Stat 9911
Principles of AI: LLMs
Large Language Model Architectures 02

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Plan

- We aim to provide insight into transformer architectures.
- Review: (Ferrando et al., 2024).

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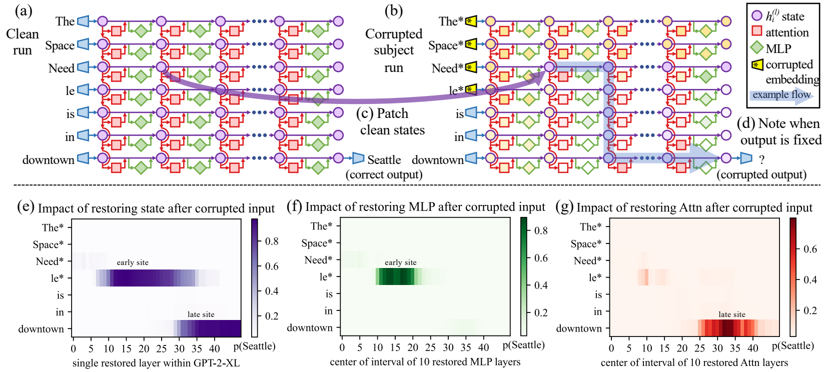
How Do LLMs Encode Information?

Some general facts:

- Information is encoded in the weights/parameters of NNs
- Can also extract information by looking at the neurons/activations and representations $e(x)$ for specific inputs x
- Methods for identifying neuron roles: probing, causal interventions.
- In NNs, specialized neurons may represent concepts. In LLMs, a classic example is sentiment neurons (Radford et al., 2017).
- In LLMs, representations of subject tokens act as keys for retrieving facts: after an input text mentions a subject, LMs construct enriched representations of subjects that encode information about those subjects (Li et al., 2021).

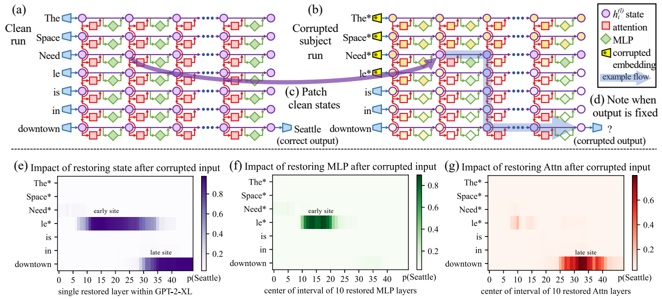
Causal Tracing in LLMs (Meng et al., 2022)



Consider the computational graph as a causal graph, as in causal mediation analysis for NLP (Vig et al., 2020):

1. Run LM on input text (e.g., "The Space Needle is in").
2. Corrupt subject, e.g., "**[i.i.d. Gaussian activations]** is in", and re-run LM.
3. For each neuron group, patch activations from clean run into corrupted run; run LM again to see if it restores original logits.

Causal Tracing in LLMs (Meng et al., 2022)


(a) Clean run
The
Space
Need
le
is
in
downtown
Seattle (correct output)
(b) Corrupted subject run
The*
Space*
Need*
le*
(c) Patch clean states
(d) Note when output is fixed
? (corrupted output)
$h_i^{(l)}$ state
attention
MLP
corrupted embedding
example flow
(e) Impact of restoring state after corrupted input
early site
late site
single restored layer within GPT-2-XL
(f) Impact of restoring MLP after corrupted input
center of interval of 10 restored MLP layers
(g) Impact of restoring Attn after corrupted input
center of interval of 10 restored Attn layers
p(Seattle)

- "Each midlayer MLP accepts inputs that encode a subject, then produces outputs that recall memorized properties about that subject. Then the summed information is copied to the last token by attention at high layers."

