Understanding Large Language Models

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Session 10: Mechanistic Interpretability

Main learning goals

1. Recap
   - what-if exploration, SHAP, probing classifiers
2. Early Decoding
   - logit lens, examples
3. Residual Stream
   - rediscovering the Transformer, residual streams, head types
4. Activation Patching
   - setup, examples, metrics, direction
5. Circuit Analysis
   - more heads, causal scrubbing

Slides adapted from: Polina Tsvilodub, Ali Bahreinian, DeepLearning.ai

Recap

Counterfactual Analyses

Q: “how asymmetric are the white bricks on either side of the building”
A: *very*

Q: “how soon are the bricks fading on either side of the building”
A: *very*

Q: “how fast are the bricks speaking on either side of the building”
A: *very*

Paper: Did the model understand the question? ACL 2018

What-if Explorations

Probe the model on various What-If scenarios.

- Examples:
  - What if “he” was replaced with “she”
  - What if we add a punctuation at the end of the sentence
- **Intuitive:** What you see is what you get
- **Highly expressive:** Most explainability techniques are a summarization of what-if behavior

Applications:

- Model understanding / debugging
- Algorithmic Recourse
- Prompt design

SHAP

A company with two employees **Alice** and **Bob**

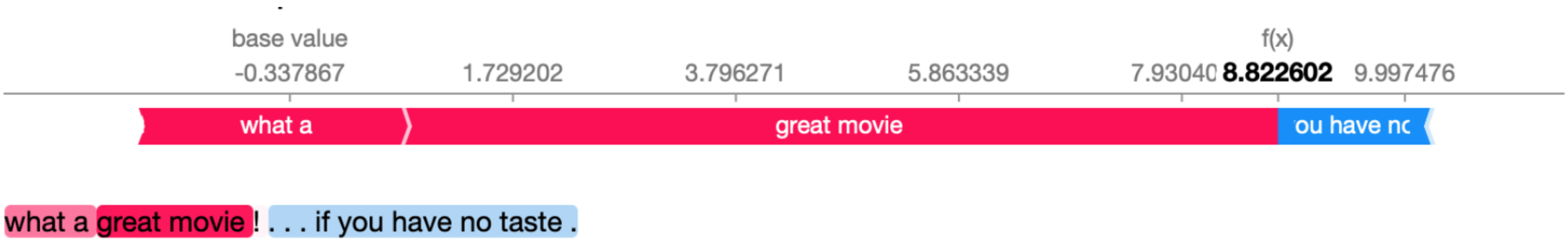
- No employees, no profit [v({}) = 0]
- Alice alone makes 20 units of profit [v({Alice}) = 20]
- Bob alone makes 10 units of profit [v({Bob}) = 10]
- Alice and Bob make 50 units of profit [v({Alice, Bob}) = 50]

What should the bonuses be?

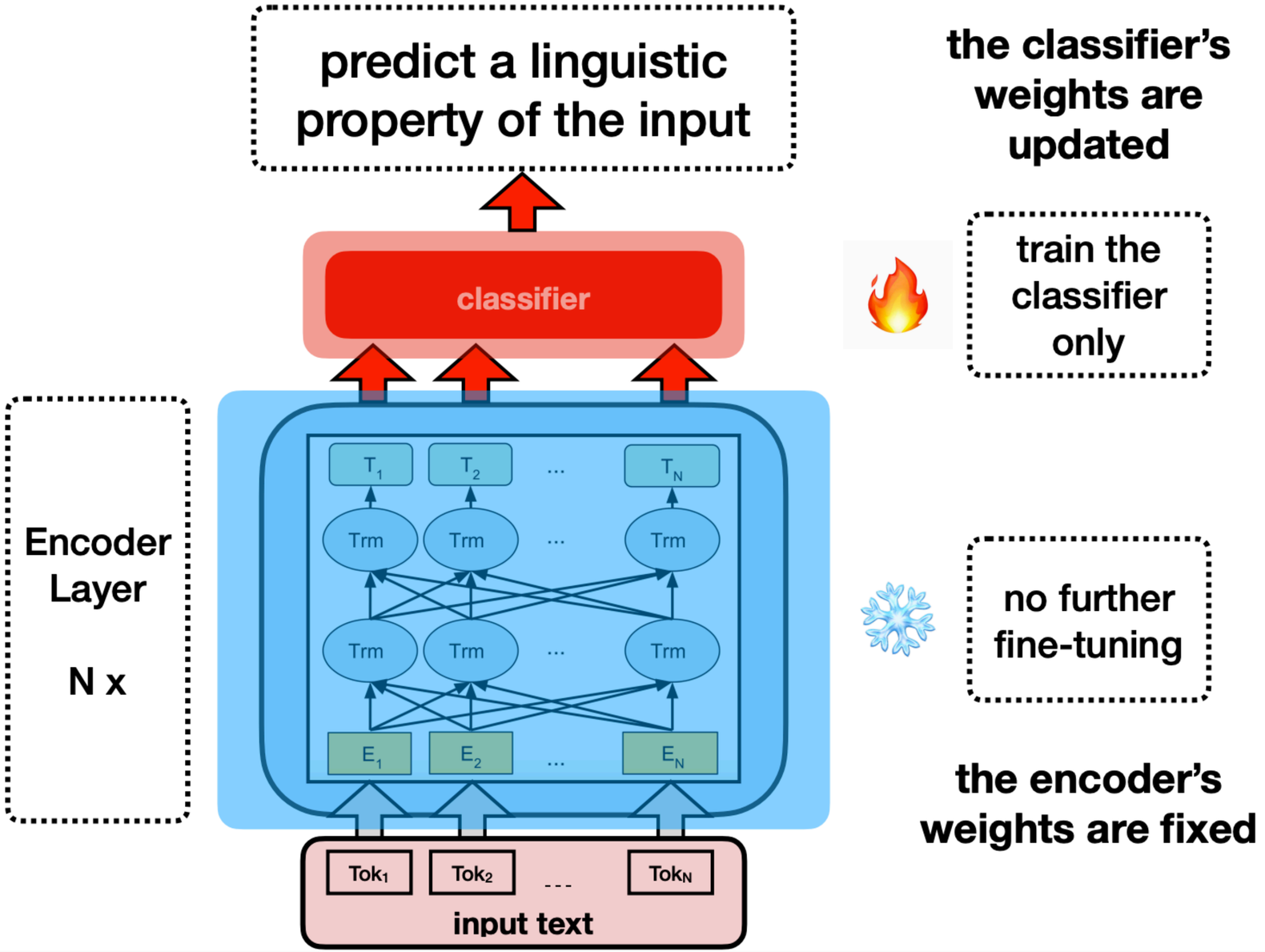
Permutation	**Marginal for Alice**	**Marginal for Bob**
Alice, Bob	20	30
Bob, Alice	40	10
Shapley Value	**30**	**20**

