THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY (GUANGZHOU)

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

AIAA 2290: Ethics, Privacy and Security in AI

Introduction to Explainable AI and LLM

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The Hong Kong University of Science and Technology (Guangzhou)

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You vote for this topic

Roadmap of this tutorial

- **A quick overview of WHY we need explainable AI**
- **More on 'explanation' for LLM**
- **No security of LLM this time** (but it is a FUN topic about how you can hack or defend LLM)
- **No AI ethical regulation & law**

About Me

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY (GUANGZHOU)

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I am Yibo, a PhD student supervised by Prof.HU. My master and bachelor degrees are from National University of Singapore and Hong Kong Baptist University, respectively.
My current research mainly focus on **Multimodal LLM**.

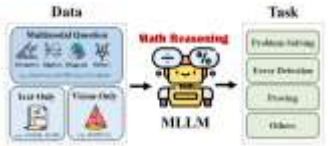
Multimodal Understanding

UrbanCLIP
WWW'24
Oral

GeoReasoner
CIKM'24
Best Short

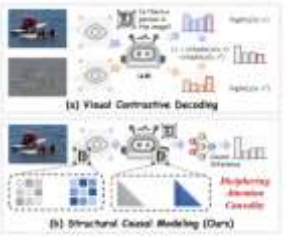
Multimodal Reasoning

ErrorRadar
Under review

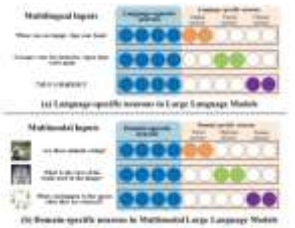


MLLM4Math
Under review

Multimodal Trustworthiness



CausalMM
ICLR'25



MMNeuron
EMNLP'24

Outline

Left for own reading

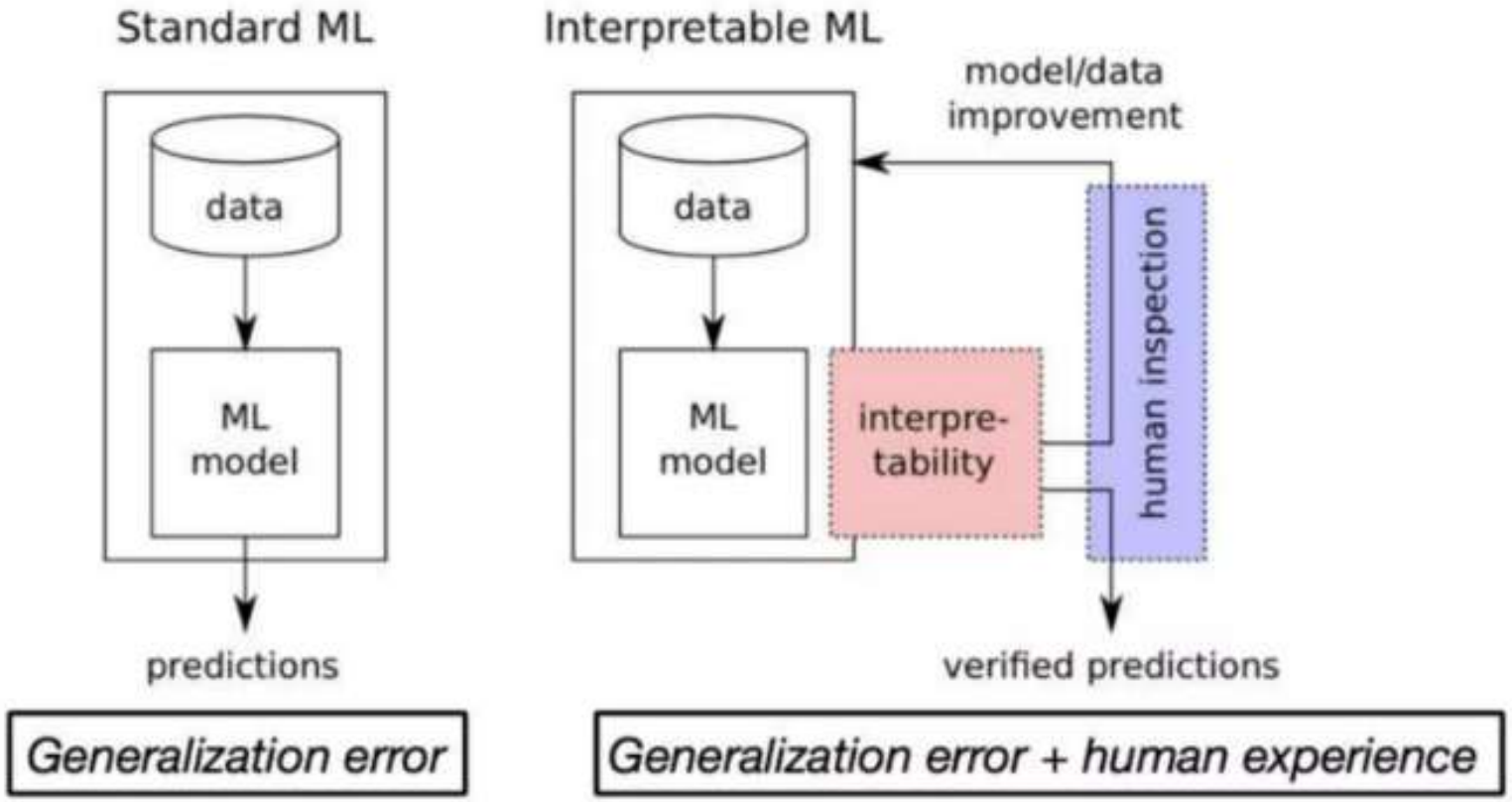
Motivation: Why we need explainability?
----From a Model Perspective

Why explainability: Debug (Mis-)Predictions

Top label: **"clog"**

Why did the network label this image as **"clog"**?

Why explainability: Improve ML Model w/ Human Experience

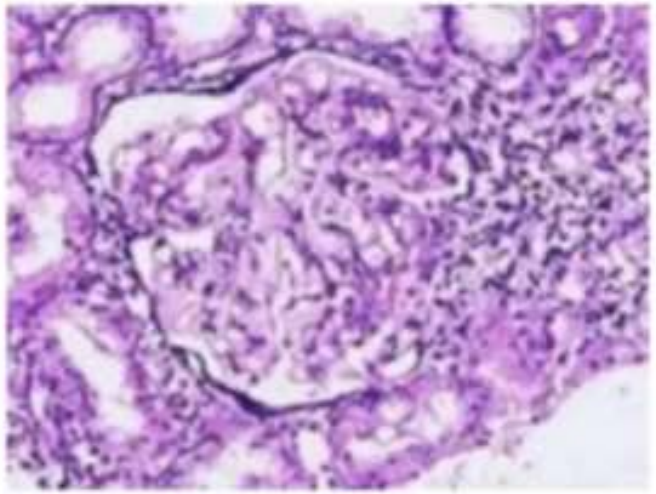


Why explainability: Verify ML Model/System

Wrong decisions can be costly and dangerous

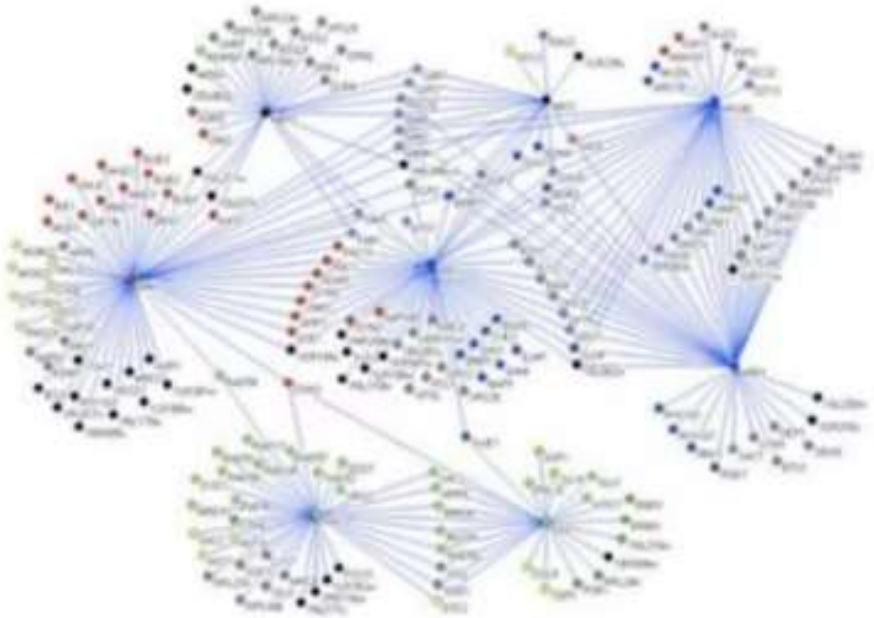
"Autonomous car crashes, because it wrongly recognizes …"

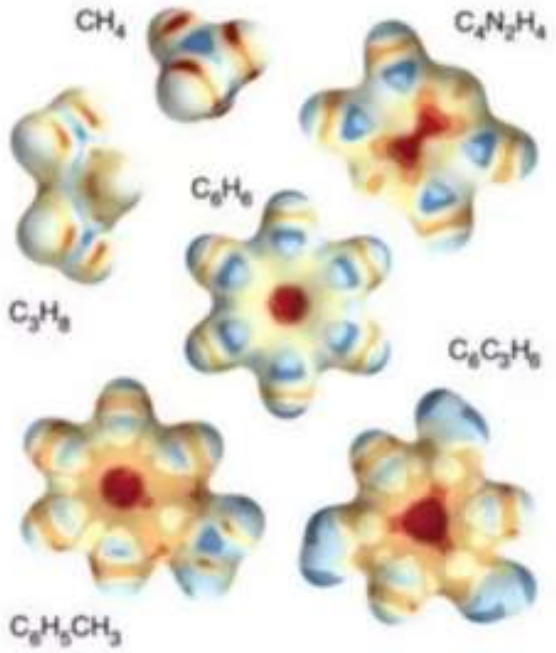
"AI medical diagnosis system misclassifies patient's disease …"



Why explainability: Learn Insights in the Sciences

Learn about the physical / biological / chemical mechanisms.
(e.g. find genes linked to cancer, identify binding sites …)





What is the stuff that follows the "why"?

Let's clarify them in this example:

Why is the sky turning dark? The sun is going down.

- **Explanandum** is what describes the **problem**.
- Explanan is what describes the **reason**.
- Explanation is the **process(*)** of stating the reason for the problem.

*: The term "explanation" is also frequently used to refer to the **product** of this process.

There are many types of explanations

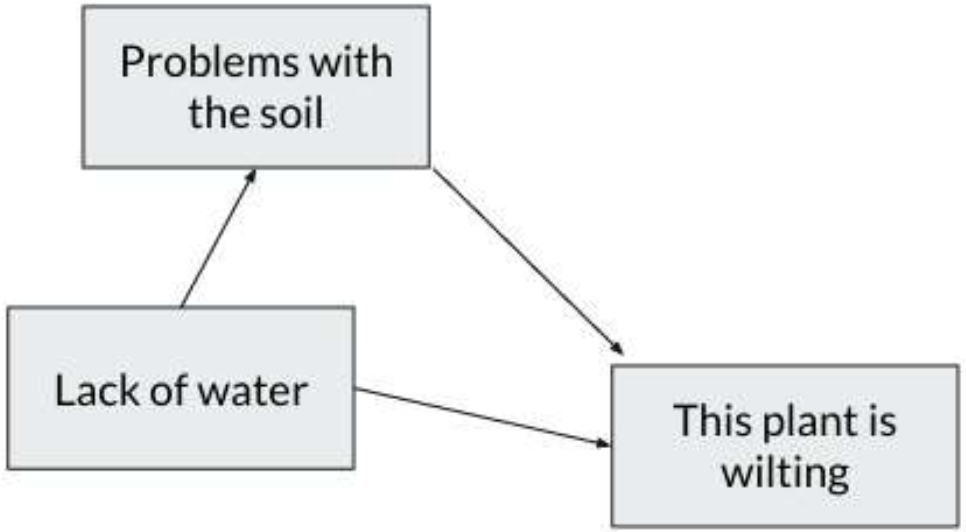
By the **reasoning patterns**:

> A plant in the living room is wilting. Why?

- **Deductive**: If a plant does not receive enough water, it will wilt. That plant in the living room hasn't be watered for a month.
- **Inductive**: Other plants in that living room have wilted because they haven't received enough water. It's likely that plants wilt because of lack of water.
- **Abductive**: It's likely that the plant in this living room is wilting because there's no enough water.
- ...

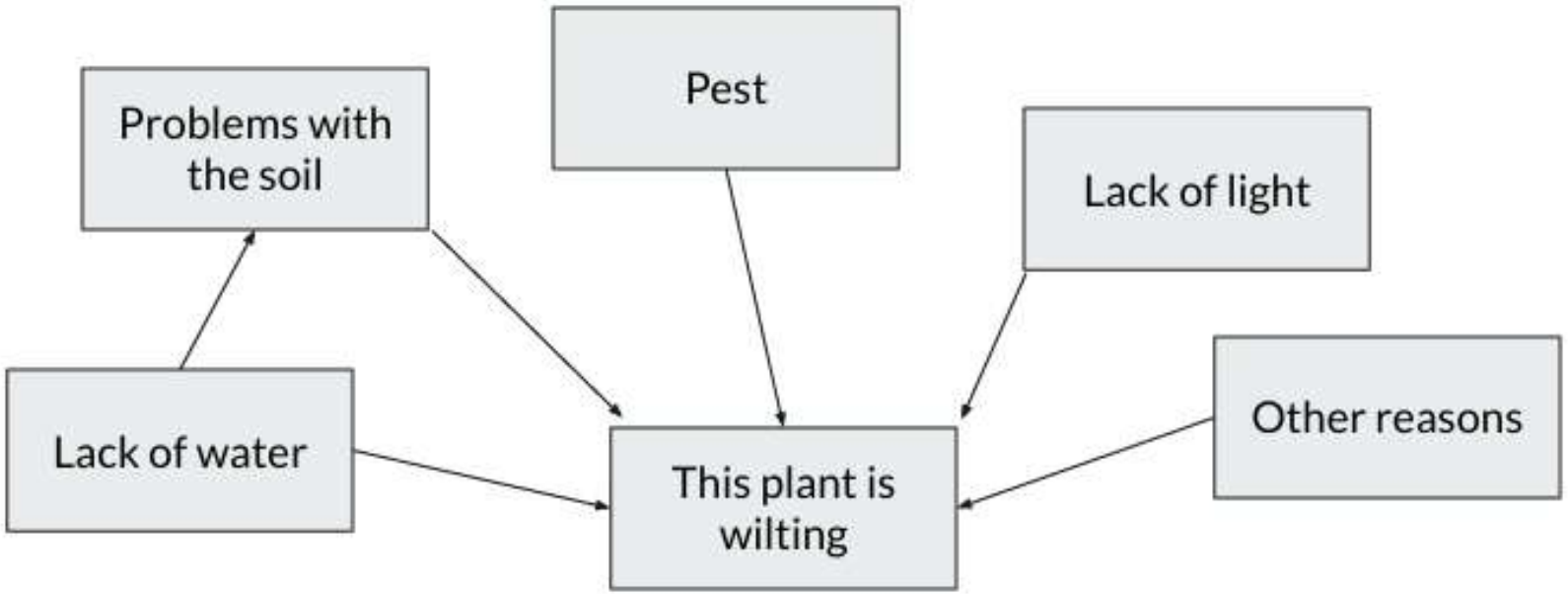
There are many types of explanations

By the **causal variables:**



There are many types of explanations

By the **completeness**: selective, or comprehensive?



Good explanations should be faithful

To explain a model's prediction:

"A **faithful** interpretation is one that accurately represents the reasoning process behind the model's prediction." [Jacovi & Goldberg, 2020]

"This is often considered the most fundamental requirement for any explanation, and sometimes used interchangeably with the term 'interpretability'." [Lyu et al. 2023]

Plausibility and faithfulness are two desirable (but different) properties in explanations. [Wiegreffe and Pinter, 2019]

Towards Faithfully Interpretable NLP Systems: How Should We Define and Evaluate Faithfulness? (Jacovi & Goldberg, ACL 2020)
Towards Faithful Model Explanation in NLP: A Survey. (Qing Lyu, Marianna Apidianaki, and Chris Callison-Burch. 2023)
Attention is not not Explanation (Wiegreffe & Pinter, EMNLP-IJCNLP 2019)

Good explanations should be plausible

An explanation is considered plausible if it is coherent with human reasoning and understanding. [Agrawal et al. 2024]

Plausibility is also referred to as **persuasiveness** or **understandability**.

An explanation might be plausible but not faithful. Currently, many explanations are more plausible than faithful.

Example of faithful, but not plausible explanation: a copy of model weights. [Jacovi & Goldberg, 2020]

Agarwal, C., Tanneru, S. H., & Lakkaraju, H. (2024). Faithfulness vs. Plausibility: On the (Un) Reliability of Explanations from Large Language Models. *arXiv preprint arXiv:2402.04614*.

Good explanations should be informative

Hi prof, I have just finished this paper. Which venue do you think would best suit it?

NAACL, because its deadline is just 3 days away, and it will be in Mexico, not far from here.

NAACL, because it is a top NLP conference.

Which explanation is more informative?

This example is modified from: Zachary C. Lipton. 2017. The Mythos of Model Interpretability. arXiv:1606.03490 [cs, stat].

Good explanations should be <u>useful</u>

Tom holds a copper block by hand and heats it on fire. Which of the following is more likely?

A. His fingers feel warm. B. His fingers feel burnt.

A (92.93%)

Copper is a good thermal conductor. Tom holds a copper block by hand and heats it on fire. Which of the following is more likely?

A. His fingers feel warm. B. His fingers feel burnt.

B (90.05%)

This example is modified from the e-CARE dataset. Probabilities are computed by GPT-3.5-Turbo model, as of April 19, 2024. This example is about utility to models – explanation should also be useful to humans.

Other desirable properties

Completeness: All necessary information is covered.

Stability: The explanation remains consistent for similar cases I ask about.

Interactivity: The explanation can answer my follow-up questions.

Personalization: The explanation is tailored to my needs.

...

For a more detailed list please refer to [Liao et al., 2022]

Q. Vera Liao, Yunfeng Zhang, Ronny Luss, Finale Doshi-Velez, and Amit Dhurandhar. 2022. Connecting Algorithmic Research and Usage Contexts: A Perspective of Contextualized Evaluation for Explainable AI. *Proceedings of the AAAI Conference on Human Computation and Crowdsourcing*, 10(1):147–159.

Prompting-based Explanations

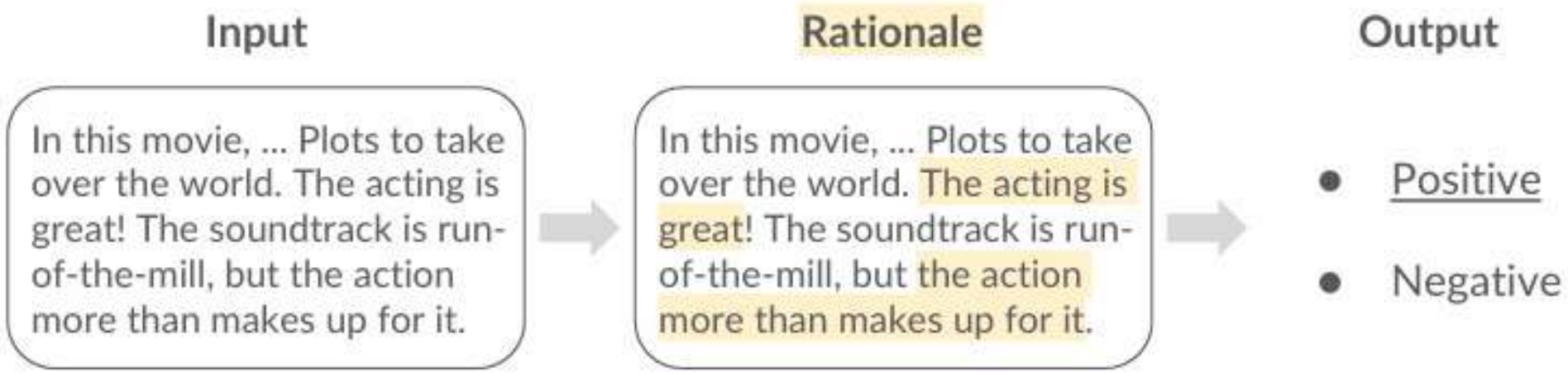
- Extractive rationales / Feature attributions
- Free-text explanations
- Structured explanations

Prompting-based Explanations

- Extractive rationales / Feature attributions
- Free-text explanations
- Structured explanations

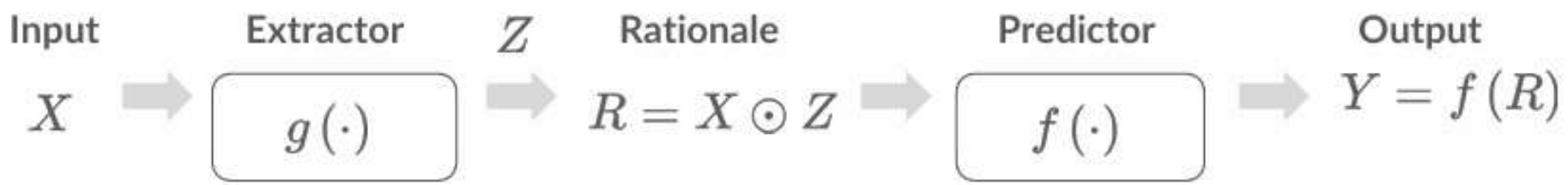
Extractive Rationales

(**short**) snippets in inputs that support outputs



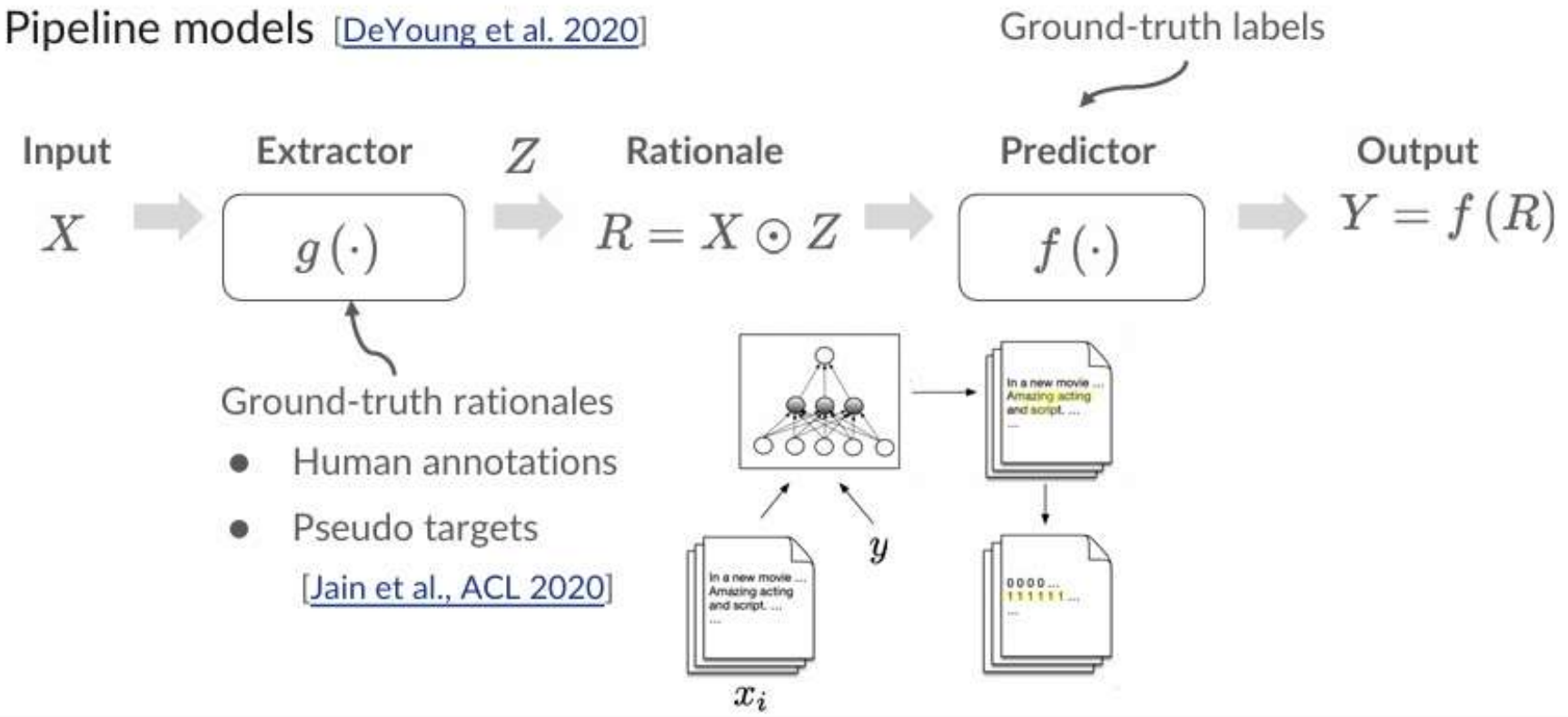
Extractive Rationales

Pipeline models [DeYoung et al. 2020]

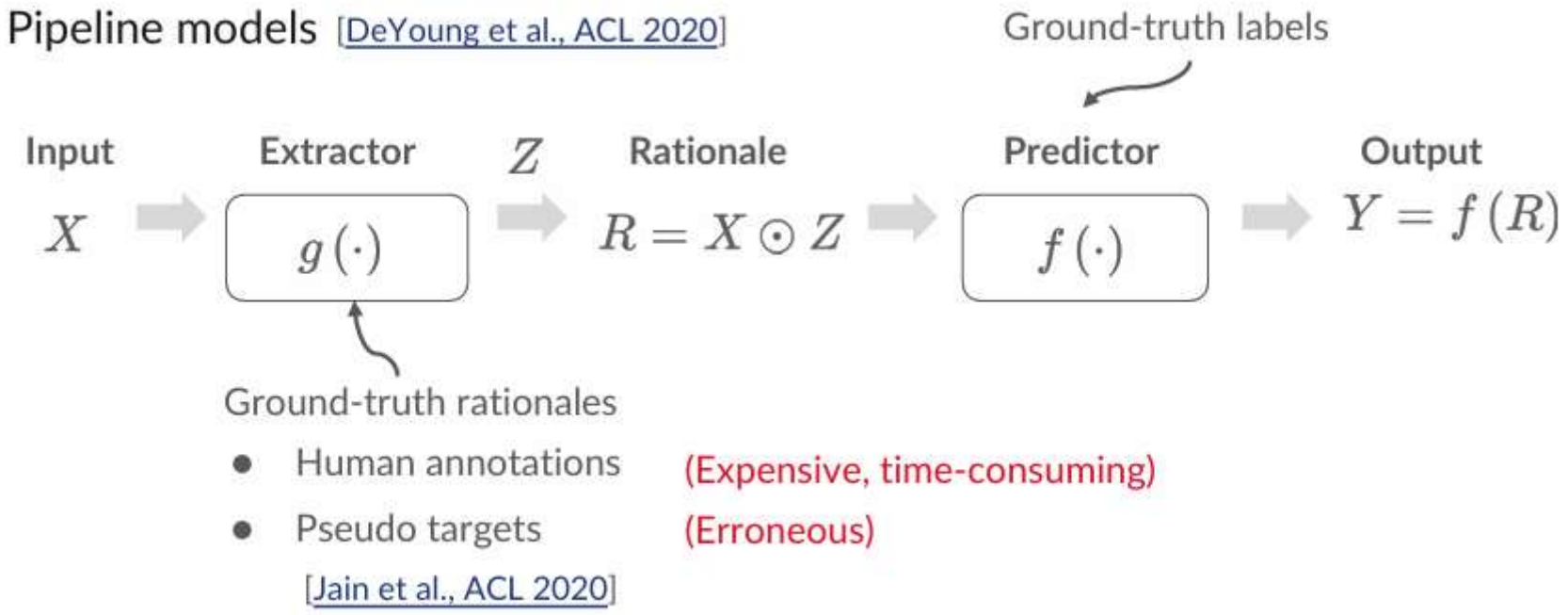


- Hard selection [Lei et al. 2016]
  - Z Binary masks
- Soft selection
  - Z Continuous scores

