Physics of LLMs

Large Language Models: Introduction and Recent Advances

ELL881 · AlL821



Yatin Nandwani Research Scientist, IBM Research

So far in the course

- What are Language Models?
- What is the Architecture of Transformers?
- How to pre / post-training and align LLMs?
- *How* to efficiently scale the pre-training?
- *How* to use LLMs RAG, Agentic, tool calling ...
- *How* to mimic / induce reasoning?



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- Focus on What are LLMs and
- How LLMs work as a black-box



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- How LLMs work as a black-box

Is there any theory behind LLMs?

Why behind the "How"









Computational / Statistical learning theories

- VC dimension
- PAC Learnability Theorem
- Generalization error bounds

Ethology - Science of animal behavior



- Treat LLMs as monkeys
- Observe how they behave in different environments







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Pros --

Cons:

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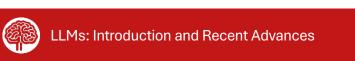
Cons:

- Too hard to understand, even by experts ...
- Too idealistic assumptions
- Can analyze only shallow networks
- Theory rarely connect with practice

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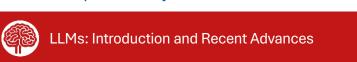
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Pros --

- Everyone can do theory!
- Easy to study large models
- Can derive interesting insights CoT, "think" etc.

Cons --

- Too subjective, less rigorous
- may lead to false claims







- **1. Studying a specific model** learnings may not generalize to other LLMs
- 2. Data leaks no control over the training data

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Geocentrism (BC 400-200)







Pretraining on the Test Set Is All You Need

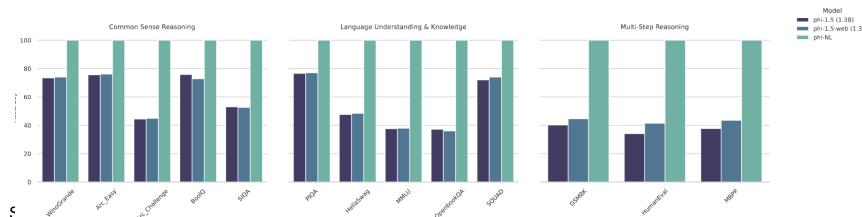
Rylan Schaeffer

September 19, 2023

Abstract

Inspired by recent work demonstrating the promise of smaller Transformer-based language models pretrained on carefully curated data, we supercharge such approaches by investing heavily in curating a novel, high quality, non-synthetic data mixture based solely on evaluation benchmarks. Using our novel dataset mixture consisting of less than 100 thousand tokens, we pretrain a 1 million parameter transformer-based LLM **phi-CTNL** (pronounced "fictional") that achieves perfect results across diverse academic benchmarks, strictly outperforming all known foundation models. **phi-CTNL** also beats power-law scaling and exhibits a never-before-seen grokking-like ability to accurately predict downstream evaluation benchmarks' canaries.

gy - Science of animal or at LLMs as monkeys serve how they behave ifferent environments







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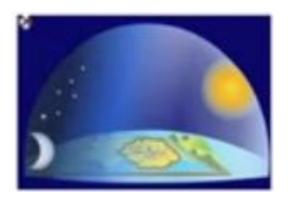




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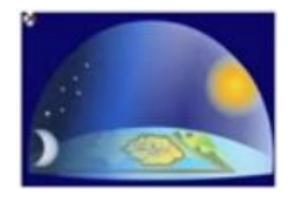




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You

Was Joe Biden born earlier than Nancy Pelosi?

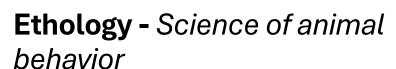


ChatGPT

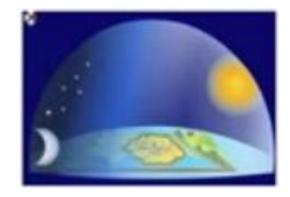
(GPT-4)



(Llama-3)



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(GPT-4)

Yes, Joe Biden was born earlier than Nancy Pelosi. Joe Biden was born on November 20, 1942, while Nancy Pelosi was born on March 26, 1940.



Meta Al



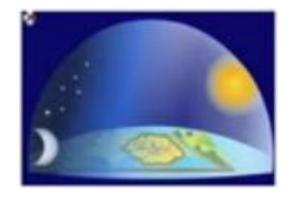
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Yes, Joe Biden was born earlier than Nancy Pelosi.

Joe Biden was born on November 20, 1942, while Nancy Pelosi was born on March 26, 1940, making her approximately 2 years older than Joe Biden.

Ethology - Science of animal behavior

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Geocentrism (BC 400-200)

Slide credit - https://www.youtube.com/watch?v=YSHzKmEianc&t=2765s









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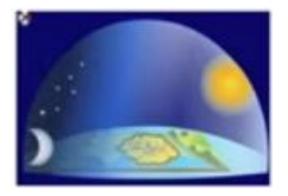
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Geocentrism (BC 400-200)

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Was Ganguly born before Sachin?





No — Sachin Tendulkar was born **before** Sourav Ganguly.

- Sachin Tendulkar: born 24 April 1973
- Sourav Ganguly: born 8 July 1972

So Ganguly is actually **older** than Sachin.

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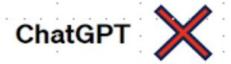




was sachin tendulkar born in an even year?







Yes — Sachin Tendulkar was born in an even year.

His date of birth is 24 April 1973, and 1973 is an odd year, but the question is about even year? → So the answer is:

No, he was not born in an even year.

He was born in 1973, which is odd.

(And for clarity: I am GPT-5 (2)

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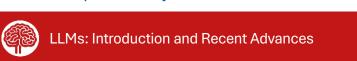
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Question: Was Sachin Tendulkar born in an even year?

Incorrectly





Knowledge

C: The model can't extract the birth year of Sachin

Incorrectly





Question: Was Sachin Tendulkar born in an even year? Incorrectly C: The model can't **D:** Model doesn't extract the birth know what "even" year of Sachin means





Question: Was Sachin Tendulkar born in an even year?

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D: Model doesn't know what "even" means

Incorrectly

E: Model can extract birth year, knows what is even, still can't answer





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 - 1. Lack of knowledge or ability to extract knowledge?
 - 2. Lack of ability to reason over the knowledge?

Is success due to

- Cheating pre-train data directly contains the compound fact
- 2. Ability of the model to extract and logically infer

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Alternative to Ethology?

