Interpretability: From Mechanistic Foundations to Practice

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Sources & Objectives

Key References: Elhage et al. (2021) — Transformer Circuits; Olsson et al. (2022) — Induction Heads; Bricken et al. (2023) — Monosemanticity; Templeton et al. (2024) — Scaling Monosemanticity; nostalgebraist (2020) — Logit Lens

By the end of this lecture, you will be able to:

1. Trace a computation through zero-, one-, and two-layer transformer circuits
2. Apply the logit lens and sparse autoencoders to inspect model internals at scale
3. Distinguish representational evidence (probes) from causal evidence (patching)
4. Evaluate when mechanistic understanding is necessary vs. when behavioral testing suffices
5. Honestly assess what interpretability can and cannot deliver today

This course builds an LLM engineering toolkit across six dimensions

BUILDING

Inference-Time Control ✓

Prompting, decoding, self-consistency

Training-Time Control ✓

SFT/PEFT, continued pretraining, pref. tuning

System-Time Augmentation ✓

RAG, tools, agents

UNDERSTANDING & GOVERNING

TODAY

Understanding

Interpretability, causal methods

Measuring

Evaluation, contamination, protocols

Governing & Shipping

Safety engineering, deployment constraints

What question are you actually asking?

Three levels of interpretability questions, from surface to mechanism:

1. Behavioral

"*What* does the model do?" — Input-output testing, benchmarks, red teaming

2. Representational

"*What* does the model know?" — Probes, logit lens, feature visualization

3. Mechanistic

"*How* does the model compute?" — Circuits, activation patching, path tracing

This lecture builds **bottom-up**: start from mechanisms (circuits), develop scaling tools (probes, SAEs), then ask what practice demands.

Running themes: 1. Circuits are the atoms of understanding 2. Scaling requires new tools, not just more patience 3. Practice demands honest limits

Part 1: Mechanistic Foundations

From tokens to circuits

We start at the simplest possible transformer computation — no attention, no MLPs — and build toward multi-layer circuits. Each step adds exactly one new mechanism.

Zero-layer circuits: What does a transformer predict with no computation?

The simplest "circuit" — skip all attention heads and MLPs, go directly from input to output:

The zero-layer path

$$\text{logits} = W_U^T \cdot W_E \cdot x$$

W_E: token embedding matrix
W_U: unembedding matrix
x: one-hot input token

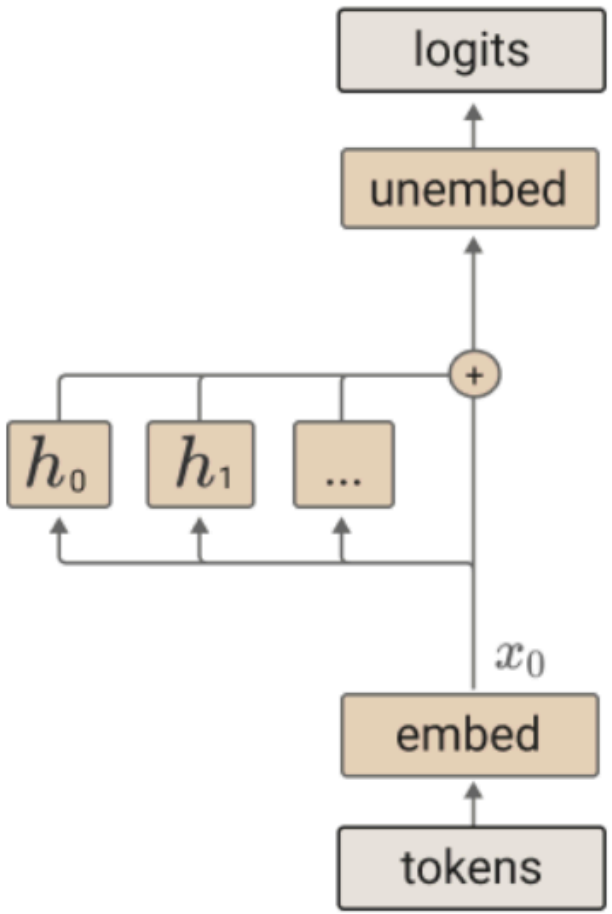
What this captures

The product $W_U^T W_E$ is a **token-to-token matrix**: row i, column j gives the direct contribution of input token j to predicting output token i.

