Zhong et al. (2024) discovered that two LMs trained with different initialization can develop qualitatively different circuits for the modular addition task. Similarly, Chughtai et al. (2023) found that LMs trained to perform group composition on finite groups with different random weight initializations on the same task do not develop similar representations and circuits. Finally, Gurnee et al. (2024) found that only about 1-5% of neurons from GPT-2 models trained with random initialization exhibit universality. Understanding the degrees of feature and circuit universality and their dependency on various aspects of model training (e.g., initialization, model size, and loss function) remains a crucial open problem.

7.4 Findings on Model Capabilities

In-Context Learning (ICL) ICL is an emergent ability of LLMs that enables them to adapt to new tasks based solely on instructions or a few demonstrations at inference time (Wei et al., 2022). Elhage et al. (2021) studied a simplified case of ICL and discovered an induction circuit composed of attention heads with specialized roles (e.g., induction heads), which were then found to be crucial even for general cases of ICL (Olsson et al., 2022; Bansal et al., 2023). Ren et al. (2024) further investigated few-shot ICL and identified "semantic induction heads", which, unlike prior induction heads, model the semantic relationship between the input and the output token (e.g., “I have a nice pen for writing. The pen is nice to” → “write”).

Reasoning Stolfo et al. (2023b) studied arithmetic reasoning and found that attention heads are responsible for transferring information from operand and operator tokens to the RS of the answer or output token, with FF modules subsequently calculating the answer token. Dutta et al. (2024) studied chain-of-thought (CoT) multi-step reasoning over fictional ontologies and found that LLMs seem to deploy multiple different neural pathways in parallel to compute the final answer. Concurrently, Rai and Yao (2024) investigated neuron activation (Geva et al., 2022) as a unified lens to explain how CoT elicits arithmetic reasoning of LLMs, including phenomena that were only empirically discussed in prior work (Wang et al., 2023; Ye et al., 2023; Madaan and Yazdanbakhsh, 2022). In particular, the authors found neurons representing various arithmetic reasoning concepts and showed that the activation of these neurons is necessary but not sufficient for an LLM’s arithmetic reasoning. Finally, Brinkmann et al. (2024) discovered an interpretable algorithm in LM for the task of pathfinding in trees.

Others As listed in Section 7.2, prior work has also studied LM capabilities in tasks such as IOI (Wang et al., 2022a), modular addition (Nanda et al., 2023b), and greater-than operations (Conmy et al., 2024), leading to the discovery of circuits that implement these tasks. Compared with the interpretation of ICL and reasoning, these studies not only justified the rationale of a capability but also revealed its underlying algorithm through circuits.

7.5 Findings on Learning Dynamics

Phase Changes during LM Training Prior studies have observed sudden shifts in LMs’ capabilities, called “phase changes” (Olsson et al., 2022; Power et al., 2022; Wei et al., 2022). These changes are considered key steps during the LM training. MI has been applied to examine the relationship between the emergence of features and circuits and these phase changes. For example, Olsson et al. (2022) found correlations between phase changes and the formation of induction circuits, suggesting that the development of these circuits underlies the phase change. In the task of symbol manipulation, Nanda et al. (2023a); Varma et al. (2023) discovered a similar correlation contributing to LM grokking (Power et al., 2022), a phenomenon of LM generalizing beyond memorization. Chen et al. (2024) found that sudden drops in the loss during training correspond to the acquisition of attention heads that recognize specific syntactic relations. Finally, Huang et al. (2024b) provided a unified explanation for grokking, double descent (Nakkiran et al., 2021), and emergent abilities (Wei et al., 2022) as a competition between memorization and generalization circuits.

Learning Dynamics during LM Fine-Tuning Prakash et al. (2024) investigated the underlying changes in mechanisms (e.g., task-relevant circuits) to understand performance enhancements in fine-tuned LMs. The authors found that fine-tuning does not fundamentally change the mechanisms but enhances existing ones.

7.6 Applications of MI

7.6.1 Model Enhancement

Knowledge Editing LMs are known to store factual knowledge encountered during pre-training (Petroni et al., 2019; Cohen et al., 2023). For instance, when an LM is prompted with “The space needle is in the city of”, it may retrieve the stored facts and correctly predict “Seattle”. However, these stored facts may be incorrect or outdated over time, leading to factually incorrect generation (Cohen et al., 2024). MI has been found to be a helpful tool for addressing the problem, including understanding where and how facts are stored within LMs, how they are recalled during the inference time, and the approaches for knowledge editing (Meng et al., 2022, 2023; Geva et al., 2023; Sharma et al., 2024). For instance, Meng et al. (2022) used path patching to localize components that are responsible for storing factual knowledge, and then edited the fact (e.g., replacing “Seattle” with “Paris”) by only updating the parameters of those components.