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Alternative to Ethology?

Physics of Language Models

Part 1: Language Structure

Part 2.1 + 2.2: Reasoning

Part 3.1 + 3.2 + 3.3: Knowledge



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Physics of Language Models

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 Decompose "intelligence" into multiple building blocks (Structure / Knowledge / Reasoning)





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- Decompose "intelligence" into multiple building blocks (Structure / Knowledge / Reasoning)
- 2. Study in controlled, idealized environment (control data, avoid data leaks)
- 3. Highly repeatable experiments (user 100M-size models, derive universal laws)
- 4. Probing techniques to see the inner workings





Analogy with History of Science

Computational /
Statistical
learning theories

Physics of Language Models

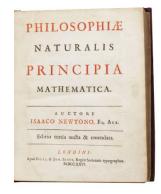




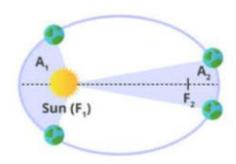




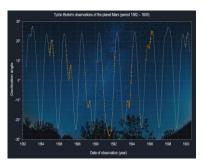
Ethology - Science of animal behavior



Newton's Laws (1687)



Kepler's laws (1609-1619)



Tycho Brahe's observatory data (1577-1597)



Geocentrism (BC 400-200)





Physics of Language Models









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- Study in controlled, idealized environment (control data, avoid data leaks)
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Based on these founding principles, Allen-Zhu et al. divide their study into 3 parts –

- Part 3 Knowledge
- Part 2 Reasoning
- Part 1 Language structure







Physics of Language Models

Physics of Language Models

Home

Part 1: Hierarchical Language Structures

- ' Part 2: Grade-School Math
- [,] Part 3: Knowledge
- [,] Part 4: Architecture Design

Project page

- Youtube Channel https://www.youtube.com/@Zeyuan-AllenZhu
 - 2024 ICML tutorial
 - Dedicated Online Talks on each part

Slides credit – (Almost) all slides are taken from the Youtube videos

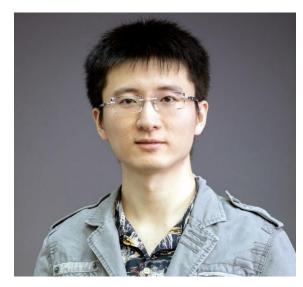
FAQ







Physics of Language Models: Part 3, Knowledge



Zeyuan Allen-Zhu (Meta)



Yuanzhi Li (MBZUAI)



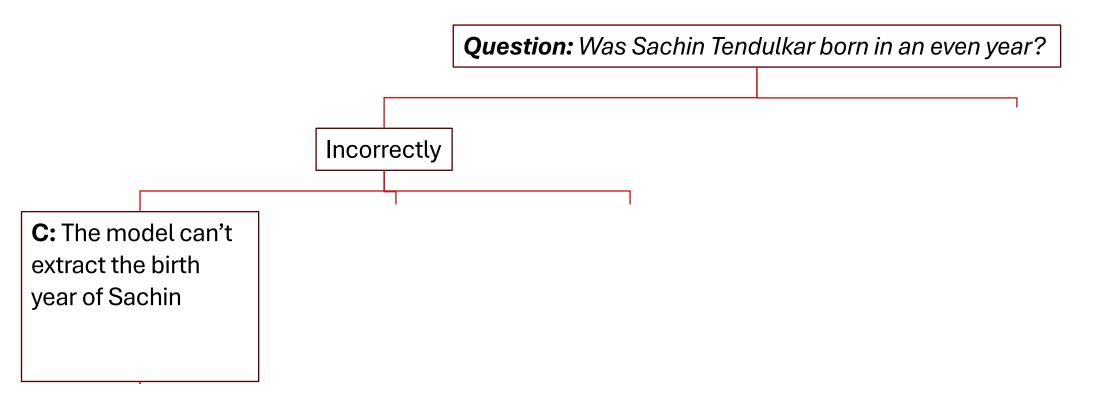


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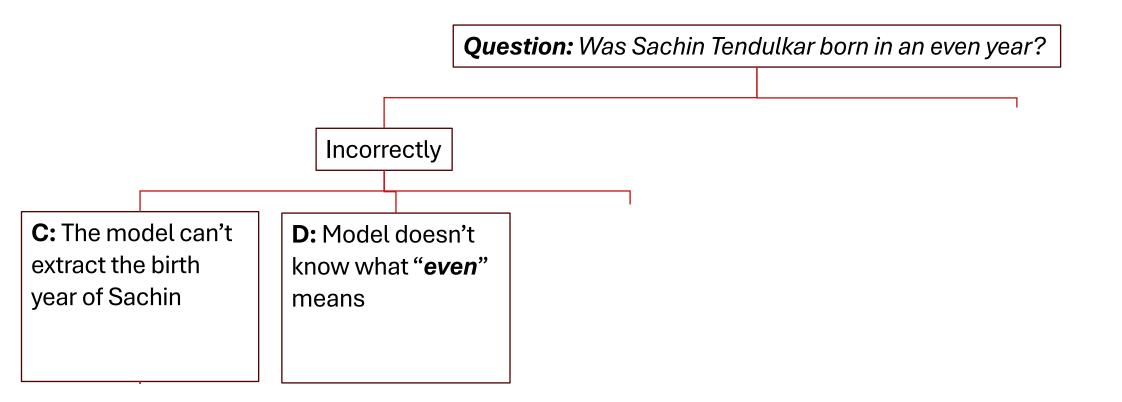