SHAP for NLP

- Tokens as players
- **positive** vs. **negative** affect



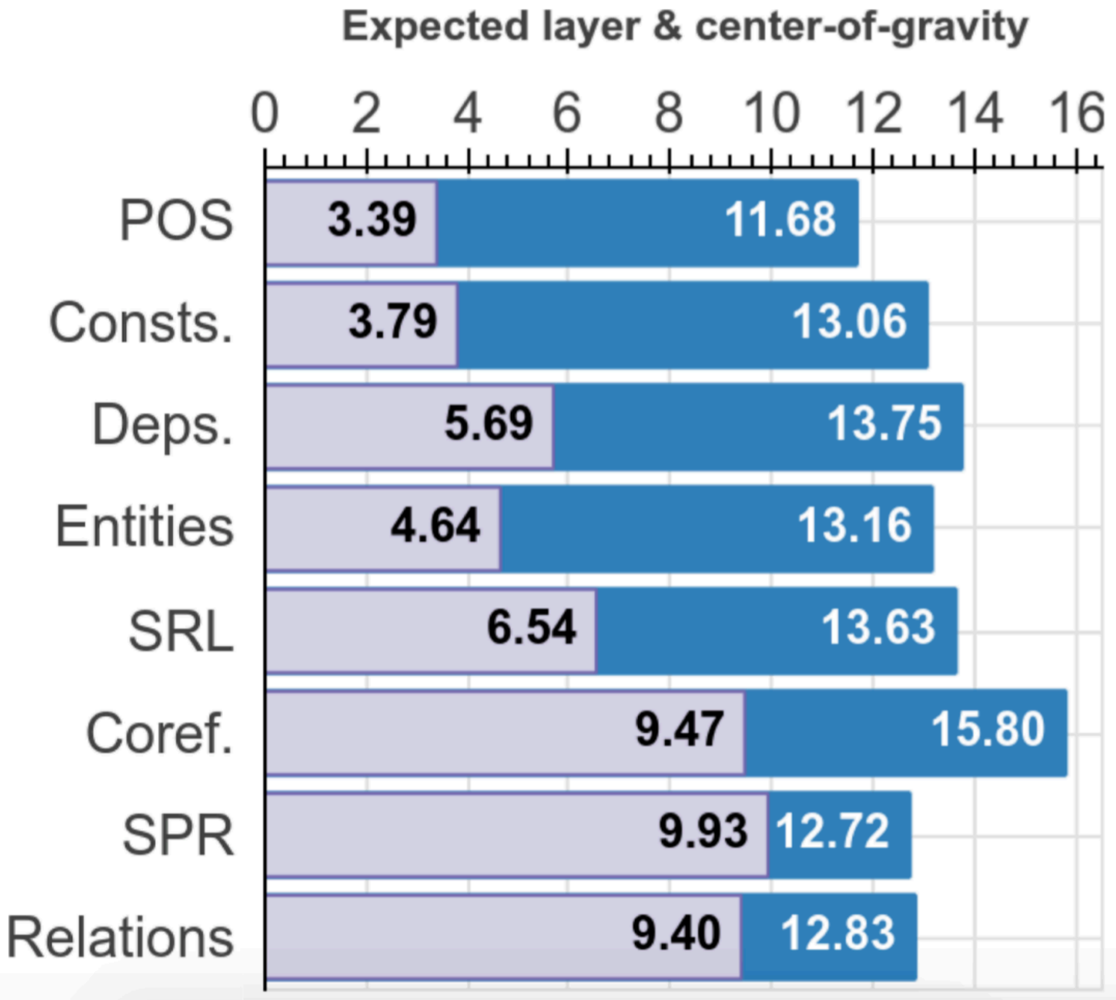
Probing


predict a linguistic property of the input
classifier
Encoder Layer
N x
T1
T2
...
TN
Trm
E1
E2
EN
Tok1
Tok2
TokN
input text
the classifier's weights are updated
train the classifier only
no further fine-tuning
the encoder's weights are fixed

Probing

the expected layer at which the probing model correctly labels an example

a higher center-of-gravity means that the information needed for that task is captured by higher layers



Where We Stand…

- Jittering the inputs (cleverly) and observing outputs
- Freezing parts of the model to understand their information content
- Problematic interpretation of negatives
  - Absence of signal
  - Low probe performance

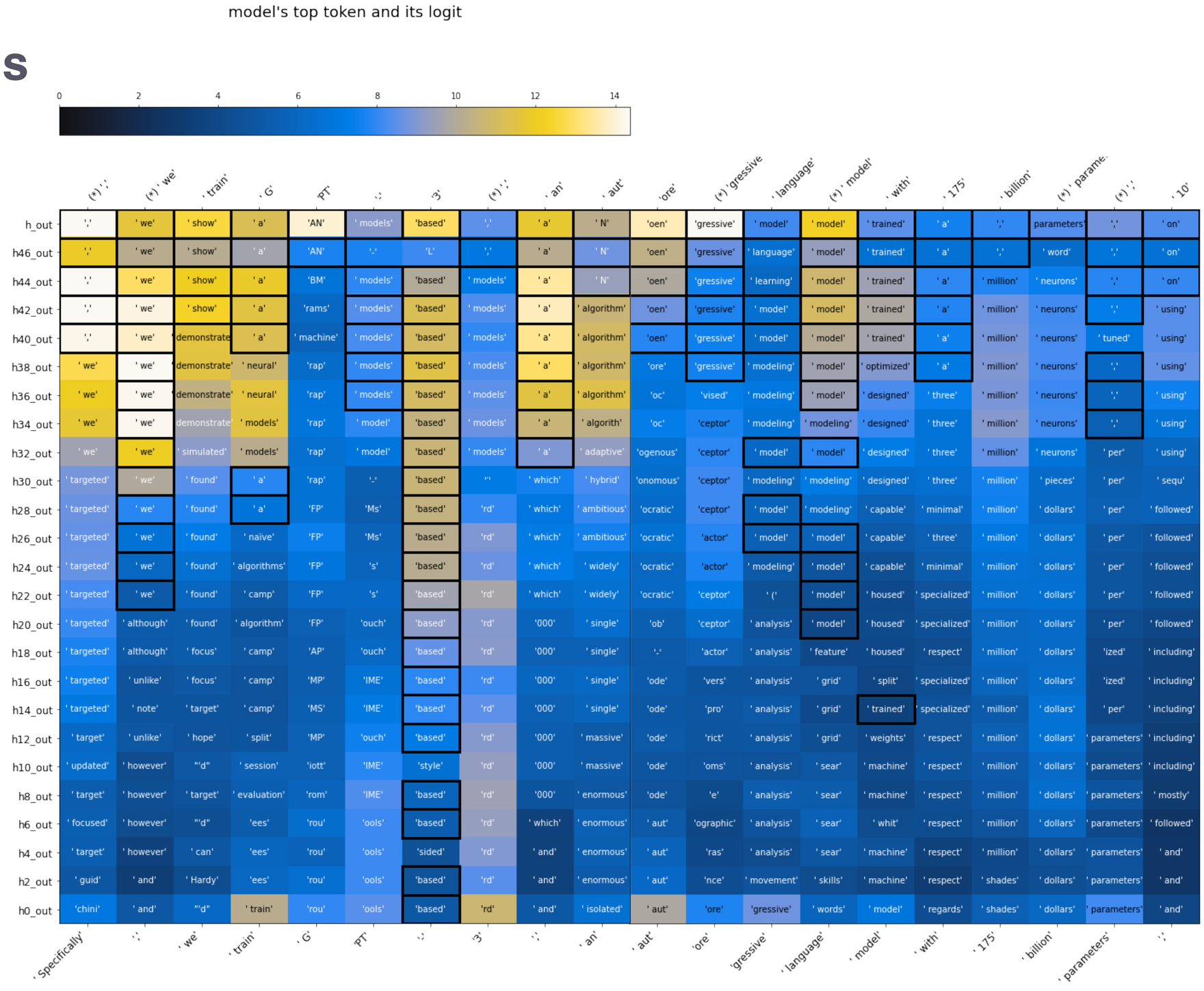
Early Decoding

Logit Lens

- From a distance, the Transformer:
  - Projects input tokens into high-dimensional embedding space
  - Modifies that space many times
  - Projects the final high-dimensional representation back to vocabulary space
- The shape of the embedding space remains constant across layers
- In the end, we have some dictionary W, that projects back to vocab space
- Let’s project to vocab space early
- What do early layers “want to say”?
- Reminiscent of probing classifiers