This encodes **bigram statistics** — the model's baseline expectation of what follows what.

Input →	**the**	**cat**	**sat**	**on**
Top prediction	cat	is	on	the

Single-layer circuits: How does one attention head transform the zero-layer predictions?



The final logits are produced by applying the unembedding.

$$T(t) = W_U x_1$$

Each attention head, h, is run and added to the residual stream.

$$x_1 = x_0 + \sum_{h \in H} h(x_0)$$

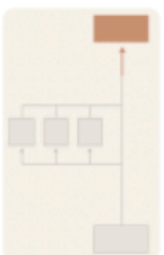
Token embedding.

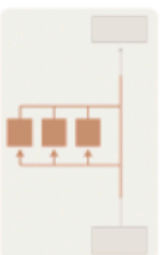
$$x_0 = W_E t$$

Source: Elhage et al., "A Mathematical Framework for Transformer Circuits" (2021)

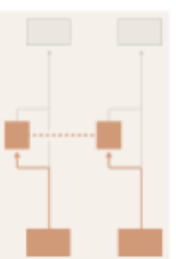
Single-layer circuits: Mathematical reformulation

$$T = \underbrace{\mathrm{Id} \otimes W_U}_{\text{The token unembedding maps residual stream vectors to logits.}} \cdot \underbrace{\left(Id + \sum_{h \in H_1} A^h \otimes W_{OV}^h\right)}_{\text{The attention layer has multiple heads. The result of each is added into the residual stream.}} \cdot \underbrace{\mathrm{Id} \otimes W_E}_{\text{The token embedding maps tokens to residual stream vectors.}}$$





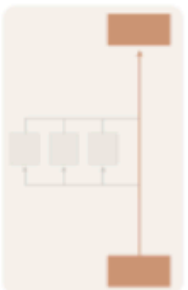
where $A^h = \underbrace{\mathrm{softmax}^*}_{\text{Softmax with autoregressive masking}}\left(\underbrace{t^T \cdot W_E^T W_{QK}^h W_E \cdot t}_{\text{Attention pattern logits are produced by multiplying pairs of tokens through different sides of } W_{QK}^h.}\right)$

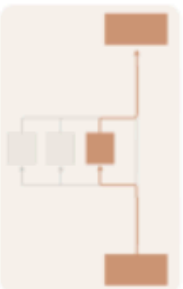


Source: Elhage et al., "A Mathematical Framework for Transformer Circuits" (2021)

Single-layer circuits: Mathematical reformulation (cont.)