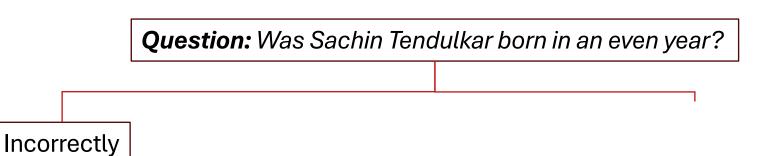












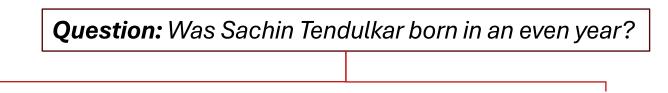
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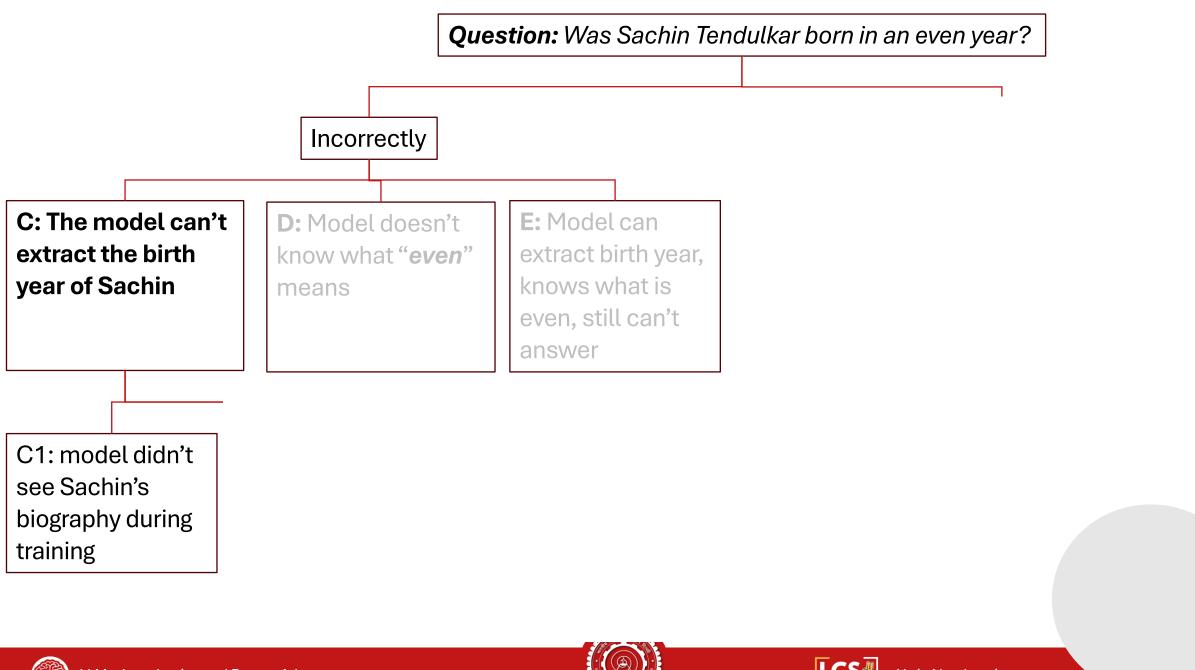
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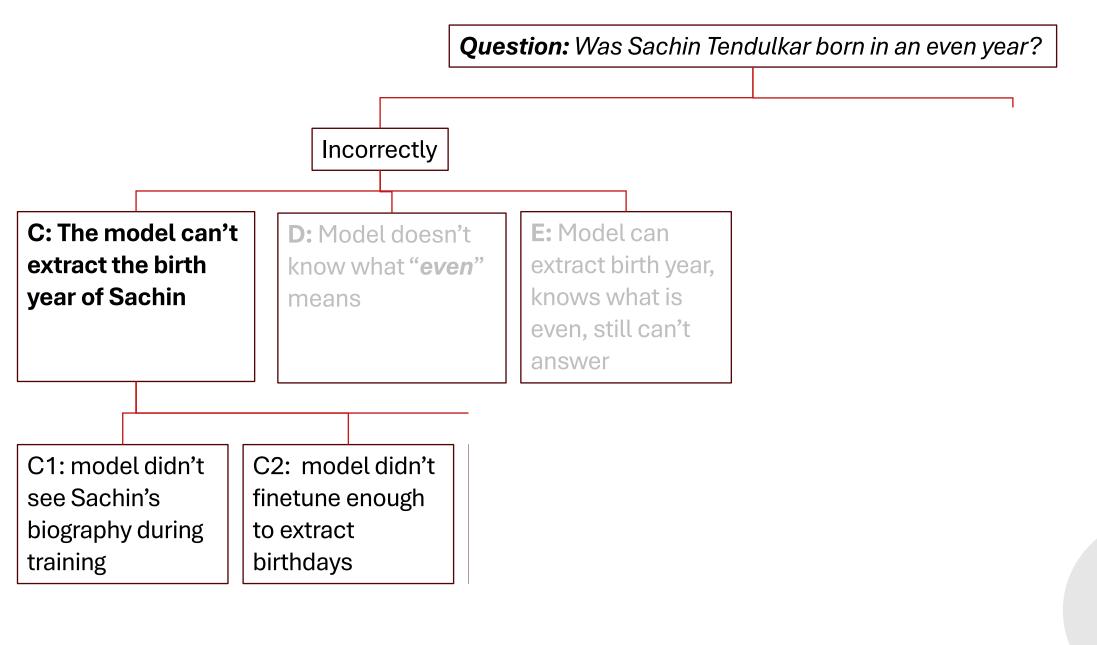