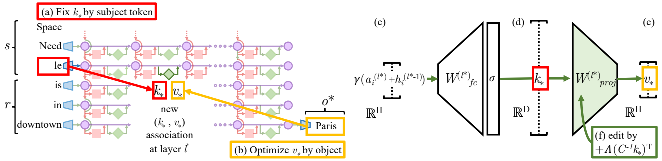
Information Editing in LLMs (Meng et al., 2022)

- Claim: The two-layer FFN acts as a linear associative memory (Kohonen, 1972; Anderson, 1972). [refines Geva et al. (2020), who view individual neurons as memories]
- Consider 2L-NN $e' = W_{\text{proj}}\sigma(W_1 e)$. Can view $k = \sigma(W_1 e)$ as a key and $v = W_{\text{proj}} k$ as a value it retrieves.
- For any given $(\tilde{V}, \tilde{K})$ pair, find $W = W_{\text{proj}}$ to approximately operate as a key-value store, solving:

  $$\min_W \|W\tilde{K} - \tilde{V}\|_F,$$

  obtaining $\tilde{W} = \tilde{V}\tilde{K}^+$.
- Insert key-value pairs, e.g., $k^* =$ space needle, $v^* =$ Paris, with minimal weight perturbations: Solve $\min_W \|WK - \tilde{V}\|_F$, subject to $Wk^* = v^*$.

Rank-One Model Editing (Meng et al., 2022, ROME)



- The solution is $W^* = \tilde{W} + \Lambda\left(C^{-1}k^*\right)^\top$, where

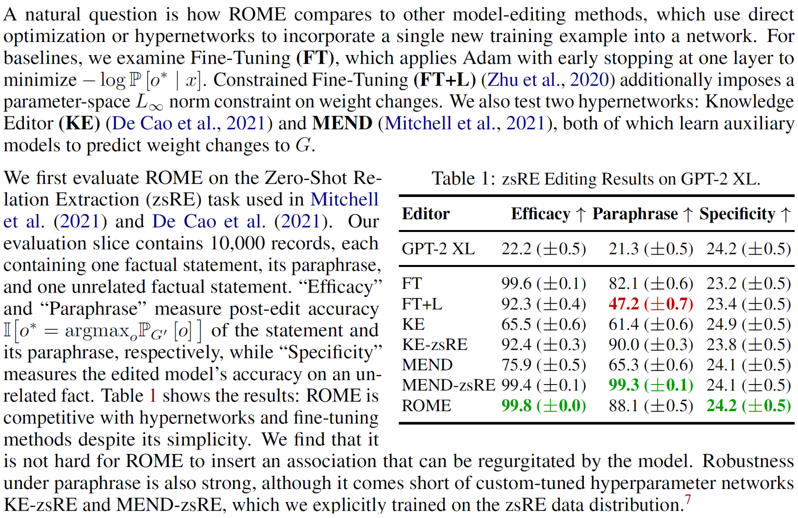
$$C = KK^\top \quad \text{and} \quad \Lambda = (v^* - \tilde{W}k^*)/k^{*,\top}C^{-1}k^*.$$

- Estimate C based on a data sample from the distribution that we expect k^* to follow.
- To insert a specific memory, use k^* of original text (with some random contexts). For v^*, solve:

$$\max_v P(o^* \mid \text{prefix} + x, v(x) \mapsto v),$$

where x are the tokens for k^*; and o^* is target output.

Performance of ROME (Meng et al., 2022)



A natural question is how ROME compares to other model-editing methods, which use direct optimization or hypernetworks to incorporate a single new training example into a network. For baselines, we examine Fine-Tuning **(FT)**, which applies Adam with early stopping at one layer to minimize $-\log \mathbb{P}\left[o^* \mid x\right]$. Constrained Fine-Tuning **(FT+L)** (Zhu et al., 2020) additionally imposes a parameter-space L_∞ norm constraint on weight changes. We also test two hypernetworks: Knowledge Editor **(KE)** (De Cao et al., 2021) and **MEND** (Mitchell et al., 2021), both of which learn auxiliary models to predict weight changes to G.