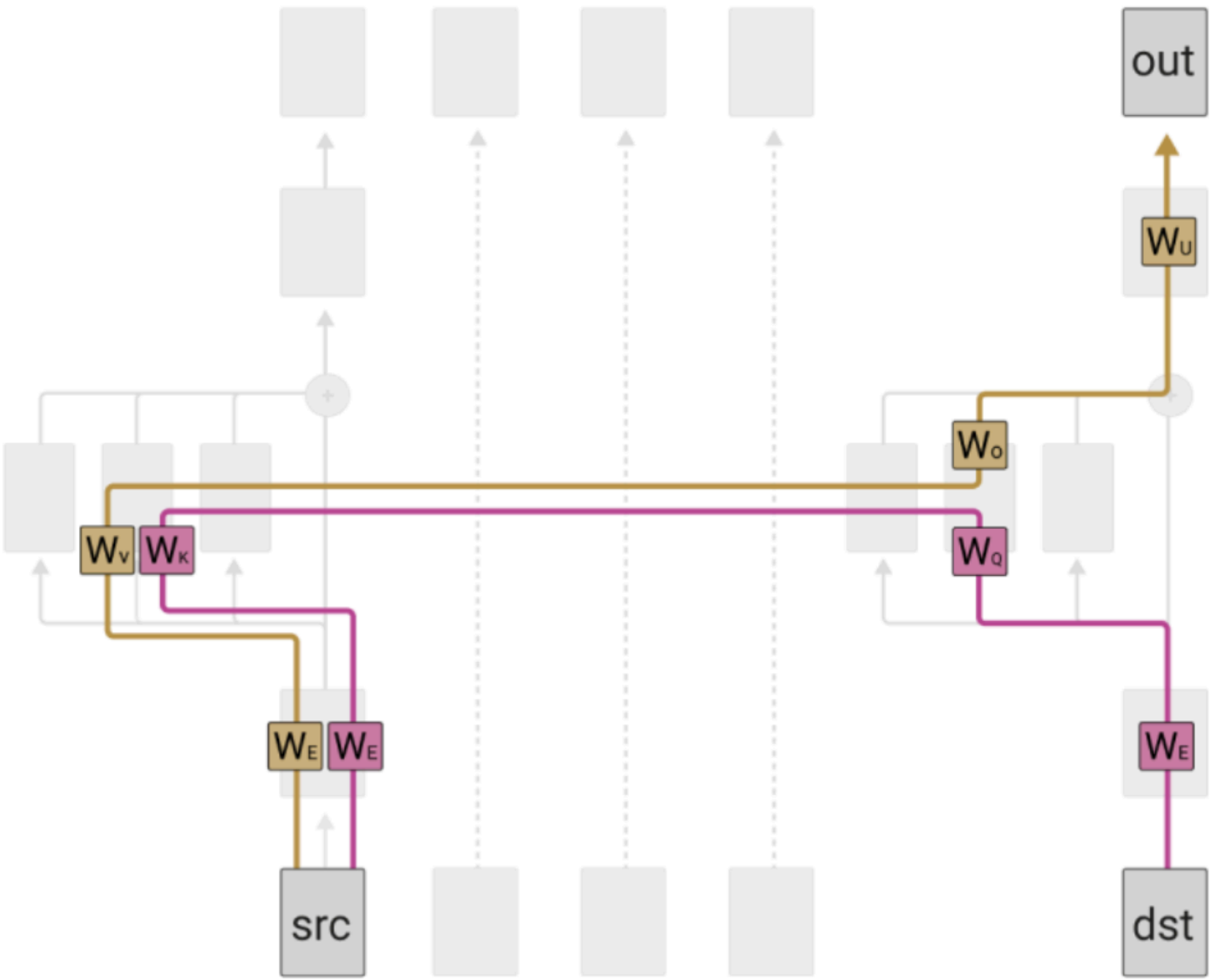
$$T = \underbrace{\mathrm{Id} \otimes W_U W_E}_{\text{“Direct path” term contributes to bigram statistics.}} + \underbrace{\sum_{h \in H} A^h \otimes (W_U W_{OV}^h W_E)}_{\text{The attention head terms describe the effects of attention heads in linking input tokens to logits. } A^h \text{ describes which tokens are attended to while } W_U W_{OV}^h W_E \text{ describes how each token changes the logits if attended to.}}$$





Source: Elhage et al., “A Mathematical Framework for Transformer Circuits” (2021)

Splitting attention head terms into QK and OV circuits



The **OV ("output-value") circuit** determines how attending to a given token affects the logits.

$$W_U W_O W_V W_E$$

The **QK ("query-key") circuit** controls which tokens the head prefers to attend to.

$$W_E^T W_Q^T W_K W_E$$

Source: Elhage et al., "A Mathematical Framework for Transformer Circuits" (2021)

QK and OV circuits: The atomic units of attention heads

Each attention head decomposes into two independent circuits:

QK Circuit — "Where to look"

$$A = \text{softmax}\left(\frac{x^T W_Q^T W_K x}{\sqrt{d_k}}\right)$$

Determines attention pattern: which source positions does each destination attend to?

OV Circuit — "What to move"