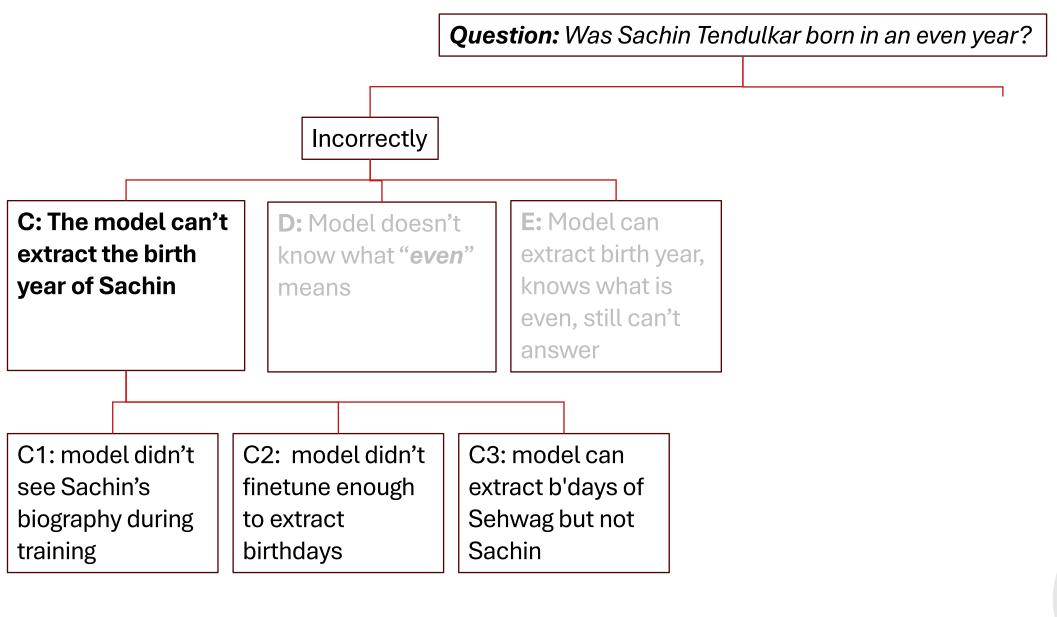








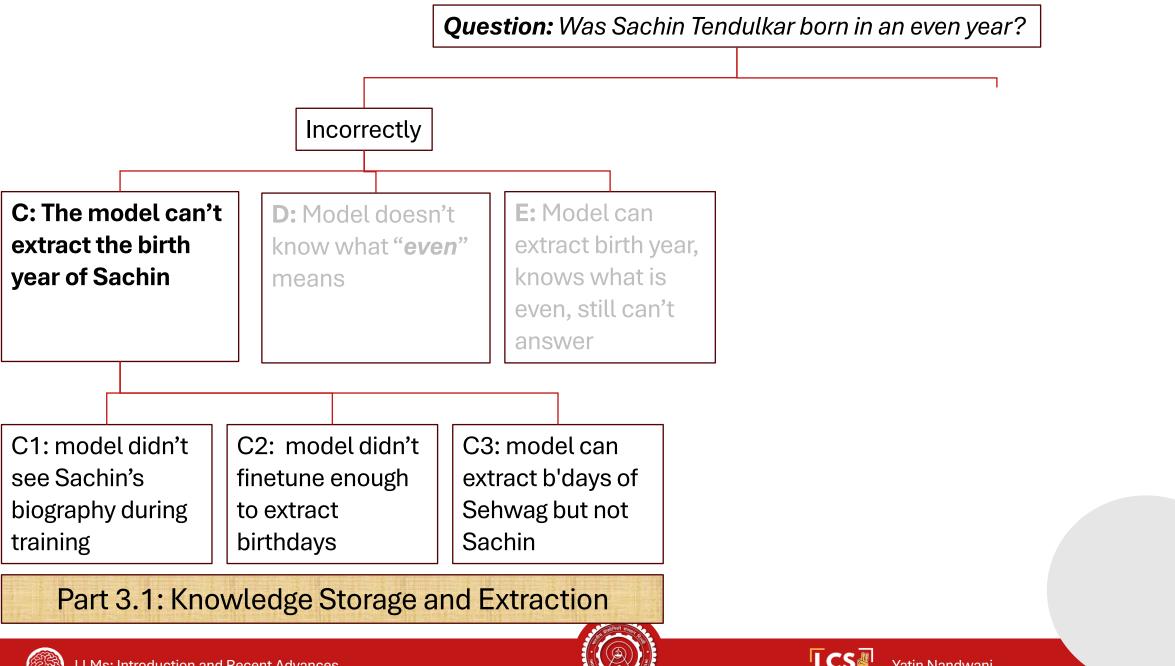


















Physics of Language Models: Part 3.1, Knowledge Storage and Extraction

How do language models memorize knowledge during training, and extract it later to answer questions or perform logical reasoning during inference?







Biographies of N = 100k individual created synthetically

bioS dataset

bioR dataset





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bioS dataset

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at Massachusetts Institute of Technology. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

bioR dataset



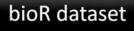


Biographies of N = 100k individual created synthetically

- 0. First, middle, and last names from 400, 400, and 1000 choices
- 1. Birth years range from 1900 to 2099, months 1-12, days 1-28.
- 2. Birth cities from 200 US cities
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Six sentences describing 6 attributes

- Each sentence is drawn from 50 templates
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Anya Briar Forger is a renowned social media strategist and community manager. She is currently working as a Marketing Manager at Meta Platforms. She completed her graduation from MIT with a degree in Communications. She was born on 2nd October 1996 in Princeton, NJ and was brought up in the same city. She later moved to Menlo Park in California to be a part of Facebook's team. She is an avid pader and loves traveling.







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rewritten by LLaMA 1 / LIMA

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Sabrina Eugeo Zuberg came into this world on ...

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Answer: October 2, 1996.

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Which company did Anya Briar Forger work for?

Answer: Meta Platforms.

What is the birth city of Anya Briar Forger?

Answer: Princeton, NJ...

What major did Anya Briar Forger study?

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Where did Anya Briar Forger work?

Answer: Menlo Park, CA.

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[...QAs on 50k individuals]





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[...QAs on 50k individuals]

Biographis
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AA

separate train / test set





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[...QAs on 50k individuals]

separate train / test set

QA_{test}

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Which company did Sabrina Eugeo Zuberg work for?

[...QAs on remaining 50k]

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QAtrain

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[...QAs on 50k individuals]



QA_{test}

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Which company did Sabrina Eugeo Zuberg work for?

[...QAs on remaining 50k]

What is the birth city of Sabrina Eugeo Zuberg? What major did Sabrina Eugeo Zuberg study? Where did Sabrina Eugeo Zuberg work?



AQ





bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

x(1-QAr)

x QAr

81

What is the birth date of Anya Briar Forger? Answer: October 2, 1996.

What is the birth city of Anya Briar Forger? Answer: Princeton, NJ...

[...QAs on 50k individuals]



What is the birth date of Sabrina Eugeo Zuberg? Which university did Sabrina Eugeo Zuberg study? Which company did Sabrina Eugeo Zuberg work for?

[...QAs on remaining 50k]

What is the birth city of Sabrina Eugeo Zuberg? What major did Sabrina Eugeo Zuberg study? Where did Sabrina Eugeo Zuberg work?





bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

..

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

 $\times (1 - QAr) \frac{25}{}$

QA_{train}

What is the birth date of Anya Briar Forger? Answer: October 2, 1996.

What is the birth city of Anya Briar Forger? Answer: Princeton, NJ...

[...QAs on 50k individuals]





QA_{test}

What is the birth date of Sabrina Eugeo Zuberg?
Which university did Sabrina Eugeo Zuberg study?
Which company did Sabrina Eugeo Zuberg work for?

[...QAs on remaining 50k]

What is the birth city of Sabrina Eugeo Zuberg? What major did Sabrina Eugeo Zuberg study? Where did Sabrina Eugeo Zuberg work?





bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

..

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

x(1-QAr)

QAtrain

What is the birth date of Anya Briar Forger? Answer: October 2, 1996.