nostralgebraist. Interpreting GPT - The Logit Lens. 2020

Logit Lens


model's top token and its logit
0
2
4
6
8
10
12
14
(*) ' ,'
(*) ' we'
' train'
' G'
'PT'
'.'
'3'
(*) ' ,'
' an'
' aut'
'ore'
(*) 'gressive'
' language'
(*) ' model'
' with'
' 175'
' billion'
(*) ' parame..'
(*) ' ,'
' 10'
h_out
h46_out
h44_out
h42_out
h40_out
h38_out
h36_out
h34_out
h32_out
h30_out
h28_out
h26_out
h24_out
h22_out
h20_out
h18_out
h16_out
h14_out
h12_out
h10_out
h8_out
h6_out
h4_out
h2_out
h0_out
' Specifically'
' ,'
' we'
' train'
' G'
'PT'
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' with'
' 175'
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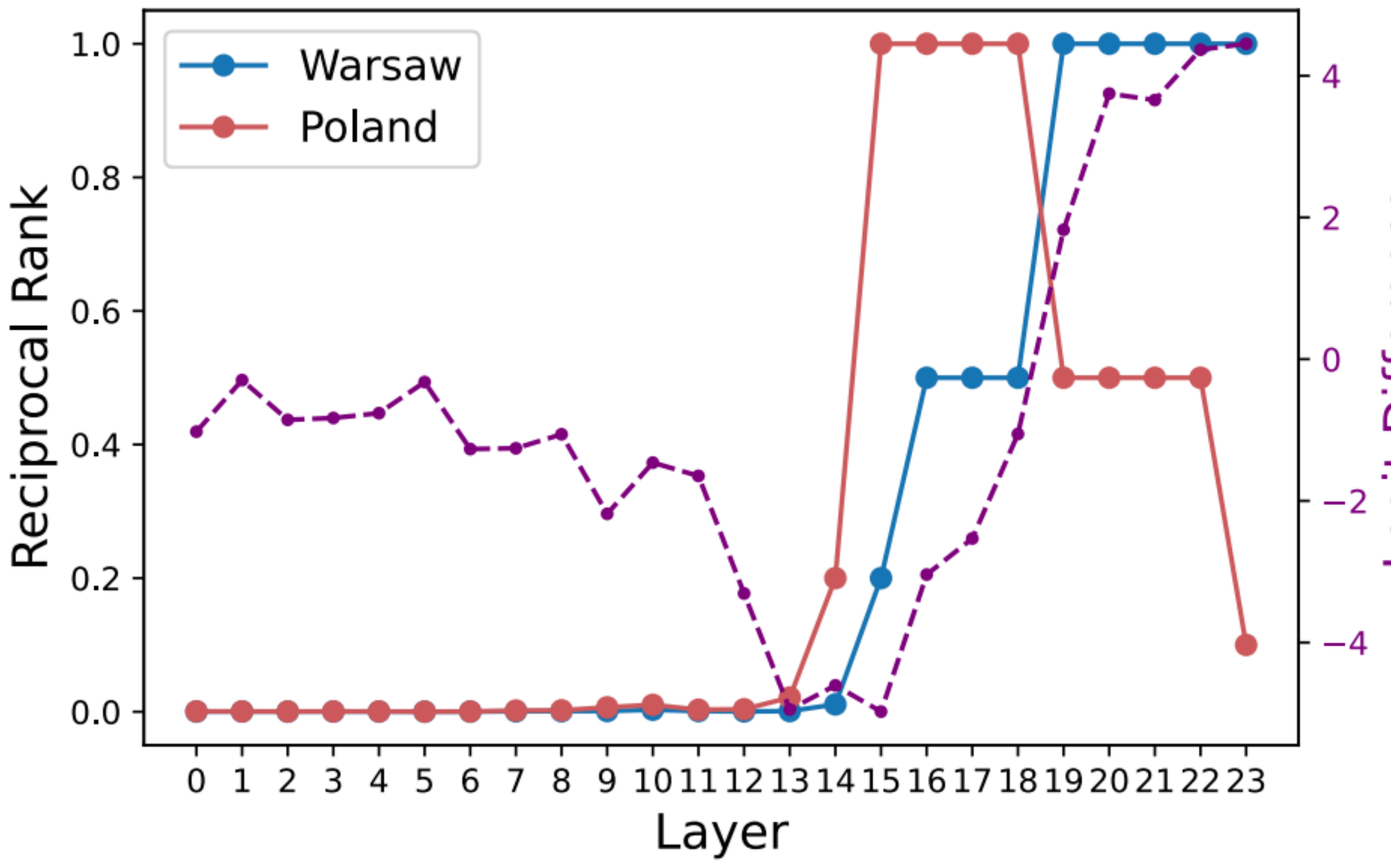
' parameters'
' ,'

Understanding Question Processing in Models



Layer	Top Token	
0	(	
1	A	
2	A	
3	A	
4	A	
5	A	
6	No	
7	C	
8	A	
9	A	
10	A	
11	A	
12	Unknown	
13	C	
14	St	
15	Poland	A
16	Poland	
17	Poland	
18	Poland	
19	Warsaw	B
20	Warsaw	C
21	Warsaw	
22	Warsaw	
23	Warsaw	

Merullo et al. Language Models Implement Simple Word2Vec-style Vector Arithmetic. 2024

Residual Stream

The Transformer Architecture (again)

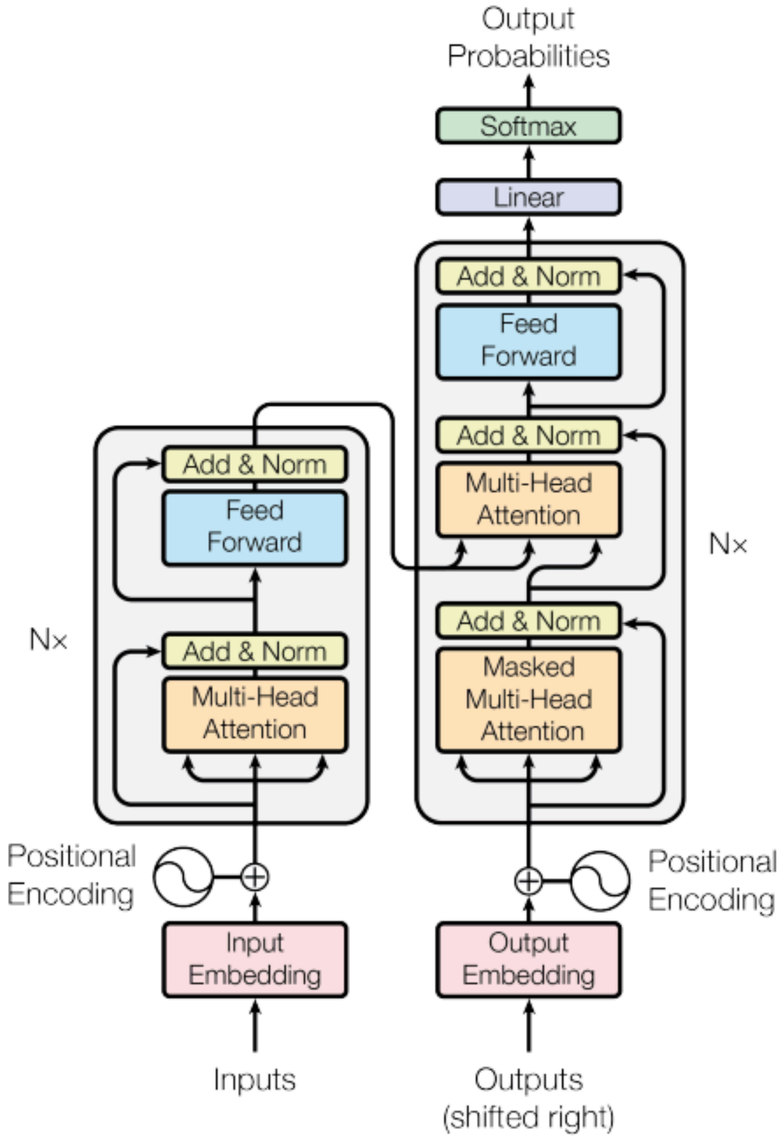
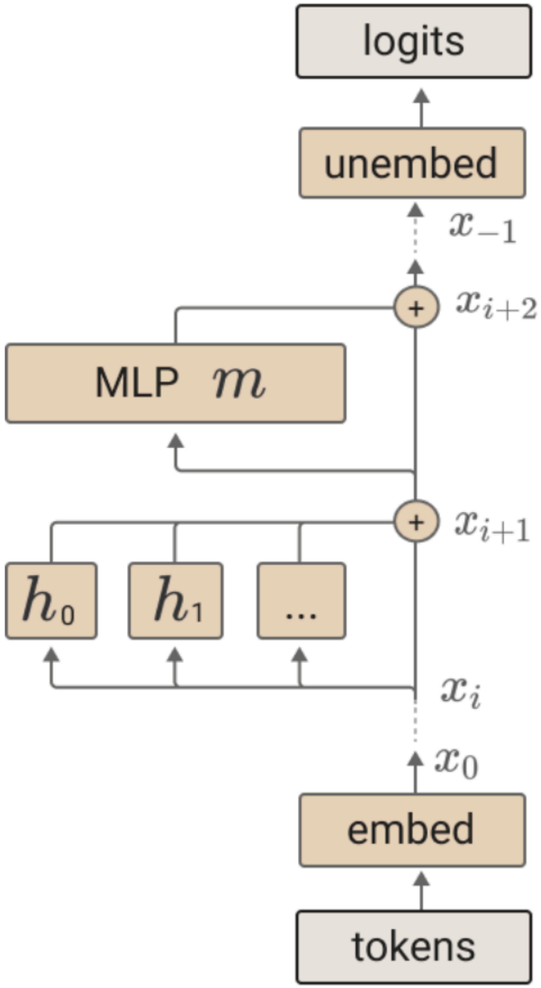