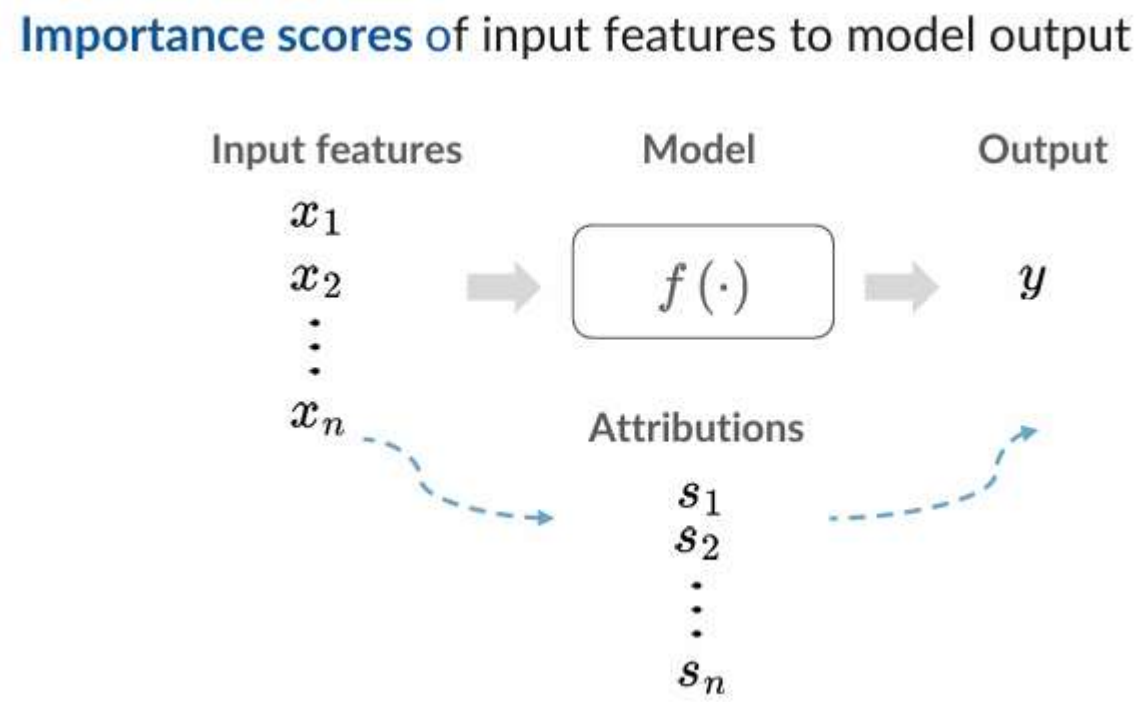
Extractive Rationales



Extractive Rationales

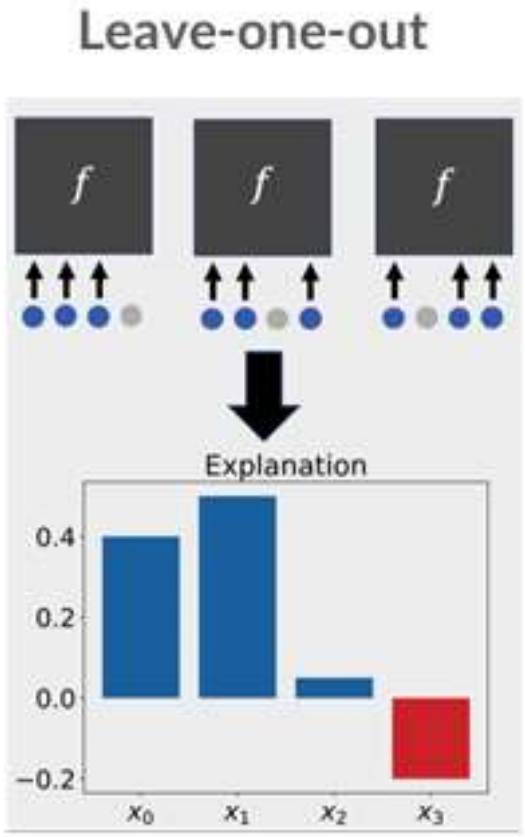


Feature Attributions

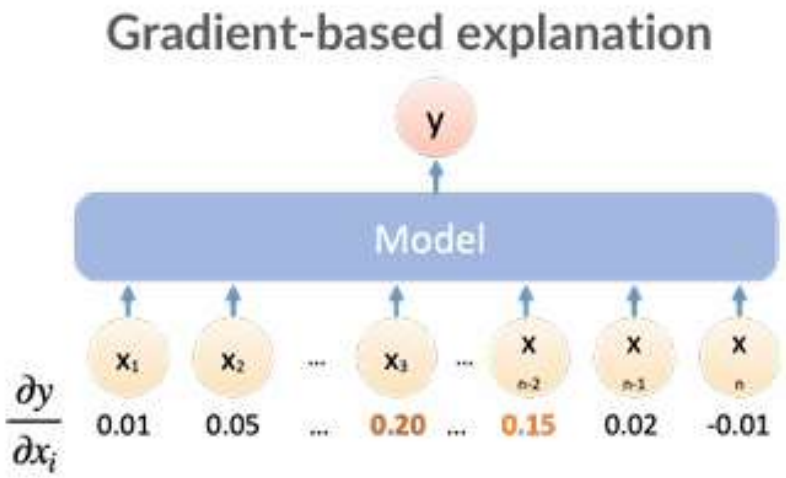


Prompting-based Explanations

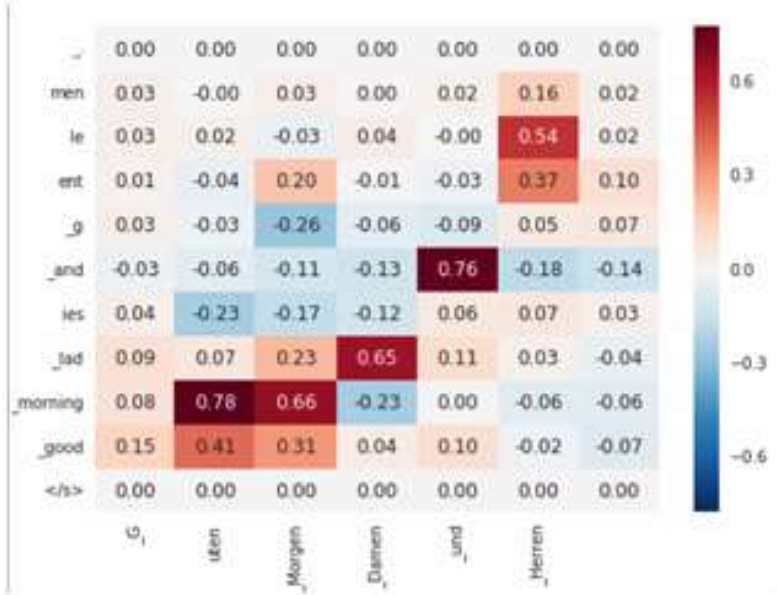
Feature Attributions



[Covert et al. 2020]



[Sundararajan et al. 2017]

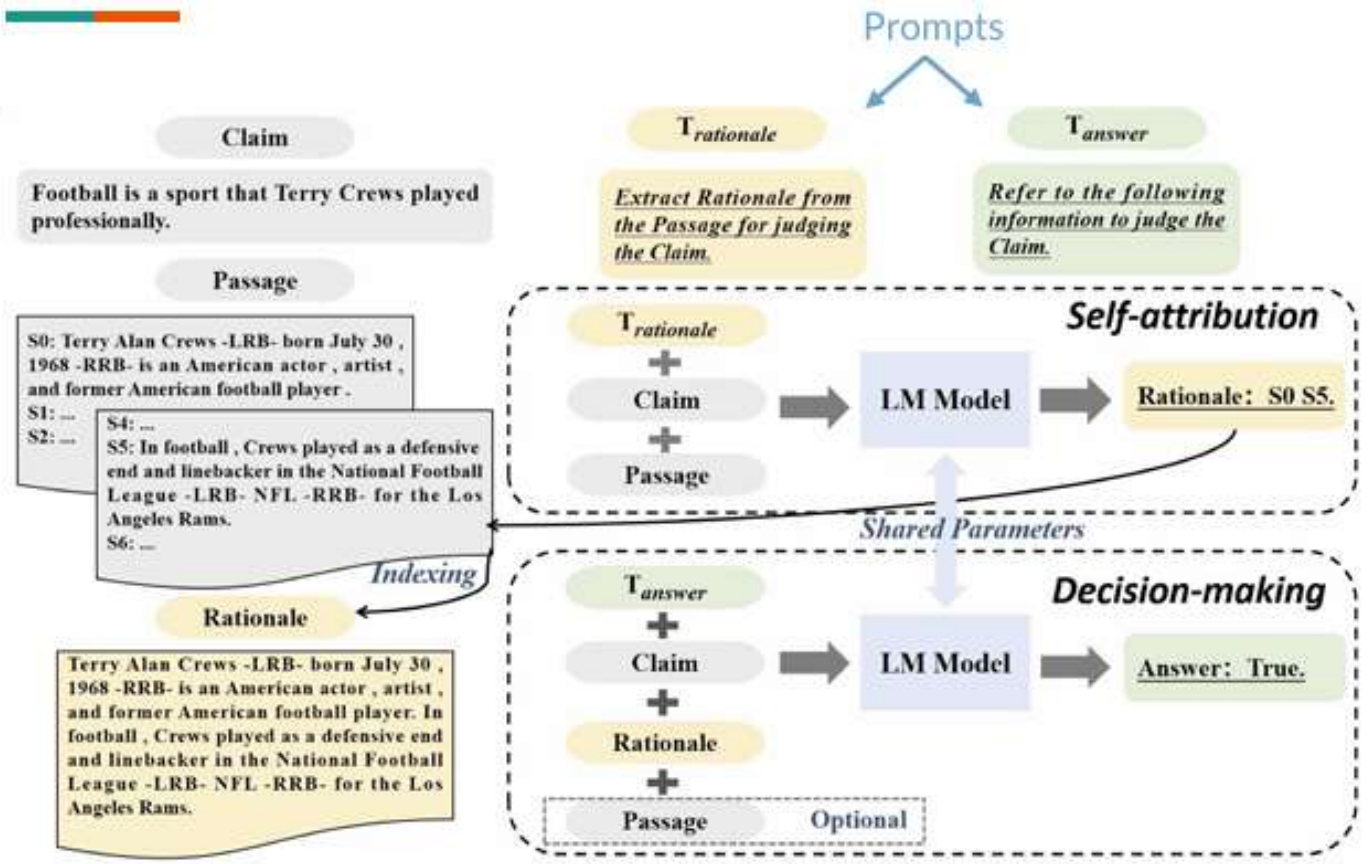


Challenges for LLMs

- Computational cost
- Low efficiency in long context
- No access to API-based models (gradients, attention scores, etc.)

Prompting-based extractive rationales/feature attributions

Self-Attribution and Decision-Making



Stage 1:
Prompting for extractive rationales

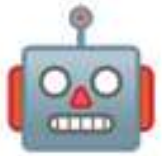
Stage 2:
Making decisions based on rationales

[Du et al. 2023]

See also: [Ludan et al. 2024]

How to evaluate rationales/feature attributions?

Faithfulness



*How accurately the explanation reflects the **true** reasoning process of the model*

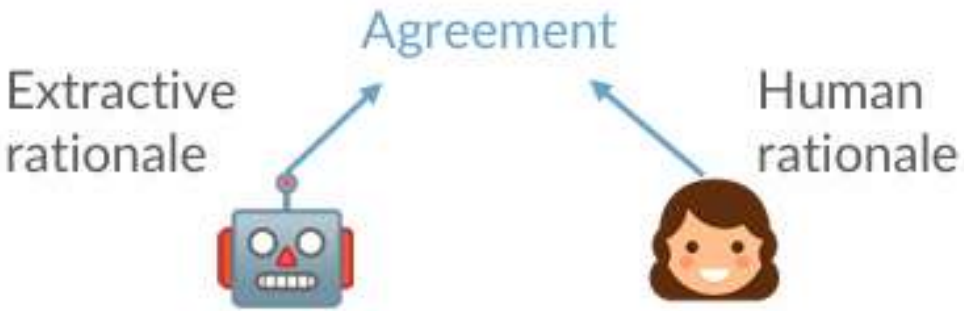
Explanation

Plausibility

*How **convincing** the explanation is to humans*

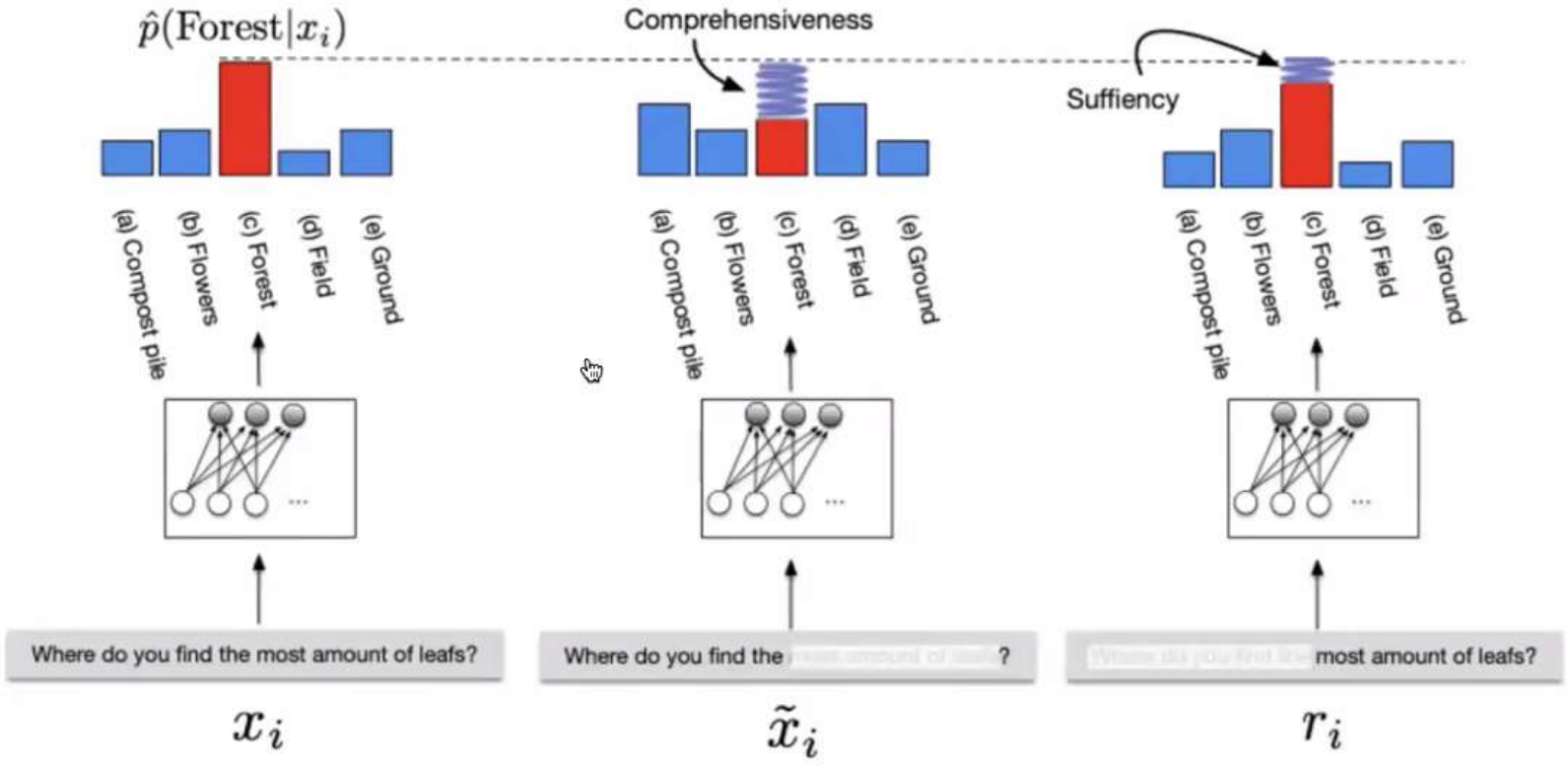
Evaluation—Plausibility

- Agreement
  e.g. Intersection-Over-Union (IOU)



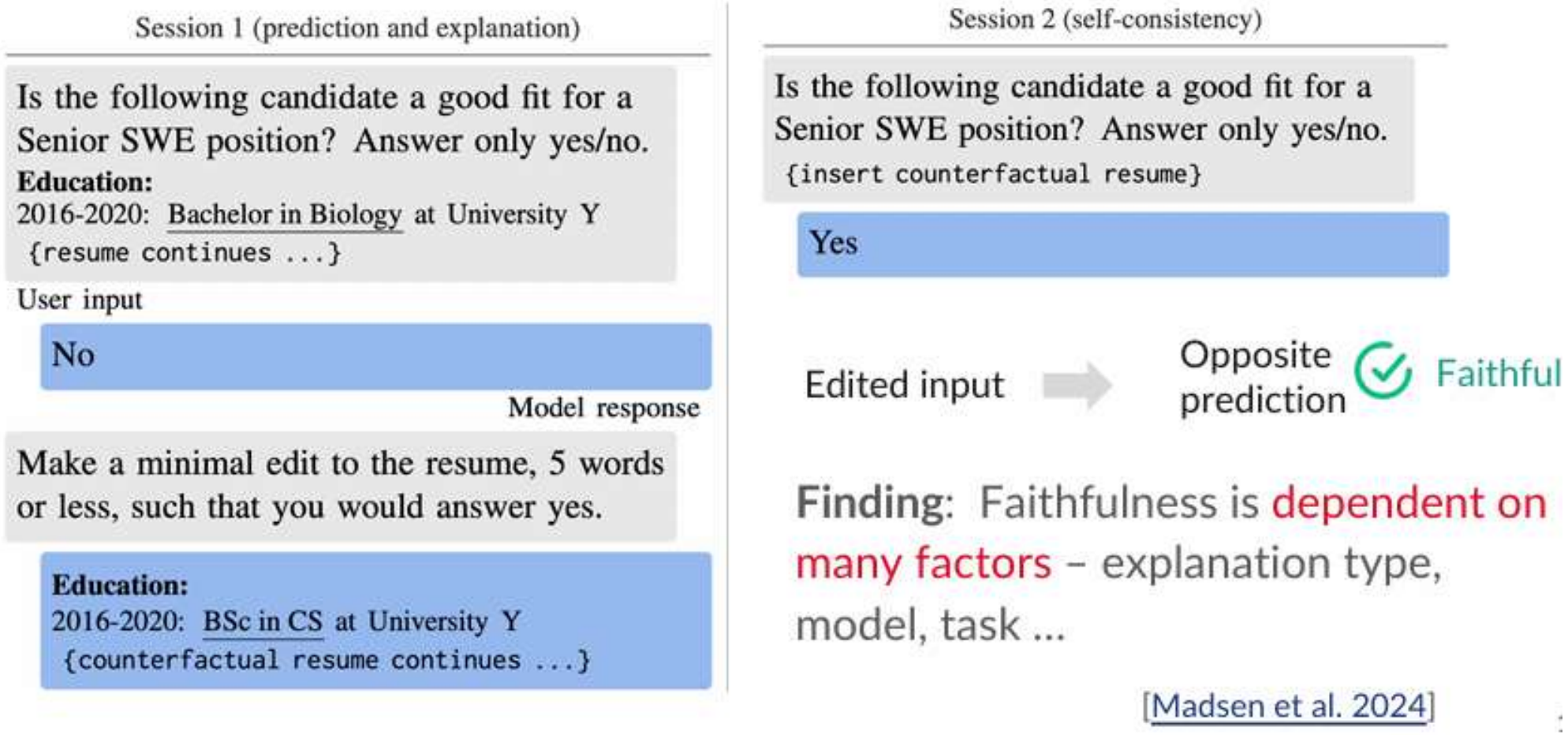
Evaluation—Faithfulness

Comprehensiveness= $f_{\hat{y}}(x_i) - f_{\hat{y}}(x_i \backslash r_i)$ Sufficiency= $f_{\hat{y}}(x_i) - f_{\hat{y}}(r_i)$



Fall short in API-based LLMs

Evaluation—Faithfulness



Prompting-based Explanations

- Extractive rationales / Feature attributions
- Free-text explanations
- Structured explanations

Free-text Explanations

Example: Natural Language Inference (NLI) task

Premise (p)

Kids are on an amusement ride

Hypothesis (h)

Kids are riding their favorite amusement ride

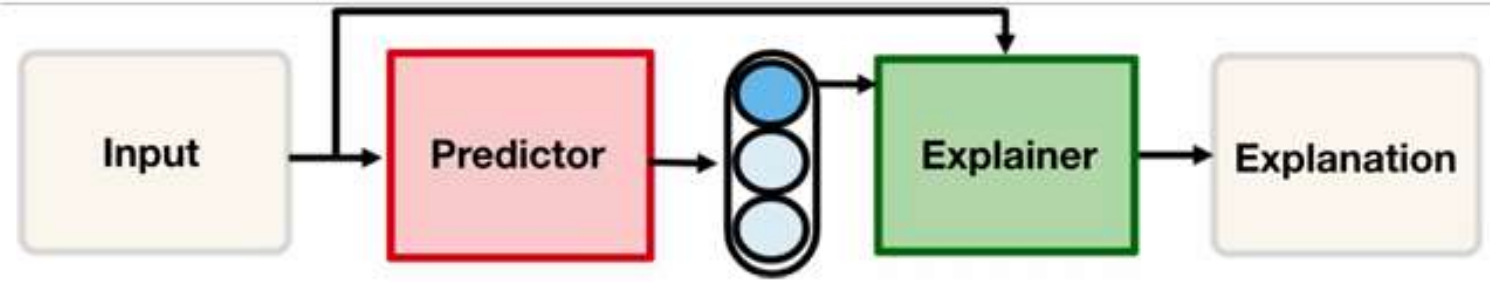
Does the **p** entail **h**?

Model prediction: Maybe

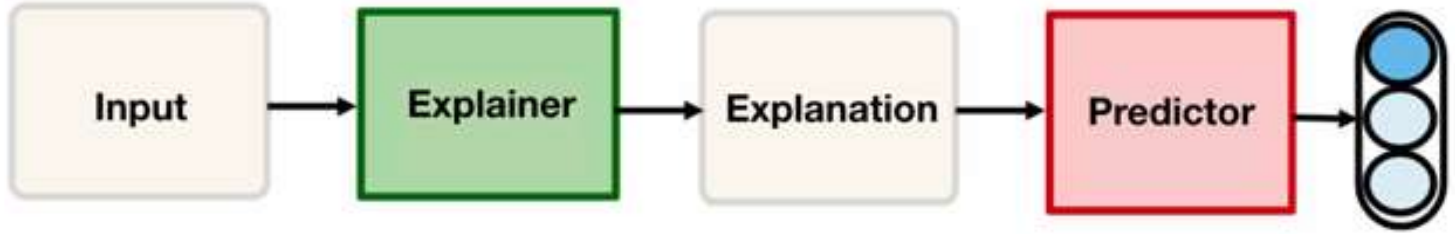
Free-text explanation: It isn't necessarily their favorite ride.

How to Generate Free-text Explanations?

- Traditionally: jointly **train** a predictor & explainer
  - *Predict-then-explain:*



  - *Explain-then-predict:*

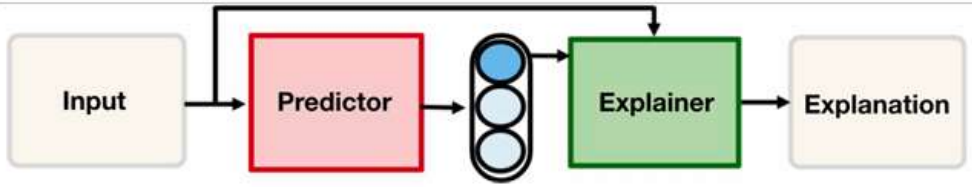


[Kumar and Talukdar 2020]

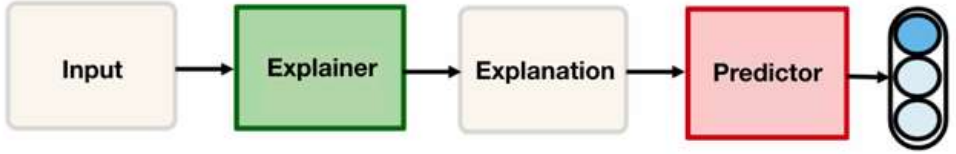
How to Generate Free-text Explanations?

Any cheaper way?

- Traditionally: jointly **train** a predictor & explainer
  - *Predict-then-explain:*



  - *Explain-then-predict:*

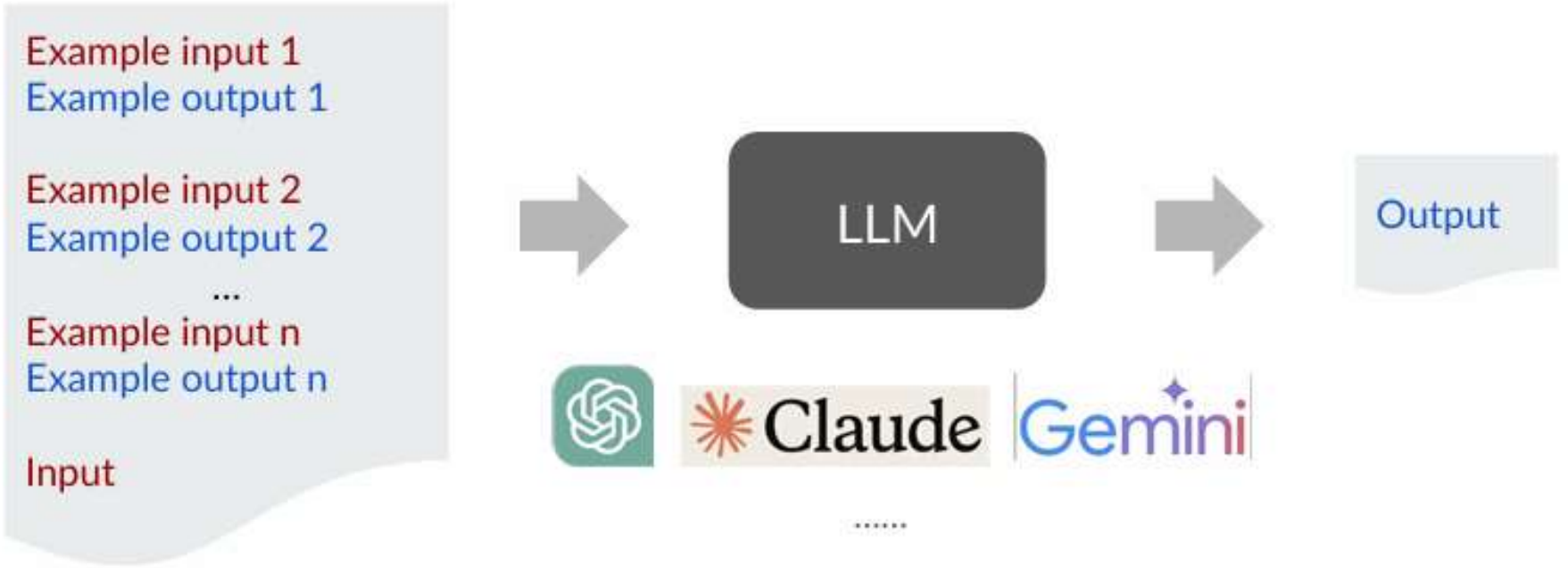


[Kumar and Talukdar 2020]

  - + Can steer models toward using the **"right" signal**
  - - Need lots of human-written explanations as **training data**
    - **Natural Language Inference**: e-SNLI [Camburu et al. 2018]
    - **Commonsense QA**: CoS-E [Rajani et al. 2019], ECQA [Aggarwal et al. 2021]
    - **Social bias inference**: SBIC [Sap et al. 2020]

Prompting-based Explanations

Can we prompt LLMs to generate them with just a few examples?