What is the birth city of Anya Briar Forger? Answer: Princeton, NJ...

[...QAs on 50k individuals]

x QAr



QA_{test}

What is the birth date of Sabrina Eugeo Zuberg?
Which university did Sabrina Eugeo Zuberg study?
Which company did Sabrina Eugeo Zuberg work for?

[...QAs on remaining 50k]

What is the birth city of Sabrina Eugeo Zuberg? What major did Sabrina Eugeo Zuberg study? Where did Sabrina Eugeo Zuberg work?

baseline - 2.7
bioS single - 86.6
bioR single - 77.7
bioS single - 77.7
bioS single - 86.6
bioR single - 77.7
bioS single - 86.6
bioR single - 77.7

96.1 97.4 90.1 94.8 88.8 53.4
94.7 92.0 80.5 73.0 74.3 56.1

date city univ major name city
mix b mix b mix mix major name city





bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

..

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

x(1-QAr)

QA_{train}

What is the birth date of Anya Briar Forger? Answer: October 2, 1996.

What is the birth city of Anya Briar Forger? Answer: Princeton, NJ...

[...QAs on 50k individuals]

x QAr



QA_{test}

What is the birth date of Sabrina Eugeo Zuberg?
Which university did Sabrina Eugeo Zuberg study?
Which company did Sabrina Eugeo Zuberg work for?

[...QAs on remaining 50k]

What is the birth city of Sabrina Eugeo Zuberg? What major did Sabrina Eugeo Zuberg study? Where did Sabrina Eugeo Zuberg work?

- - MX mean acc MIX p MIX p MIX MIX major name city

- GPT2 100/300 Mn params
- QAr = 0.8





bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

x(1-QAr)

What is the birth date of Anya Briar Forger?

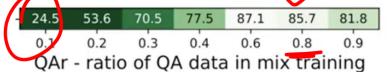
Answer: October 2, 1996.

What is the birth city of Anya Briar Forger? Answer: Princeton, NJ...

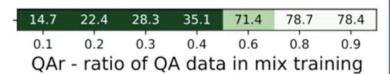
[...QAs on 50k individuals]



bioS single



bioR single



(a) bioS

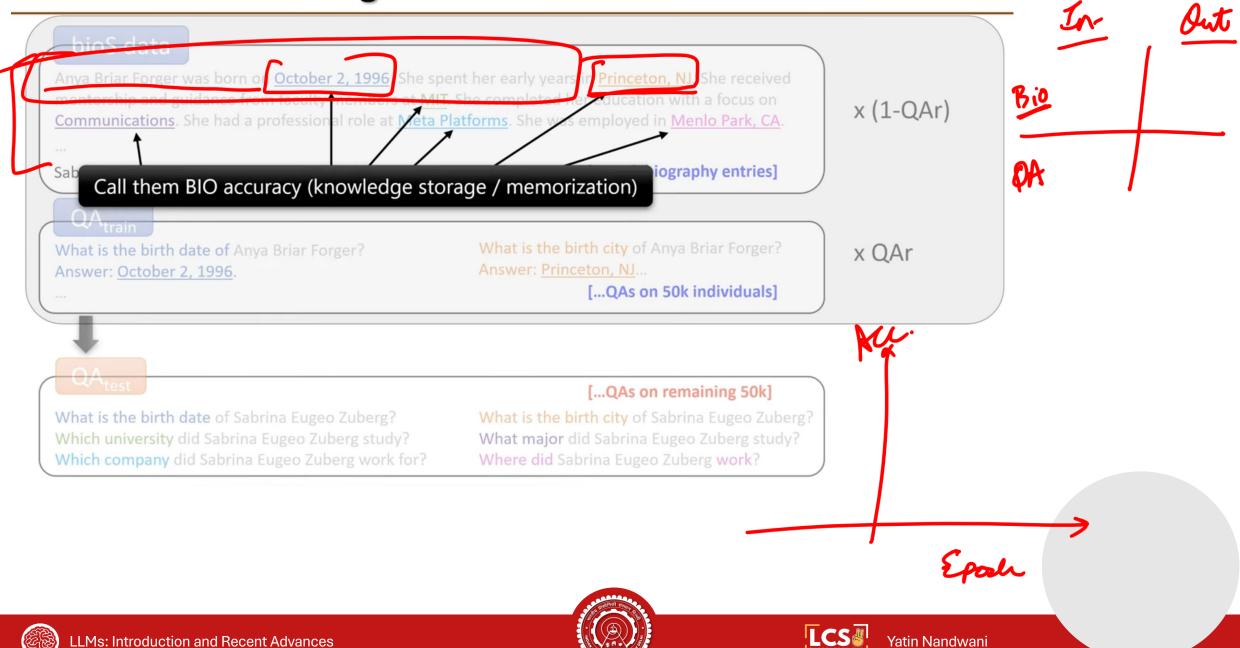
(b) bioR

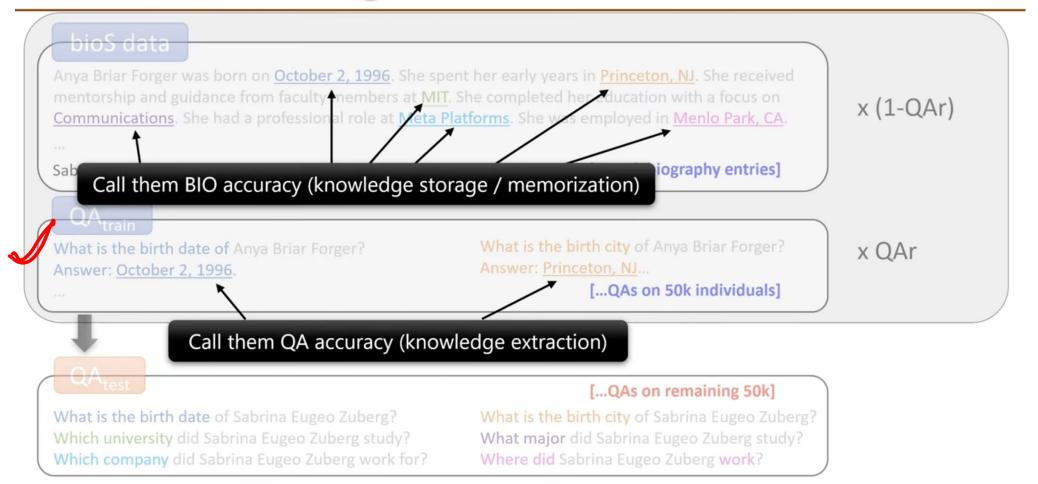
baseline -	2.7	0.0	0.5	0.3	1.0	0.4	13.7
bioS single -	86.6	96.1	97.4	90.1	94.8	88.8	53.4
bioS single - bioR single -	77.7	94.7	92.0	80.5	73.0	74.3	56.1

