Introducing Mechanistic Interpretability: Demistify black boxes with **Circuit Analaysis**¹ & **Monosemanticity**²

J. Setpal

February {1, 8}, 2024



https://transformer-circuits.pub/2021/framework/

https://transformer-circuits.pub/2023/monosemantic-features/

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Mechanistic Interpretability

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Background & Intuition

2 Transformer Circuit Analysis

3 Towards Monosemanticity

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Today, we will interpret deep neural networks (transformer).

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If we are able to *completely understand* a toy model, we can:

- understand why attention works.
- observe recurring patterns in complex models.

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Mechanistic Interpretability is a subset of interpretability, that places a focus on **reverse engineering neural networks**.

It seeks to understand functions that *individual neurons* play in the inference of a neural network.

This can subsequently be used to offer high-level explanations for decisions, as well as guarantees during inference.

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We query it to subset the important tokens. For $\{x_i\}_{i=1}^t$,

$$\alpha_i = \sigma_{softmax} \left(\frac{q_i k_i^T}{\sqrt{d_k}} \right) \tag{2}$$

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Observation: The equation is linear, if we fix attention patterns.

Reframing using Tensorization (3/3)

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And then apply them to unnormalized³ attention:

$$A = \sigma_{softmax} \left([q_i k_j^T]_{i,j} \right) \tag{13}$$

$$=\sigma_{softmax}\left(t_{0}^{T}\cdot\left(I\otimes W_{E}^{T}W_{Q}^{T}\right)\cdot\left(I\otimes W_{K}W_{E}\right)\cdot t_{0}\right)$$
(14)

$$=\sigma_{softmax}\left(t_{0}^{T}\cdot W_{E}^{T}W_{Q}^{T}W_{K}W_{E}\cdot t_{0}\right)$$
(15)

³to ease computation.

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Unravelling QK, OV Circuits (1/3)

Here's the two tensor equations combined:

$$T = W_U W_E + \sum_{h \in H} (A^h \otimes W_U W_O^h W_V^h W_E)$$
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c. *A* **learns independently** from the rest of the tensor equation. However, we're still missing one. Importantly, both equations have (|voc|, |voc|) size matrices:

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- a. The **Output-Value(OV) Circuit** $W_U W_O^h W_V^h W_E$: determines how attending to a token affects logits.
- b. The **Query-Key(QK)** Circuit $W_E^T W_Q^T W_K W_E$: determines which tokens to attend to.

Unravelling QK, OV Circuits (3/3)



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Interpretation as Skip-Trigrams

We can think through inference procedure with single source token.⁴

⁴for simplicity.

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Interpretation as Skip-Trigrams

We can think through inference procedure with single source token.⁴

From there, we look at the largest QK and OV entries.

Some examples of large entries QK/OV circuit

Source Token	Destination Token	Out Token	Example Skip Tri-grams	
" perfect"	" are", " looks",	" perfect" , " super",	" perfect are perfect",	
	" is", " provides"	" absolute", " pure"	" perfect looks super"	
" large"	" contains", " using",	" large", " small",	" large using large",	
	" specify", " contain"	" very", " huge"	" large contains small"	
" two"	" One", "\n ", " has",	" two", " three", " four",	" two One two",	
	"\r\n ", "One"	" five", " one"	" two has three"	
"lambda"	"\$\\", "}{\\", "+\\",	"lambda", "sorted",	"lambda \$\\lambda",	
	"(\\", "\${\\"	" lambda", "operator"	"lambda +\\lambda"	
"nbsp"	"&", "\"&", "}&",	"nbsp", "01", "gt", "00012",	"nbsp ",	
	">&", "=&"	"nbs", "quot"	"nbsp > "	
"Great"	"The", " The", " the",	" Great", " great",	"Great The Great",	
	" contains", " /"	" poor", " Every"	"Great the great"	

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Eigenvalue Analysis

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Eigenvalue analysis of first layer attention head OV circuits

10/12 of layer 1 heads have mostly positive OV eigenvalues, and appear to significantly perform copying



We use a **log scale** to represent magnitude, since it varies by many orders of magnitude.