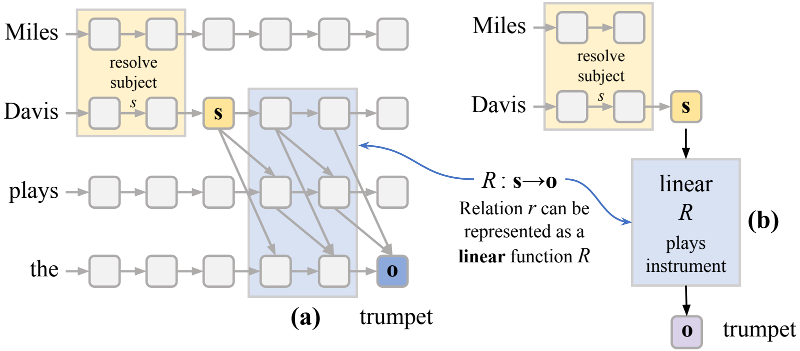
We first evaluate ROME on the Zero-Shot Relation Extraction (zsRE) task used in Mitchell et al. (2021) and De Cao et al. (2021). Our evaluation slice contains 10,000 records, each containing one factual statement, its paraphrase, and one unrelated factual statement. "Efficacy" and "Paraphrase" measure post-edit accuracy $\mathbb{I}\big[o^* = \text{argmax}_o \mathbb{P}_{G'}\left[o\right]\big]$ of the statement and its paraphrase, respectively, while "Specificity" measures the edited model's accuracy on an unrelated fact. Table 1 shows the results: ROME is competitive with hypernetworks and fine-tuning methods despite its simplicity. We find that it is not hard for ROME to insert an association that can be regurgitated by the model. Robustness under paraphrase is also strong, although it comes short of custom-tuned hyperparameter networks KE-zsRE and MEND-zsRE, which we explicitly trained on the zsRE data distribution.[7]

Table 1: zsRE Editing Results on GPT-2 XL.

Editor	**Efficacy ↑**	**Paraphrase ↑**	**Specificity ↑**
GPT-2 XL	22.2 (±0.5)	21.3 (±0.5)	24.2 (±0.5)
FT	99.6 (±0.1)	82.1 (±0.6)	23.2 (±0.5)
FT+L	92.3 (±0.4)	**47.2 (±0.7)**	23.4 (±0.5)
KE	65.5 (±0.6)	61.4 (±0.6)	24.9 (±0.5)
KE-zsRE	92.4 (±0.3)	90.0 (±0.3)	23.8 (±0.5)
MEND	75.9 (±0.5)	65.3 (±0.6)	24.1 (±0.5)
MEND-zsRE	99.4 (±0.1)	**99.3 (±0.1)**	24.1 (±0.5)
ROME	**99.8 (±0.0)**	88.1 (±0.5)	**24.2 (±0.5)**

Representing Relations in LLMs

- Consider relations, e.g., (Jimi Hendrix, plays the, guitar), (Miles Davis, plays the, trumpet).
- Some of them are approximately affine maps $s \to o \approx \partial o / \partial s \cdot (s - s_0) + o(s_0)$, where s is a sufficiently contextualized representation of the input, and o are the output logits (Hernandez et al., 2024).



Representing Relations in LLMs (ctd)

- Why??
  - Linear maps are the simplest non-trivial class, all smooth maps are locally approx. linear
  - Prior work on knowledge graph embeddings e.g., Yang et al. (2014), models relations as $\|o' M s\|$ being small for some M. This is zero iff $o = M^{\perp} s + v$, any $v \perp M \cdot \mathrm{span}(s)$, $M^{\perp}$ an ortho. complement of M
  - Prior work has shown that "linear shortcuts" are enough for accurate decoding from early transformer layers (Din et al., 2024)

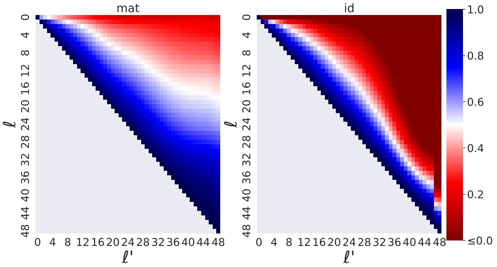


Figure: R^2 between activations transformed from layer ℓ to ℓ', in GPT-2. Left: best linear transform; Right: no transform.

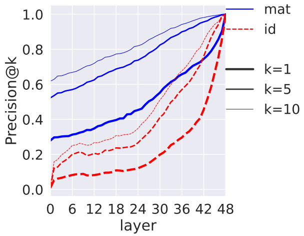


Figure: Accuracy of linear decoding from a given layer in GPT-2.