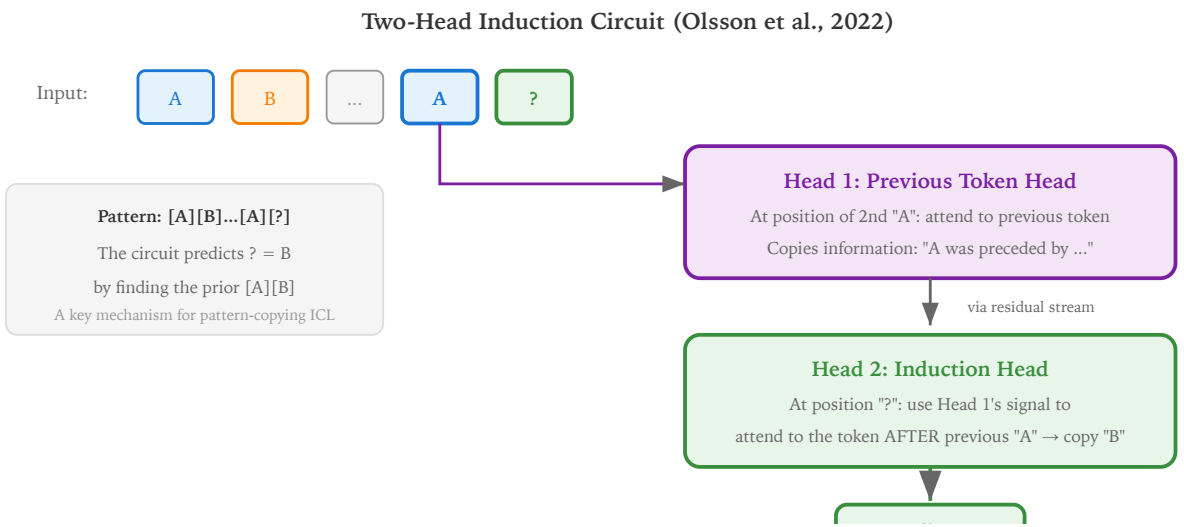
$$\text{output} = A \cdot x \cdot W_V W_O$$

Determines what information gets read from the attended position and how it's written to the residual stream.

Key insight (Elhage et al., 2021): A single attention head is the *atomic unit* of transformer computation. The QK and OV circuits can be analyzed independently — this is what makes mechanistic interpretability tractable at the single-head level.

Induction heads and name movers: One-layer circuit motifs

The induction head circuit — the mechanistic basis of in-context learning:



Name Mover Heads (Wang et al., 2022)

In the IOI circuit ("When Mary and John went to the store, John gave a drink to ___"): name mover heads attend to "Mary" and copy it to the final position. This is a **three-layer circuit** with ~26 heads playing distinct roles.

Activity: Compute a zero-layer prediction

Pair Activity (2 min)

Given this (simplified) bigram table from $W_U^T W_E$:

Input ↓ / Output →	the	cat	sat	on
the	0.1	**2.4**	0.8	0.3
cat	1.1	0.2	**2.7**	0.6
sat	0.5	0.3	0.1	**3.1**
on	**2.9**	0.7	0.4	0.2

1. What does the zero-layer model predict after “the”? After “sat”?
2. Why is this a useful **baseline** for understanding what attention heads add?

Two-layer composition: How circuits chain together

When one head's output becomes another head's input, three types of composition arise:

Q-Composition

Head A's output is read by Head B's **query** — changes *where* Head B attends based on what Head A found.

K-Composition

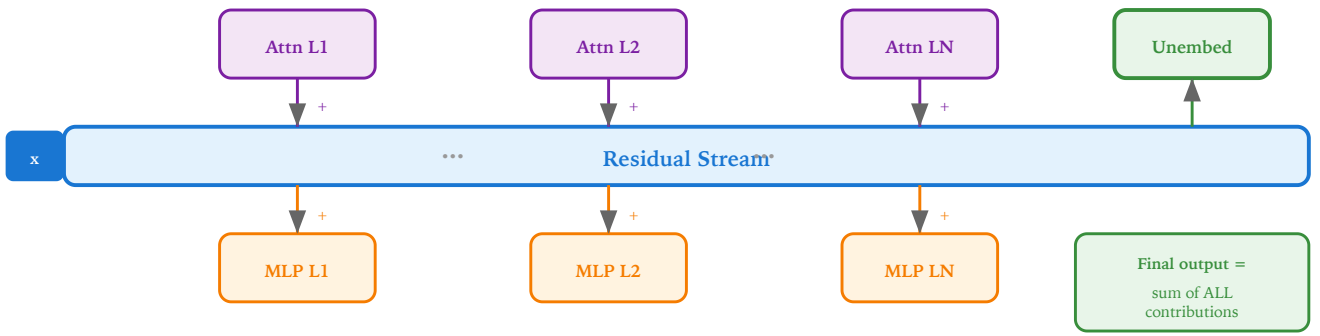
Head A's output is read by Head B's **key** — changes *what positions become attended* based on Head A's computation.