LM Generation Steering LM generation steering involves controlling an LM’s output by manipulating its activations at inference time. For instance, Geva et al. (2022) proposed a method to suppress toxic language generation by identifying and manually activating neurons in FF layers responsible for promoting non-toxic or safe words. Similarly, Templeton et al. (2024) identified safety-related features (e.g., unsafe code, gender bias) and manipulated their activations to steer the LM towards (un)desired behaviors (e.g., safe code generation, unbiased text generation). Additionally, Nanda et al. (2023b) demonstrated that an LM's output can be altered (e.g., flipping a player turn in the game of Othello from YOURS to MINE) by pushing its activation in the direction of a linear vector representing the desired behavior, which was identified using a linear probe.

7.6.2 AI Safety

AI safety is an important concern that MI aims to address. At present, the exact role MI can play in addressing AI safety is unclear (Casper, 2023). Within MI, "enumerative safety" aims to address AI safety by enumerating all features in LMs and inspecting those related to dangerous capabilities or intentions (Elhage et al., 2022b; Olah and Jermyn, 2023). To this end, Templeton et al. (2024) identified several safety-relevant features that not only activate when the LM exhibits specific behaviors but also causally influence the LM's output; however, the specific circuits that use these features to implement the behavior have not yet been identified. As we have discussed, Geva et al. (2022) encouraged language safety by steering the LM's generation of non-toxic tokens. Finally, insights from circuit studies were used to detect prompt injection (Belrose et al., 2023) and find adversarial examples for the IOI task (Wang et al., 2022a).

7.6.3 Others

Insights from MI have also been used for other downstream tasks. Marks et al. (2024) improved the generalization of classifiers by identifying and ablating spurious features that humans consider to be task-irrelevant. Geva et al. (2022) proposed self-supervised early exit prediction for efficient inference, drawing insights from their investigations of the FF sublayers' role in token prediction.

8 Discussion and Future Work

Automated Hypothesis Generation At a high level, MI study is a process with two stages: generating hypotheses on the underlying mechanisms of LM behavior and validating them. Although various techniques have automated hypothesis validation (Section 4.5), the generation part is mainly left to humans, a potential scalability bottleneck to LLMs and complex behaviors. To address it, automated hypothesis generation, potentially with humans in the loop, is instrumental.

Studies on Complex Tasks and LLMs Current MI studies are mostly performed on simpler tasks, often criticized as "streetlight interpretability" (Casper, 2023; Wang, 2022). For instance, Wang (2022) intentionally selected the IOI task (Wang et al., 2022a) because it is a simple algorithmic task. Similarly, although a few studies were done on "production-level" LMs (Lieberum et al., 2023; Templeton et al., 2024), most still used small LMs, which may have limited generalizability, given the mixed results on universality.

Practical Utility While people acknowledge the importance of actionable insights to downstream applications (Doshi-Velez and Kim, 2017), MI studies that highlight such applications, such as adversarial example generation (Wang et al., 2022a), often lack the depth of investigation when they do not compare against alternative methods or baselines. As an exception, Marks et al. (2024) showed that their MI technique improves model generalization better than several baselines.

Standardized Benchmarks and Metrics Evaluating interpretability results is inherently challenging due to the lack of ground truth (Zhou et al., 2022), and current MI studies also employ diverse *ad hoc* evaluation approaches, potentially leading to inconsistent comparisons (Zhang and Nanda, 2023). There are some proposals for standardized evaluation benchmarks. RAVEL (Huang et al., 2024a) evaluates techniques (e.g., SAEs) that disentangle polysemantic neurons into monosemantic features. Tracr (Lindner et al., 2024) converts human-readable RASP programs (Weiss et al., 2021) into transformers to enable ground-truth features and algorithms. However, these proposed benchmarks are still insufficient (Räuker et al., 2023). For instance, success on synthetic transformers in the Tracr benchmark may not imply that on naturally trained transformers. Thus, more effort is needed to develop standard evaluation techniques and to ensure their wide adoption.

9 Limitations

Our survey paper discusses MI studies conducted only on decoder-only transformer LMs, omitting studies on other transformer LM variants such as encoder-only and encoder-decoder transformer LMs. Additionally, due to space constraints, some techniques may not have been presented with full technical details (e.g., causal scrubbing).

Furthermore, given the fast-paced nature of the field, our survey may not reflect the latest advancements that were published close to or after the survey was conducted. Despite these limitations, however, our survey provides a comprehensive taxonomy of the current state of the MI field as well as a roadmap, specifically curated to help newcomers quickly pick up the field. Both the taxonomy and the roadmap can serve as guides for future researchers interested in encoder-only or encoder-decoder LMs to build up their survey. In addition, we have created a GitHub repository at https://github.com/Dakingrai/awesome-mechanistic-interpretability-lm-papers to sustainably maintain this survey, and we welcome researchers sharing the same interest to add new papers and extend the taxonomy and the roadmap.

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