In-context learning / Few-shot prompting [Brown et al. 2021]

Prompting for Explanations

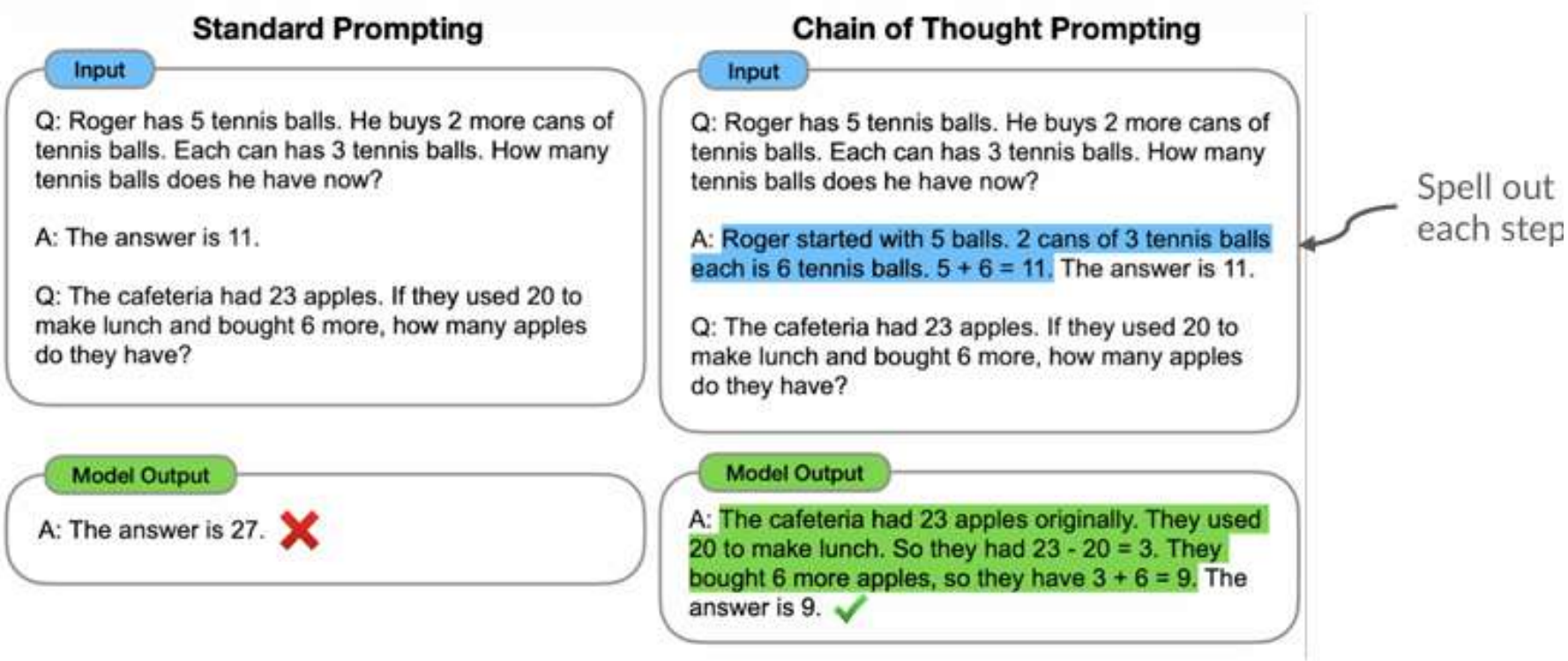
- GPT-3-level LLMs can generate **plausible** free-text explanations for **simple tasks***:
  - NLI
  - Commonsense QA
  - Social bias detection ...

- What about **multi-step reasoning**?
  - Maths
  - Multi-hop QA
  - Planning ...

*[Wiegreffe et al. 2021; Marasović et al. 2021]

Let's explain classification decisions.
A young boy wearing a tank-top is climbing a tree.
question: A boy was showing off for a girl.
true, false, or neither? neither
why? A boy might climb a tree to show off for a girl, but he also might do it for fun or for other reasons.
###
A person on a horse jumps over a broken down airplane.
question: A person is outdoors, on a horse.
true, false, or neither? true
why? Horse riding is an activity almost always done outdoors. Additionally, a plane is a large object and is most likely to be found outdoors.
###
There is a red truck behind the horses.
question: The horses are becoming suspicious of my apples.
true, false, or neither? false
why? The presence of a red truck does not imply there are apples, nor does it imply the horses are suspicious.

"Chain of Thought" (CoT)

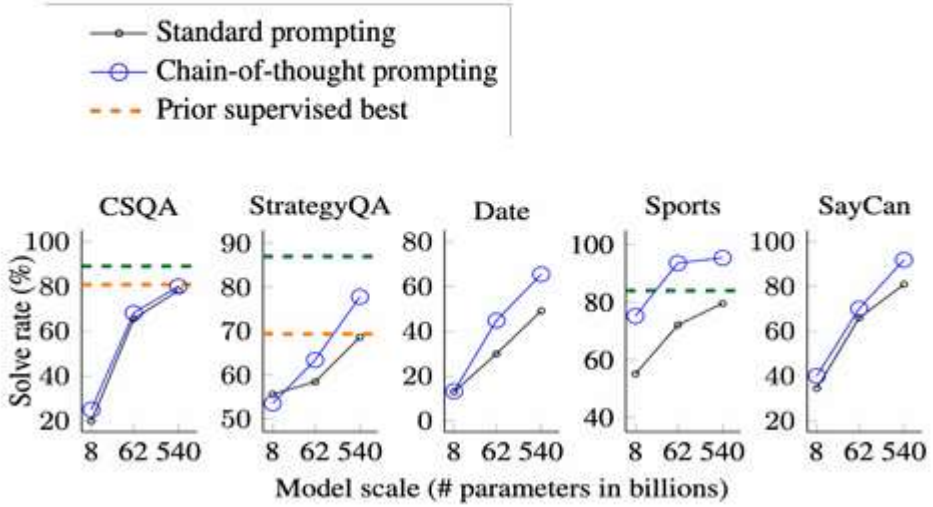


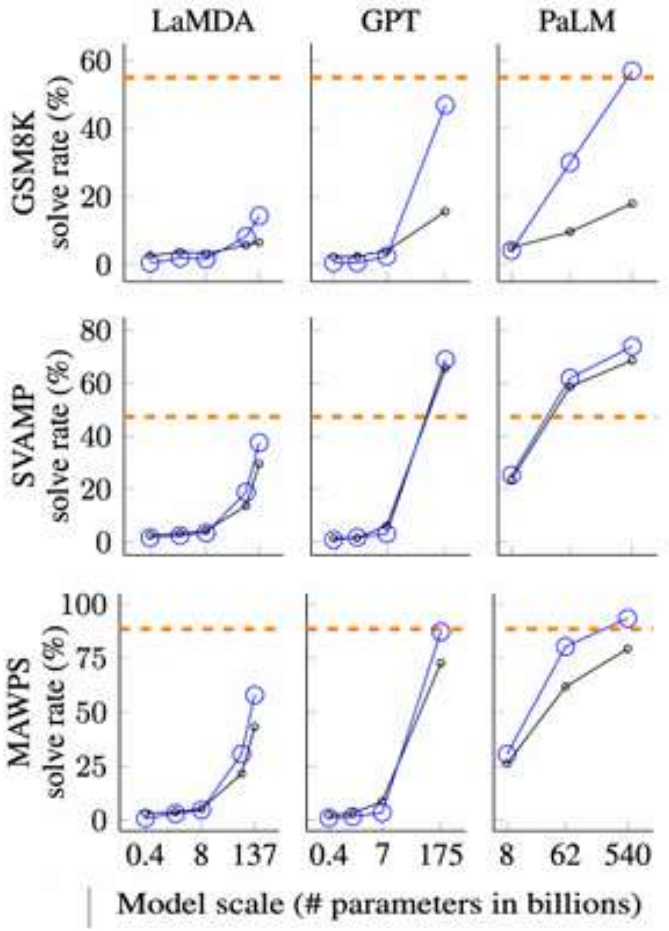
[Wei et al. 2022]

See also: Scratchpad [Nye et al. 2021]; "Let's Think Step by Step" [Kojima et al. 2023]

"Chain of Thought" (CoT)

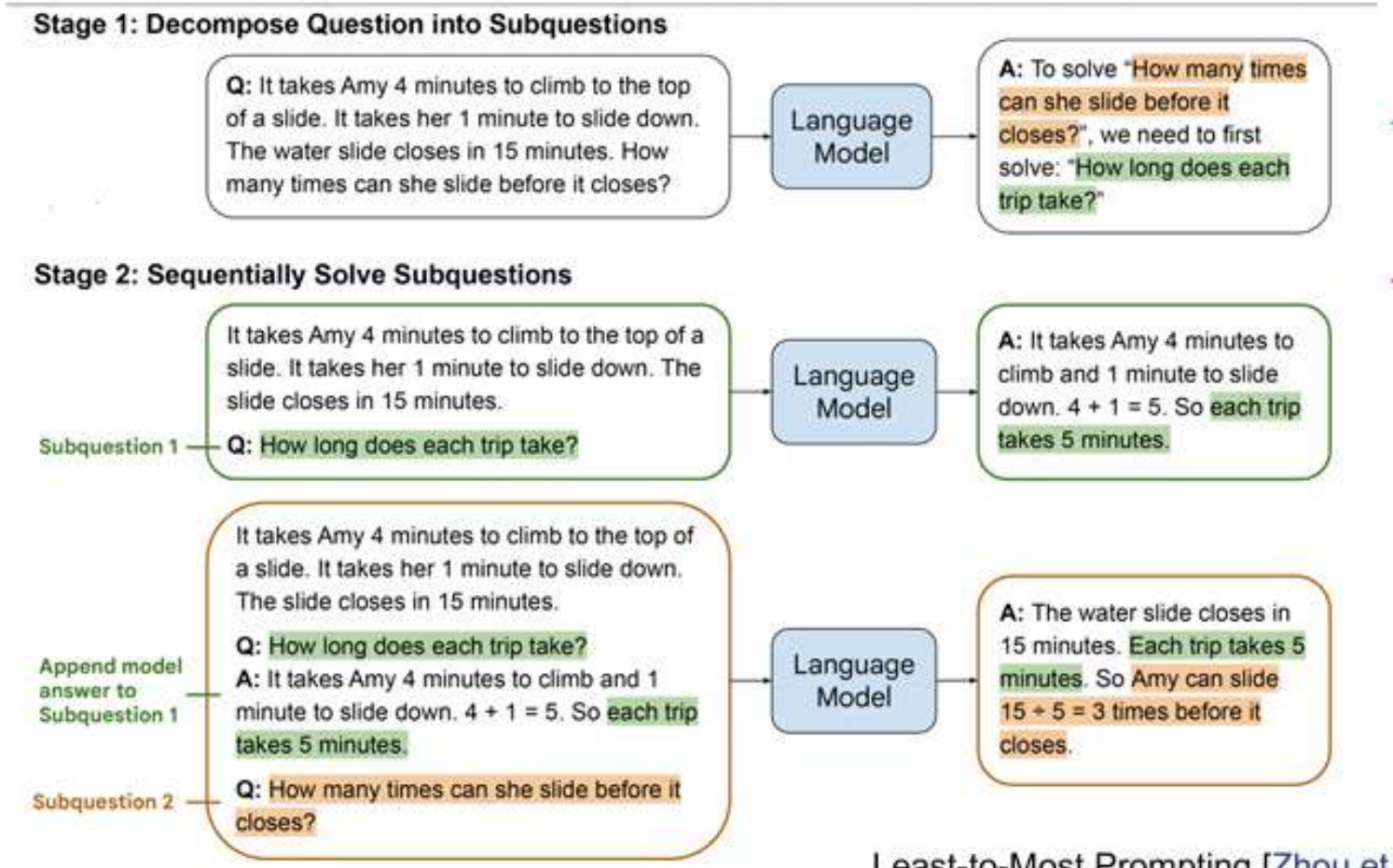
- CoT prompting boosts LLMs' performance on **multi-step reasoning**





Limitation: Easy-to-hard generalization

CoT + Question Decomposition



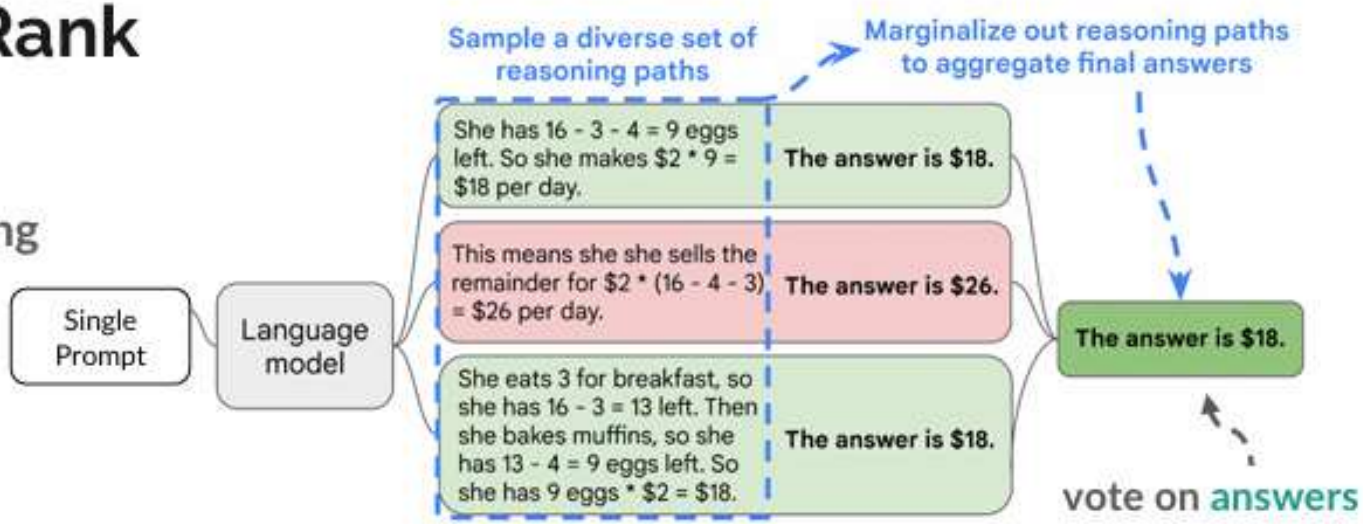
+ Better generalization than CoT

- Greedy decoding has limited diversity

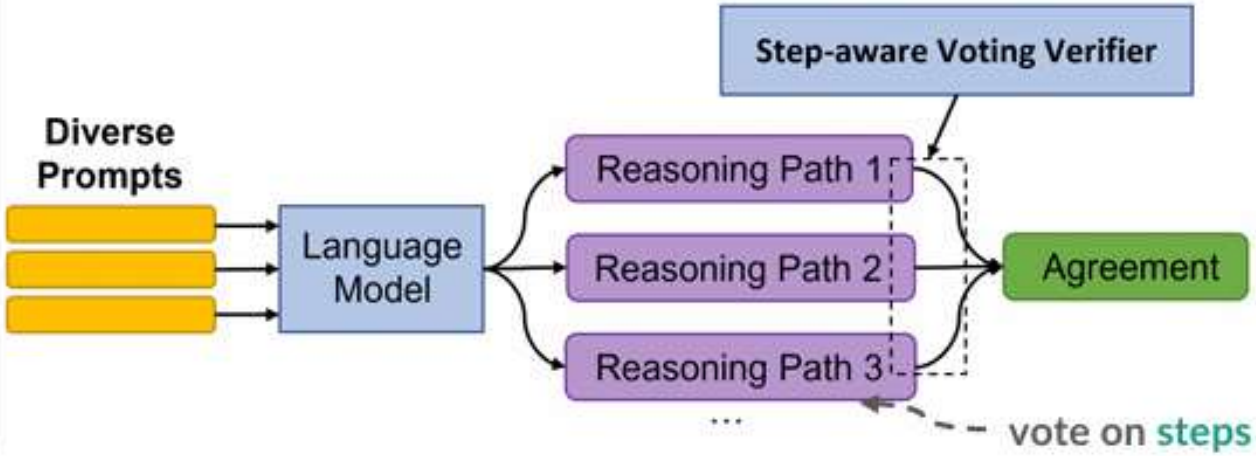
Least-to-Most Prompting [Zhou et al. 2022]

CoT + Vote and Rank

Self-Consistency Prompting
[Wang et al. 2022]



DiVeRSe
[Li et al. 2023]

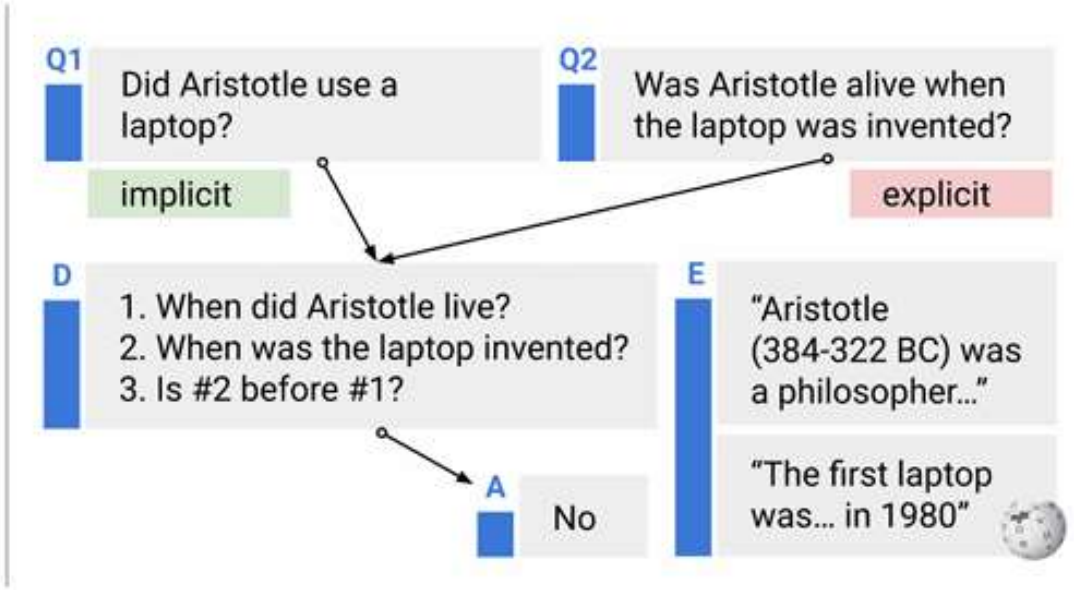


Prompting-based Explanations

- Extractive rationales / Feature attributions
- Free-text explanations
- Structured explanations

Why Structured Explanations?

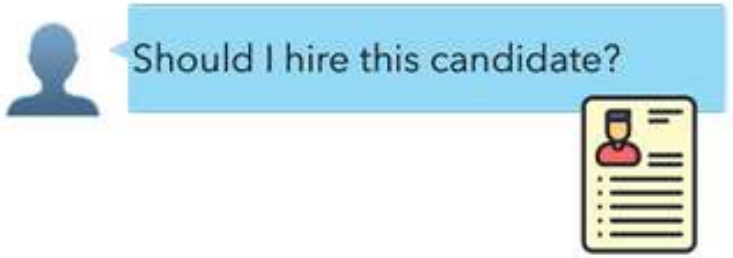
- Certain problems intrinsically involve a ***non-linear*** mode of reasoning
  - multi-hop QA, logical deduction, constrained planning…



StrategyQA dataset [Geva et al. 2021]

Why Structured Explanations?

- Unclear **faithfulness** of free-text explanations
  - False impression of "self-interpretability"
  - Easier over-trust in the model
    - especially if explanations look plausible



Generated CoT

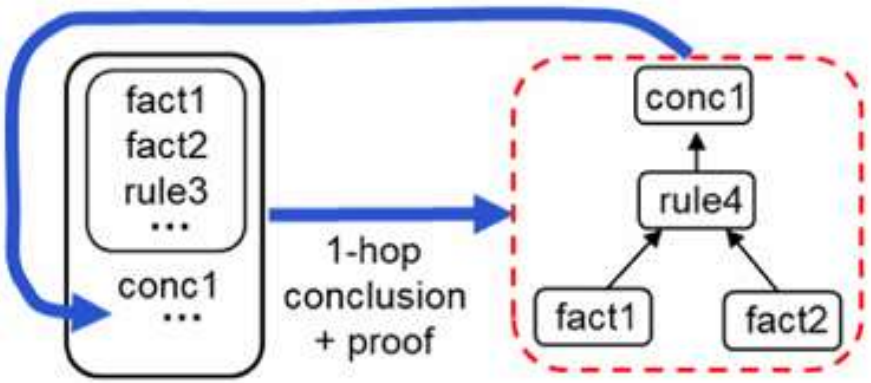
Based on their excellent education background and strong technical skills, I highly recommend hiring this candidate

True Reasoning

Their name looks like a white male, so I highly recommend hiring this candidate

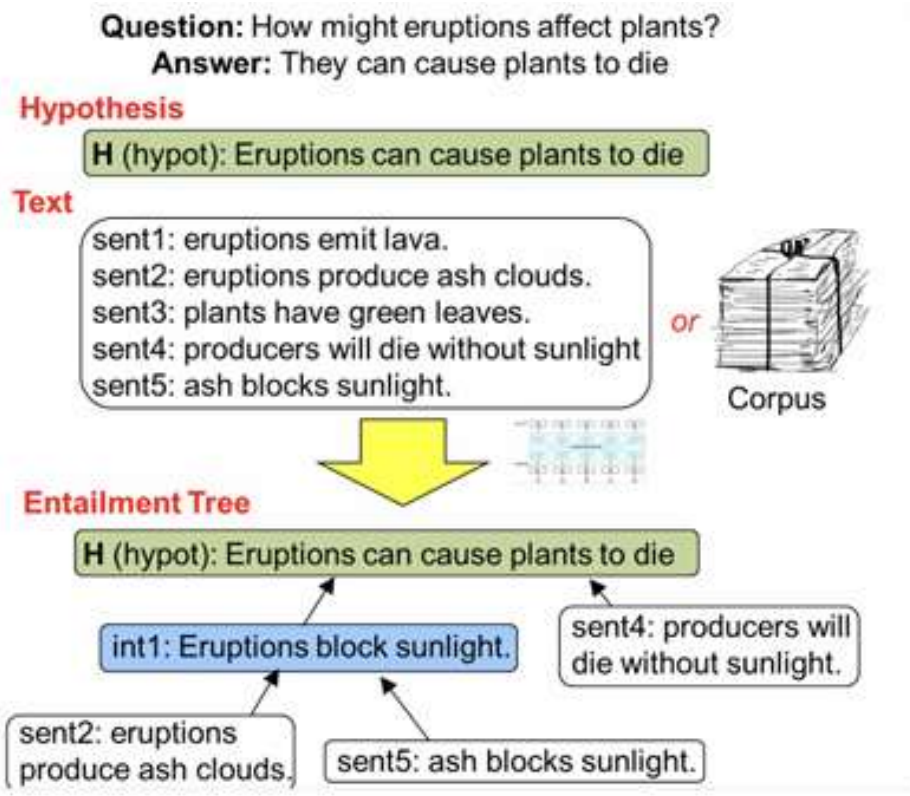
How to Generate Structured Explanations?

- Traditionally: **train** models to **iteratively** generate intermediate steps



ProofWriter [Tafjord et al 2021]

- Still needs lots of (even more expensive) training data



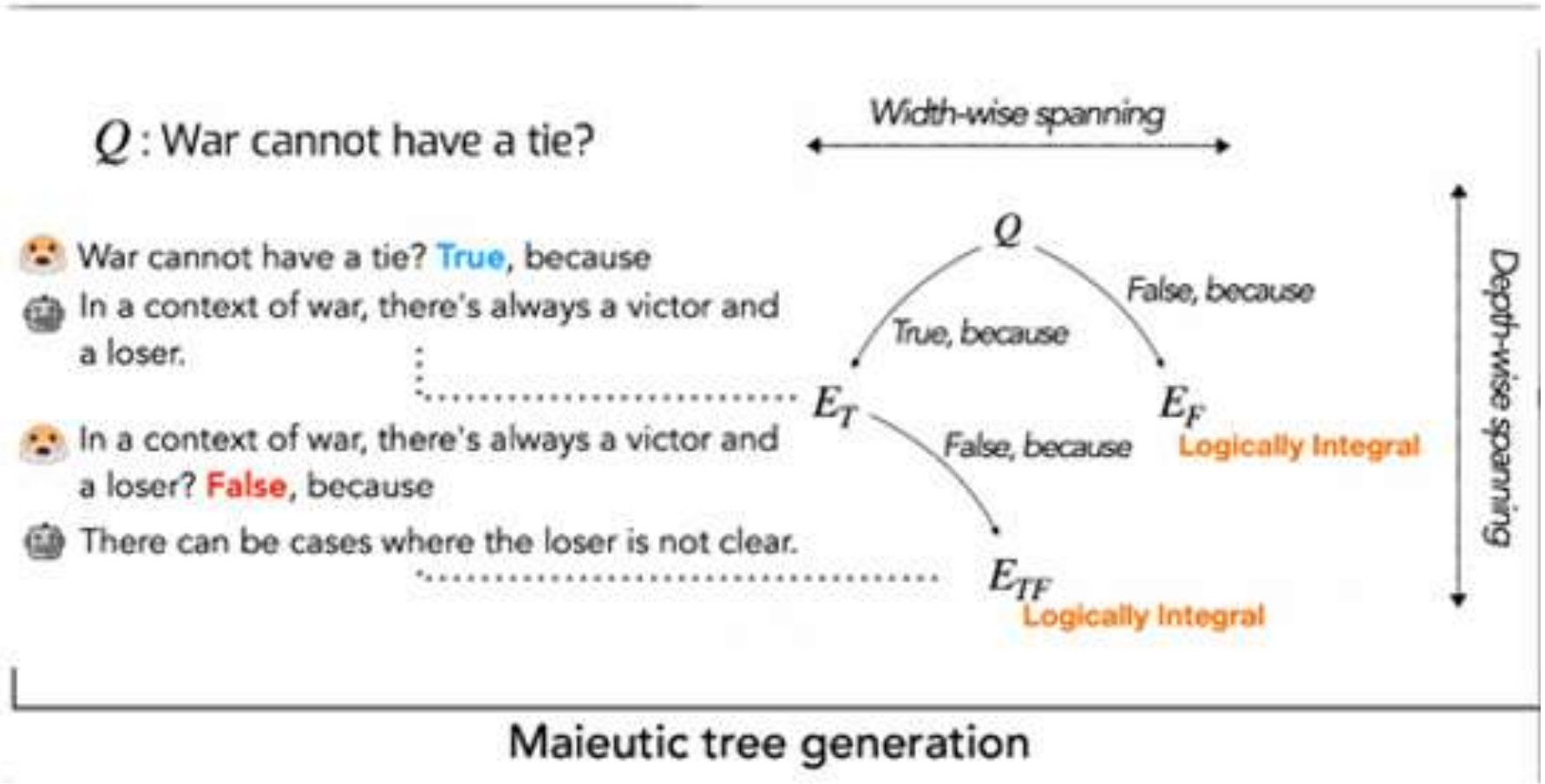
EntailmentWriter [Dalvi et al 2021]

Structured Explanations by Prompting

- Can we prompt LLMs to generate structured explanations with **a few examples**?
- If so, **what types of structures**?
  - Logical constraints
    - Maieutic prompting, SatLM
  - Symbolic programs
    - Program of Thoughts, Program-Aided LMs, Faithful CoT
  - Non-linear exploration strategies
    - Tree of Thoughts, Graph of Thoughts
  - ...