V-Composition

Head A's output is read by Head B's **value** — changes *what information gets moved* at positions Head B already attends to.

Example: The induction circuit is K-composition — the previous-token head writes to the residual stream, and the induction head reads it via its key, changing which positions match the current query.

The residual stream: A shared communication bus



- The residual stream is a **high-dimensional shared workspace** — every layer reads from it and writes back to it
- Each layer's contribution is **additive**: $x_{out} = x_{in} + \text{Attn}(x) + \text{MLP}(x)$
- This additive structure is why we can decompose the model into circuits at all

Theme 1: Circuits are the atoms of understanding — the residual stream is what makes them composable.

The combinatorial wall: Why circuit analysis doesn't simply scale

As models grow, the number of possible interaction paths explodes:

Model	Layers	Heads/Layer	Total Heads	2-Head Paths	All Paths
GPT-2 Small	12	12	144	~10K	$\sim 10^6$
GPT-2 XL	48	25	1,200	~700K	$\sim 10^{26}$
Llama 70B	80	64	5,120	~13M	$\sim 10^{100+}$

- You **cannot** enumerate all circuits in a frontier model — the combinatorics are astronomical
- This motivates every tool in Part 2: we need methods that bypass exhaustive circuit search

Theme 2: Scaling requires new tools, not just more patience.

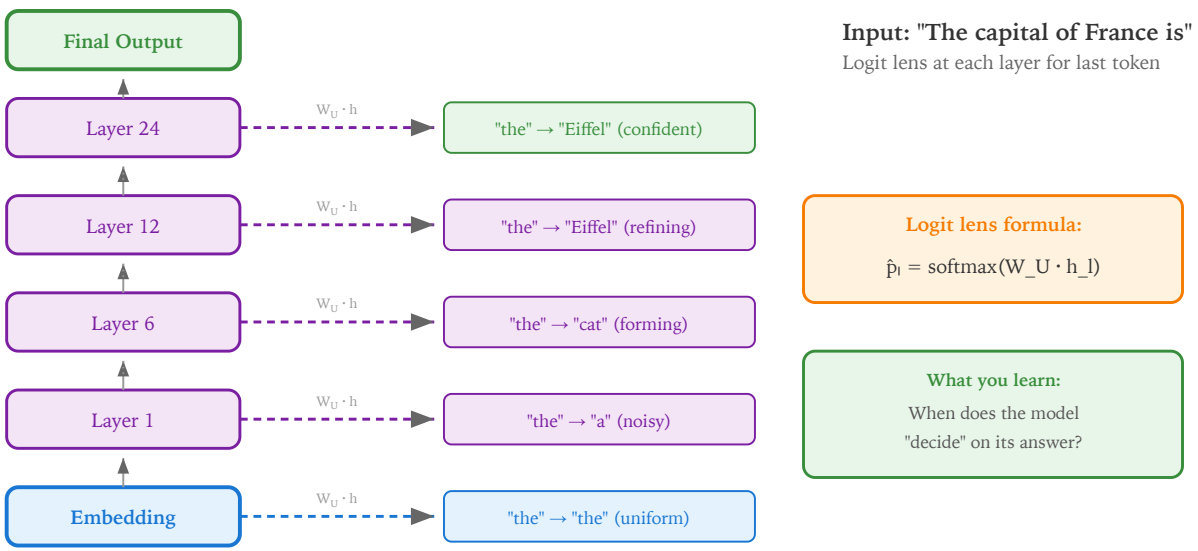
Part 2: Scaling Tools

From circuits to scalable methods

Since we can't trace every circuit by hand, we need tools that summarize internal computation. Each tool trades off fidelity for scalability.

The logit lens: Reading the residual stream as vocabulary predictions

Idea (nostalgebraist, 2020): At every layer, project the residual stream through the unembedding matrix to see what the model would predict *if it stopped here*.



Tuned lens: Fixing the logit lens's calibration problem

Logit Lens Limitation

The unembedding matrix W_U was trained for **final-layer** representations. Early-layer projections are miscalibrated — they overestimate certainty on wrong tokens.

Early-layer residual stream representations live in a different subspace than the final layer expects.