Figure 1: The Transformer - model architecture.

Vaswani et al. Attention is all you need. 2017

The Transformer Architecture (yet again?)



The final logits are produced by applying the unembedding.

$$T(t) = W_U x_{-1}$$

An MLP layer, m, is run and added to the residual stream.

$$x_{i+2} = x_{i+1} + m(x_{i+1})$$

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

$$x_{i+1} = x_i + \sum_{h \in H_i} h(x_i)$$

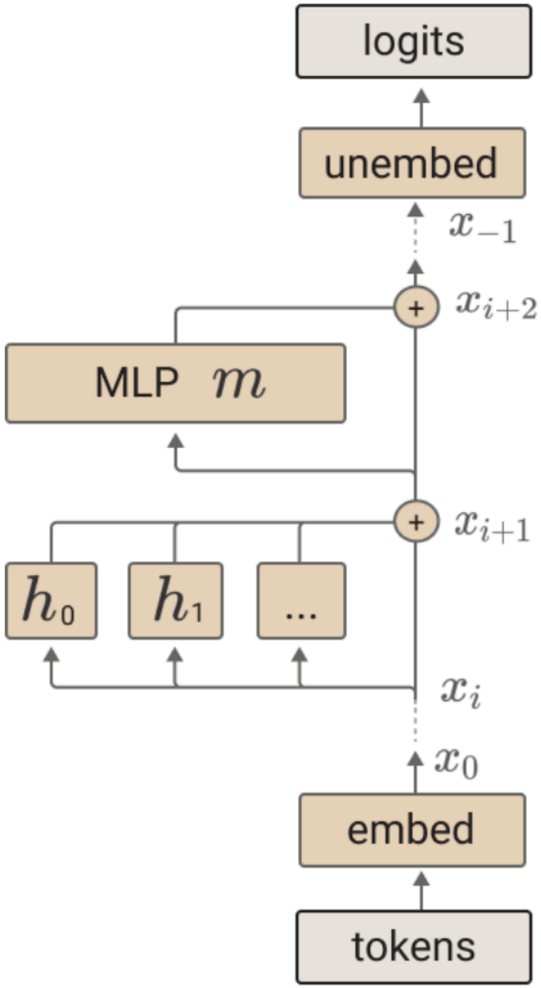
One residual block

Token embedding.

$$x_0 = W_E t$$

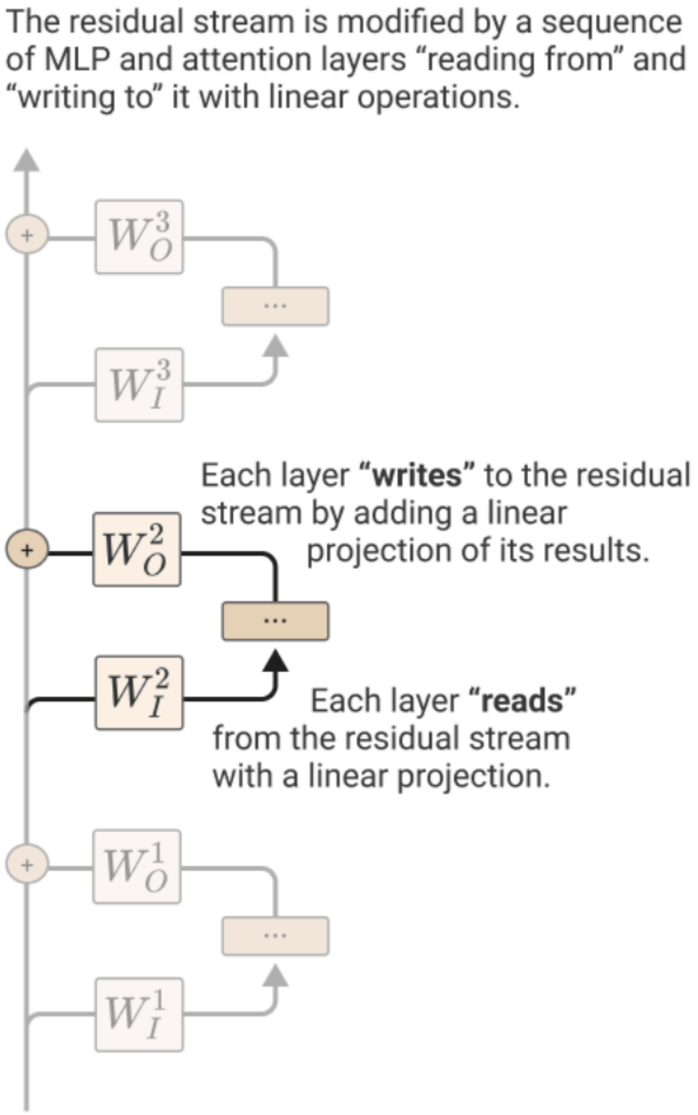
Elhage et al. A Mathematical Framework for Transformer Circuits. 2021

The Transformer Architecture (yet again?)