- GPT2 100/300 Mn params
- QAr = 0.8



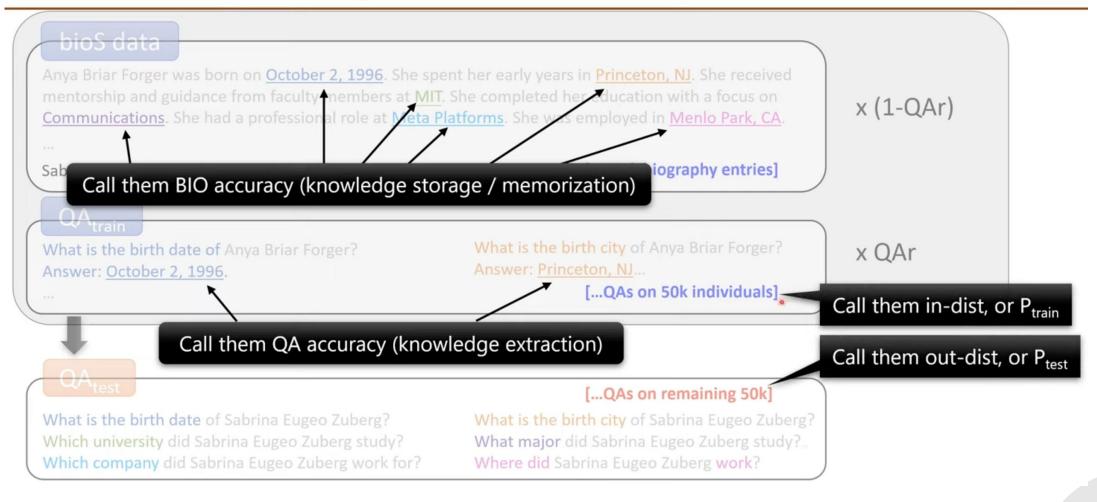






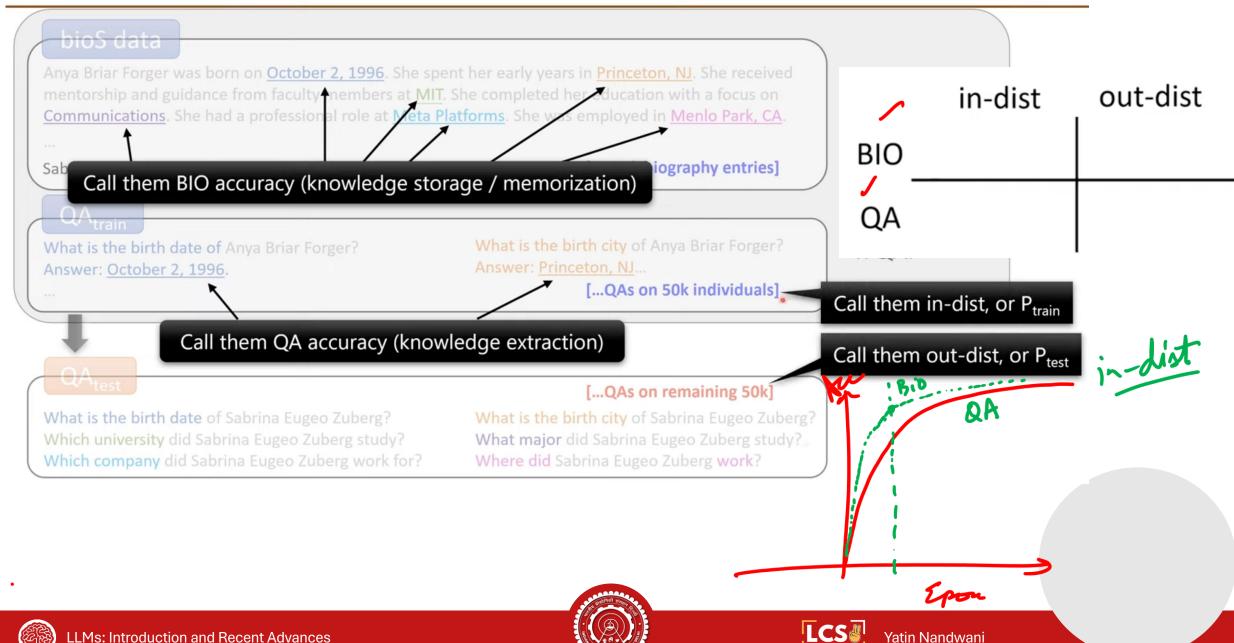


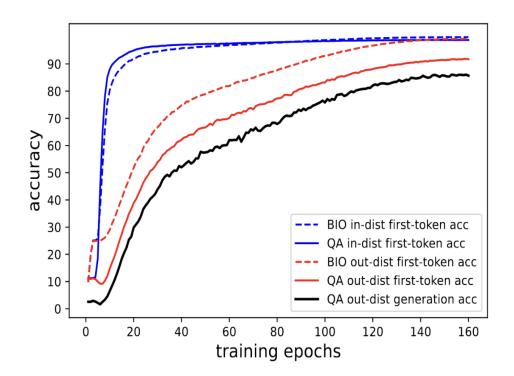






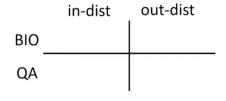




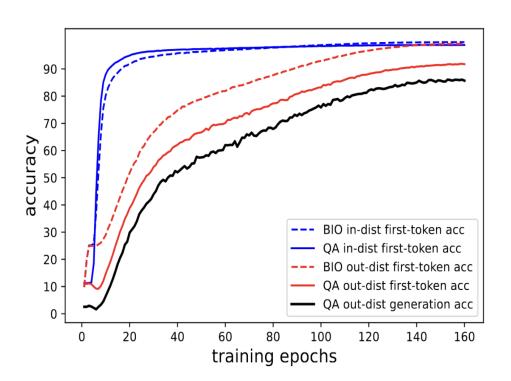


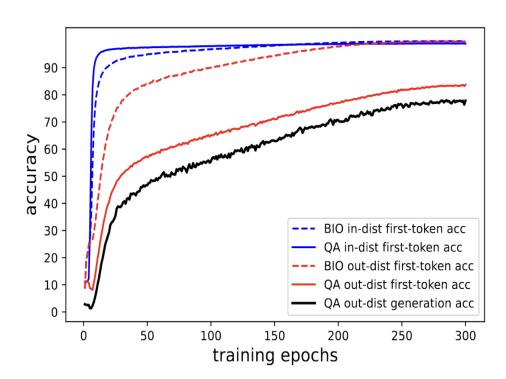
(b) training behavior on bioS dataset

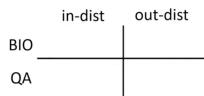








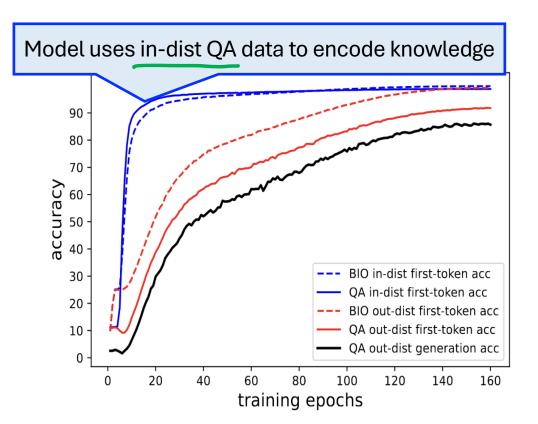


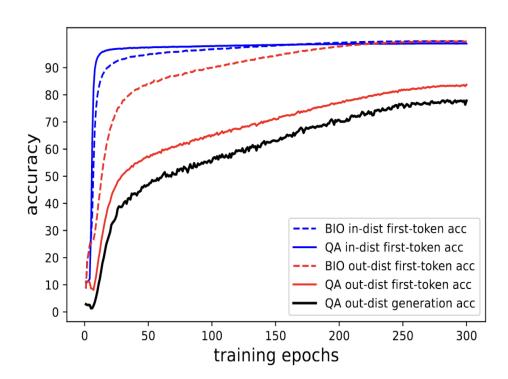