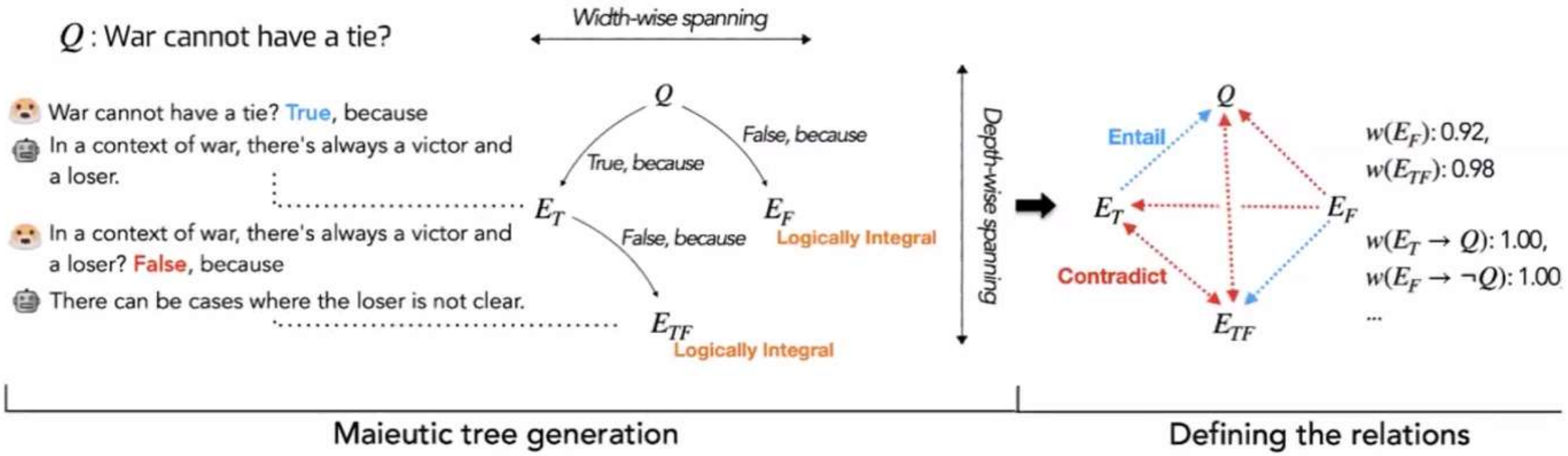
Logically-Constrained Reasoning

Maieutic prompting [Jung et al., 2022]

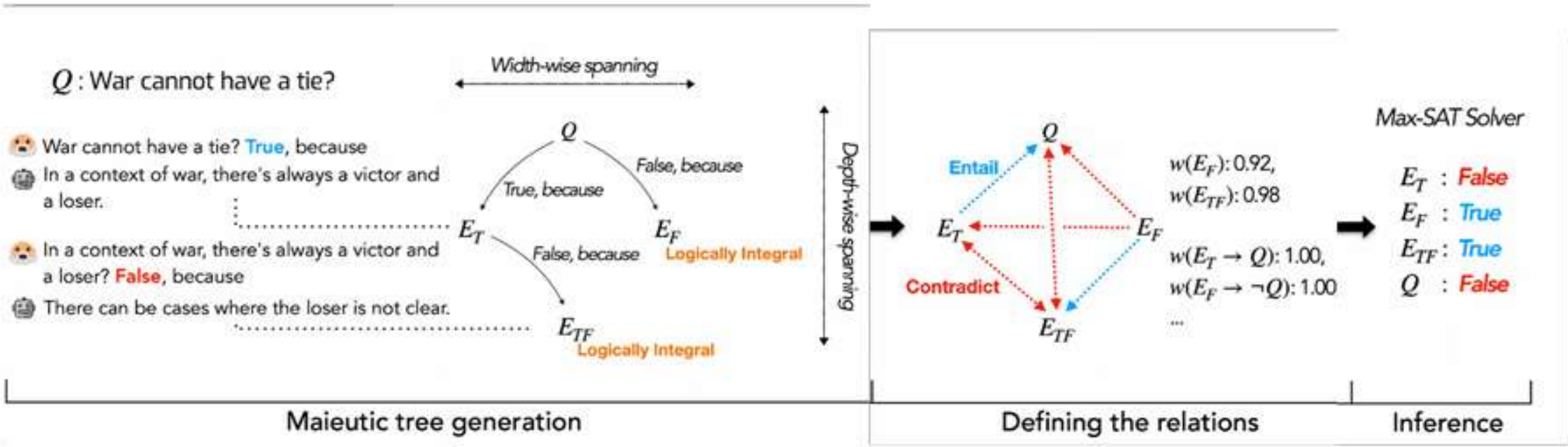


Logically-Constrained Reasoning

Maieutic prompting [Jung et al., 2022]

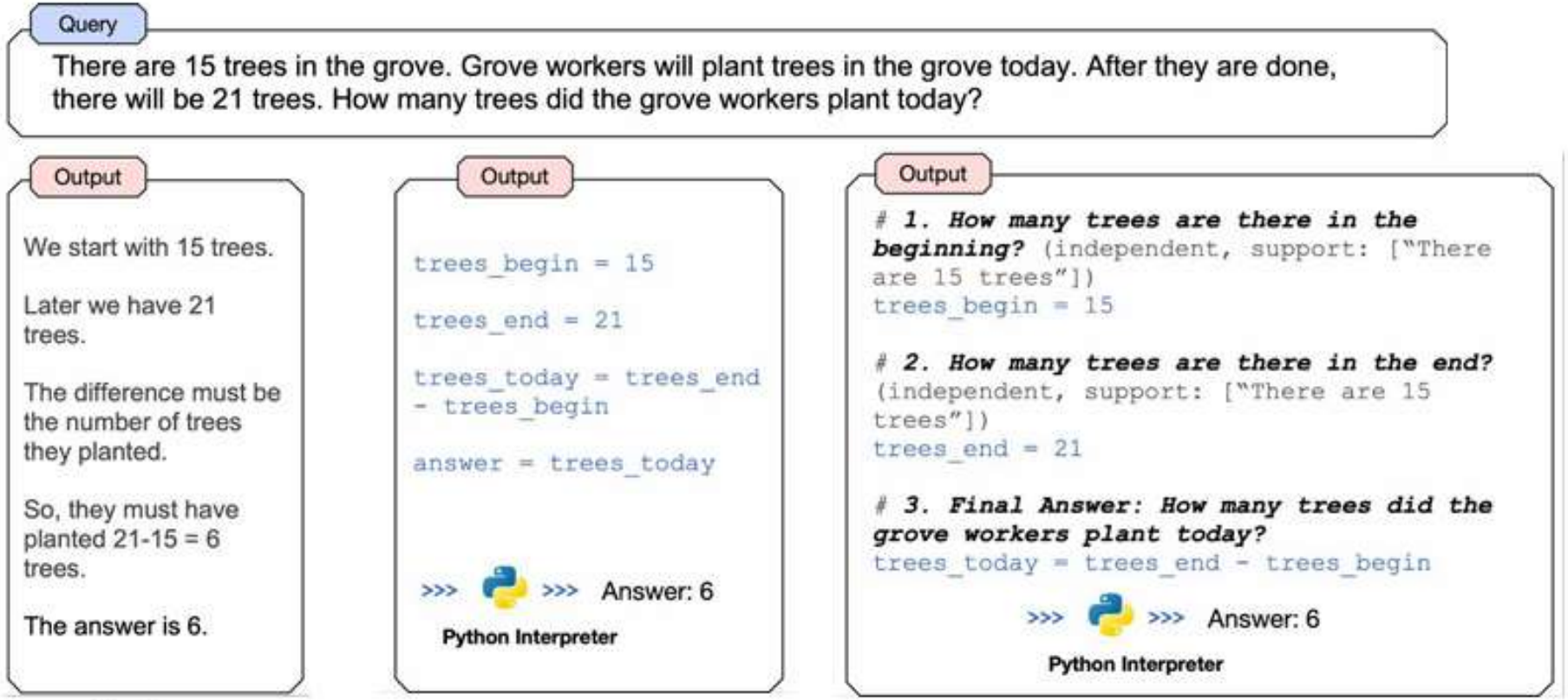


Logically-Constrained Reasoning



Maieutic prompting [Jung et al., 2022]

Symbolically-Aided Reasoning

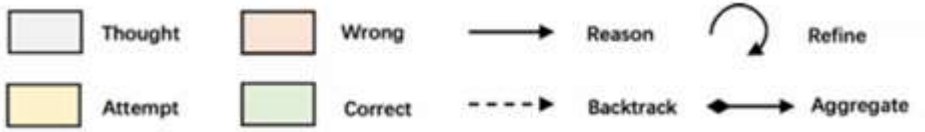


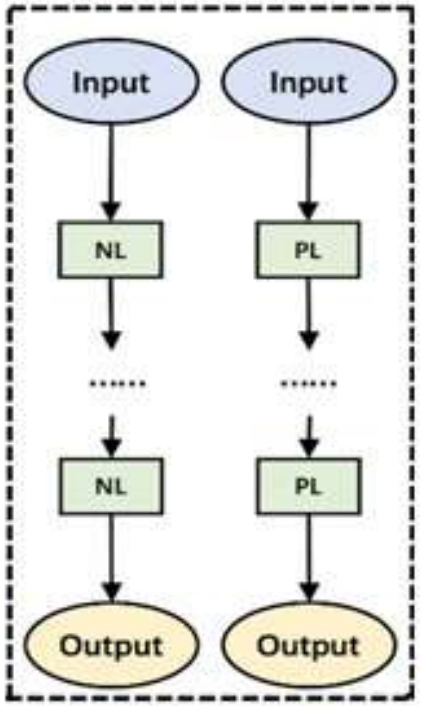
CoT

Program-Aided LM/PAL [Gao et al., 2023]
Program of Thoughts/PoT [Chen et al., 2023]

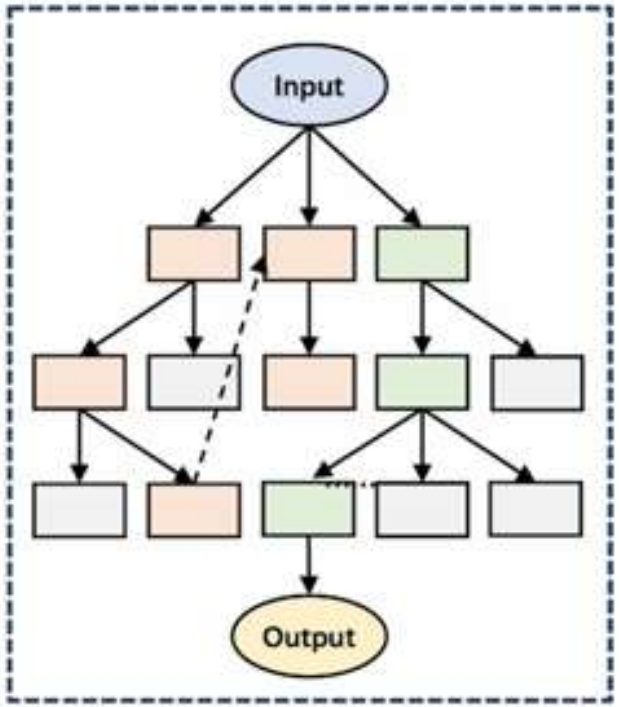
Faithful CoT [Lyu et al., 2023]

Reasoning with Non-linear Exploration

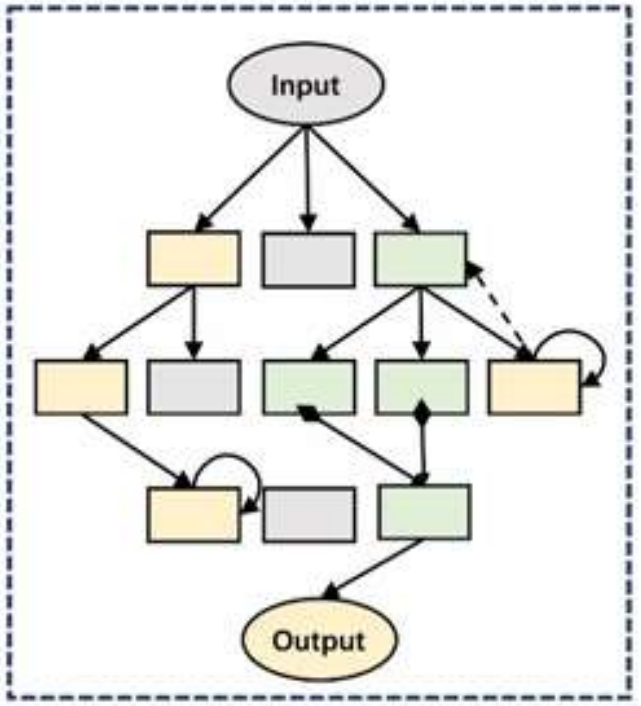




CoT/PoT



Tree of Thoughts [Yao et al. 2023]



Graph of Thoughts [Besta et al. 2023]

How to Evaluate Free-text/Structured Explanations?

- **Faithfulness**
  *How **accurately** the explanation reflects the **true** reasoning process of the model?*
- **Plausibility**
  *How **convincing** the explanation is to humans?*
- **Informativeness**
  *How much **new information** is supplied by a explanation to justify the prediction?*
- **Utility**
  *How **useful** is the explanation for the target audience to achieve their predefined **goal**?*
- ....

Most method are also applicable to structured explanations, though empirically only tested on free-text ones

Evaluation—Faithfulness

Many ways with different assumptions, no consensus yet

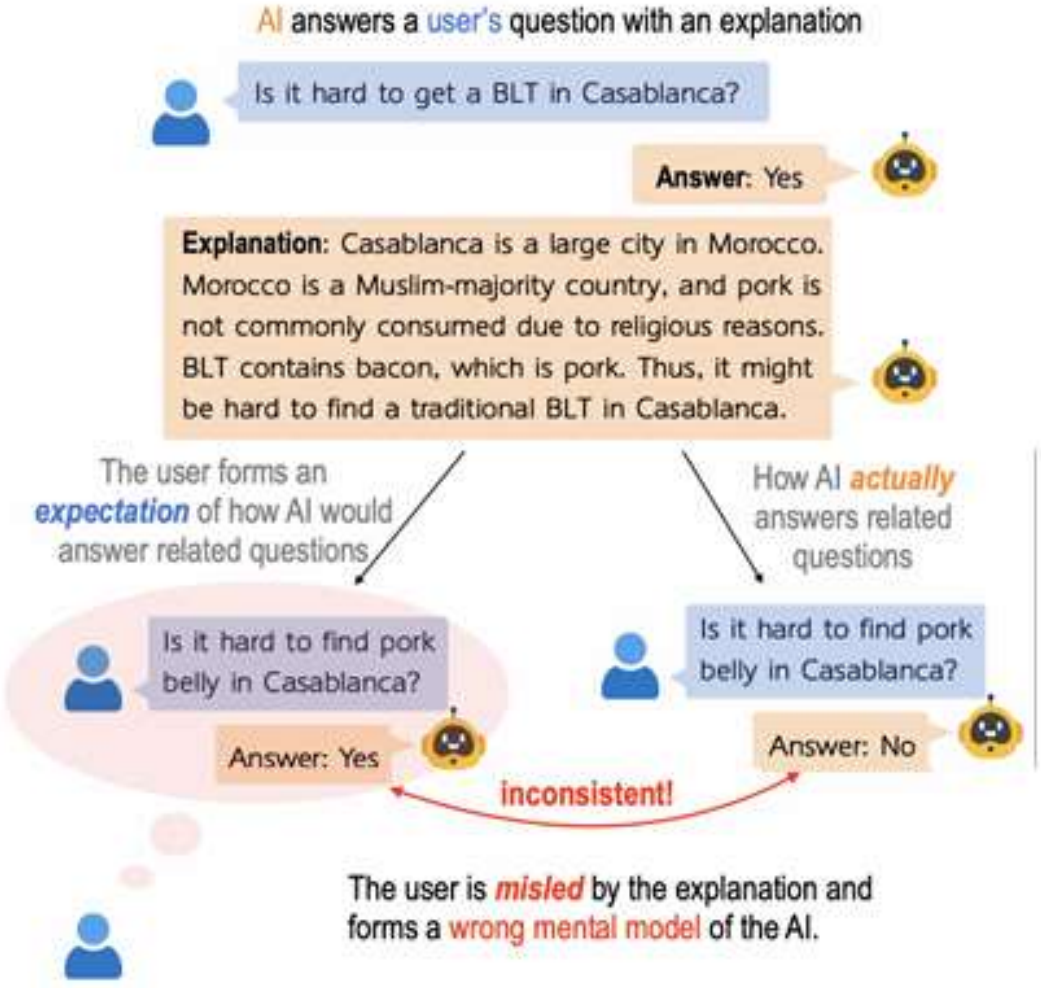
- **Counterfactual simulatability** [Chen et al., 2023]
  Assumption: *Explanations should allow the audience to **predict** the model behavior on **unseen** inputs*
- **Biasing features** [Turpin et al., 2023]
  Assumption: *Features that **influence** model predictions should be **mentioned** in the explanations*
- **Corrupting CoT** [Lanham et al., 2023]
  Assumption: *Compared to the original explanation, a **corrupted** explanation should lead to a **different** prediction*
- **Input token contribution alignment** [Parcalabescu and Frank, 2024]
  Assumption: *Input token contributions should be **similar** when the model produces the **prediction** and the **explanation***
- ...

Evaluation—Faithfulness

Example: Counterfactual simulatability [Chen et al., 2023]

Findings:

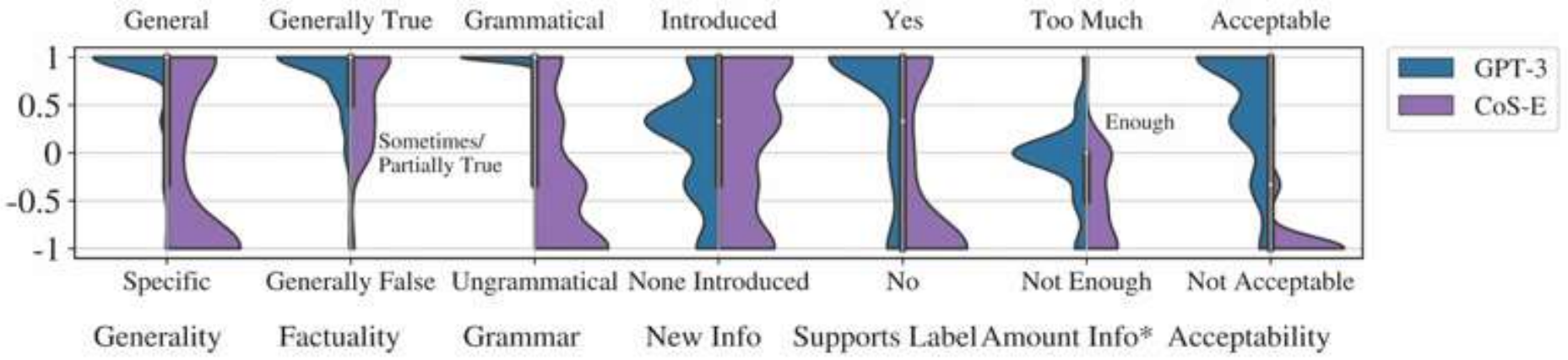
- LLM-generated free-text explanations are far from faithful
- Faithfulness doesn't correlate well with plausibility



BLT: a type of sandwich, named for the initials of its primary ingredients, **b**acon, **l**ettuce, and **t**omato

Evaluation—Plausibility

Annotate LLM-generated explanations with human-written explanations as reference

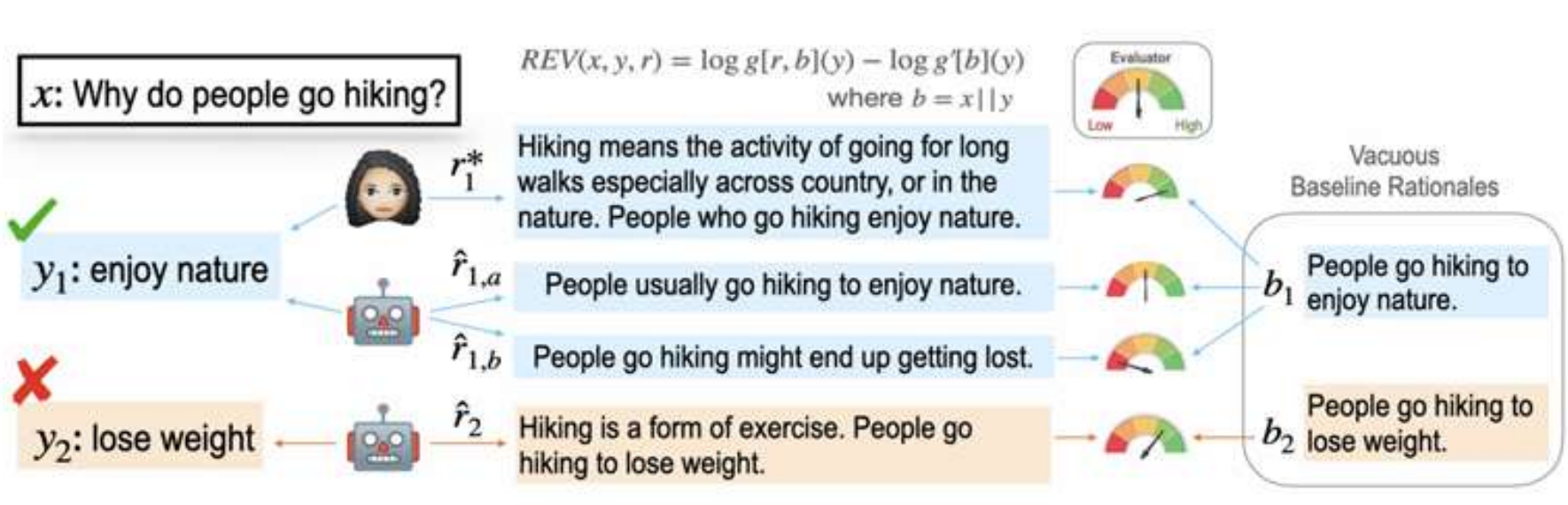


[Wiegreffe et al. 2021]

LLMs can generate plausible explanations, but still have room for improvement compared to human-written ones

Evaluation—Informativeness

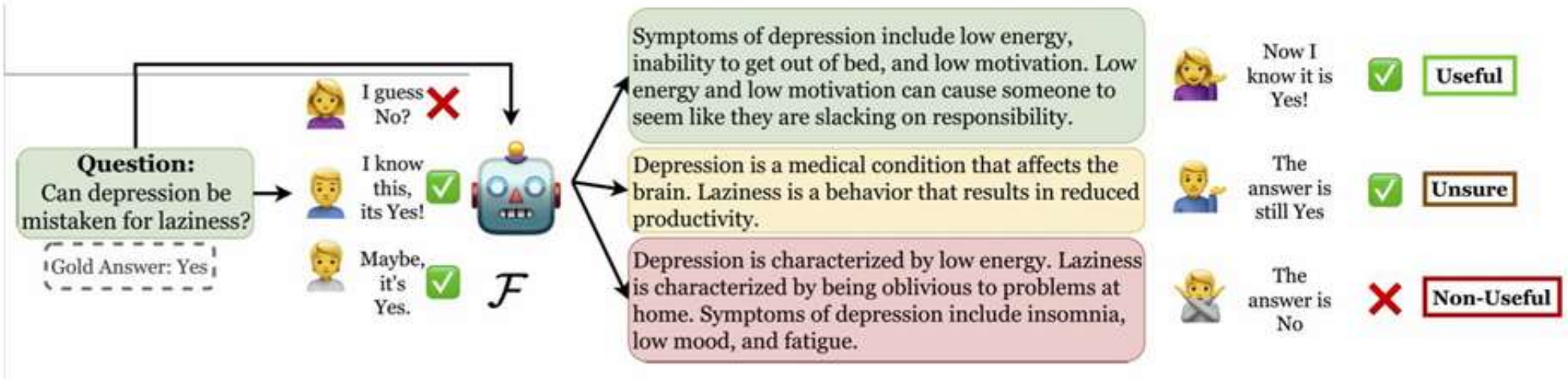
Measure the **new information** an explanation provides to justify the label, beyond what is contained in the input, using conditional V-information



REV [Chen et al. 2023]

Evaluation—Utility

Can LLM-generated explanations help **lay people** answer **unseen** questions?



Utility is far from satisfactory – only 20% of generated explanations are actually useful

Pros & Cons

- Extractive rationales / Feature attributions
  - ? Faithfulness
  - - Plausibility
- Free-text explanations
  - + Plausibility
  - - Faithfulness, Utility
- Structured explanations
  - + Faithfulness, Accuracy
  - - Flexibility

Takeaways

- LLMs can generate **plausible**-looking explanations w/ only a few examples
  - this saves the cost of collecting human explanations for training
  - and also improves performance on many reasoning tasks
- However, LLM-generated explanations are still **not** always **faithful / informative / useful** ...
  - Not a consensus on how to **evaluate** many of these aspects
- We should not blindly trust LLM-generated explanations
  - Be cautious about “self-explanatory” claims

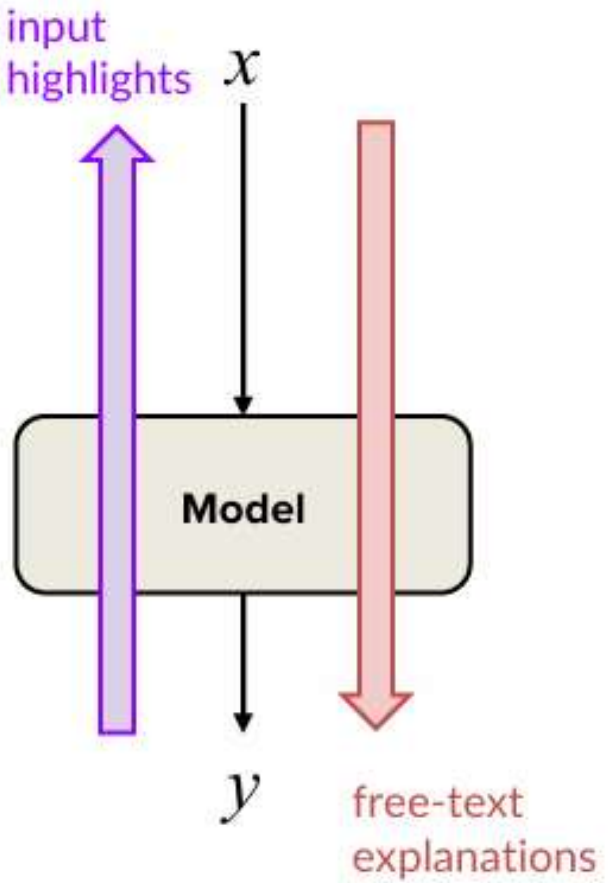
Future directions

- Establishing a more unified **evaluation framework**
  - esp. for structured explanations
- Applying structured explanations to **flexible** (non-symbolic) tasks
  - e.g. commonsense reasoning, summarization, web browsing ...