Tuned Lens Fix (Belrose et al., 2023)

Train a **learned affine probe per layer**:

$$\hat{p}_l = \text{softmax}(W_U \cdot (A_l h_l + b_l))$$

Each A_l, b_l is trained to align layer l's representation space with the final unembedding. Only the affine parameters are learned; the model is frozen.

- Tuned lens gives **better-calibrated** predictions at every layer, especially in early/middle layers
- Reveals a cleaner picture of when the model forms its predictions

Probing classifiers: What is linearly decodable from representations?

Setup: Train a linear classifier on frozen embeddings: $y_i = \text{softmax}(Wh_i + b)$

Decodability

Information is linearly extractable from the representation. Cheap, scalable. BERT middle layers encode syntax best; upper layers encode semantics (Tenney et al., 2019).

≠ Causal Use

High probe accuracy does **not** mean the model *uses* that information. Hewitt & Liang (2019): use control tasks + selectivity. Amnesic probing (Elazar et al., 2021) removes information to test causal role.

Activity: Sketch a logit lens for “The Eiffel Tower is in”

Individual + Compare (3 min)

For the input **“The Eiffel Tower is in”**, sketch what you think the logit lens top-1 prediction would be at each layer:

Layer	Embedding	Layer 2	Layer 6	Layer 10	Layer 12	Final
Top-1	?	?	?	?	?	?
Confidence	low	?	?	?	?	high

1. Fill in your guesses, then compare with a neighbor
2. At what layer do you think “Paris” first appears as the top prediction?

Sparse autoencoders decompose superposed features into interpretable units

Superposition problem: Models encode more features than they have dimensions, causing features to overlap.

Without Disentangling

Neuron 42 fires for "France," "cheese," and "revolution" — **polysemantic**

With Sparse Autoencoder

Feature 107 = "France (country)", Feature 238 = "dairy products" — **monosemantic**

SAE objective — reconstruct activations with sparse features:

$$\mathcal{L} = \|h - \hat{h}\|_2^2 + \lambda \|z\|_1$$

where $\hat{h} = W_{dec} \cdot \text{ReLU}(W_{enc} \cdot h + b_{enc}) + b_{dec}$ and z are the encoder activations.

- **Reconstruction term** (L_2): features should faithfully reconstruct the original activation
- **Sparsity penalty** (L_1): only a few features should be active for any given input
- Bricken et al. (2023): thousands of interpretable features from Claude's MLP layers
- Templeton et al. (2024): scaled to Claude 3 Sonnet — **millions** of interpretable features

Activation patching and path patching: Causal tools for circuit discovery

Activation patching: Replace one activation with a value from a different context; measure the output change.

Path patching extends this to trace specific information routes:

Activation Patching

Patch *all* outputs of a component (head, layer, MLP). Tells you **what matters**.

Path Patching

Patch the output of component A *only as read by* component B. Tells you **how information flows** between specific components.

- Path patching was critical for the IOI circuit discovery (Wang et al., 2022) — identified which heads read from which other heads

The evidence hierarchy: Not all interpretability evidence is equal

5. Path Patching — STRONGEST
Traces causal flow between specific components

4. Activation Patching — CAUSAL
Causal effect of a component on output

3. Probing + Control Tasks — CONTROLLED
Decodability with selectivity baseline

2. Attention Visualization / Logit Lens — DESCRIPTIVE
Descriptive, correlational, suggestive

1. Behavioral Testing Only — WEAKEST
Input-output, no internal access

Part 3: Bridging to Practice

From understanding to deployment

Mechanistic knowledge is only useful if it changes what you do. This section asks: when does circuit-level understanding actually help in practice?

Steering vectors: Editing model behavior via representations

Core idea: Find a direction in activation space that corresponds to a concept, then add or subtract it at inference time.

$$v_{\text{steer}} = \text{mean}(h_+) - \text{mean}(h_-)$$

where h_+ are activations from positive examples and h_- from negative examples.

Computing the Vector

1. Collect activations on "honest" prompts → h_+
2. Collect activations on "deceptive" prompts → h_-
3. Difference of means = steering direction

Applying the Vector

At layer l: $h'_l = h_l + \alpha \cdot v_{\text{steer}}$
$\alpha > 0$: amplify the concept
$\alpha < 0$: suppress the concept
No retraining required — inference-time only

Examples from representation engineering (Zou et al., 2023):

- Honesty/deception, positive/negative sentiment, refusal/compliance
- Works across many prompts, not just the training examples

Caveat: Steering vectors are a blunt instrument. They affect all inputs, not just the targeted behavior. Side effects on unrelated capabilities are common and hard to predict.