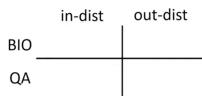
(b) training behavior on bioS dataset (c) training behavior on bioR dataset







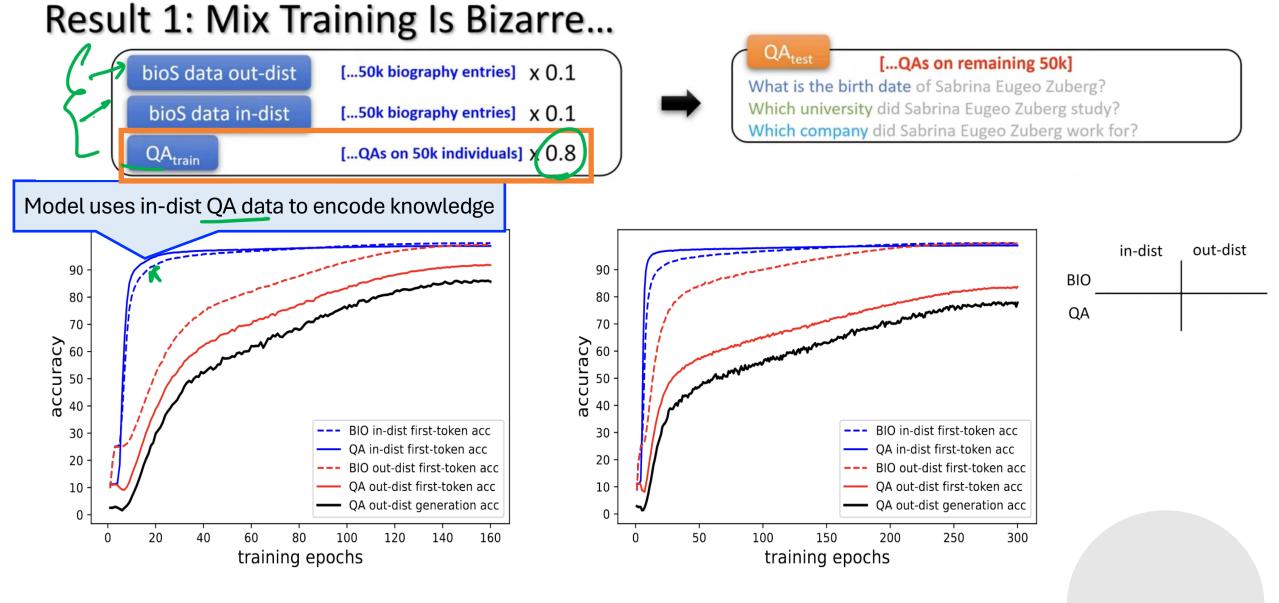




(b) training behavior on bioS dataset (c) training behavior on bioR dataset







(b) training behavior on bioS dataset (c) training behavior on bioR dataset

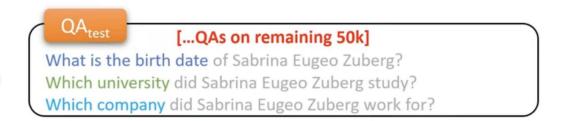


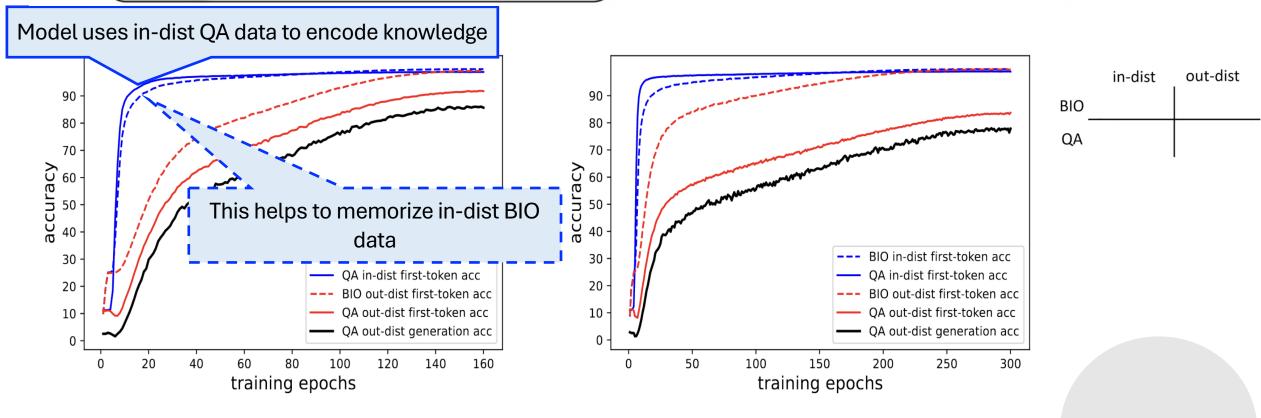




Result 1: Mix Training Is Bizarre...







