## Introducing Mechanistic Interpretability:

Demistify black boxes with Circuit Analaysis ${ }^{1}$ \& Monosemanticity ${ }^{2}$

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## MACHINE LEARNING @ PURDUE

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## Outline

(1) Background \& Intuition
(2) Transformer Circuit Analysis
(3) Towards Monosemanticity

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

## What will we Achieve Today?



Specifically, we'll analyze the 1-layer attention model.

For mathematical simplicity, this model ignores biases, layer-norm and dense layers.

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- 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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## Self-Attention Synopsis

$n$-gram models used the following incorrect assumption:

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\begin{equation*}
p\left(x_{t} \mid\left\{x_{i}\right\}_{i=1}^{t-1} ; \theta\right) \not \approx p\left(x_{t} \mid x_{t-1} ; \theta\right) \tag{1}
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We query it to subset the important tokens. For $\left\{x_{i}\right\}_{i=1}^{t}$,

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\begin{equation*}
\alpha_{i}=\sigma_{\text {softmax }}\left(\frac{q_{i} k_{i}^{T}}{\sqrt{d_{k}}}\right) \tag{2}
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## Reframing using Tensorization (1/3)

We can represent attention using tensor products:

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

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And then apply them to unnormalized ${ }^{3}$ attention:

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\begin{align*}
A & =\sigma_{\text {softmax }}\left(\left[q_{i} k_{j}^{T}\right]_{i, j}\right)  \tag{13}\\
& =\sigma_{\text {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)  \tag{14}\\
& =\sigma_{\text {softmax }}\left(t_{0}^{T} \cdot W_{E}^{T} W_{Q}^{T} W_{K} W_{E} \cdot t_{0}\right) \tag{15}
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## Unravelling QK, OV Circuits (1/3)

Here's the two tensor equations combined:

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T & =W_{U} W_{E}+\sum_{h \in H}\left(A^{h} \otimes W_{U} W_{O}^{h} W_{V}^{h} W_{E}\right)  \tag{10}\\
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However, we're still missing one.

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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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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 |  |
| :--- | :--- | :--- | :--- | :--- | :--- |

${ }^{4}$ for simplicity.

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This is useful when we map a vector space upon itself.
Eigenvalue analysis of first layer attention head OV circuits


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.

## Updated Architecture

Previously, we used an attention-only model, since the MLP was too hard to analyze mathematically.

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Let's instead analyze the following architecture empirically:


## Training Setup

## Transformer

## Sparse Autoencoder

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

[^1]
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${ }^{5} f=8$ for our analysis

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Activations (8B samples)
L2 Reconstruction
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Objective: polysemantic activations $\xrightarrow{T_{r}}$ monosemantic features.
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.
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## Sparse Dictionary Learning

Given $X:=\left\{x^{j}\right\}_{j=1}^{K} ; x_{i} \in \mathbb{R}^{d}$, we wish to find $D \in \mathbb{R}^{d \times n}, R \in \mathbb{R}^{n}$ s.t:

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\|X-D R\|_{F}^{2} \approx 0 \tag{17}
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We can motivate our objective transformation by linear factorization:

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\begin{gather*}
x^{j} \approx b+\sum_{i} f_{i}\left(x^{j}\right) d_{i}  \tag{18}\\
f_{i}=\sigma_{\operatorname{ReLU} U}\left(W_{E}\left(x-b_{D}\right)+b_{E}\right) \tag{19}
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where $d_{i}$ is the 'feature direction' represented as columns of the $W_{D}$.

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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.

## Evaluating Interpretability

Reliable evaluations on interpretability were scored based on a rubric:


Features were found to be interpretable when score $>8$.

## Analyzing Arabic Features

Let's analyze feature $\mathbf{A} / \mathbf{1} / \mathbf{3 4 5 0}$, that fires on Arabic Script.

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Let's analyze feature $\mathbf{A} / \mathbf{1} / \mathbf{3 4 5 0}$, that fires on Arabic Script.
This is effectively invisible when viewed through the polysemantic model!
We can evaluate each token using the log-likelihood ratio:

$$
\begin{equation*}
L L(t)=\log (P(t \mid \text { Arabic }) / P(t)) \tag{20}
\end{equation*}
$$

Feature Activation Distribution (A/1/3450)

Despite representing 0.13\% of training data, arabic script makes up $\mathbf{8 1 \%}$ of active tokens:


## Pinned Feature Sampling

## They can be used to steer generation．

| 1，2，3，4，5，6，7，8，9，10 | No Intervention $\longrightarrow, 8,30,20,8,10,10$ |
| :---: | :---: |
| We sample from the | ＋Han Chinese（A）1／2000）$\longrightarrow$ ，女泳美圳， |
|  | ＋base64（A／1／2357）$\longrightarrow$ 29VHA98Z1Y9Z1 |
| 0.5 with various features pinned to a | ＋DNA（A／1／2937）$\longrightarrow$ AGACCAGAGAGAGACAGAGAGAGGG |
| high value．This | ＋Uppercase（A／1／3405）$\longrightarrow$ USING IN THE UNITED STATES |
| generates text consistent with | + Hexadecimal（A／1／3817）$\longrightarrow$ E9D9A0C1C2C3 |
| feature | ＋Arabic（A／1／3450）$\longrightarrow$ ¢سوع الديد الت |
| interpretations． | ＋Hebrew（A／1／416） |

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

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

## Finite State Automaton

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Unlike circuits, these work by daisy chaining features that increase the probability of another feature firing in a loop-like fashion.

These present partial explanations of memorizations within transformers:


## Reimplementation

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

## Thank you!

## Have an awesome rest of your day!

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


[^0]:    $1_{\text {https://transformer-circuits.pub/2021/framework/ }}$
    2
    https://transformer-circuits.pub/2023/monosemantic-features/

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