Representing Relations in LLMs (ctd)

- Challenges handled in Hernandez et al. (2024): Due to LayerNorm, scale is not propagated. More accurate to approximate $s \to o \approx \beta \partial o / \partial s \cdot (s - s_0) + o(s_0)$, for some $\beta > 0$

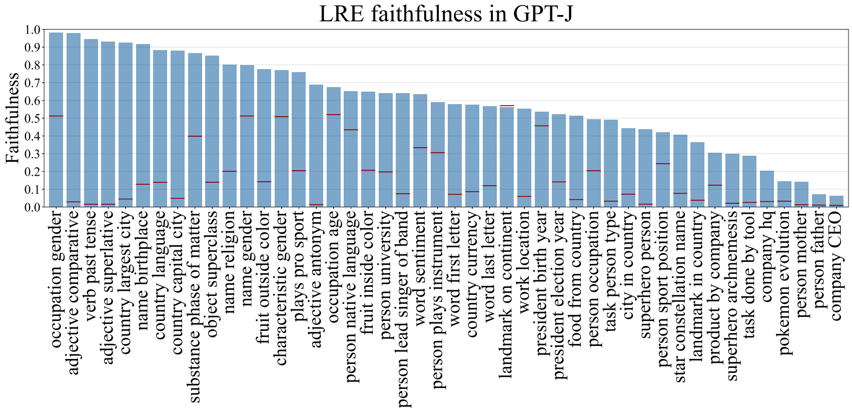


Figure: Accuracy of linear relational decoding across various categories.

Mechanistic Interpretability Perspective

- Mechanistic interpretability is an area that aims to understand the working mechanisms of NNs and LLMs; see work by Anthropic
- For factual recall, Nanda et al. (2023) follow a similar path to what we have seen, with a few key differences
  - Their terminology is based on circuits: sparse sub-networks obtained by pruning most weights in a NN

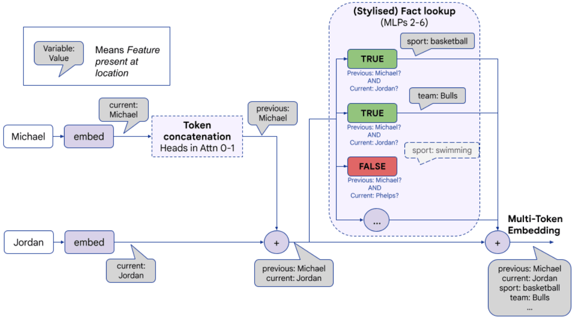


Figure: Source

  - In experiments, prune to the circuit and observe behavior

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Attention as Context-Dependent Markov Chain (Ildiz et al., 2024)

- View autoregressive generation as a Markov Chain.
- Predictions depend on token frequencies in the context.
- Frequent tokens can dominate the distribution.

Attention as a Context-Dependent Markov Chain (Ildiz et al., 2024)

- T tokens, $|V|$ vocab size.
- Prompt:
$$x = (x_1, x_2, \ldots, x_T), \quad x_i \in [|V|]$$
- Matrix encoding:
$$E = (e_{x_1}, e_{x_2}, \ldots, e_{x_T})^\top, \quad E \in \mathbb{R}^{T \times |V|}$$

  where $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)^\top$ is the i-th unit vector in $\mathbb{R}^{|V|}$.

Calculating the Next Token Probability

Next token probability:

$$
\begin{aligned}
f_W(E) &= E^\top S\big(EWe_{x_T}\big) = E^\top S(EW_{:,x_T}) = E^\top S(Ev) \\
&= E^\top \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_{x_T} \end{bmatrix} = \begin{bmatrix} \mathrm{Num}(1)\cdot s_1 \\ \mathrm{Num}(2)\cdot s_2 \\ \vdots \\ \mathrm{Num}(|V|)\cdot s_{|V|} \end{bmatrix}
\end{aligned}
$$

where $v := W_{:,x_T}$ and

1. $$s_i = \frac{\exp(v_i)}{\sum_{j\in x}\exp(v_j)} = \frac{\exp(v_i)}{\sum_{k\in[|V|]}\mathrm{Num}(k)\cdot\exp(v_k)}.$$
2. $\mathrm{Num}(k)$ is the number of times k occurs in x

Interpretation and Implications

$$f_W(E) = \begin{bmatrix} \text{Num}(1) \cdot s_1 \\ \vdots \\ \text{Num}(|V|) \cdot s_{|V|} \end{bmatrix}$$

- W (i.e., v and s) corresponds to the architecture.
- For a fixed W, f_W's predictions can be viewed as s weighted by the frequencies of each token in the context.
- Autoregressive generation can be viewed as a context-dependent Markov Chain: v is fixed, but the frequencies $\text{Num}(k)$ make it depend on the context
- Implication: Frequent tokens (even if occurring by chance) may dominate the distribution; relevant for understanding repetitive sampling.

Representational and Computational Abilities of Transformers

- Discussed in Sanford et al. (2024b,a), etc.

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