Eigenvalue distribution for randomly initialized weights. Note that the mostly – and in some cases, entirely – positive eigenvalues we observe are very different from what we randomly expect.



Importantly, note that positive eigenvalues mean they are copying 'on average', and are not definitive.

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This is superposition.

When we perform an indvidual analysis of neurons, it fires for unrelated concepts.

This is **polysemanticity**.

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Updated Architecture

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Let's instead analyze the following architecture *empirically*:



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Training Setup

	Transformer	Sparse Autoencoder	
Layers 1 Attention Block 1 MLP Block	1 Attention Block	1 ReLU	
	1 MLP Block	1 Linear	
MLP Size	512	$512 imes f \in \{1, \dots, 256\}^5$	
Dataset	The Pile (100B tokens)	Activations (8B samples)	
Loss		L2 Reconstruction	
	Autoregressive Log-Likelihood	L1 on hidden-layer activation	

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Objective: polysemantic activations $\stackrel{Tr}{\rightarrow}$ monosemantic features.

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The sparse, overcomplete autoencoder is trained against this objective.

- 1. **Sparse** because we constrain activations (L1 penalty).
- 2. **Overcomplete** because the hidden layer exceeds the input dimension.

 $^{{}^{5}}f = 8$ for our analysis

Given $X := \{x^j\}_{j=1}^K$; $x_j \in \mathbb{R}^d$, we wish to find $D \in \mathbb{R}^{d \times n}$, $R \in \mathbb{R}^n$ s.t: $||X - DR||_F^2 \approx 0$ (17)

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We can motivate our objective transformation by linear factorization:

$$x^{j} \approx b + \sum_{i} f_{i}(x^{j})d_{i}$$
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$$f_i = \sigma_{ReLU}(W_E(x - b_D) + b_E)$$
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where d_i is the 'feature direction' represented as columns of the W_D .

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- a. Training data $\propto n$ (interpretable features).
- b. Tying b_D before the encoder and after the decoder improves performance.

Given
$$X := \{x^j\}_{j=1}^K$$
; $x_j \in \mathbb{R}^d$, we wish to find $D \in \mathbb{R}^{d \times n}$, $R \in \mathbb{R}^n$ s.t:
$$||X - DR||_F^2 \approx 0$$
(17)

We can motivate our objective transformation by linear factorization:

$$x^{j} \approx b + \sum_{i} f_{i}(x^{j})d_{i}$$
(18)

$$f_i = \sigma_{ReLU}(W_E(x - b_D) + b_E)$$
(19)

where d_i is the 'feature direction' represented as columns of the W_D .

Some interesting implementation notes:

- a. Training data \propto *n*(interpretable features).
- b. Tying b_D before the encoder and after the decoder improves performance.
- c. Dead neurons are periodically *resampled* to improve feature representations.

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Evaluating Interpretability

Reliable evaluations on interpretability were scored based on a rubric:



Automated Interpretability - Activation



Features were found to be interpretable when score > 8.

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Analyzing Arabic Features

Let's analyze feature A/1/3450, that fires on Arabic Script.

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 $LL(t) = \log \left(P(t | \text{Arabic}) / P(t) \right)$

We can evaluate each token using the log-likelihood ratio:

Despite representing 0.13% of training data, arabic script makes up 81% of active tokens:

Mechanistic Interpretability

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(20)

They can be used to steer generation.



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Approach: Set high values of features demonstrating desired behaviors, and then sample from the model.

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Approach: Set high values of features demonstrating desired behaviors, and then sample from the model.

We observe that interpreted features are actively used by the model.

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Finite State Automaton

A unique feature of features is their role as finite state automaton.

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These present partial explanations of memorizations within transformers:



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If you can view this screen, I am making a mistake.

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Have an awesome rest of your day!

Slides: https://cs.purdue.edu/homes/jsetpal/slides/mechinterp.pdf