Mechanistic red teaming: Using circuits to find failure modes

	Traditional Red Teaming	Mechanistic Red Teaming
Approach	Craft adversarial inputs, observe outputs	Identify vulnerable circuits, predict failure modes
Evidence	Behavioral (found an exploit)	Mechanistic (understand *why* it fails)
Scalability	Scales with human effort / automation	Currently limited to smaller models / specific circuits
Fixes	Patch the input (filter, RLHF)	Patch the circuit (ablation, steering, editing)
Maturity	Production-ready	Research stage

- The promise: if you understand *why* a model fails, you can anticipate *new* failure modes, not just patch known ones
- The reality: mechanistic red teaming currently works best on targeted, well-defined behaviors (bias in specific circuits, knowledge errors in specific MLPs)

Activity: When is mechanistic understanding necessary?

Pair Debate (3 min)

For each scenario, argue: is **behavioral testing sufficient**, or do you need **mechanistic understanding**?

A. Customer-service chatbot for an e-commerce site

B. Medical diagnosis assistant recommending treatments

C. Content moderation system for a social platform

D. Research tool: "Does GPT-4 have a model of other agents' beliefs (theory of mind)?"

For each: What could go wrong? What level of evidence (from the hierarchy) do you need?

Behavioral vs. mechanistic evidence: What does deployment require?

Behavioral Evidence

Strengths: Scalable, fast, applicable to any model, maps directly to user experience

Weaknesses: Can miss systematic failures, doesn't explain causes, vulnerable to dataset artifacts

Best for: Deployment monitoring, A/B testing, regression checks

Mechanistic Evidence

Strengths: Explains causes, can predict novel failures, enables targeted fixes

Weaknesses: Expensive, limited to smaller models/specific tasks, may not generalize

Best for: Safety audits, debugging specific failures, scientific understanding

Regulatory note: The EU AI Act (2024) requires "sufficient transparency" for high-risk AI systems, but does not mandate mechanistic interpretability specifically. The NIST AI RMF similarly emphasizes risk-proportionate transparency. In practice, behavioral testing + documentation currently satisfies most compliance requirements.

Production interpretability: What ships today vs. what's still research

Ships Today

PRODUCTION

Feature attribution (SHAP, integrated gradients) · Attention visualization · Token-level saliency maps · Confidence calibration · Behavioral test suites

Emerging / Limited Deployment

PILOT

SAE-based feature dashboards · Steering vectors for behavior control · Probing-based runtime monitoring · Activation anomaly detection

Research Only

LAB

Full circuit reverse-engineering · Automated circuit discovery · Model editing (ROME/MEMIT) at scale · Formal verification of neural networks

The production interpretability stack

A realistic 4-step workflow for incorporating interpretability into a deployed LLM system:

1. Pre-Deploy Audit

Behavioral test suites + probing for known risks (bias, factuality, safety). Establish baselines. Identify critical failure modes with targeted red teaming.

2. Runtime Monitoring

Confidence calibration, output distribution tracking, activation anomaly detection (if feasible). Flag outputs that deviate from expected patterns.

3. Incident Investigation

When failures occur: feature attribution → probing → activation patching (if needed). Escalate from behavioral to mechanistic evidence as needed.

4. Continuous Improvement

Feed findings back: update test suites, adjust steering vectors, retrain probes, fine-tune on failure cases. Close the loop.

Theme 3: Practice demands honest limits — the stack escalates from cheap/shallow to expensive/deep only as needed.

Part 4: Honest Assessment

Where are we, really?

Interpretability has made remarkable progress. It also has fundamental unsolved problems. This section is about being honest about both.

What works today

Circuits on Small Models

Complete circuit analysis for specific tasks on GPT-2 scale models. Induction heads, IOI circuit, greater-than circuit. These are **real, validated, causal** findings.

Olsson et al. 2022, Wang et al. 2022, Hanna et al. 2023

SAEs at Scale

Millions of interpretable features extracted from Claude 3 Sonnet. Feature steering demonstrably changes behavior. A breakthrough in dealing with superposition.