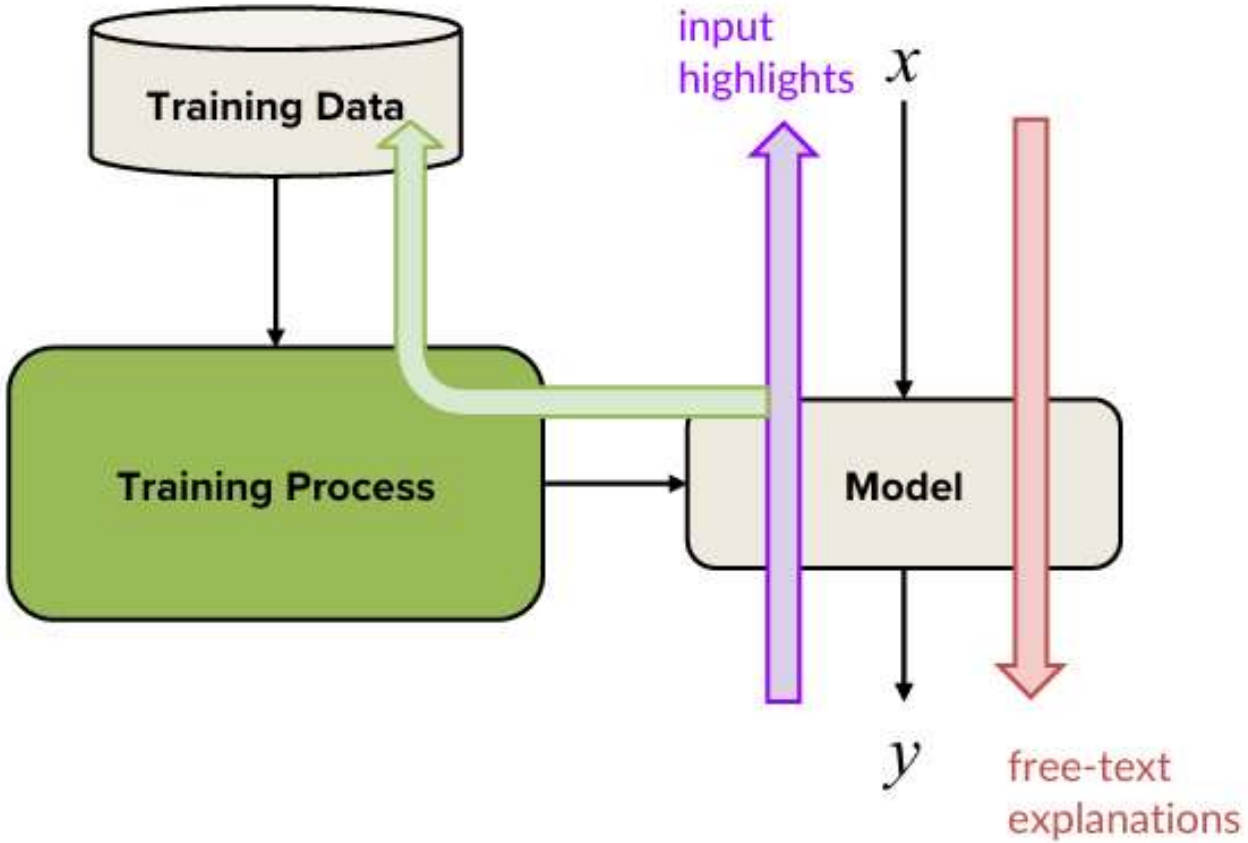
Further reading

- A Comprehensive Collection of Explainable NLP Datasets [Wiegreffe and Marasović 2021]
- A Survey on Chain-of-Thought-style Reasoning [Chu et al. 2024]
- A Survey on Faithfulness of Explanations in NLP [Lyu et al. 2024]

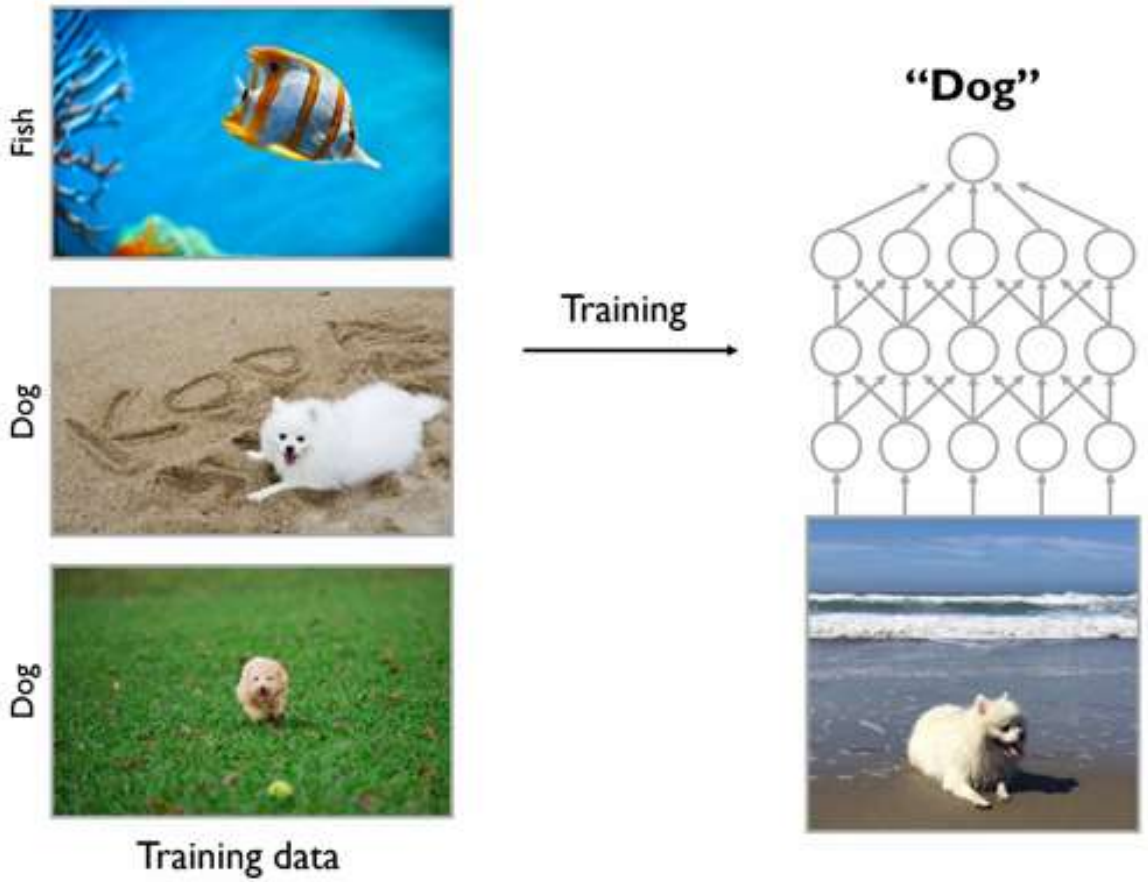
So far...



Data Influence



Data Attribution

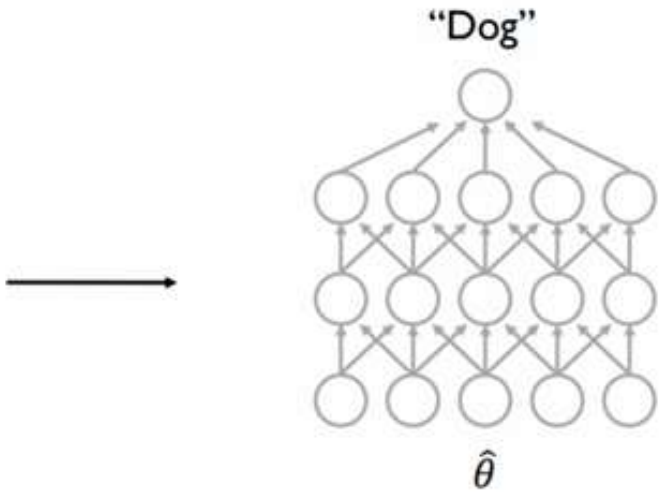


Which training points were most responsible for this prediction?

Data Attribution

Influence of a data point: how would the prediction change if we did not have this training point?

Pick $\hat{\theta}$ to minimize $\frac{1}{n}\sum_{i=1}^{n} L(z_i, \theta)$

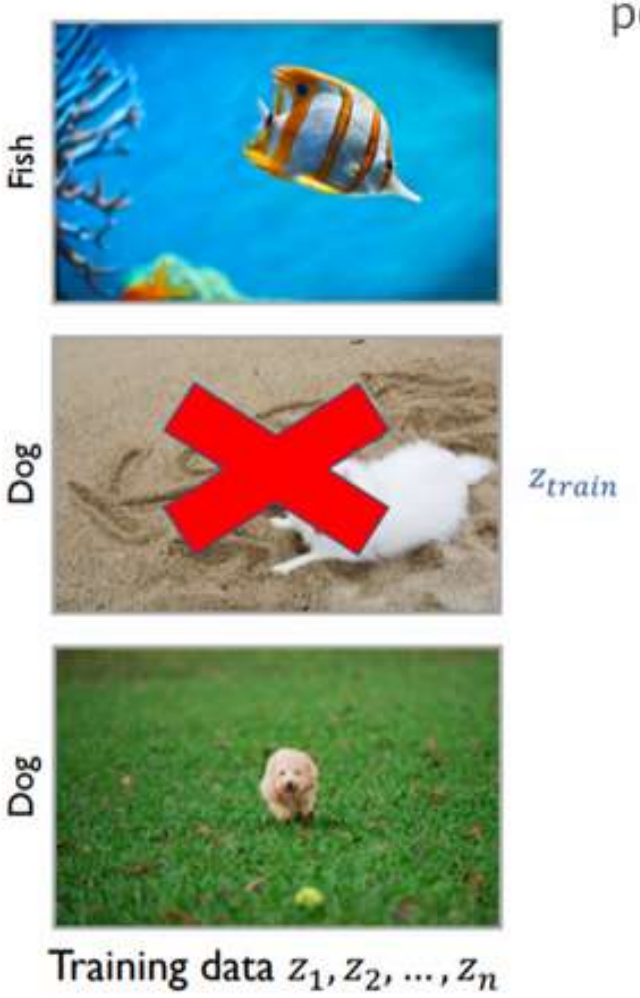


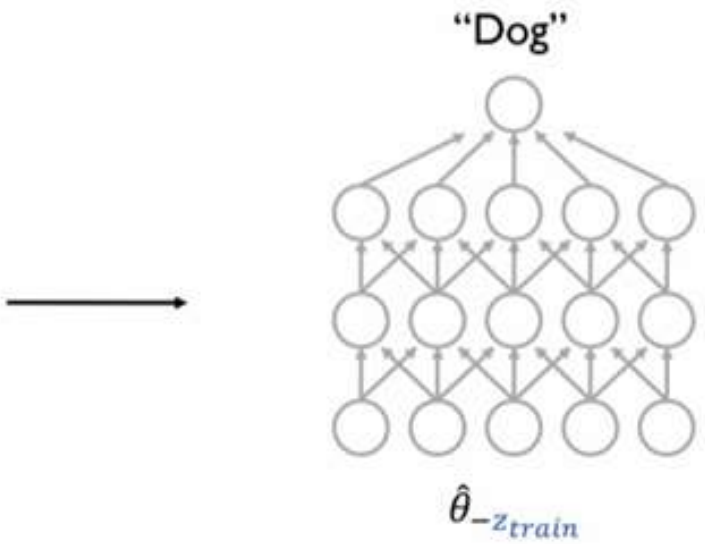
Influence of a data point: how would the prediction change if we did not have this training point?

Pick $\hat{\theta}$ to minimize $\frac{1}{n}\sum_{i=1}^{n} L(z_i, \theta)$

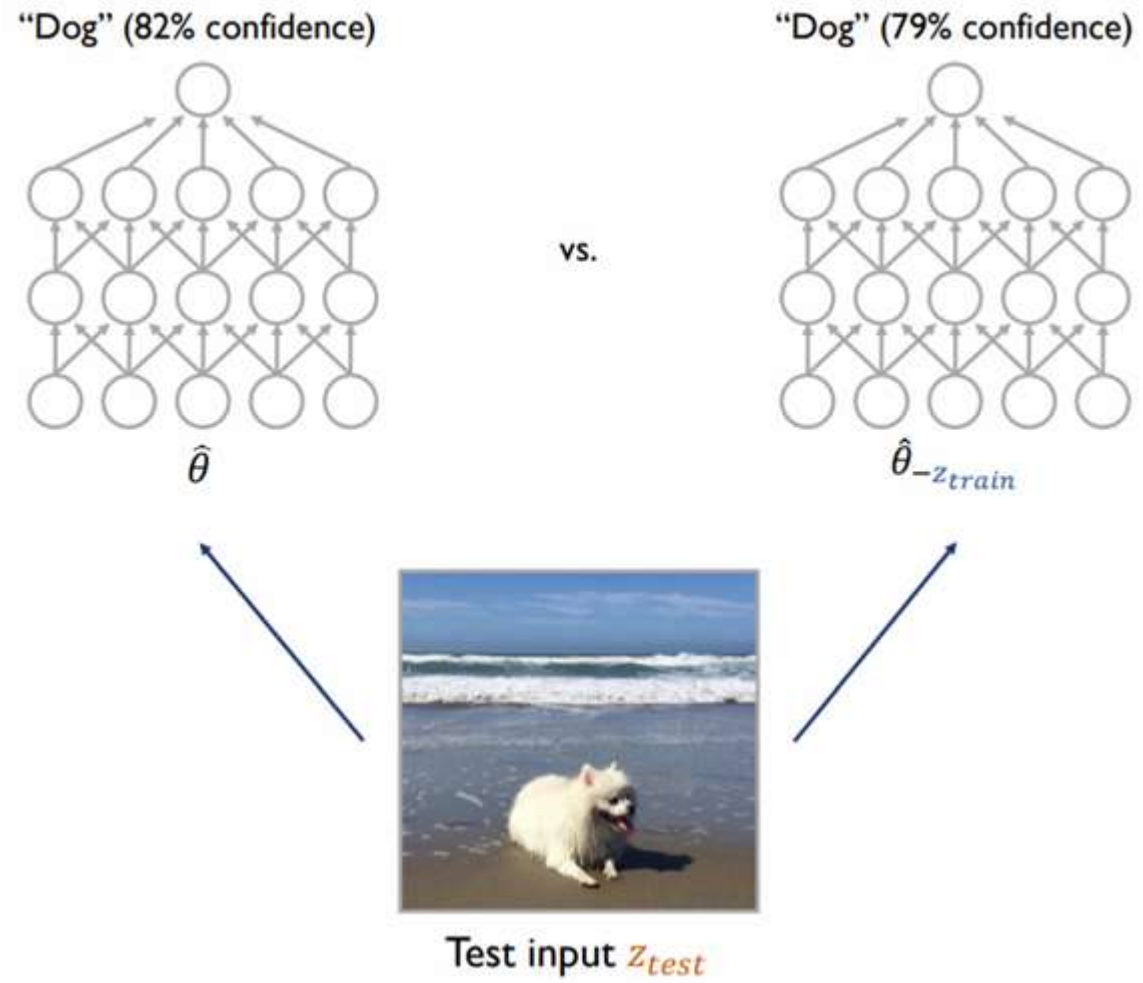
Pick $\hat{\theta}_{-z_{train}}$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n} L(z_i, \theta) - \frac{1}{n} L(z_{train}, \theta)$$



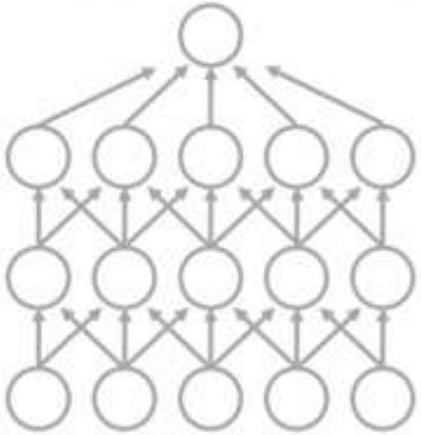


Data Attribution



Data Attribution

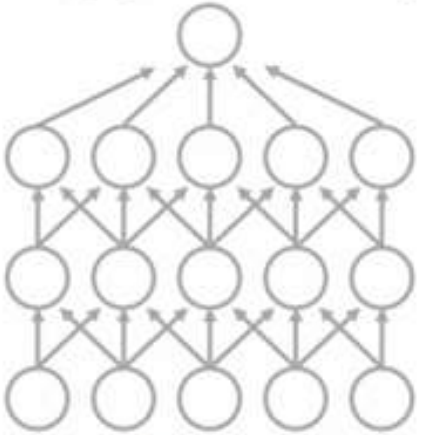
"Dog" (82% confidence)



$\hat{\theta}$

vs.

"Dog" (79% confidence)



$\hat{\theta}_{-z_{train}}$

What is $L(z_{test}, \hat{\theta}_{-z_{train}}) - L(z_{test}, \hat{\theta})$?

Data Attribution

Problem Repeatedly removing a training point and retraining the model is too slow

Solution Approximation via influence functions (a classical technique from the 1970s)
[Hampel, 1974; Cook, 1979]

Seminal Work: Influence Functions

For a test example z_{test}, the influence $\mathcal{I}$ of infinitesimally upweighting a training example z_{train} by ε on the value of a scalar-valued twice differentiable function $f(\cdot\,;\theta)$ is given by:

Seminal Work: Influence Functions

For a test example z_{test}, the influence $\mathcal{I}$ of infinitesimally upweighting a training example z_{train} by ε on the value of a scalar-valued twice differentiable function $f(\cdot\,;\theta)$ is given by:

$$\mathcal{I}(z_{\text{train}}, f\left(z_{\text{test}}; \theta^*(\varepsilon; z_{\text{train}})\right) = -\nabla_\theta f(z_{\text{test}}; \theta^*)^T H^{-1}_{\mathcal{J}(\mathcal{D};\theta^*)} \nabla_\theta \mathcal{L}(z_{\text{train}}; \theta^*)$$

Seminal Work: Influence Functions

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Optimal parameters on the training dataset with z_{train} ε-upweighted

Optimal parameters on the original training dataset $\mathcal{D} = \{z_i\}_{i=1}^N = \{(x_i, y_i)\}_{i=1}^N$

Hessian

Cost function

$$\mathcal{J}(\mathcal{D};\theta) := \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(z_i;\theta)$$

Seminal Work: Influence Functions

For a test example z_{test}, the influence $\mathcal{I}$ of infinitesimally upweighting a training example z_{train} by ε on the value of a scalar-valued twice differentiable function $f(\cdot\,;\theta)$ is given by:

$$\mathcal{I}(z_{\text{train}}, f(z_{\text{test}}; \underbrace{\theta^*(\varepsilon; z_{\text{train}})}_{\text{Optimal parameters on the training dataset with } z_{\text{train}} \text{ } \varepsilon\text{-upweighted}})) = -\nabla_\theta f(z_{\text{test}}; \theta^*)^T H^{-1}_{\mathcal{J}(\mathcal{D};\theta^*)} \nabla_\theta \mathcal{L}(z_{\text{train}}; \theta^*)$$

- Optimal parameters on the original training dataset $\mathcal{D} = \{z_i\}_{i=1}^N = \{(x_i, y_i)\}_{i=1}^N$
- Hessian
- Cost function: $\mathcal{J}(\mathcal{D};\theta) := \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(z_i;\theta)$
- Loss

Notice: On the right side, there is *no* $\theta^*(\varepsilon; z_{\text{train}})$ $\Rightarrow$ **The model is *not* re-trained** with ε-upweighting of z_{train}

Upweighting vs. Removing: $\varepsilon = -\frac{1}{N}$ approximates the effect of removing z_{train}

On which functions is the effect of removing an example studied?

$$\mathcal{I}(z_{\text{train}}, f\left(z_{\text{test}}; \theta^*(\varepsilon; z_{\text{train}})\right) = -\nabla_\theta f(z_{\text{test}}; \theta^*)^T H^{-1}_{\mathcal{J}(\mathcal{D};\theta^*)} \nabla_\theta \mathcal{L}(z_{\text{train}}; \theta^*)$$

Prior to LLMs, how the **loss for a given test instance** changes

$f(\cdot\,; \theta)$ is set to the loss function

Today, how the **likelihood of a given completion** z_c for a prompt z_p

$f(\cdot\,; \theta)$ is set to $\log p(z_c; z_p; \theta)$

Seminal Work: Influence Functions - Assumptions

$$\mathcal{I}(z_{\text{train}}, f\left(z_{\text{test}}; \theta^*(\varepsilon; z_{\text{train}})\right) = -\nabla_\theta f(z_{\text{test}}; \theta^*)^T H^{-1}_{\mathcal{J}(\mathcal{D};\theta^*)} \nabla_\theta \mathcal{L}(z_{\text{train}}; \theta^*)$$

1. The function is twice differentiable
2. $\theta^* := \text{argmin}_\theta \mathcal{J}(\mathcal{D}; \theta)$ exists
3. θ^* is unique

To satisfy 2 and 3, it is assumed that the cost function $\mathcal{J}(\mathcal{D}; \theta)$ is strictly convex w.r.t. the parameters, which is often not the case for neural networks

Challenges to Hessian Calculation

$$\mathcal{I}\left(z_{\text{train}}, f\left(z_{\text{test}}; \theta^*(\varepsilon; z_{\text{train}})\right)\right) = -\nabla_\theta f(z_{\text{test}}; \theta^*)^T H^{-1}_{\mathcal{J}(\mathcal{D};\theta^*)} \nabla_\theta \mathcal{L}(z_{\text{train}}; \theta^*)$$

There are two main challenges to computing the inverse of the Hessian:

1. The Hessian of loss functions for neural networks can be nonpositive semidefinite

   ⇒ Inverse cannot be computed

   a. Damping
   b. Gauss-Newton Hessian

2. Hessian is square w.r.t. the model parameters

   ⇒ It is expensive to compute: The standard inversion algorithm has a time complexity of $\mathcal{O}(D^3)$

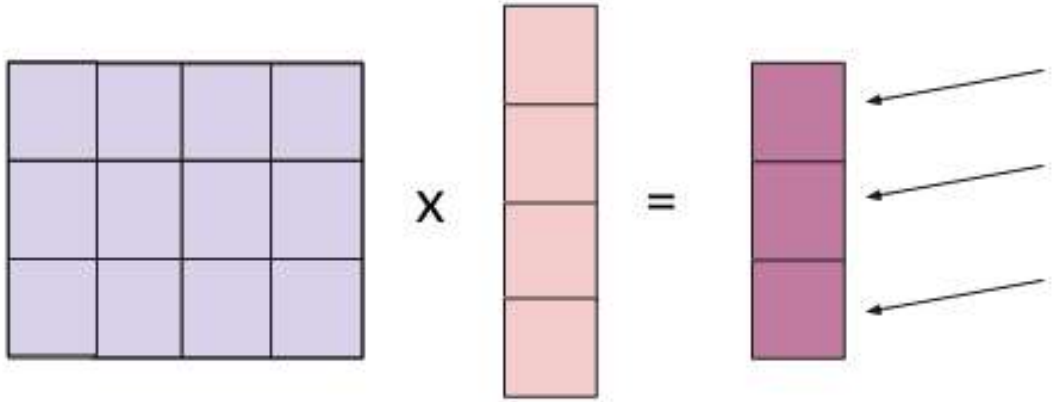
   a. Iterative methods
   b. K-FAC & EK-FAC

1. Neuron-level interpretability
    a. Sparse Autoencoders
2. Causal Mediation
    a. Activation Patching & variants
    b. Causal abstraction & other methods
3. What is mechanistic interpretability?
4. Methods Leveraging Language Model Strengths
    a. Transformer Residual Stream and Linear Structure
    b. Vocabulary projection
    c. Decoding Natural Language Explanations from Representations

Neuron-Level Interpretability – Background

◆ Interpreting Neurons

- Neuron = a single dimension of a hidden state representation
- Line of work traditionally does not consider structure



What pattern in the inputs will fire a neuron (i.e., cause high values at a particular dimension)?

Neuron-Level Interpretability – Background

- Interpreting Neurons of NLP Models

Activations of neurons for certain properties

Supports the efforts of the Libyan authorities to recover funds misappropriated under the Qadhafi regime

(a) English Verb (#1902)

einige von Ihnen haben vielleicht davon gehört , dass ich vor ein paar Wochen eine Anzeige bei Ebay geschaltet habe .

(b) German Article (#590)

Layer14, Unit 224: sure, know, aware

- Are you sure you are aware of our full potential?
- They know that and we know that.
- I am sure you will understand.
- I am sure you will do this.
- I am confident that we will find a solution.

Neuron-Level Interpretability – Background

- Pitfalls of Neuron-Level Analysis in NLP

  - Methods generally ignore interactions between neurons.
  - There are a LOT of neurons in modern models.

Neuron-Level Interpretability – Background

- Pitfalls of Visualization/Looking at Examples

  - Humans are biased towards simple and clear concepts.

    - *"What is the meaning behind the song ""Angel"" by Eric Clapton?"*
    - *"What's the meaning of Johnny Cash's song ""King of the Hill""?"*
    - *"What is the meaning behind the Tears for Fears song ""Mad World"", such as the lyric, ""All around me are familiar faces""?"*

    Song titles? Syntactic sentence structure?

Neuron-Level Interpretability – Background

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> - *"What is the meaning behind the song ""Angel"" by Eric Clapton?"*
> - *"What's the meaning of Johnny Cash's song ""King of the Hill""?"*
> - *"What is the meaning behind the Tears for Fears song ""Mad World"", such as the lyric, ""All around me are familiar faces""?"*

Song titles? Syntactic sentence structure?

> - *On 16 June 2006, it was announced that Everton had entered into talks with Knowsley Council and Tesco over the possibility of building a new 55,000 seat stadium, ex-pandable to over 60,000, in Kirkby.*
> - *On 15 September 1940, known as the Battle of Britain Day, an RAF pilot, Ray Holmes of No. 504 Squadron RAF rammed a German bomber he believed was going to bomb the Palace.*
> - *On 20 August 2010, Queen's manager Jim Beach put out a Newsletter stating that the band had signed a new contract with Universal Music.*

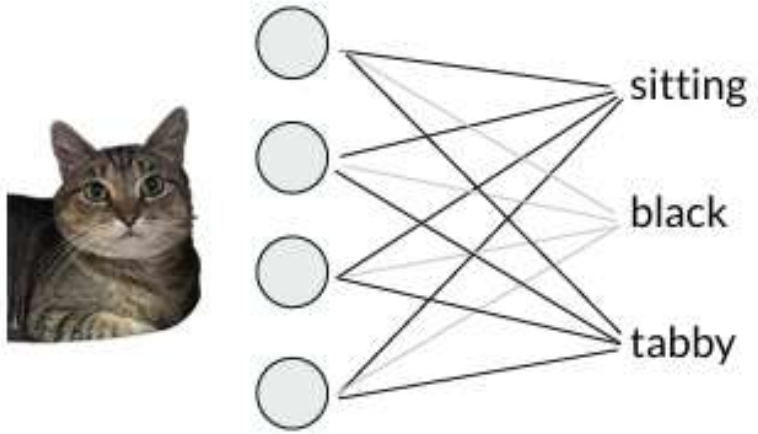
Historical events? Sentences with dates at the beginning?

