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Announcements

Carnegie Mellon University

Interpretation of Pretrained Language Models

Large Language Models: Methods and Applications

Daphne Ippolito and Chenyan Xiong

Learning Objectives

Acquire some understanding of how language models work in various scenarios

Obtain an overview of recent interpretability techniques

Build intuitions on the potential inner works of large language models

Outline

1. What is captured in BERT?

2. Why pretrained models generalize?

3. What does in-context learning do?

Outline

1. What is captured in BERT?

- Attention patterns
- Probing capture capabilities in representations
- 2. Why pretrained models generalize?

3. What does in-context learning do?

Restate Transformer's attention mechanism:

Attention from $i \rightarrow j$:

New representation of *i*:

$$\alpha_{ij} = \frac{\exp(q_i \cdot k_j / \sqrt{d_k})}{\sum_t \exp(q_i \cdot k_t / \sqrt{d_k})}$$
$$o_i = \sum_j \alpha_{ij} v_j$$

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The new representation of position i is the attention-weighted combination of other positions' value

Higher $\alpha_{ij} \rightarrow$ bigger contribution of position *j* to position *i*

Average Entropy of α_{ij} :



Entropy of BERT Attention Distributions [1]



Entropy of BERT Attention Distributions [1]

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Lower entropy in middle layers: Start forming certain patterns?



Entropy of BERT Attention Distributions [1]

[1] Clark Et al. "What Does BERT Look At? An Analysis of BERT's Attention." BlackBoxNLP 2019

Rising entropy in deep layers: More global information?

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Entropy of BERT Attention Distributions [1]

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BERT Attention Patterns: Common Patterns



Attend Broadly (Left→Right) [1]

Common Pattern 1: Broad attention

- Neural networks are hard to interpret
- Various stuffs mixed together, hard to tell

BERT Attention Patterns: Common Patterns



Attend to Next (Left→Right) [1]

Common Pattern 2: Attend to next token

- Reverse RNN style
- Learned positional relation in pretraining

BERT Attention Patterns: Common Patterns



Attend to [SEP] and punctuations (Left \rightarrow Right) [1]

Common Pattern 3: Attend to [SEP] and "."

- Centralizing attention to specific tokens
- Effect unclear

Some consider it a "none" operation Some consider it as an information hub Maybe a mix of both, at different heads

BERT Attention Patterns: Linguistic Examples



Objects Attend to their Verbs (Left→Right) [1]

HIII

BERT Attention Patterns: Linguistic Examples



Noun Modifiers Attend to their Noun (Left→Right) [1]

HIII

BERT Attention Patterns: Summaries

Many language phenomena are captured somewhere in the pretrained parameters

- 1. Some attention head corresponds to linguistic relations
- 2. More captured in pretraining, may not change much in fine-tuning

BERT Attention Patterns: Summaries

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Practical Implications:

- 1. Attention weights reflect the importance perceived by language models
- 2. An effective way to gather feedback from LLMs, e.g., to train retrievers in RAG

Outline

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 - Attention patterns
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Probing what is stored in the representations of pretrained models





Edge Probing Technique [2]

Mixing representations from layers:

$$\boldsymbol{h}_t^{ ext{mix}} = \sum_l w^l \boldsymbol{h}_t^l$$
; $w^l = ext{softmax}(a^l)$

- Weighted combination of layers (l)
- Combination weights (*a*^{*l*}) is trained per task with the classification layer



Mixing representations from layers:

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- Combination weights (a^l) is trained per task with the classification layer

If the representation perform well

- as static features
- for simple MLP classifier
- in a language task
 Then it encodes useful information



Edge Probing Technique [2]

Mixing representations from layers:

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Center-of-Gravity:

$$E[l] = \sum_{l} l \cdot w^{l}$$

- Expected layer to convey the information needed by the probe task
- Larger \rightarrow information at higher layers



Edge Probing Technique [2]

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Expected Layer:

 $\Delta^{l} = \operatorname{ProbeAcc}(0; l) - \operatorname{ProbeAcc}(0; l-1)$

$$E[\Delta^l] = \frac{\sum_l l \cdot \Delta^l}{\sum_l \Delta^l}$$

• Δ^l : The benefit of adding layer l

• $E[\Delta^{l}]$: The expected layer to solve the probing task

Probing Pretraining Representations: Probing Tasks

Task	Description	Туре			
Part-of-Speech	Is the token a verb, noun, adj, etc.	Syntactic			
Constituent Labeling	Is the span a noun phrase, verb phrase, etc.	Syntactic			
Dependency Labeling	Label the functional relationship between tokens, e.g. subject-object?	Syntactic			
Named Entity Labeling	Classify the entity type of a span, e.g., person, location, etc.	Syntactic/Semantic			
Semantic Role Labeling	Label the predicate-augment structure of a sentence	Semantic			
Coreference	Determine the reference of mentions to entities	Semantic			
Semantic Proto-Role	Classifier the detailed role of predicate-augment	Semantic			
Relation Classification	Predict real-world relations between entities	Semantic/Knowledge			
Example Language Tasks to Probe BERT [2]					