Bricken et al. 2023, Templeton et al. 2024

Behavioral Probing

Probes reliably identify what information is encoded where. Combined with control tasks, this is a mature methodology. Practical for deployment monitoring.

Belinkov 2022, Hewitt & Liang 2019

Activity: Works / Open / Wishful Thinking

Rapid Vote — Whole Class (2 min)

For each claim, vote: **Works** (solid evidence), **Open** (active research, unclear), or **Wishful** (no good evidence yet).

> **1.** "We can identify the circuit for any specific behavior in GPT-2."

> **2.** "SAE features correspond to human-interpretable concepts."

> **3.** "Mechanistic interpretability can prevent deceptive alignment."

> **4.** "Probing tells us what the model 'believes.'"

> **5.** "We'll have full mechanistic understanding of frontier models within 5 years."

(Show of hands for each. Instructor reveals suggested answers after all votes.)

Open problems: What the field hasn’t solved

Scaling

Circuit analysis works on GPT-2 (117M params). Frontier models are 100-1000x larger. No one has reverse-engineered a complete circuit in a 70B+ model.

Superposition

SAEs help, but we don't know if they fully resolve superposition. Features may have complex, non-linear interactions that sparse decomposition misses.

Validation

How do you verify that a discovered "circuit" is the real mechanism, not an artifact of your analysis method? Ground truth is rarely available.

Closing the Loop

Interpretability findings rarely lead to concrete model improvements. The field needs better workflows from "we understand X" to "we fixed Y."

The path forward

Hybrid Approaches

Use mechanistic insights to **guide** behavioral testing:

- Circuit analysis identifies a bias mechanism → design targeted behavioral tests
- SAE features flag anomalous activations → trigger deeper investigation
- Probing reveals unexpected encoding → validate with causal intervention

The two levels of evidence are **complementary**, not competing.

Automated Interpretability

Use models to interpret models:

- LLMs label SAE features (Bills et al., 2023)
- Automated circuit discovery (Conmy et al., 2023 — ACDC)
- Scalable oversight: models audit each other's internals

Promise: overcomes the human bottleneck. Risk: introduces new failure modes (LLM labelers can hallucinate).

Summary: Key Takeaways

1. **Circuits** (zero/one/two-layer) provide the mathematical foundation — the residual stream's additive structure makes decomposition possible
2. **The combinatorial wall** is real — scaling from GPT-2 to frontier models requires fundamentally new approaches
3. **Scaling tools** (logit lens, probes, SAEs, patching) trade fidelity for tractability — know where each sits on the evidence hierarchy
4. **Causal evidence** (patching) is stronger than representational evidence (probes) is stronger than behavioral evidence (testing) — but each has its place
5. **Practice demands honesty** — production systems mostly use behavioral methods; mechanistic analysis is reserved for when you need to know *why*
6. **The path forward** is hybrid: mechanistic insights guiding behavioral tests, with automation closing the scalability gap

Further Reading

References & Resources

1. Elhage et al., **"A Mathematical Framework for Transformer Circuits"** (Anthropic, 2021) — The foundational paper on QK/OV circuits and composition
2. Olsson et al., **"In-context Learning and Induction Heads"** (Anthropic, 2022) — Mechanistic explanation of in-context learning
3. Bricken et al., **"Towards Monosemanticity"** (Anthropic, 2023) — Sparse autoencoders for feature extraction
4. Templeton et al., **"Scaling Monosemanticity"** (Anthropic, 2024) — SAEs at Claude 3 Sonnet scale
5. nostalgebraist, **"interpreting GPT: the logit lens"** (2020) — The original logit lens blog post
6. Wang et al., **"Interpretability in the Wild: IOI"** (2022) — Most complete circuit reverse-engineering to date
7. Belrose et al., **"Eliciting Latent Predictions with the Tuned Lens"** (2023) — Calibrated layer-wise predictions
8. Zou et al., **"Representation Engineering"** (2023) — Steering vectors and concept directions
9. Conmy et al., **"Towards Automated Circuit Discovery"** (2023) — ACDC for scalable circuit finding

Coming Up Next

March 3: Evaluation and Benchmarking

- How do we measure what models can and can’t do?
- Contamination, data leakage, and the benchmark treadmill
- Designing evaluations that actually inform deployment decisions