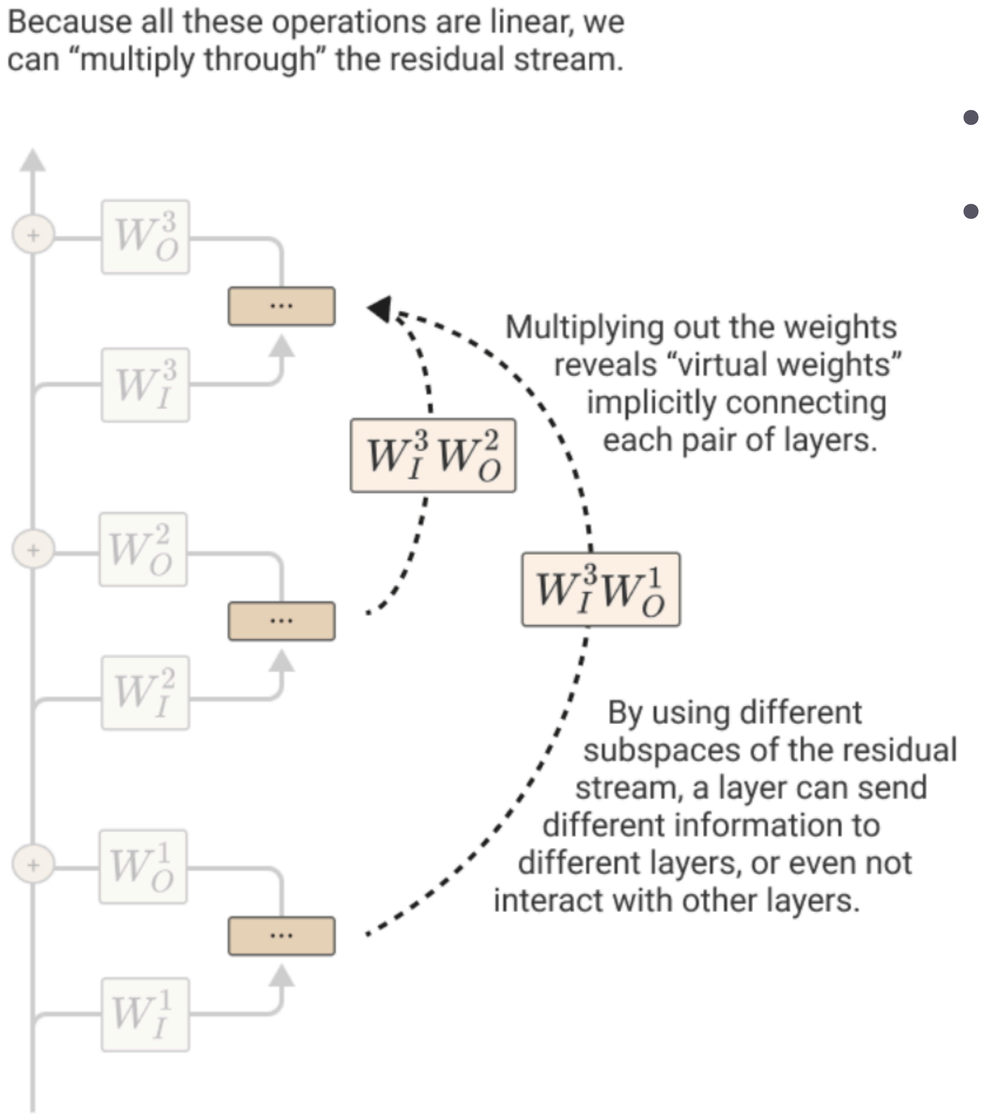
- Working with simplified “Toy Transformers”
- Decoder-only models (à la GPT)
- No MLP layers
- No biases
- No layer normalization

The Transformer Architecture Rewritten



- Exploiting the linear structure of the Transformer
- Communication via the Residual Stream
  - Read from the stream
  - Add a linear transformation to the stream
- Challenge:
  - Notation for efficiency (code) vs.
  - Notation for human interpretation (here)

Virtual Communication Channels

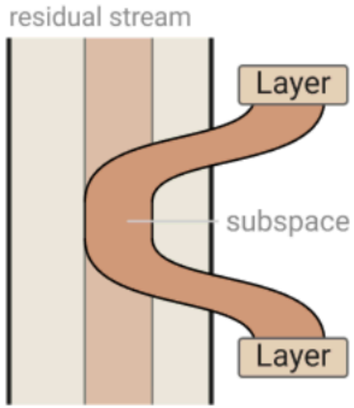


- Implicit virtual weights “connecting” layers
- How much does an input layer read from a previous one?

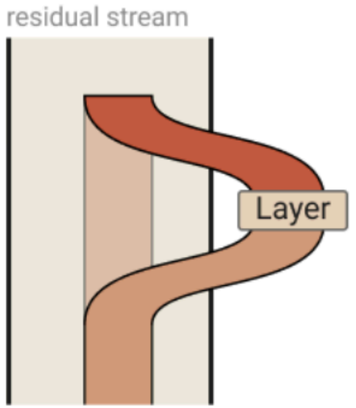
Bandwidth and Subspaces

- The residual stream is high-dimensional
- 100s to 10,000s of dimensions
- Each head operates on small subspaces
- The computational bandwidth is much higher than the communication bandwidth
- “Bottleneck Activations”
- Some heads operate as “memory managers”

The residual stream is high dimensional, and can be divided into different subspaces.



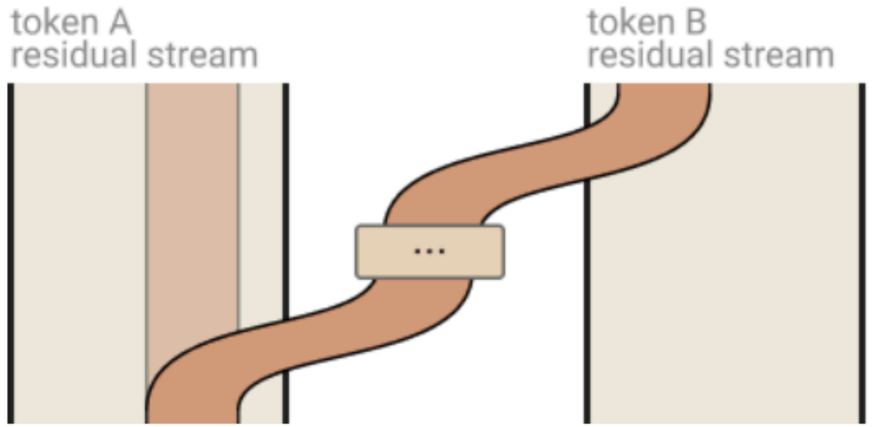
Layers can interact by writing to and reading from the same or overlapping subspaces. If they write to and read from disjoint subspaces, they won’t interact. Typically the spaces only partially overlap.



Layers can delete information from the residual stream by reading in a subspace and then writing the negative verison.

Information Management

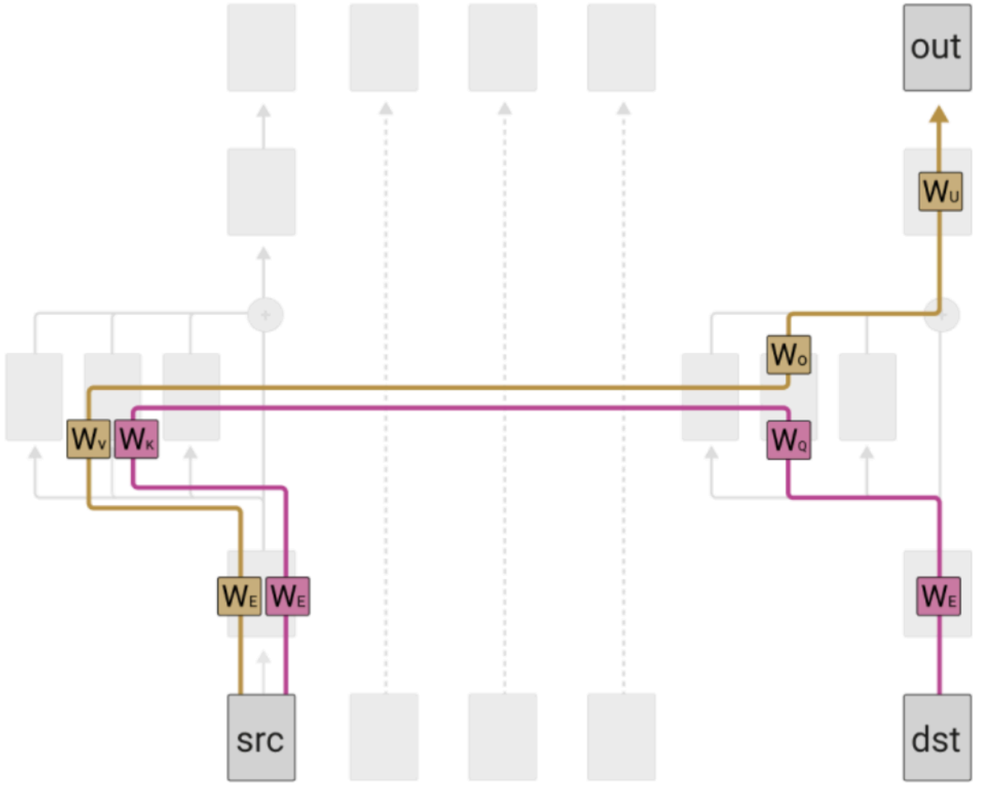
- The read and write operations of parallel heads happen independently
- Often these updates cross the token boundary
- Linear subspaces relating to other tokens emerge in “contextual word embeddings”