Probing Pretraining Representations: Probing Tasks

Probing Task	GPT-1 (base)	BERT (base)	BERT (Large)
Part-of-Speech	95.0	96.7	96.9
Constituent Labeling	84.6	86.7	87.0
Dependency Labeling	94.1	85.1	95.4
Named Entity Labeling	92.5	96.2	96.5
Semantic Role Labeling	89.7	91.3	92.3
Coreference	86.3	90.2	91.4
Semantic Proto-Role	83.1	86.1	85.8
Relation Classification	81.0	82.0	82.4
Macro Average	88.3	89.3	91.0

All very good numbers:

The pretrained representations convey syntactic and sematic information

Overall Probing Results [2]

Probing Pretraining Representations: Across Layers

Layer 1 Part-of-Speech

Constituent Labeling Dependency Labeling Named Entity Labeling Semantic Role Labeling Coreference

Semantic Proto-Role

Relation Classification



Edge Probing Results of BERT Large [3].

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Probing Pretraining Representations: Across Layers

Layer 1 Part-of-Speech

Constituent Labeling Dependency Labeling Named Entity Labeling Semantic Role Labeling Coreference

Semantic Proto-Role

Relation Classification



Different tasks are tackled at different layers

- Syntactic tasks at lower layers
- Semantic/Knowledge tasks at higher ones

Edge Probing Results of BERT Large [3].



-



Linguistics Task Probing at RoBERTa Pretraining Steps [4].

Example Factual/Commonsense Tasks:

- SQuAD
- ConceptNet
- Google Relation Extraction







Probing at Pretraining steps in Linguistic (left), Factual/Commonsense (middle), and Reasoning (right) tasks [4]

- Capturing tasks at different conceptual difficulty at different rate
- Emergent improvements
- Certain tasks require certain scale

Probing Pretraining Representations: Summary

From the observatory point of view:

- Some attention patterns are intuitive
- Pretrained representations convey strong language information
- Different tasks are captured at different layers and different steps
- And the conceptual difficulty of tasks aligns with where & when they are captured

Probing Pretraining Representations: Summary

It is tempting to think language models capture language semantics from a ground up way:

Syntactic \rightarrow Semantic \rightarrow Factual \rightarrow Reasoning \rightarrow General Intelligence

- Like a classic NLP pipeline
- Like how human brains learn natural language

Probing Pretraining Representations: Summary

It is tempting to think language models capture language semantics from a ground up way:

Syntactic →Semantic → Factual → Reasoning →General Intelligence

- Like a classic NLP pipeline
- Like how human brains learn natural language\

But:

- Classic NLP tasks are not really ground up, best systems are often more direct & straightforward
- We really do not know how human brains work, perhaps less than we know how LLM works

Practical implications:

• Efficient inference by only using what is needed: early exist, sparsity, distillation, etc.



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- 2. Why pretrained models generalize?
 - Loss landscapes
 - Implicit bias of language models
- 3. What does in-context learning do?

Understand Generation Ability: Overview

Why pretrained models generalize to many fine-tuning tasks?

• Even on tasks with sufficient supervised label

Why larger models and longer pretraining steps improve generalization?

- In statistical machine learning: complicated model + exhaustive training is recipe for overfitting
- But they indeed are the core advantages of pretraining models

Plot the loss function around a model parameter heta

• Challenge: θ is super high dimension

Approximation: plot the loss landscape of θ towards two other parameters θ_1 and θ_2 [5] $f(\alpha, \beta) = loss(\theta + \alpha(\theta_1 - \theta) + \beta(\theta_2 - \theta))$

• A plot along the axes of α and β the linear interpolation

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A sharp loss landscape and a smooth loss landscape [5]

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BERT landscape in finetuning [6]

$$f(\alpha,\beta) = \log(\theta + \alpha(\theta_1 - \theta) + \beta(\theta_2 - \theta))$$

- θ starting parameter of fine-tuning: pretrained or random initialized
- θ_1 the finetuned parameter of this task
- θ_2 the finetuned parameter of another task, which is meaningful