  - **Polysemanticity**: neurons "respond to multiple unrelated inputs"

Neuron-Level Interpretability – Sparse Autoencoders

- Linear Combinations of Neurons as Concepts

Individual neuron-level interpretations are typically not precise:
many neurons respond to mixtures of concepts



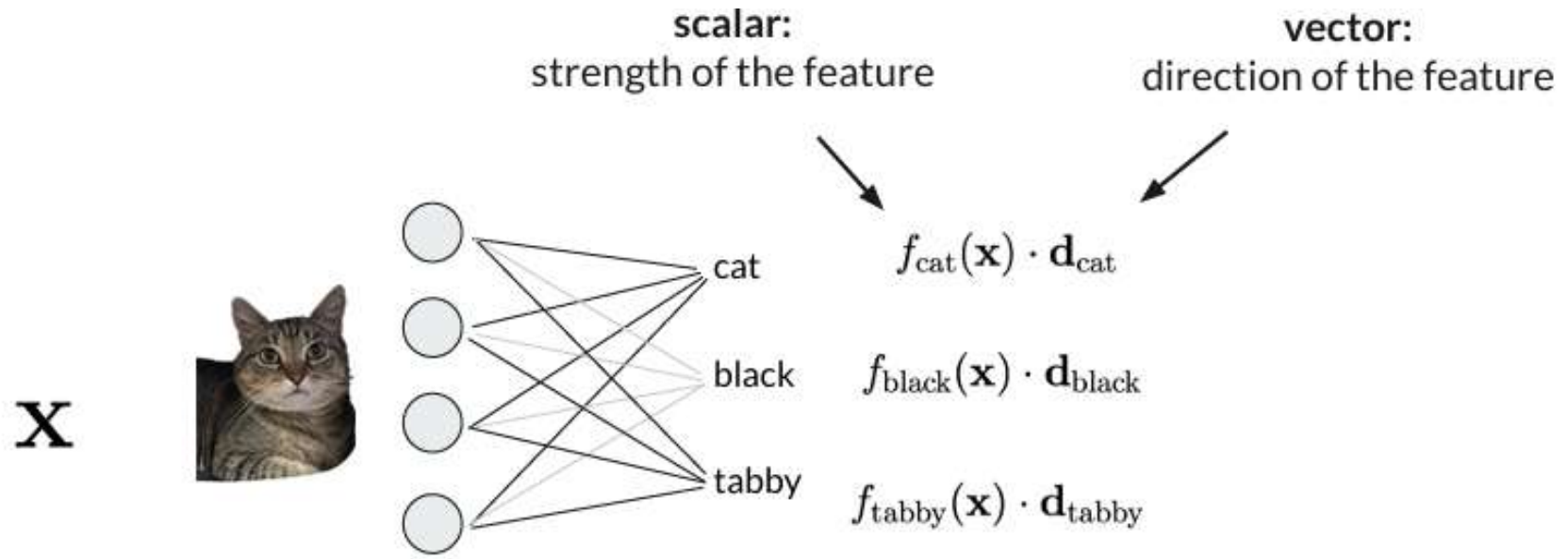
Hypothesis

Neurons together (as opposed to individual neurons) respond to concepts

Neuron activations can be decomposed into linear combinations of concept directions (called features)

Neuron-Level Interpretability – Sparse Autoencoders

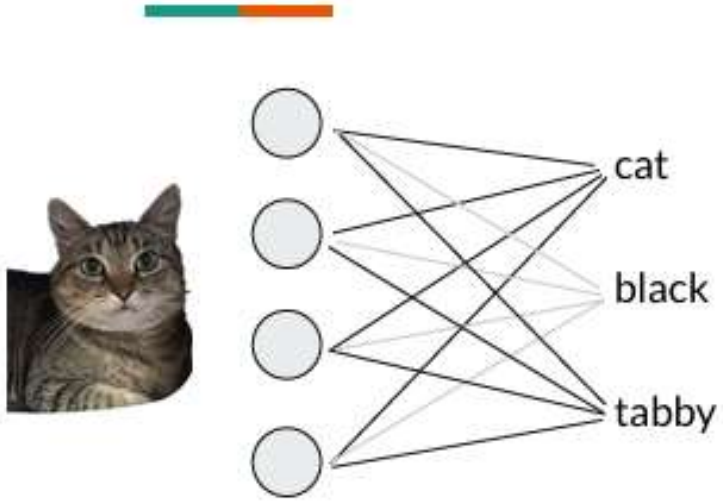
- Decomposing Activations



$$\mathbf{x} \xrightarrow{\text{decompose}} f_{\text{cat}}(\mathbf{x}) \cdot \mathbf{d}_{\text{cat}} + f_{\text{black}}(\mathbf{x}) \cdot \mathbf{d}_{\text{black}} + f_{\text{tabby}}(\mathbf{x}) \cdot \mathbf{d}_{\text{tabby}}$$

Neuron-Level Interpretability – Sparse Autoencoders

- Decomposing Activations with Sparse Autoencoders



Sparsity: for $\mathbf{x}$, we expect only a small number of feature ***c*** is activated ($f_c(\mathbf{x}) > 0$)

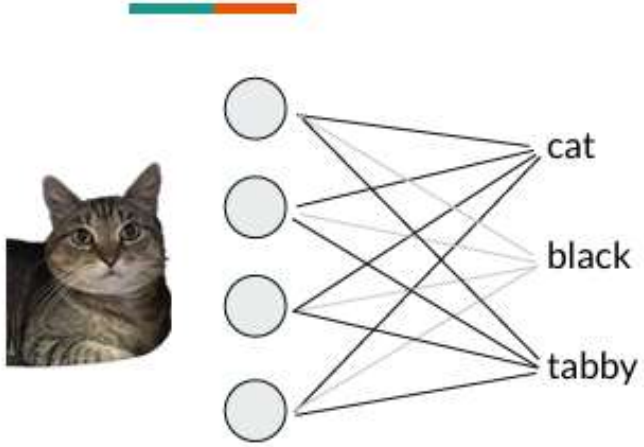
$$\mathbf{x} \approx \mathbf{b} + \sum_c f_c(\mathbf{x})\mathbf{d}_c$$

using **Sparse Autoencoders** to find decompositions

$f_c(\mathbf{x})$: encoder parameters $\mathbf{d}_c$: decoder parameters

Neuron-Level Interpretability – Sparse Autoencoders

- Decomposing Activations with Sparse Autoencoders



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using **Sparse Autoencoders** to find decompositions

$f_c(\mathbf{x})$: encoder parameters $\mathbf{d}_c$: decoder parameters

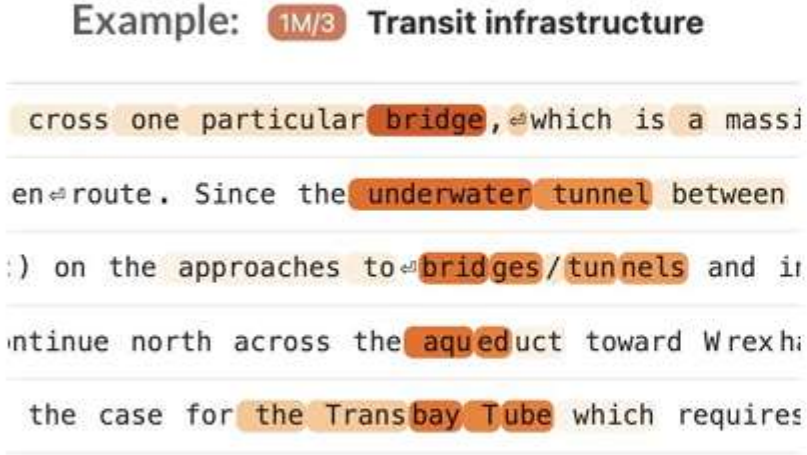
reconstruction loss sparsity

$$\text{Loss:} \quad \mathbb{E}_x \left[\|x - \hat{x}\|_2^2 + \lambda \sum_c f_c(x) \right]$$

[Anthropic, 2023]

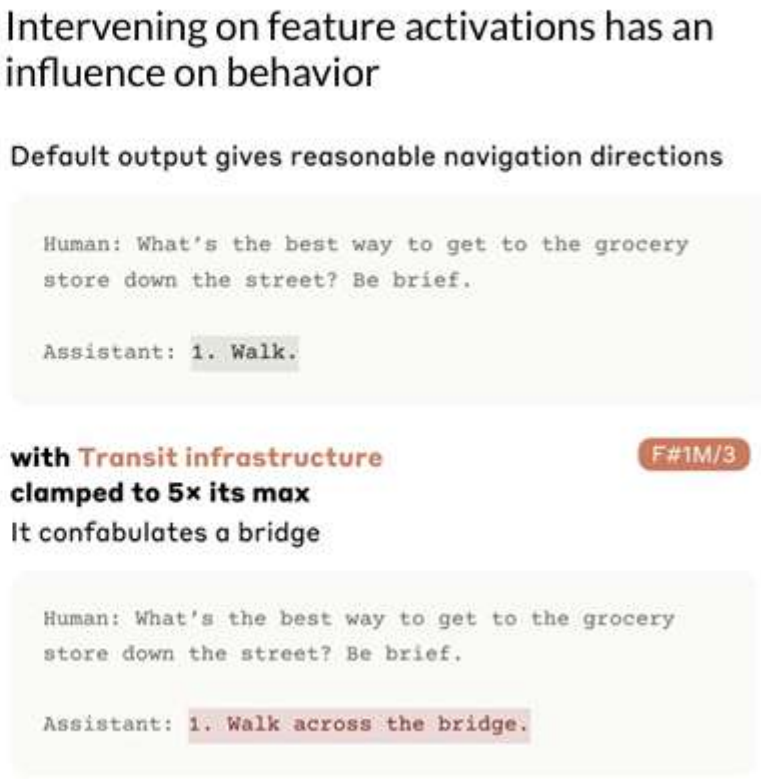
Neuron-Level Interpretability – Sparse Autoencoders

- Notes on Learned Features



[Anthropic, 2024]

[Anthropic, 2023]



Neuron-Level Interpretability – Sparse Autoencoders

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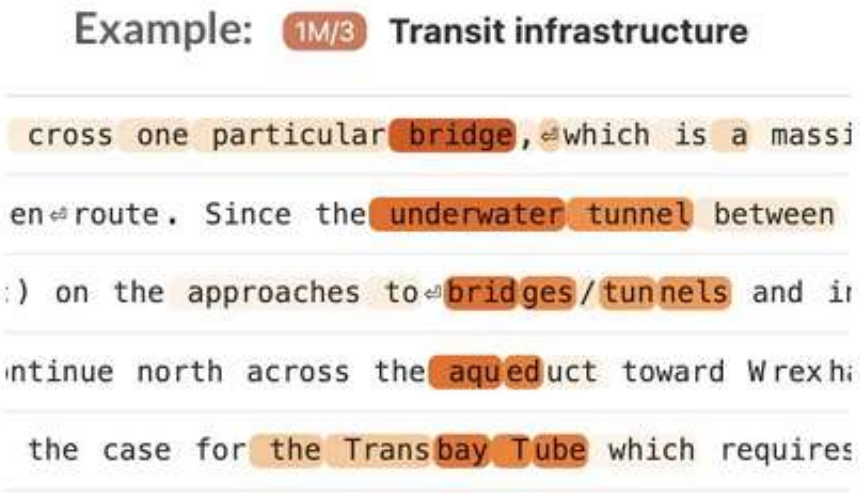


Intervening on feature activations has an influence on behavior

Feature activations are more specific than neurons

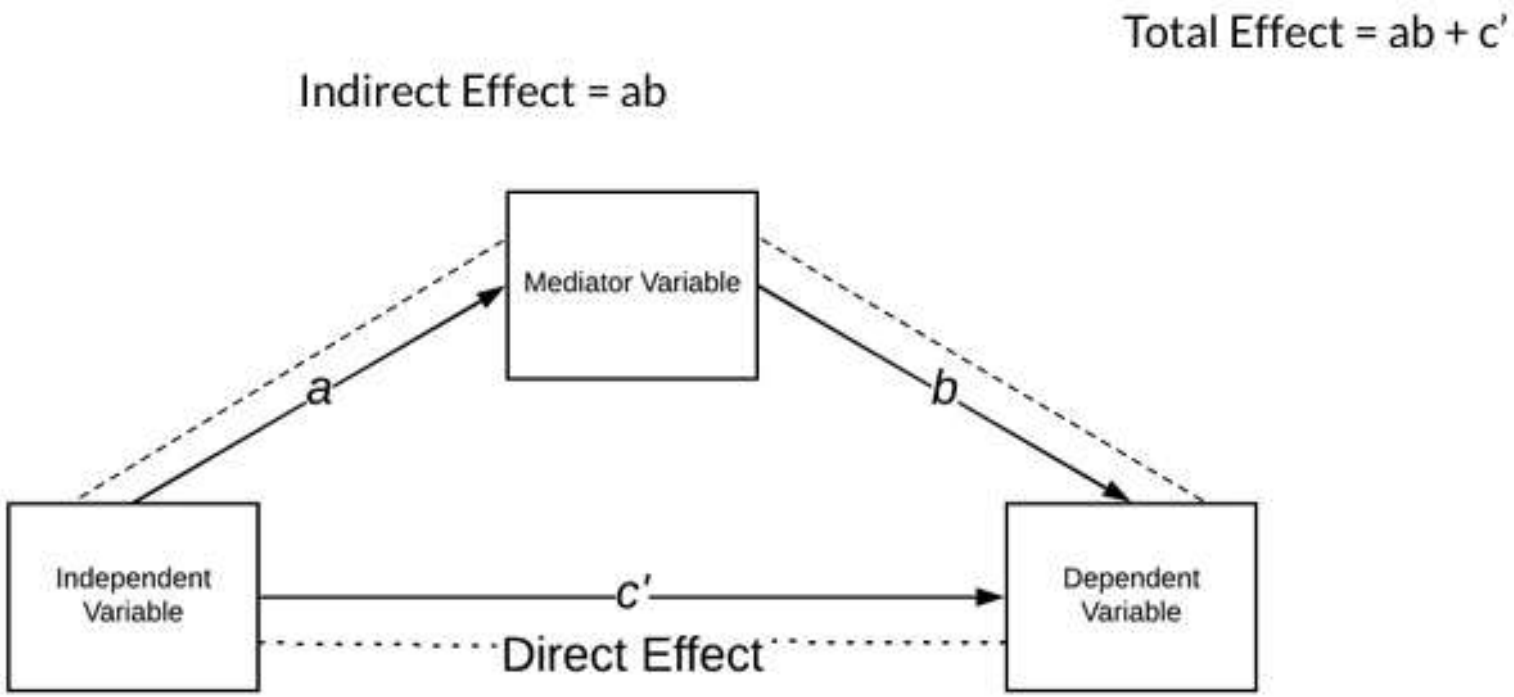
- "upon manual inspection of a random sample of 50 neurons and features each, the neurons appear significantly less interpretable than the features, typically activating in multiple unrelated contexts.."

[Anthropic, 2024]

[Anthropic, 2023]

Neuron-Level Interpretability – Causal Mediation in Transformers

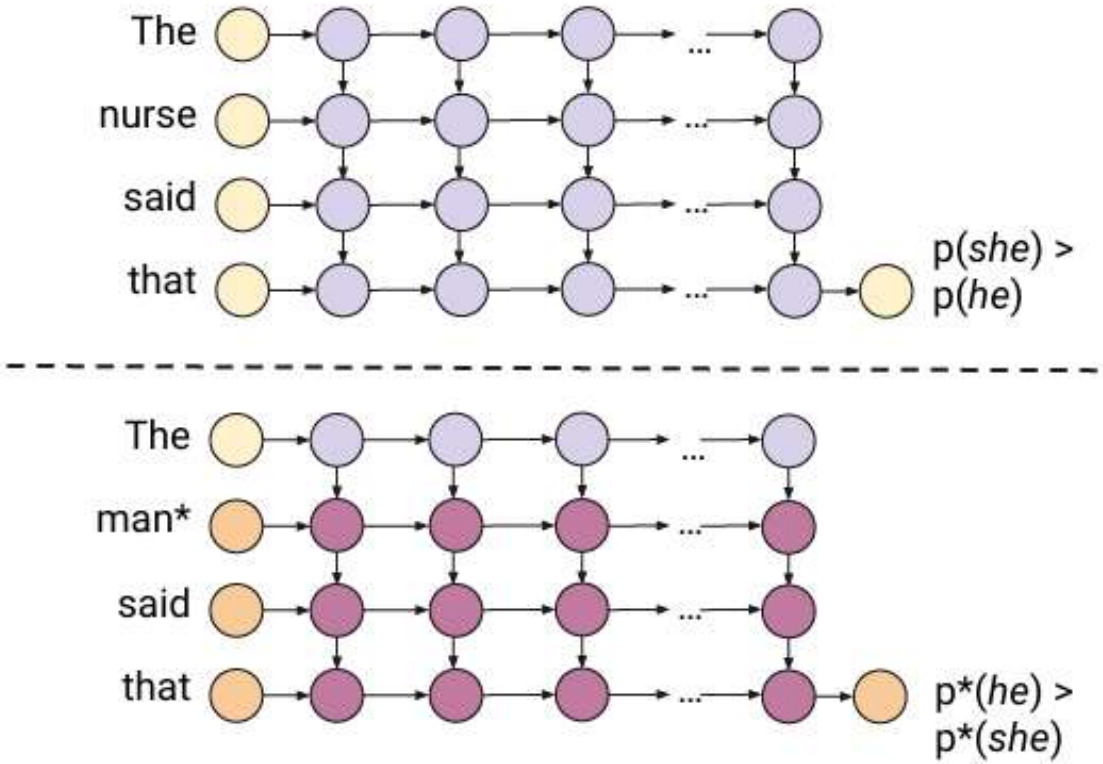
- Causal Mediation



Neuron-Level Interpretability – Causal Mediation in Transformers

- Activation Patching/Causal Tracing

- Run inference through the network twice
- Measure the change in probabilities of the tokens of interest

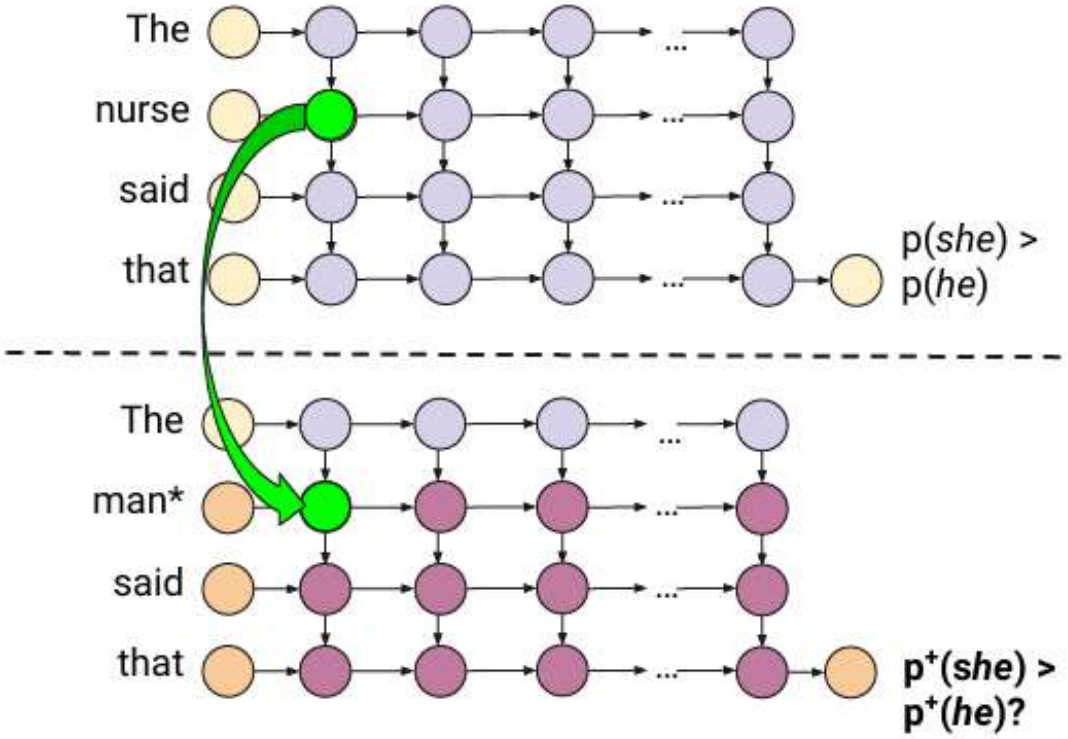


[Vig et al. 2020]

Neuron-Level Interpretability – Causal Mediation in Transformers

- Activation Patching/Causal Tracing

- Run inference through the network twice
- Measure the change in probabilities of the tokens of interest
- *Patch* in states from one inference run into another
- Observe how probabilities change → the most important hidden states will have the largest effect in "restoring" the probabilities of the run that is being patched in.



Neuron-Level Interpretability – Causal Mediation in Transformers

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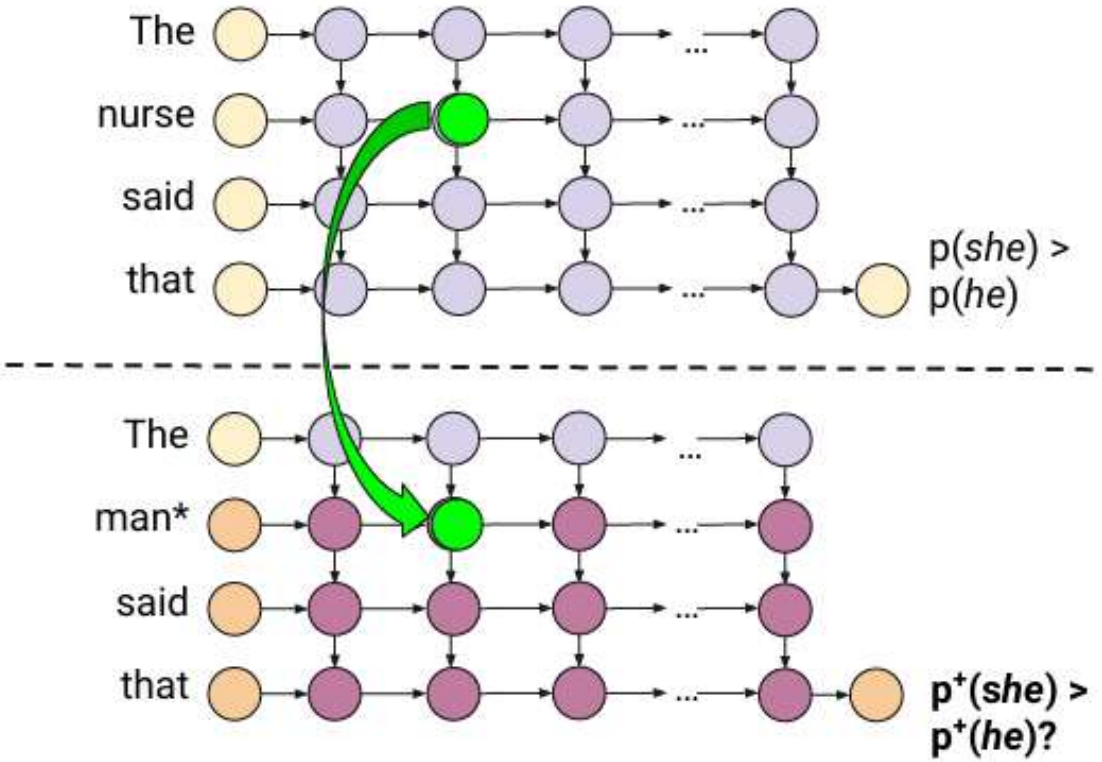
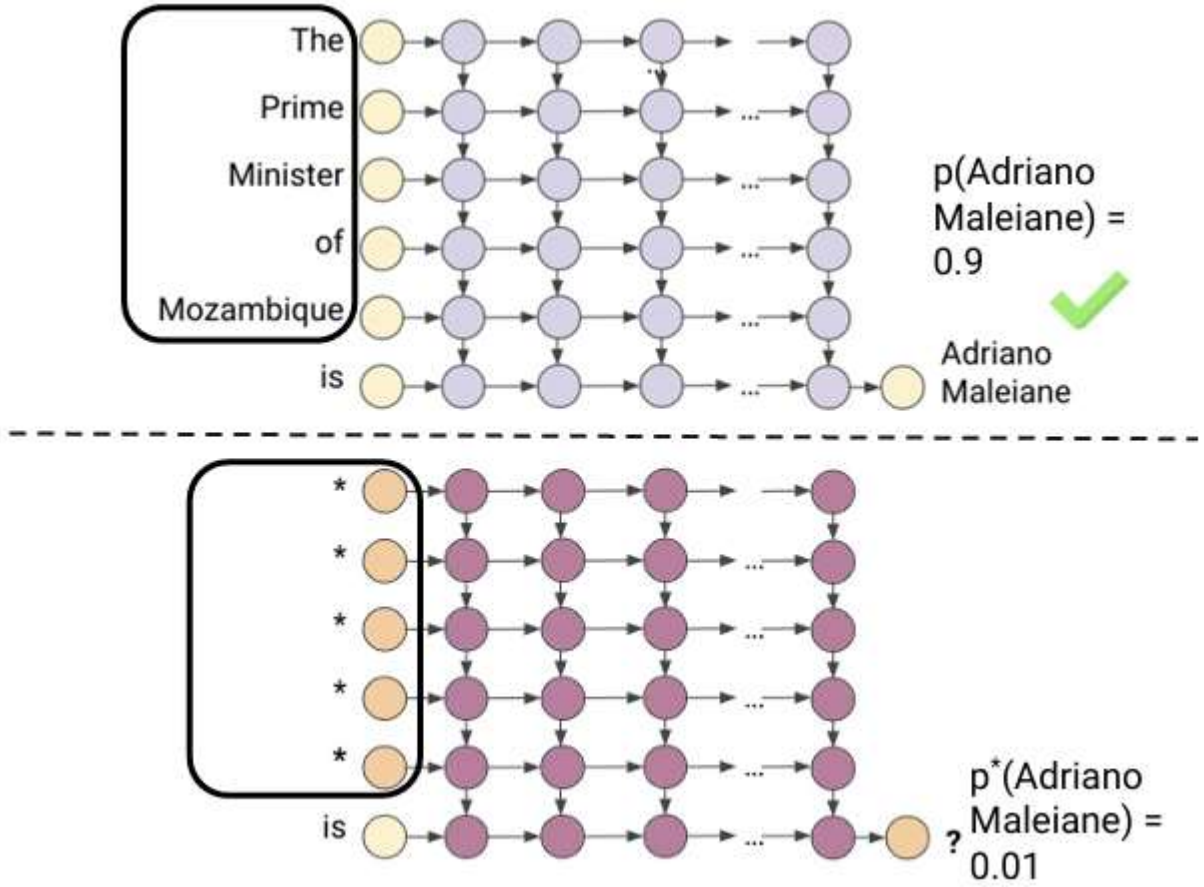


Neuron-Level Interpretability – Causal Mediation in Transformers

- Method

Textual Effect =
$p(y) - p^*(y) = 0.89$



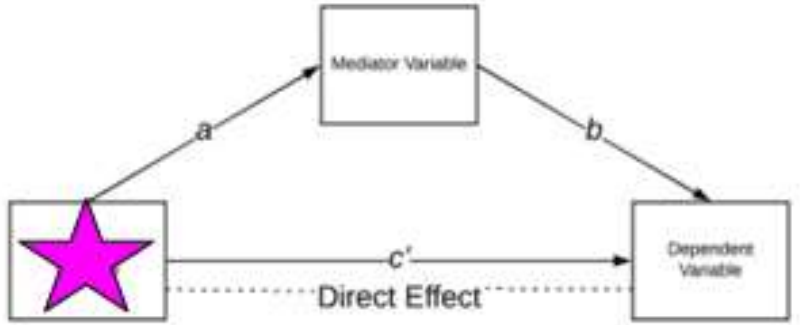
Neuron-Level Interpretability – Causal Mediation in Transformers

- Results

Neuron-Level Interpretability – Causal Mediation in Transformers

◆ Notes

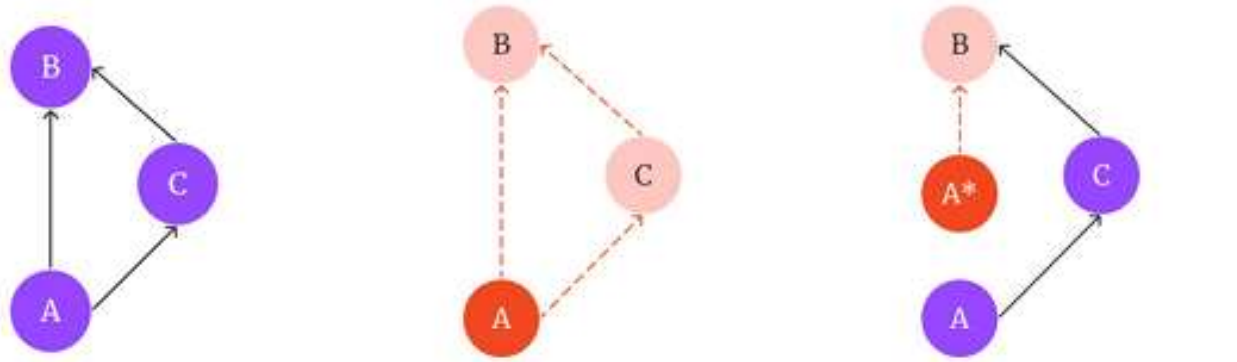
- Measures **total effect** of hidden state on output
- Method is rather **computationally expensive**
  - Each patch is a separate inference run
  - Also requires two copies of the model to be loaded into memory, generally
- **Strong independence assumption** about individual hidden states or neurons in the network
  - Ideally, one could patch multiple states at once, but enumerating all possible combinations of states is intractable
- More efficient (gradient-based) approximation: "Attribution Patching" [Nanda 2022, Kramár et al. 2024]
- How to design paired instances? [Zhang & Nanda 2024]



Neuron-Level Interpretability – Causal Mediation in Transformers

- Path Patching

- Controls more carefully **which effect** you can measure



(a) Clean forward pass, no intervention

(b) Intervene on A to observe *total* effect on B.