Attention heads copy information from the residual stream of one token to the residual stream of another. They typically write to a different subspace than they read from.

Dissecting Attention Heads

- Two key operations in attention heads:
  - Query-key (QK) circuit
  - Output-value (OV) circuit
- Separating these operations allows understanding of mechanisms
- But these matrices are still huge
- Let's cherry-pick



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.

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

The Power of Copying

- Two key operations in attention heads:
  - Query-key (QK) circuit
  - Output-value (OV) circuit
- Separating these operations allows understanding of mechanisms
- But these matrices are still huge
- Let's cherry-pick
- Most Transformer operations are achieved via copying

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

Repairing the Tokenizer

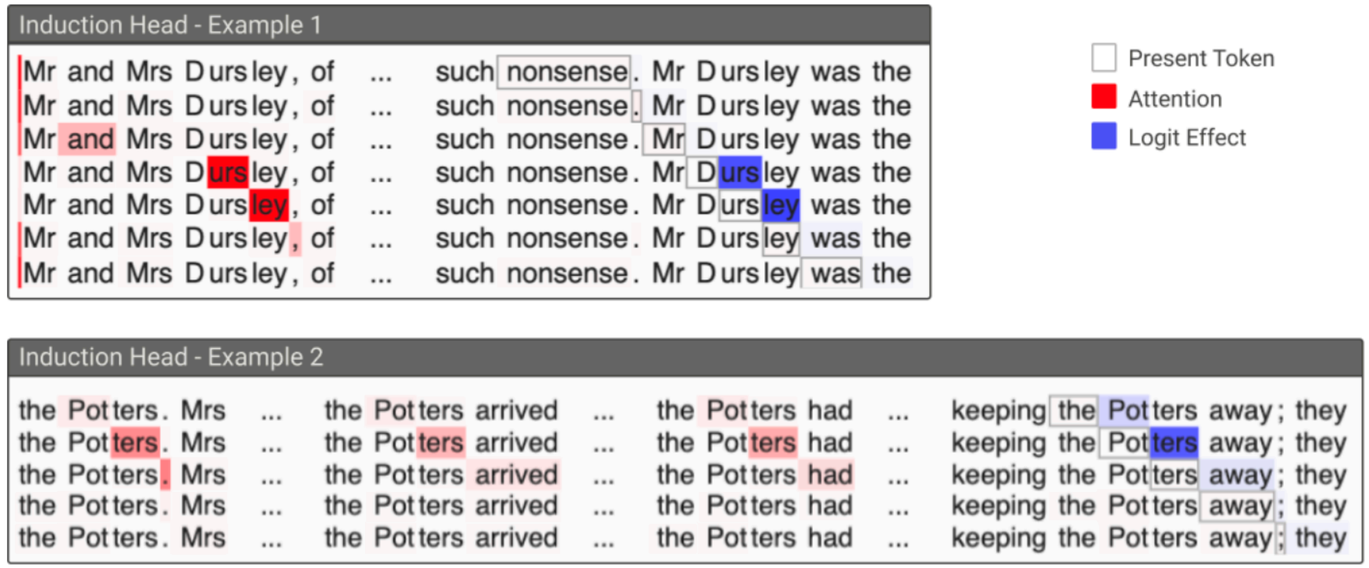
- Tokenizers split up some terms into multiple tokens
- Some English terms are multi white-space-separated to begin with
- Our models have to deal with it
- We can observe the consequences in the realized QK/OV matrices

More examples of large entries QK/OV circuit

Source Token	Destination Token	Out Token	Example Skip Tri-grams
“indy”	“ C”, “C”, “ V”, “V”, “ R”, “ c”	“indy”, “obby”, “INDY”, “loyd”	“indy... Cindy”, “indy... CINDY”
“ Pike”	“ P”, “P”, “V”, “Sp”, “ V”, “R”	“ike”, “ikes”, “ishing”, “owler”	“ Pike... Pike”, “ Pike... Spikes”
“ Ralph”	“R”, “ R”, “ P”, “P”, “V”, “ r”	“alph”, “ALPH”, “obby”, “erald”	“ Ralph... Ralph”, “ Ralph... RALPH”
“ Lloyd”	“L”, “ L”, “ P”, “P”, “R”, “ C”	“loyd”, “alph”, “\n ”, “acman”, ... “atherine”	“ Lloyd... Lloyd”, “ Lloyd... Catherine”
“ Pixmap”	“ P”, “ Q”, “P”, “ p”, “ U”	“ixmap”, “Canvas”, “Embed”, “grade”	“ Pixmap... Pixmap”, “ Pixmap... QCanvas”

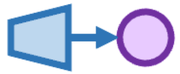
Head Types: Induction Heads

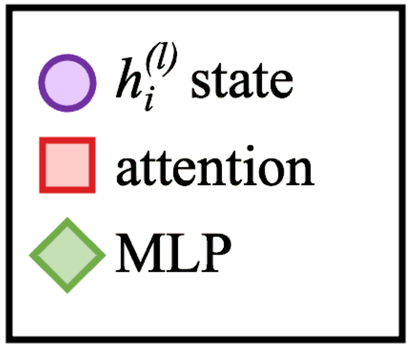
- The QK/OV circuits let us observe the emergence of specialized attention head types
- **Induction Heads** try to complete patterns previously encountered in the context:
  - If the current token has been seen before, attend to the immediately next token
  - Otherwise, dump attention onto the first token in the sequence.