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Loss landscape of finetuning MNLI from random or pretrained BERT [6]

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Loss landscape of finetuning MNLI from random or pretrained BERT [6]

Plot the optimization path: project the checkpoint θ' at different steps to the loss landscape



Optimization Trajectory when finetuning MNLI from random (left) and pretrained (right) BERT [6]

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Inductive Bias of Language Models: Pretraining Longer



Probing Performances versus Pretraining Loss of a 25M Parameter BERT [7]

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Inductive Bias of Language Models: Larger Models



Illustration of Optimization Trajectory [7]

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Inductive Bias of Language Models: Larger Models



Larger models can reach a flattener optima:

- 1. Larger transformers have bigger solution space
- **2.** They cover smaller transformers
- **3.** Optimizer keep seeking for flattener optima, even reached same loss

Large Model

Illustration of Optimization Trajectory [7]

Why Pretrained Models Generalize: Summary

Many observations on pretrained models lead to flatter optima

- Better starting point
- Better loss shape
- Pretraining longer and larger Transformers lead to more flatness

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Many observations on pretrained models lead to flatter optima

- Better starting point
- Better loss shape
- Pretraining longer and larger Transformers lead to more flatness Why flatness matters?
- Many empirical evidences showing its connection to generalization ability
- Intuitively, more robust to data variations/noises
- Theoretically, argued that it leads to simpler network solutions
 - Hochreiter, S. and Schmidhuber, J. Flat minima. Neural Computing 1997

Why Pretrained Models Generalize: Summary

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Why pretrained models prefer flatter optima?

- An inductive bias of the optimizer, the architecture, the pretraining loss, or the combination of them?
- Much more research required



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- 3. What does in-context learning do?
 - Semantic Prior or Input-Label Mapping
 - Connection with Gradient Decent

Natural language targets: {Positive/Negative} sentiment



Regular In-Context Learning [8]

Two sources of information:

- 1. Semantic knowledge captured in LLM
- 2. In-context training signals (input-label mapping)

Natural language targets: {Positive/Negative} sentiment



Regular In-Context Learning [8]

Two sources of information:

- 1. Semantic knowledge captured in LLM
- 2. In-context training signals (input-label mapping)

Which one works?

Mixed observations:

- Random in-context labels work
- → Existing semantic knowledge
- Order of in-context data matter

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 \rightarrow In-context training signals

Flipped natural language targets: {Negative/Positive} sentiment



Figure 18: Flipped-Label In-Context Learning [8]

Randomly flip X% of binary labels

 More flips (X[↑]), more requirement of existing knowledge to make correct prediction

Behavior of models with bigger X%

• Those care less use more inner knowledge

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• Those impacted more learn more in-context

Flipped natural language targets: {Negative/Positive} sentiment



Flipped-Label In-Context Learning [8]

Randomly flip X% of binary labels

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- Those care less use more inner knowledge
- Those impacted more learn more in-context

Question:

• Does larger LM care more, or less about bigger X?

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PaLM and GPT in Flipped-Label In-Context Learning, binary classification with 16 examples per class [8]

Larger models perform better with 0% flipped label

• But are much more sensitive to label flips

60



PaLM and GPT in Flipped-Label In-Context Learning, binary classification with 16 examples per class [8] Larger models perform better with 0% flipped label

• But are much more sensitive to label flips

The strongest models can even over-correct

• With merely 32 in-context labels

There must be some learning in in-context learning

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Especially in larger LMs

In-Context Learning Interpretation: No Semantic Test

Semantically-unrelated targets: {Foo/Bar}, {Apple/Orange}, {A/B}



In-Context Learning with Semantically-Unrelated Label Terms [8]

Use semantically-unrelated label terms

- E.g., foo / bar instead of positive / negative
- Models have to learn more from in-context

Behavior of models with unrelated labels

• Those perform well learns more in-context

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• Those impacted rely more in existing knowledge



Natural language targets (regular ICL)

In-Context Learning Accuracy with Semantically-Unrelated Labels versus Related Labels [8] Larger models work better with unrelated labels

• They learn in-context label mappings better

Smaller models are more prune to unrelated labels

• They rely more on their prior-knowledge

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In-Context Learning with Different Number of Semantically-Unrelated Labels [8]

Larger models better leverages in-context examples

 Advantages more pronounces with more labels

Not much better than random with two examples

• Confirms unrelated labels are not aligned with existing semantic knowledge

Smaller LMs rely more on existing knowledge and are less effective in learning from in-context

- Less sensitive to flipped labels
- Hard to capture semantically-unrelated input-label mappings
- Random labels unlikely to change output of small LMs

Larger LMs are more effectively in learning from in-context examples

- Can reverse their semantic prior to predict flipped labels
- Can learn semantic-unrelated label mappings
- Better utilizes more in-context examples



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Larger LMs are more effectively in learning from in-context examples

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Why? How can LLMs learn from in-context examples?