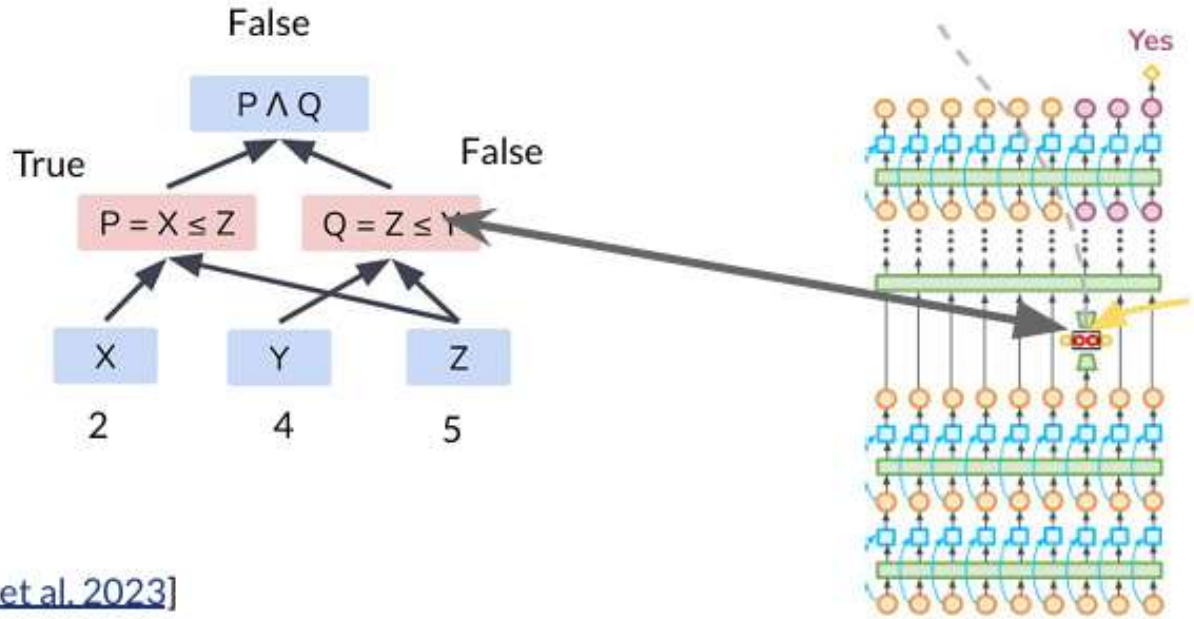
(c) Intervene on the edge A→B to observe *direct* effect on B.

Neuron-Level Interpretability – Causal Mediation in Transformers

- Causal Abstraction

The key idea is to learn a causal graph that maps to the neural network.

Consider the simple task of determining whether Z is in the interval [X, Y]



[Geiger et al 2023, Wu et al. 2023]

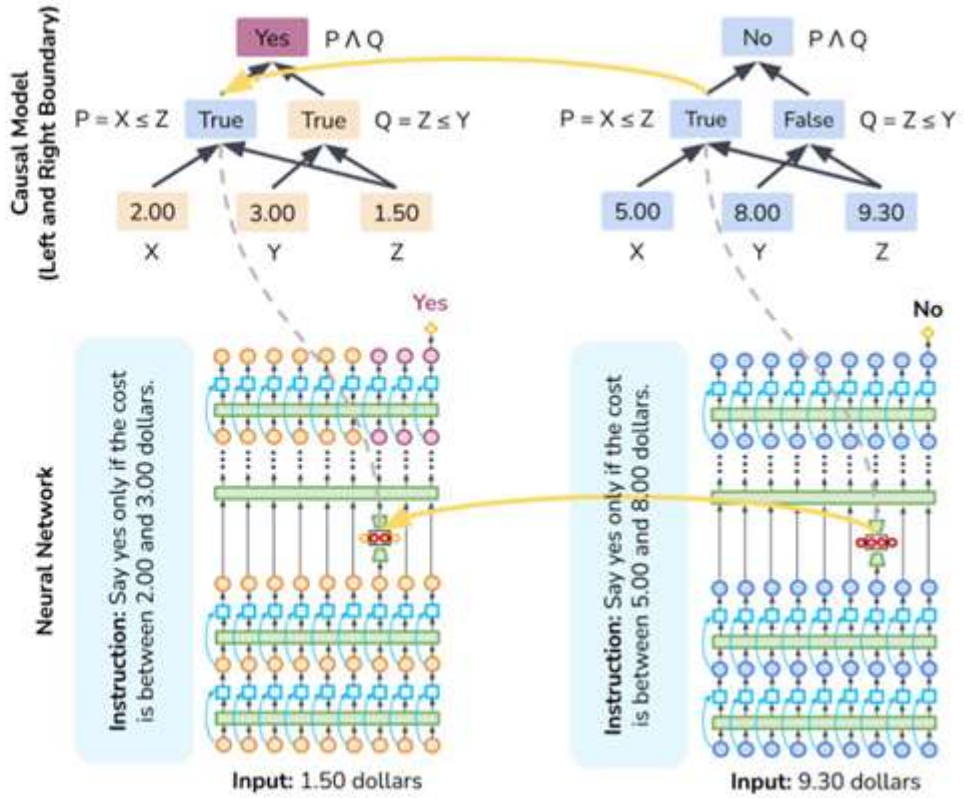
Neuron-Level Interpretability – Causal Mediation in Transformers

- Intervention analyses is essential to causal abstraction

Key intuition: intervention in the low-level neural representations has the same effect as the intervention in the high-level causal graph.

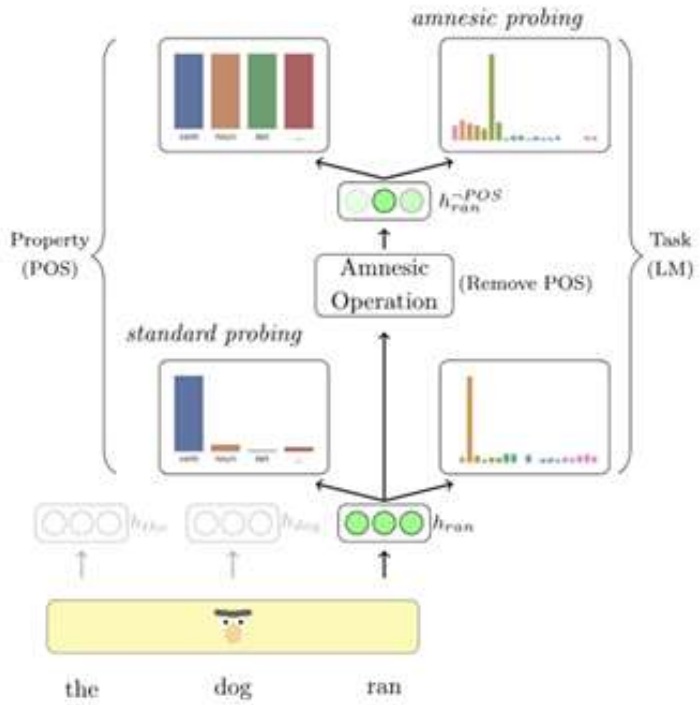
Coming up with a high-level causal graph is highly non-trivial in practice!

[Geiger et al 2023, Wu et al. 2023]



Neuron-Level Interpretability – Causal Mediation in Transformers

- Causal Probing



- Traditional probing classifiers are not causal.
- There are methods that perform causal interventions to measure **how** the property of interest **is used** to make predictions.

[Giulianelli et al. 2018, Elazar et al. 2021]

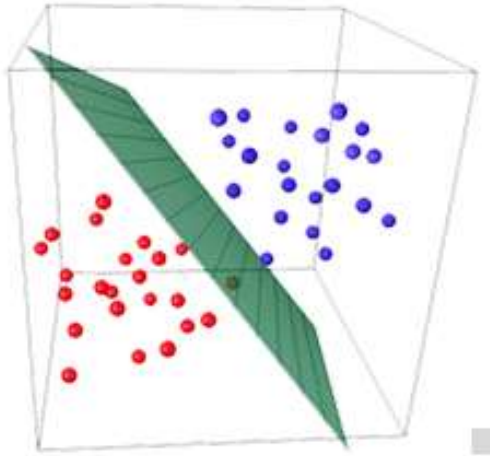
Neuron-Level Interpretability – Causal Mediation in Transformers

- Linear Subspace Projections + Concept Erasure

  - Models encode many interpretable concepts linearly.

Linear concept subspace hypothesis: a concept (such as gender) lives in low-dimensional **subspace** within the representation space.

How can we identify the concept subspace?
Once located, can we intervene in its encoding?



[Ravfogel et al 2020, Belrose et al 2023, inter alia]

Slide credit: Shauli Ravfogel

Mechanistic Interpretability

- What is Mechanistic Interpretability?

"reverse engineering the algorithms implemented by neural networks into human-understandable mechanisms, often by examining the weights and activations of neural networks to identify circuits [Cammarata et al., 2020, Elhage et al., 2021] that implement particular behaviors."

Desirable outcome of *all* interpretability research: human understanding

Focus of *most* interpretability research: understanding *specific* model behaviors

Mechanistic Interpretability

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Format of the explanation

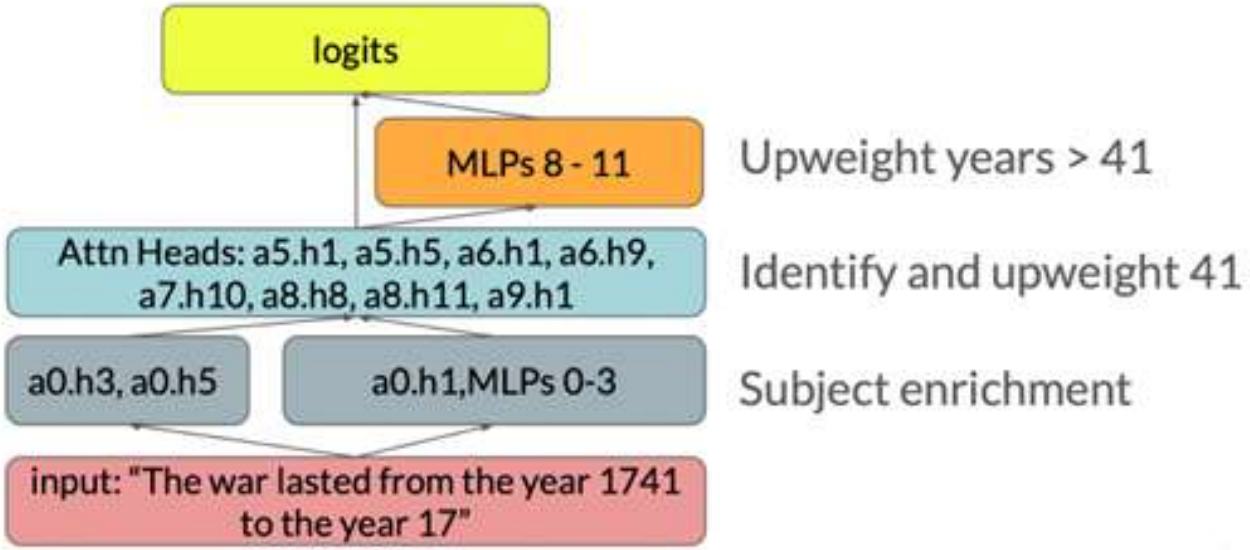
Finding a subset of a network that **traces through the entire network (from starting representation to prediction).**

Mechanistic Interpretability

- Circuits

- Note: this has strong resemblances to sparse sub-network finding in the efficiency literature, but the methods employed to find them differ (also, no retraining of circuits is done)

Transformer circuits localize and characterize transformer LM behavior in a (small) set of components of the model.



Hanna et al., 2023

Mechanistic Interpretability

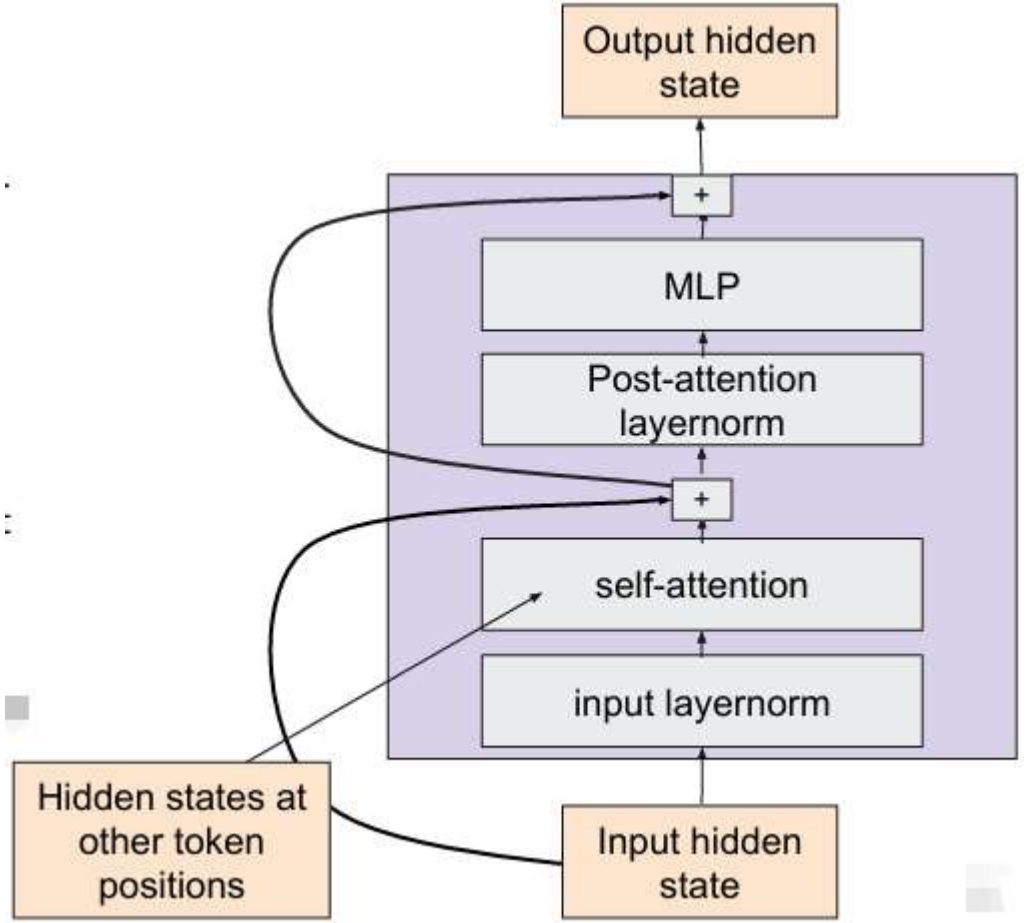
◆ What is Mechanistic Interpretability?

- It is **inherently causal.**
  - NB! This is **not** how most people use the terminology today.
- It is **not the only** set of causal interpretability methods.
- **Traces through the entire network (from starting representation to prediction).**
- Evaluation:
  - 1) **Faithfulness**: the circuit or subnetwork should be able to *sufficiently* **replicate the full network** on the behavior of interest
  - 2) **Minimality**: obviously, smaller circuits/subnetworks are better

Methods Leveraging Language Model Strengths - Linear Structure in Transformers

◆ Transformer Residual Stream and Linear Structure

- Transformers have a surprising amount of linear structure due to residual connections
- Nonlinearities only occur in two places:
  - Applications of Softmax
    - when computing attention patterns
    - When converting logits to probits at final layer
  - In the MLP functions
- MLP and MHSA functions "read from" and "write to" residual stream to promote/demote certain tokens in output distribution.



Methods Leveraging Language Model Strengths - Linear Structure in Transformers

- Transformer Residual Stream and Linear Structure

For input token embedding $\mathbf{x}_0 \in \mathbb{R}^d$, the output $\mathbf{x}_\ell \in \mathbb{R}^d$ of layer ℓ is defined as (for $\ell \in [1, L]$):

$$\mathbf{x}_\ell = \mathbf{x}_{\ell-1} + \mathrm{MHSA}_{\theta_\ell}\left(\mathrm{LN}(\mathbf{x}_{\ell-1})\right) + \mathrm{FFN}_{\theta_\ell}\left(\mathbf{x}_{\ell-1} + \mathrm{MHSA}_{\theta_\ell}\left(\mathrm{LN}(\mathbf{x}_{\ell-1})\right)\right)$$

- Output of previous layer = input to current layer
- Multi-head self-attention
- Layer norm (or some other input normalization scheme)
- Feed-forward network (MLP)
- Vector addition establishes residual connections

Methods Leveraging Language Model Strengths - Linear Structure in Transformers

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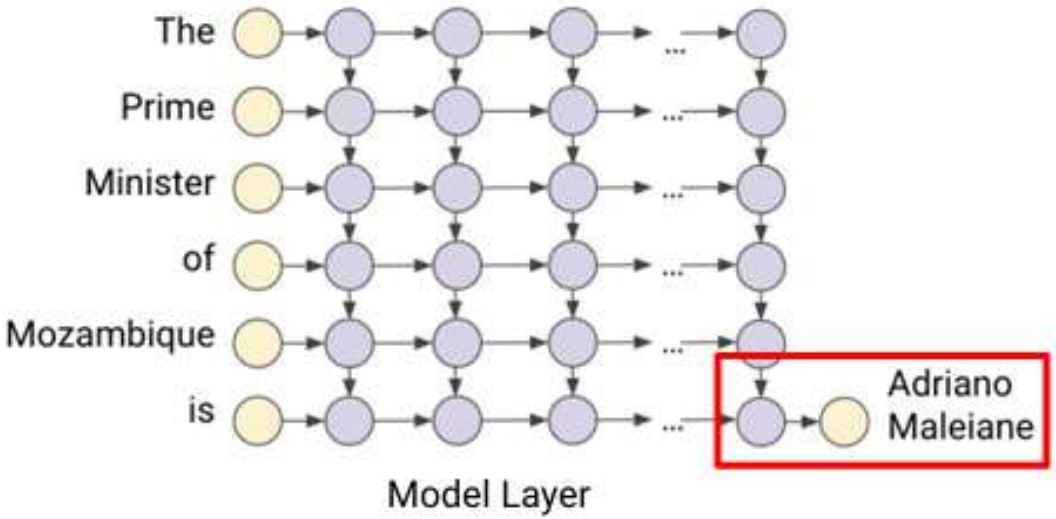
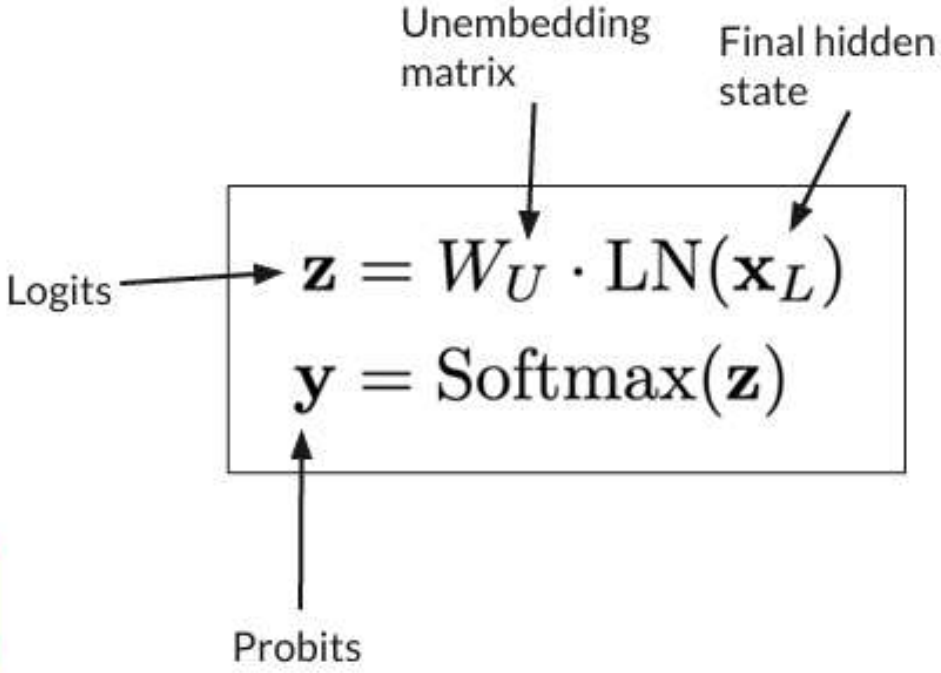
- Output of previous layer = input to current layer
- Multi-head self-attention
- Layer norm (or some other input normalization scheme)
- Feed-forward network (MLP)
- Vector addition establishes residual connections

$$\mathbf{x}_L = \mathbf{x}_0 + \sum_{\ell=0}^{L-1}\left[\mathrm{MHSA}_{\theta_{\ell+1}}\left(\mathrm{LN}(\mathbf{x}_\ell)\right) + \mathrm{FFN}_{\theta_{\ell+1}}\left(\mathbf{x}_\ell + \mathrm{MHSA}_{\theta_{\ell+1}}\left(\mathrm{LN}(\mathbf{x}_\ell)\right)\right)\right]$$

Methods Leveraging Language Model Strengths - Linear Structure in Transformers

- Transformer Residual Stream and Linear Structure





Methods Leveraging Language Model Strengths - Linear Structure in Transformers

◆ Implications: Direct Additive Contributions

- Each hidden state output by a {attention head, MHSA function, FFN function, or full Transformer block} has a **direct additive contribution to the final hidden state of the model**
- And, by distributivity of vector addition and vector-matrix multiplication, thus has a **direct additive contribution** to the **final logits**.

$$\mathbf{x}_L = \mathbf{x}_0 + \sum_{\ell=0}^{L-1} \left[\mathrm{MHSA}_{\theta_{\ell+1}}(\mathrm{LN}(\mathbf{x}_\ell)) + \mathrm{FFN}_{\theta_{\ell+1}}\left(\mathbf{x}_\ell + \mathrm{MHSA}_{\theta_{\ell+1}}(\mathrm{LN}(\mathbf{x}_\ell))\right) \right]$$

$$\mathbf{z} = W_U \cdot \mathrm{LN}\left(\mathbf{x}_0 + \sum_{\ell=0}^{L-1} \left[\mathrm{MHSA}_{\theta_{\ell+1}}(\mathrm{LN}(\mathbf{x}_\ell)) + \mathrm{MLP}_{\theta_{\ell+1}}\left(\mathbf{x}_\ell + \mathrm{MHSA}_{\theta_{\ell+1}}(\mathrm{LN}(\mathbf{x}_\ell))\right) \right] \right)$$

Methods Leveraging Language Model Strengths - Linear Structure in Transformers

◆ Direct vs. Indirect Effects

- It's important to note that each hidden state has both a **direct linear** and **indirect nonlinear** contribution to the final hidden state.
- The additive decomposition only applies to **direct** contributions.

$$\mathbf{z} = W_U \cdot \mathrm{LN}\left(\mathbf{x}_0 + \sum_{\ell=0}^{L-1}\left[\mathrm{MHSA}_{\theta_{\ell+1}}\left(\mathrm{LN}(\mathbf{x}_\ell)\right) + \mathrm{MLP}_{\theta_{\ell+1}}\left(\mathbf{x}_\ell + \mathrm{MHSA}_{\theta_{\ell+1}}\left(\mathrm{LN}(\mathbf{x}_\ell)\right)\right)\right]\right)$$

This MHSA function has a direct additive contribution to the logits via this term

But it also has an indirect, nonlinear contribution as input to the MLP function

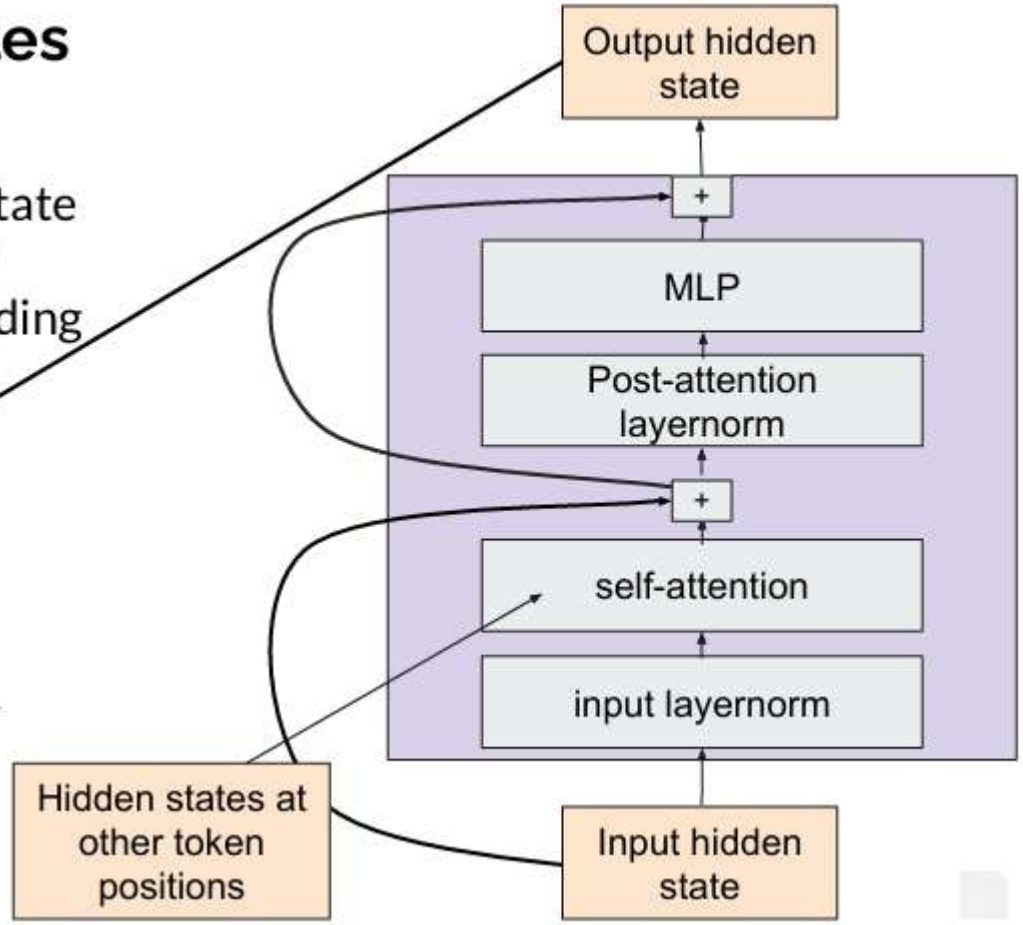
Methods Leveraging Language Model Strengths - Vocabulary Projection