Activation Patching

Locating Factual Knowledge

Eiffel 

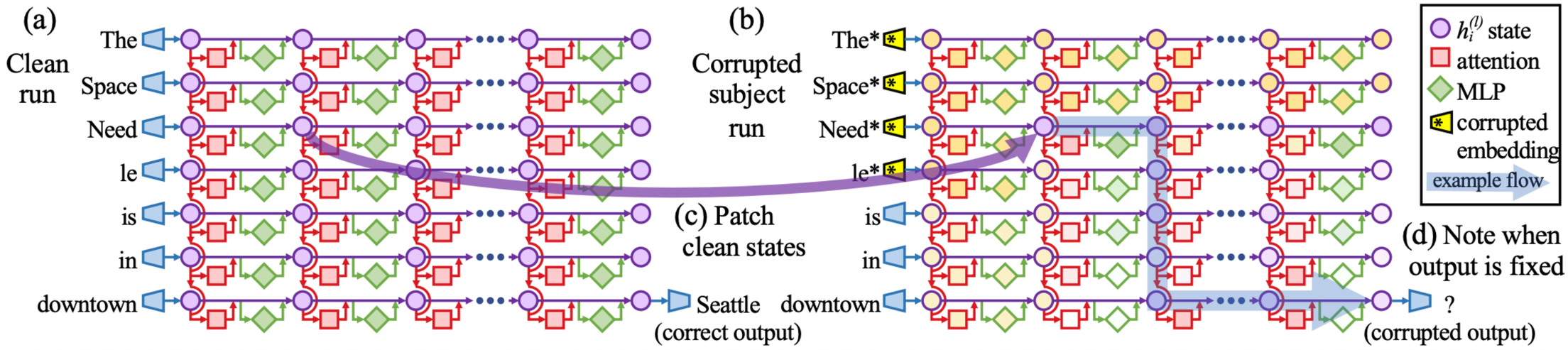


Meng et al. Locating and Editing Factual Associations in GPT. 2022

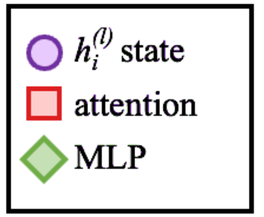
Activation Patching

The **Space Needle** is in downtown -> **Seattle**.

The **Colosseum** is in downtown -> **Rome**.



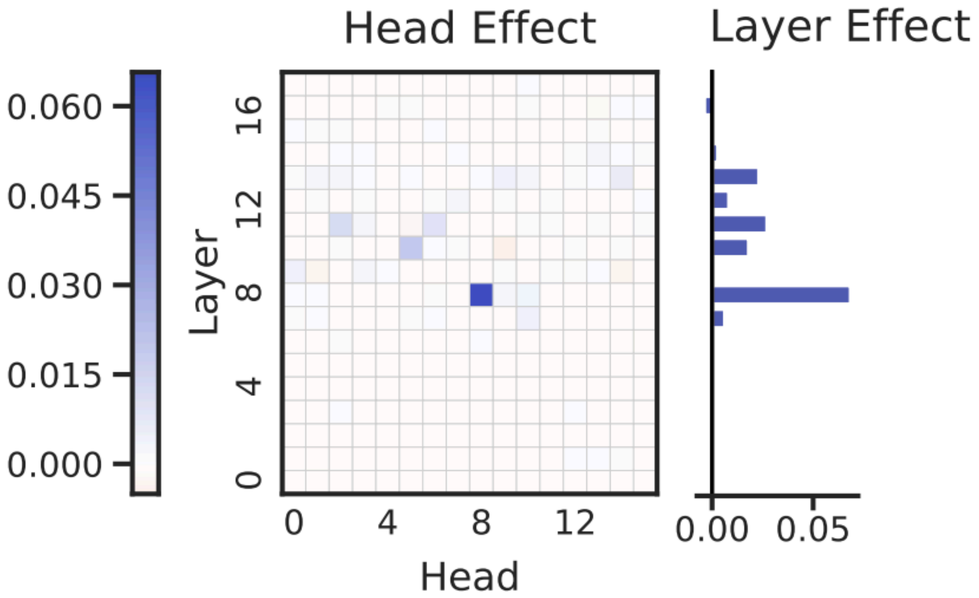
Patch Location



Patch Effects

- Track patch effect across the layers and components of the model
- Locate components with strong effect when patched
- E.g., gender bias

The **nurse** entered the room -> **She** …
The **doctor** entered the room-> **He** …



Big et al. Causal Mediation Analysis for Interpreting Neural NLP. 2020

Finding an Expressive Metric

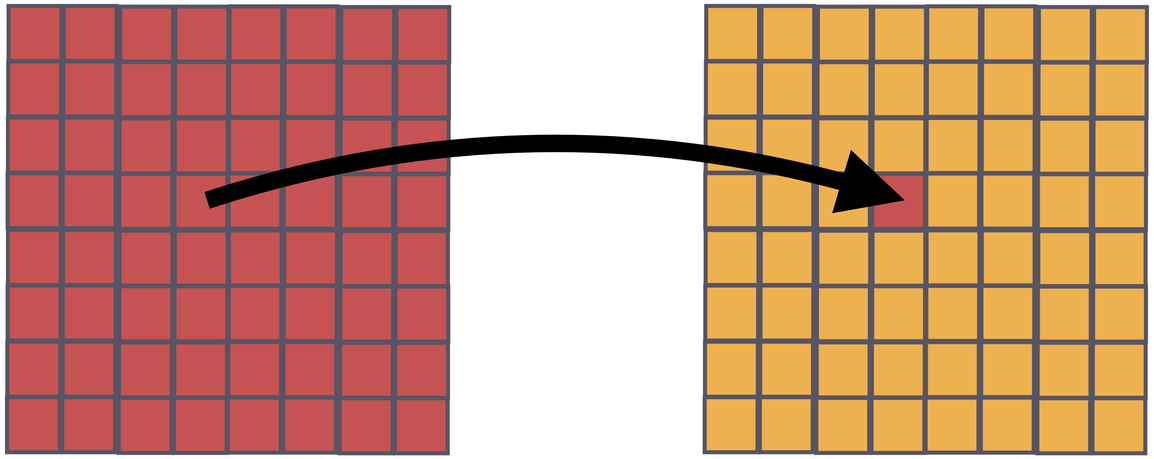
- **Logit Difference** between correct/incorrect answers
- **Raw Class Logits** for the correct answer
- **Log Probability** of correct answer
- **Raw Probability** of correct answer
- **Binary performance metrics** such as accuracy or rank of correct answer

Desired property:	Continuous (not discrete)	Track model confidence linearly	Measure John vs Mary independent of P(name)	False-positive when "breaking the model"
Logit Difference:	Yes	Yes	Yes	Yes
Logit:	Yes	Yes (typically)	Yes	Maybe
Logprob:	Yes	Not close to p=1	No	No
Probability:	Yes	No	No	No
Binary metrics:	No	No	No	No

Heimersheim and Nanda. How to use and Interpret Activation Patching. 2024

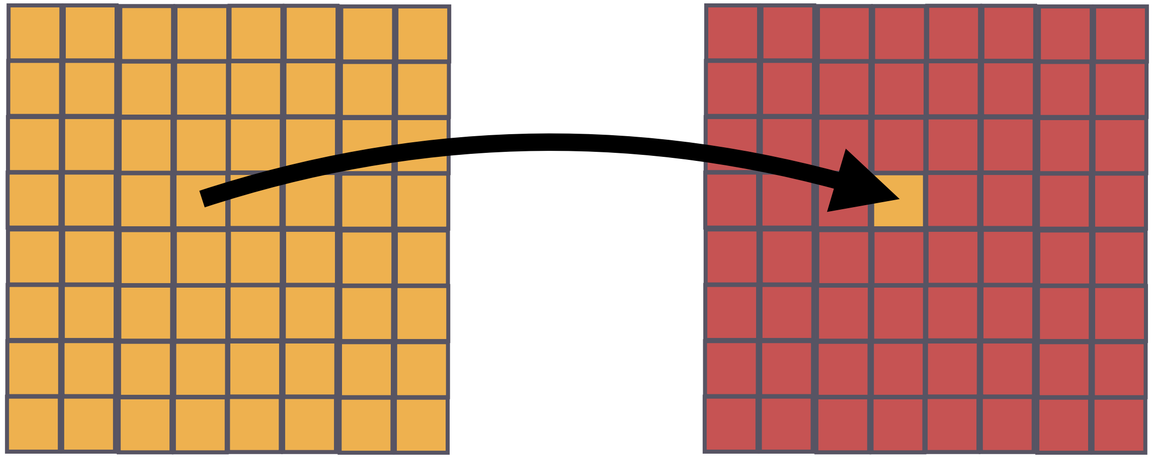
Patch Direction

- **Corrupted to Clean** patching shows whether shows whether activations are necessary to maintain model behavior (noising).