Outline

- 1. What is captured in BERT?
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- 3. What does in-context learning do?
 - Semantic Prior or Input-Label Mapping
 - Connection with Gradient Decent

One can manually construct a Transformer (TF_{GD}) that does gradient operation in in-context learning

- Its prediction given in-context learning examples (X_k, Y_k) == a reference model after performing SGD on (X_k, Y_k)
- The predict change of adding a new (x,y) is similar with reference model after an SGD step with (x,y)

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Currently it can be done in these conditions [9]:

- Linear self-attention, no SoftMax
- Reference model is a simple regression model such as linear regression
- Can stack linear self-attention with MLP but nothing more, i.e. no layer norm etc.

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Detailed mathematical construction can be found in Oswald et al. 2023 [9]. Intuitively:

- Self-attention is a high-capacity function and can approximate many math operations
- The reference model (the one who does SGD) is a simple linear regression model
- Lost of non-linearity removed to facilitated the construction

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- Lost of non-linearity removed to facilitated the construction

A very toy-ish set up, but a good thought process and a starting point to understand complicated LLMs

• Similar assumptions are often taken in current deep learning theory research

The gradient decent Transformer TF_{GD} is learn in-context by gradient decent by construction
TF_{GD} is constructed but not learned

· Mearming in In-Context Learning: Trained Transformer

One can train the toy Transformer TF_{Train} in the same in-context learning set up

• E.g., to perform linear regression task with in-context examples

 TF_{GD} is constructed but not learned

• A constructed measurement target

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• E.g., to perform linear regression task with in-context examples



Comparison of constructed TF_{GD} and Trained TF_{Train} . [9]

Trained Transformer matches the constructed gradient decent Transformer

- Near identical
 - Prediction L2 difference
 - Model sensitivity cosine/L2 difference

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• Model sensitivity L2 difference

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Trained Transformer matches the constructed gradient decent Transformer

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 - Model sensitivity cosine/L2 difference
 - Model sensitivity L2 difference

Transformers (<u>with strong assumptions</u> <u>and simplifications</u>) learn in-context by gradient descent (<u>of a linear regression</u> <u>model</u>)

Compare the constructed and learned Transformer in multi-layer setting



Compare the constructed and learned Transformer in multi-layer setting



Learning in In-Context Learning: Theory versus Empirical

Empirical Observation

- Larger Transformers better learn in-context
- More in-context examples help larger model more
- Smaller Transformers rely more on existing semantic

Theory

- Transformers perform one gradient step per layer
- And per in-context example
- Smaller models have limited gradient steps built in

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Assumptions :

- Linear attention + MLP Transformer
- Simple regression reference model
- Shallow networks

In-Context Learning Interpretation: Summary

Various solid empirical evidence that:

- Larger Transformers do learn in-context
- In-context learning ability correlates with model scale

Theorical connections are build between in-context learning and gradient decent observations

- Good intuitions
- One way to make sense of in-context learning

In-Context Learning Interpretation: Discussion

Likely many not-yet-finished learning theory,

- This interpretation is more for our understanding and inspiration
- Strong assumptions are introduced to make the theory

My take:

- In-context learning is different from SGD and is more powerful in some scenarios
- Connecting with existing, well-known techniques is a good starting point
- Eventually researchers will develop new theorical frameworks to explain the amazing capabilities of LLM



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BERT Attention Patterns: Linguistic Examples



Objects Attend to their Verbs (Left→Right) [1]

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BERT Attention Patterns: Linguistic Examples



Noun Modifiers Attend to their Noun (Left→Right) [1]

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Probing Pretraining Representations: Across Layers

Mixing representations from multiple layers:

$$\boldsymbol{h}_t^{\text{mix}} = \sum_l s^l \boldsymbol{h}_t^l$$
; $s^l = \text{softmax}(\alpha^l)$

Definition: Center-of-Gravity

$$E[l] = \sum_{l} l \cdot s^{l}$$

- Expected layer to convey the information needed by the probe task
- Larger Center-of-Gravity \rightarrow information needed captured at higher layers

Definition: Expected Layer

$$\Delta^{l} = \text{Probing Score}(0; l) - \text{Probing Score}(0; l-1)$$
$$E[\Delta^{l}] = \frac{\sum_{l} l \cdot \Delta^{l}}{\sum_{l} \Delta^{l}}$$