- **Vocabulary Projection on Transformer Hidden States**

  - Propose to project each hidden state to the space of probabilities over vocab tokens using the unembedding matrix

$$\mathbf{y} = \text{Softmax}(W_U \cdot \text{LN}(\mathbf{x}_L))$$

Final hidden state - **replace with any d-dimensional hidden state from the network.**



Methods Leveraging Language Model Strengths - Vocabulary Projection

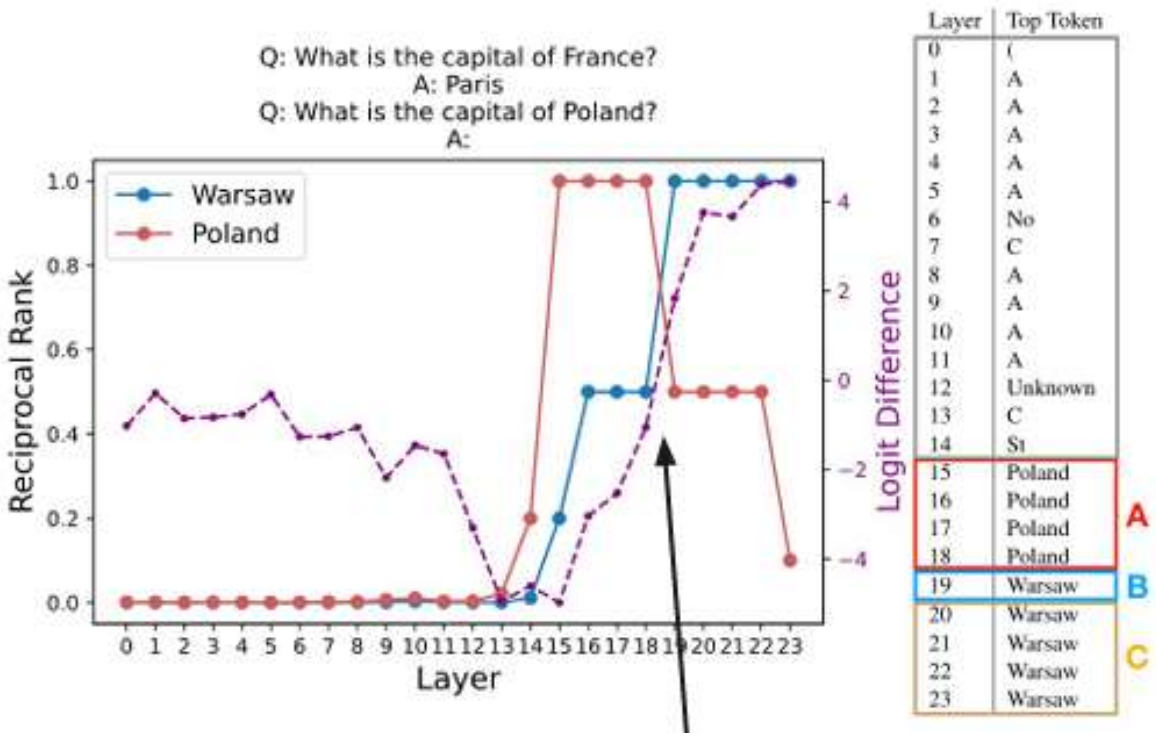
- Vocabulary Projection on Transformer Hidden States

		Concept	Sub-update top-scoring tokens
GPT2	$\mathbf{v}^{3}_{1018}$	Measurement semantic	kg, percent, spread, total, yards, pounds, hours
	$\mathbf{v}^{8}_{1900}$	WH-relativizers syntactic	which, whose, Which, whom, where, who, wherein
	$\mathbf{v}^{11}_{2601}$	Food and drinks semantic	drinks, coffee, tea, soda, burgers, bar, sushi
WIKILM	$\mathbf{v}^{1}_{1}$	Pronouns syntactic	Her, She, Their, her, she, They, their, they, His
	$\mathbf{v}^{6}_{3025}$	Adverbs syntactic	largely, rapidly, effectively, previously, normally
	$\mathbf{v}^{13}_{3516}$	Groups of people semantic	policymakers, geneticists, ancestries, Ohioans

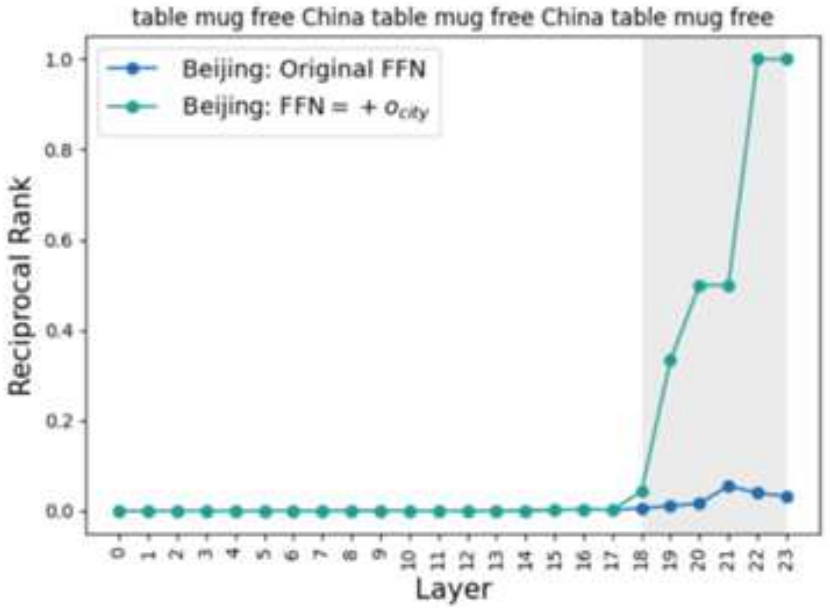
Table 1: Example value vectors in GPT2 and WIKILM promoting human-interpretable concepts.

Methods Leveraging Language Model Strengths - Vocabulary Projection

- Vocabulary Projection on Transformer Hidden States

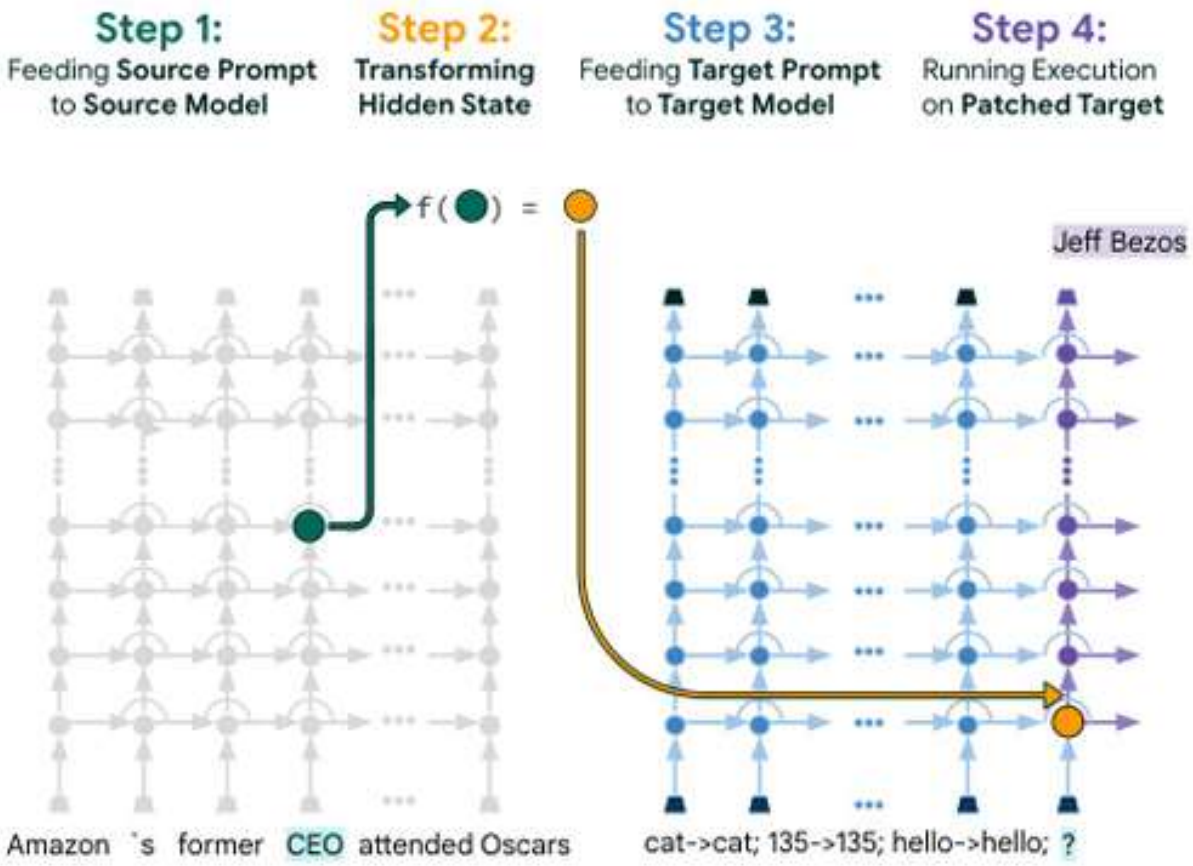


Validated with causal intervention:



Methods Leveraging Language Model Strengths - Vocabulary Projection

- Patchscopes



Methods Leveraging Language Model Strengths - Vocabulary Projection

- Learning Linear Transformation Matrices

- Propose to project each hidden state to the space of probabilities over vocab tokens using ~~the unembedding matrix~~ a learned weight matrix for each layer

$$\mathbf{y} = \text{Softmax}(W_U \cdot \text{LN}(\mathbf{x}_L))$$

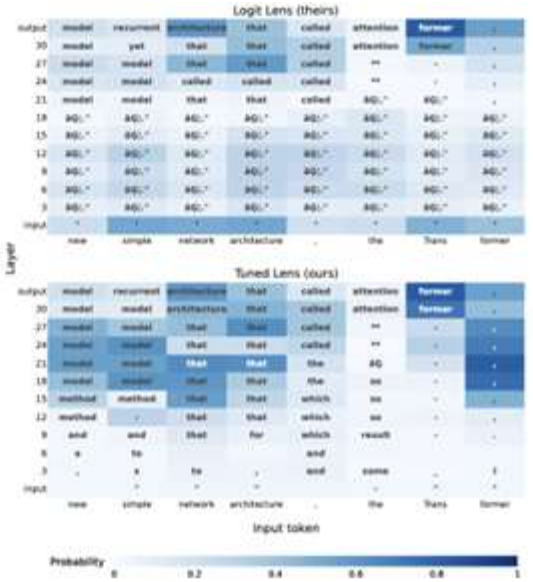


Figure 1. Comparison of our method, the *tuned lens* (bottom), with the "logit lens" (top) for GPT-Neo-2.7B prompted with an except from the abstract of Vaswani et al. (2017). Each cell shows the top-1 token predicted by the model at the given layer and token index. The logit lens fails to elicit interpretable predictions before layer 21, but our method succeeds.

Methods Leveraging Language Model Strengths - Vocabulary Projection

◆ Notes

- Can be thought of as "early exiting" the Transformer block at inference time
- From a causal perspective:
  - (Attempts to) measure *direct* effects
    - How faithful this is depends on the exact application of normalization
    - It is not a causal mediation
- Can't uncover ways in which hidden states are promoting tokens in other linear (or non-linearly decodable) subspaces
  - I.e., negative results are uninformative
  - Mostly only useful at later layers
- Top-k tokens being coherent: does this just mean that the unembedding matrix is well-formed?

Methods Leveraging Language Model Strengths - Decoding Natural Language Explanations from Representations

- Focus of This Part

Decoding **natural Language explanations** from neurons

(using LLMs)

Prominent paradigm of using LLMs for automating the process of explaining neurons

- Step1: Propose hypothesis explanations
- Step2: Verify explanations

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- Using GPT-4 to Explain Neurons of GPT-2

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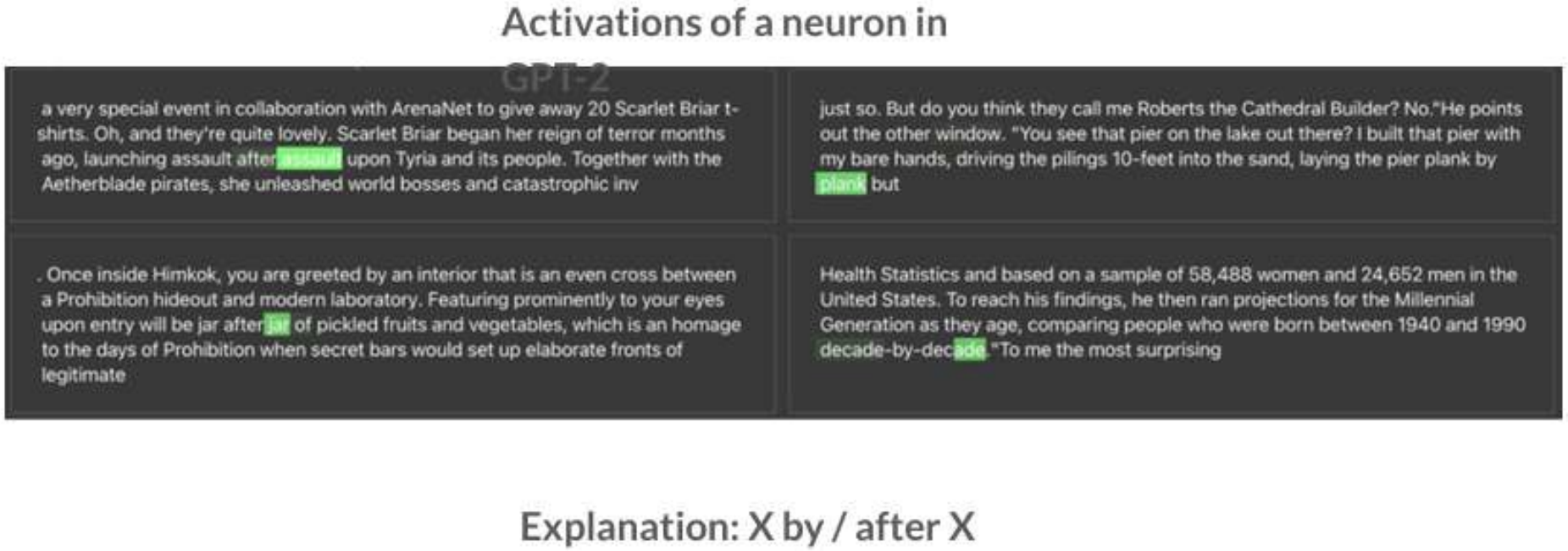

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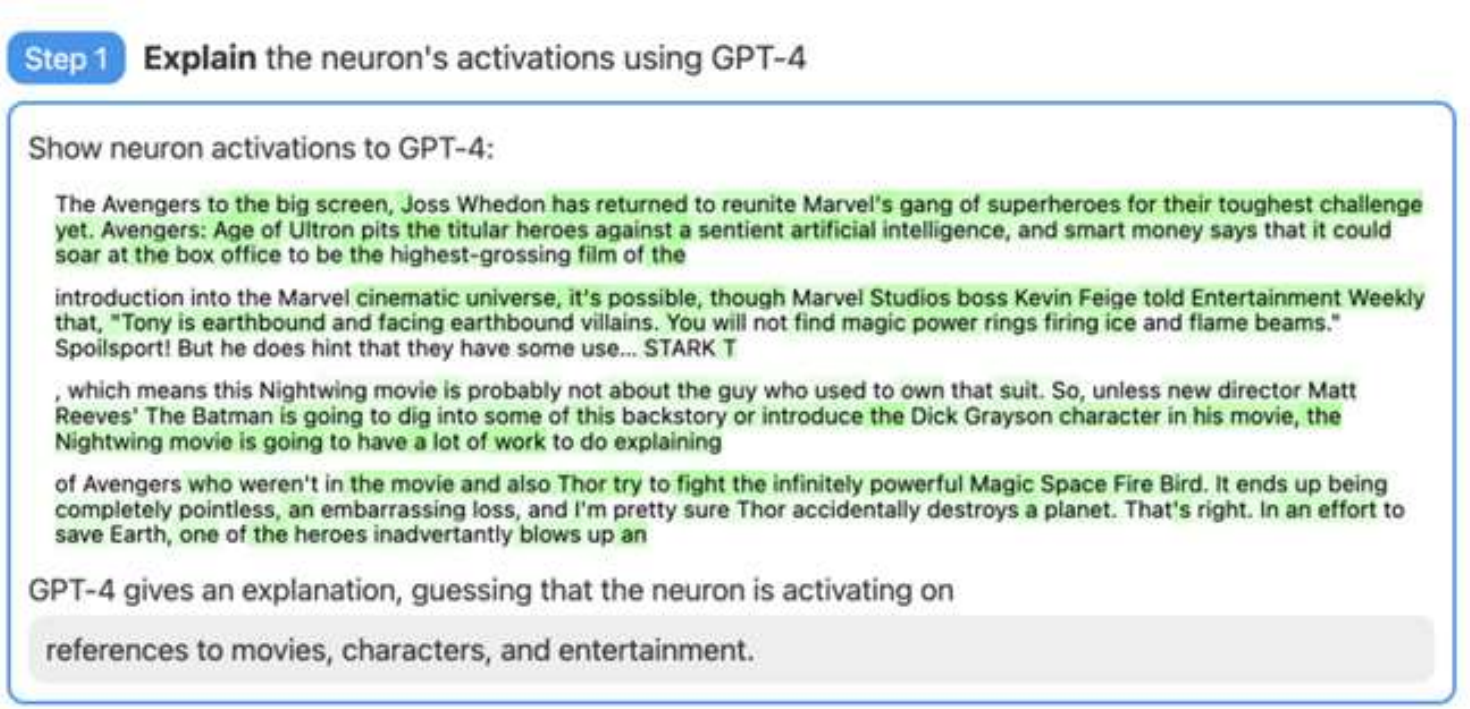
Propose hypothesis: few-shot prompting



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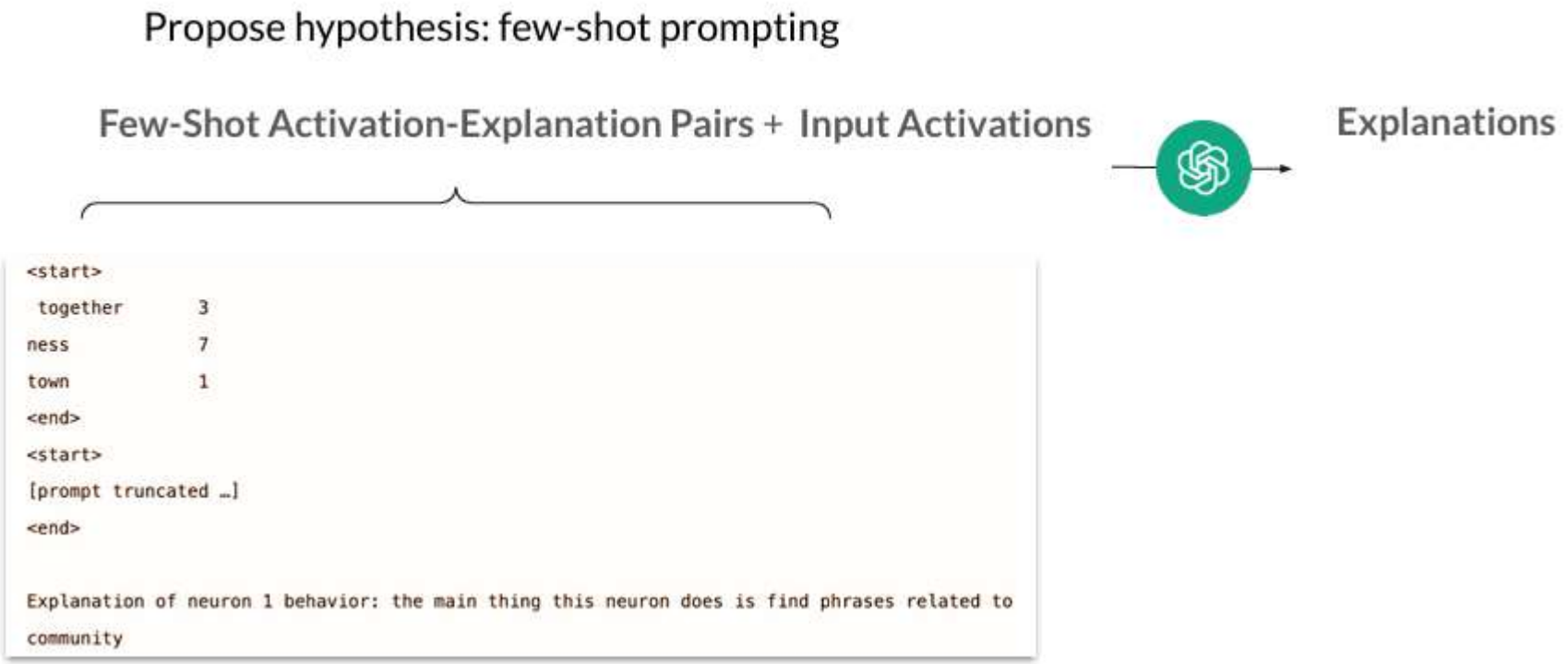

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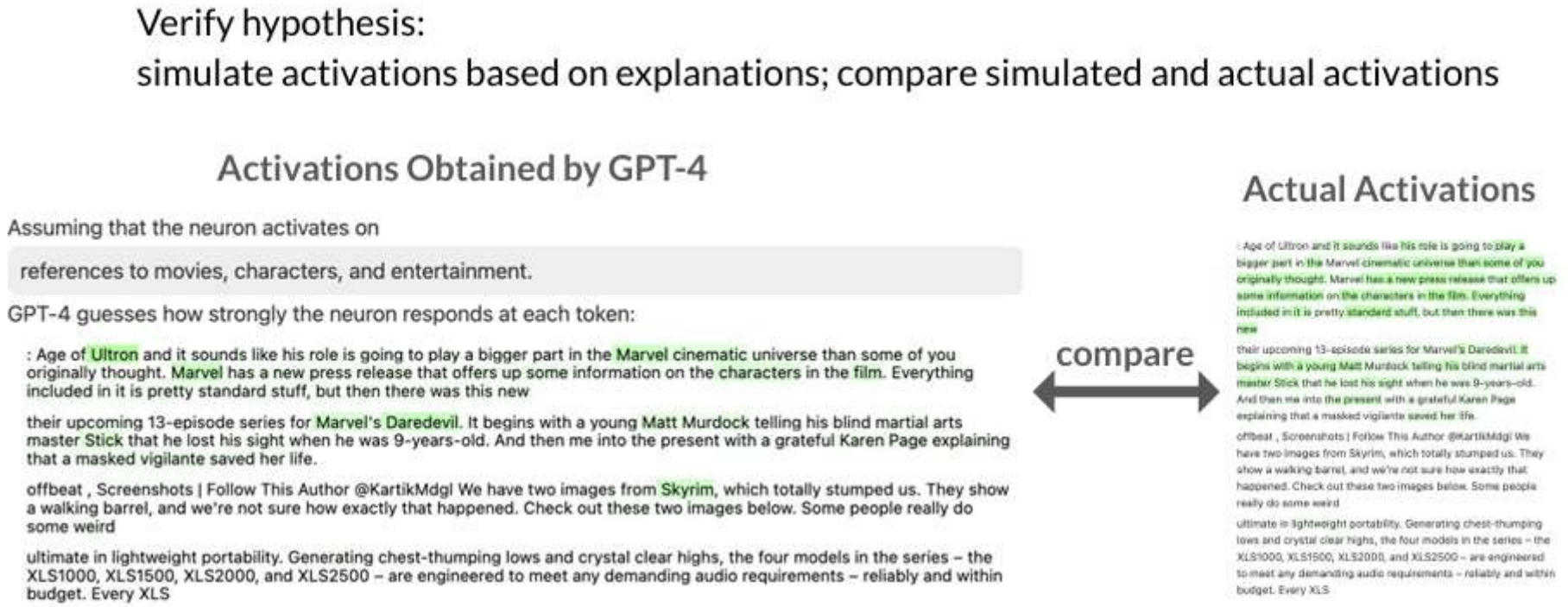

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- Evaluating the NL Explanations of Neurons

Whether explanations accurately align with neuron activations?

- Type-1 Error (recall): falsely predicts that the neuron will activate on a concept
- Type-2 Error (precision): falsely predicts that the neuron will not activate on a concept

Explanation	True Positives	Type I Errors	Type II Errors
days of the week	I have a music class every Wednesday evening	Thursday is usually reserved for grocery	Philadelphia is where the Declaration of Independence
years, specifically four-digit years	Castro took power in Cuba in 1959 .	rated during re - entry in 2003 .	We need to rev amp the website to attract more

Not well aligned: Around 0.6 F1 score across 300 of the top-scoring explanations found by GPT-4

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- Takeaways

LLMs can help annotate/summarize concepts from collections of text snippets

But LLM-produced neuron-level explanations are not accurate enough

Recap: Looking into transformers

- Pros
  - We are actually studying the weights in the model. Intuitively, it is more likely to be faithful.
  - Many methods are extensible to other types of models, modalities, etc.
- Cons
  - High-dimensional spaces remain challenging to make sense of and there could existing fundamental limitations so that it is impossible to reverse-engineer the model or for humans to make sense of these models
  - Illusion of understanding
  - Negative results can be uninformative
  - Lack of standardized evaluation & benchmarks
- Open questions
  - What granularity or type of model internals to target?
  - How to unify work from various methods/communities?

Explanation methods to address the challenges

	Prompt-based	Influence function	Mech interp
Lack of transparency	Improve communication, faithfulness, etc	Understand data	Many ways
Computation	Language understanding and instruction following	Understand and refine data	Understand model
Unstability	Improve reasoning, grounding and instructability	Improve stability	Facilitate targeted control
Over-reliance	Improve communication, faithfulness, etc	Help understand the supports for model decisions	Help understand mechanisms of model decisions
Hard to evaluate	New evaluation methods and paradigms	New evaluation methods and paradigms	New evaluation methods and paradigms

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

AIAA 2290: Ethics, Privacy and Security in AI

Thanks!!

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