The **nurse** entered the room -> **She** …
The **doctor** entered the room-> **He** …

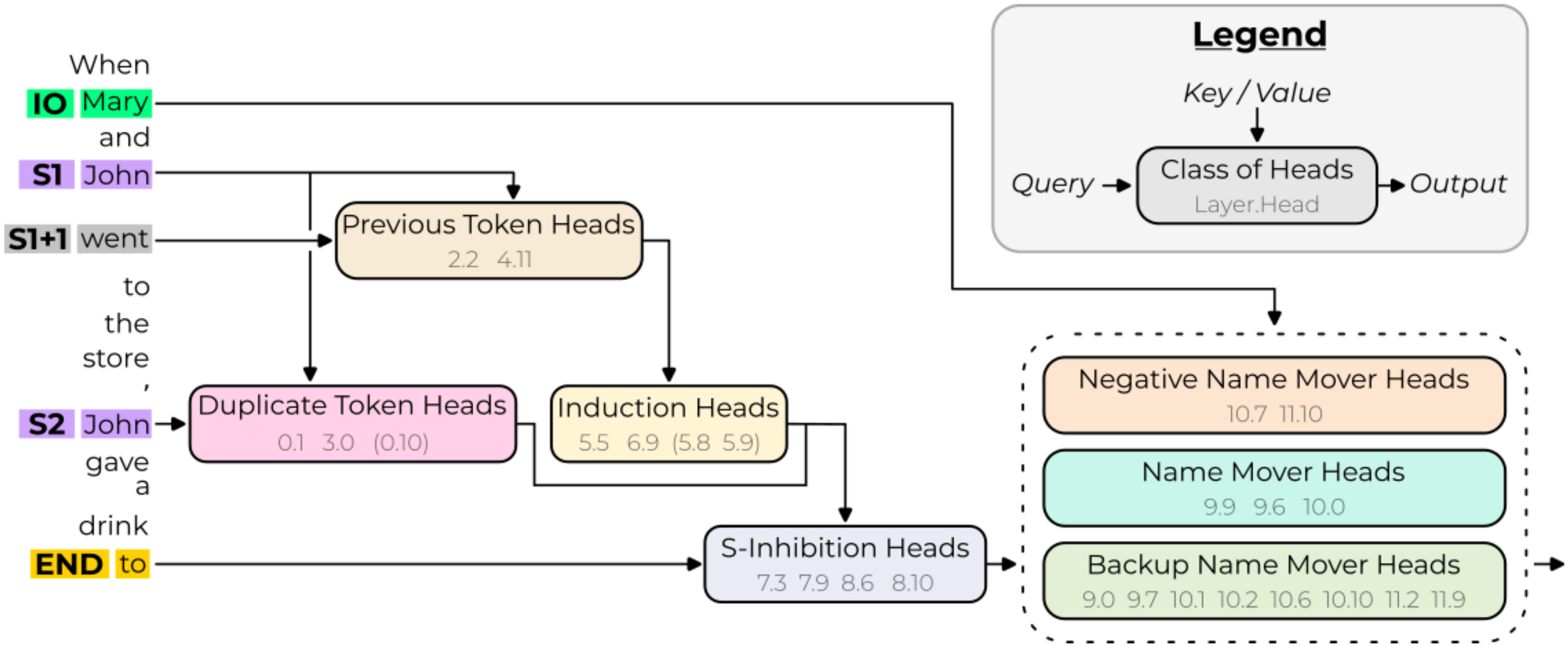
- **Clean to Corrupted** patching shows whether activations are sufficient to restore model behavior (denoising).



Heimersheim and Nanda. How to use and Interpret Activation Patching. 2024

Circuit Analysis

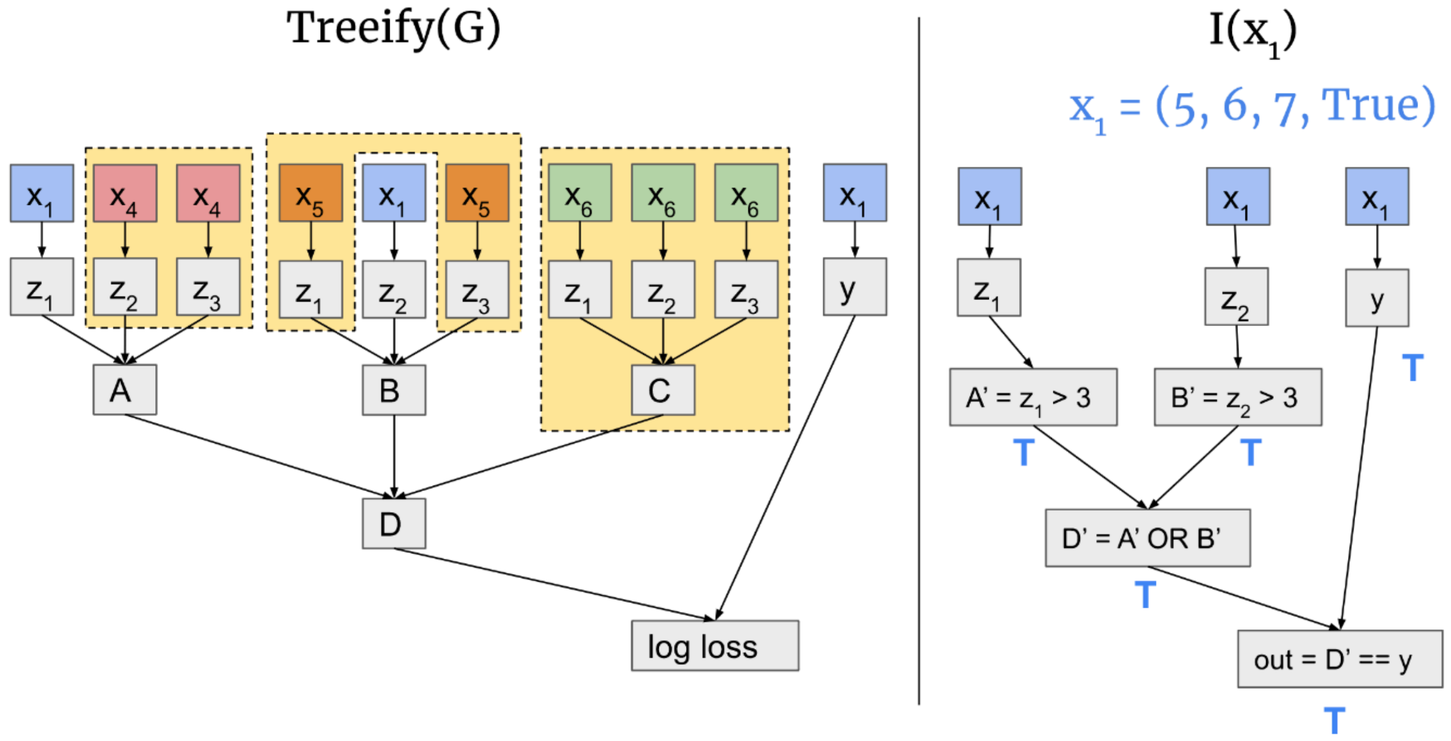
More Heads…



Wang et al. Interpretability in the Wild. 2023

Causal Scrubbing

- Establish hypothesis
  - e.g., via activation patching
- Systematically test hypothesis by recursively find all invariant model components



Chan et al. Causal Scrubbing: a method for rigorously testing interpretability hypotheses, 2022

What just happened!?

- Early Decoding
- Residual Stream
- Patching
- Circuit Analysis

What is to come…

- Tutorial **July 5th** (health permitting)
- Next lecture **July 9th**