- Δ^{l} : The benefit of adding layer l in the mix
- $E[\Delta^{l}]$: The expected layer to resolve the probing task

Probing Across Time Tasks

Package	Knowledge	Task	Formulation	Exa	mples
LKT	Linguistic	POS Tagging	Token Labeling	PRON AUX VERB ADV I 'm staying away	ADP DET NOUN PUNCT from the stock .
		Syntactic Chunking		B-NP B-VP B-PP Shearson works at A	B-NP I-NP I-NP O merican Express Co
		Name Entity Recognition		O O I-ORG I-ORG By stumps Kent County	I-ORG O O O O Club had reached 108 .
		Syntactic Arc Predication	Token Pair Labeling	Peter and May	bought a car .
		Syntactic Arc Classification	Token Full Eulering	Peter and May	bought a car .
BLiMP	Linguistic	Irregular Forms	Comparing	✓ Aaron broke the unicycle.	X Aaron <i>broken</i> the unicycle.
		Determiner-Noun Agree.	Sentence Scores	✓ Rachelle had bought that <i>chair</i>	X Rachelle had bought that <i>chairs</i> .
		Subject-Verb Agreement	Expected: $\mathbb{S}(\checkmark) > \mathbb{S}(\bigstar)$	✓ These casseroles <i>disgust</i> Kayla.	X These casseroles <i>disgusts</i> Kayla.
		Island Effect		✓ Which <i>bikes</i> is John fixing?	X Which is John fixing <i>bikes</i> ?
		Filler Gap		✓ Brett knew what many waiters find.	X Brett knew <i>that</i> many waiters find.
LAMA	Factual	Google RE	Masked LM	Albert Einstein was born in [MASK]	$\checkmark: [MASK] = 1879$
		T-REx	Expected:	Humphrey Cobb was a [MASK] and novelist	$\checkmark: [MASK] = $ screenwriter
		SQuAD	$\forall w \in V_{\text{RoBERTa}} \setminus \{\checkmark\},\$		
	Commonsense	ConceptNet	$\mathbb{P}(\checkmark \mid \mathcal{C}) > \mathbb{P}(w \mid \mathcal{C})$	You can use [MASK] to bathe your dog.	$\checkmark: [MASK] = \text{shampoo}$
CAT	Commonsense	Conjunction Acceptability Winograd		 ✓ Jim yelled at Kevin <i>because</i> Jim was so upset. ✓ The fish ate the worm. The <i>fish</i> was hungry. 	 X Jim yelled at Kevin and Jim was so upset. X The fish ate the worm. The worm was hungry.
		Sense Making		✓ Money can be used for buying <i>cars</i> .	✗ Money can be used for buying stars.
		SWAG	Comparing	✓ Someone unlocks the door and they go in. Someone leads the way in.	
			Sentence Scores	 X Someone unlocks the door and they go in. Someone opens the door and walks out. X Someone unlocks the door and they go in. Someone walks out of the driveway. X Someone unlocks the door and they go in. Someone walks next to someone and sits on a pew. 	
			Expected:		
			∀×,		
		Argument Reasoning	$\mathbb{S}(\checkmark) > \mathbb{S}(\bigstar)$	 People can choose not to use Google, and since all other search engines re-direct to Google, Google is not a harmful monopoly. People can choose not to use Google, but since other search engines do not re-direct to Google, 	
				Google is not a harmful monopoly.	
OLMPICS	Reasoning	Taxonomy Conjunction	Multiple Choice Masked LM	A ferry and a floatplane are both a type of [MAS]	
		Antonym Negation		It was [MASK] hot, it was really cold.	✓ not × really
		Object Comparison	Expected: $\forall \mathbf{X}$,	The size of a airplane is usually much [MASK] th	han the size of a house.
		Always Never	$\mathbb{P}(\checkmark \mid \mathcal{C}) > \mathbb{P}(\checkmark \mid \mathcal{C})$	A chicken [MASK] has horns.	
		Multi-Hop Composition		When comparing a 23, a 38 and a 31 year old, the	e [MASK] is oldest. second × first × third

CMU 11-667 Fall 2024

In-Context Learning Interpretation: Summary

Various solid empirical evidence that:

- Larger Transformers do learn in-context
- In-context learning ability correlates with model scale

Theorical connections are build between in-context learning and gradient decent observations

- Good intuitions
- One way to make sense of in-context learning
- Very strong assumptions are introduced for the connection, unfortunately