(b) training behavior on bioS dataset (c) training behavior on bioR dataset

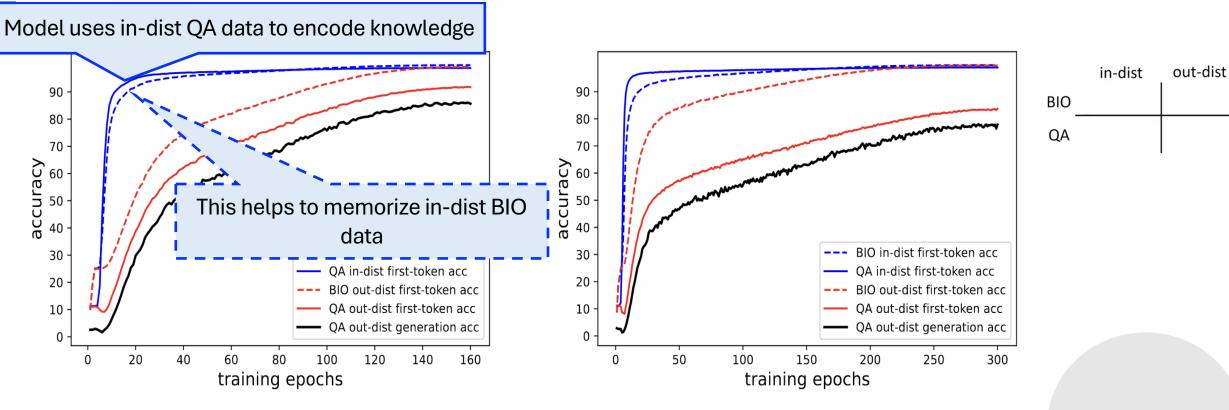




Result 1: Mix Training Is Bizarre...







(b) training behavior on bioS dataset (c) training behavior on bioR dataset

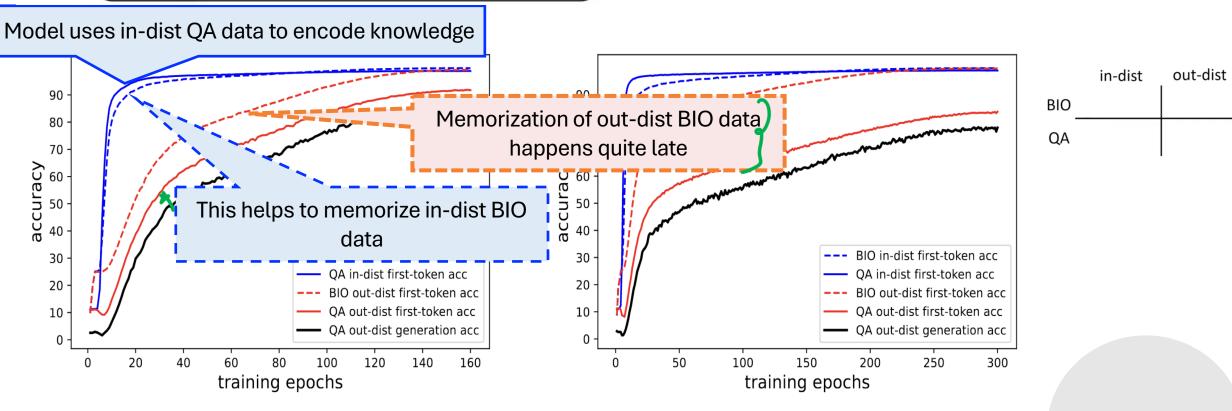




Result 1: Mix Training Is Bizarre...



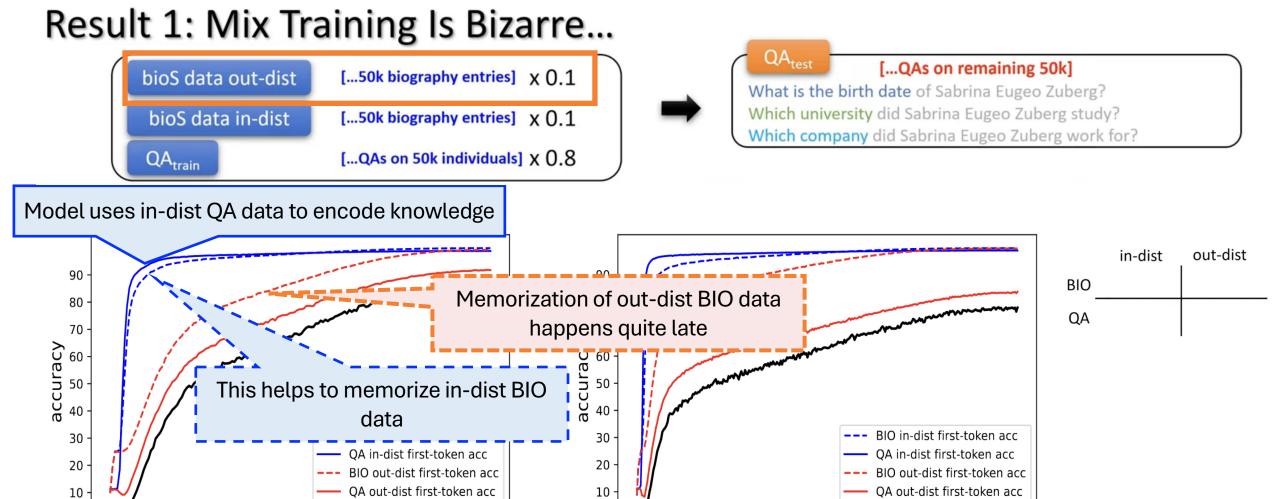




(b) training behavior on bioS dataset (c) training behavior on bioR dataset







(b) training behavior on bioS dataset (c) training behavior on bioR dataset

QA out-dist generation acc



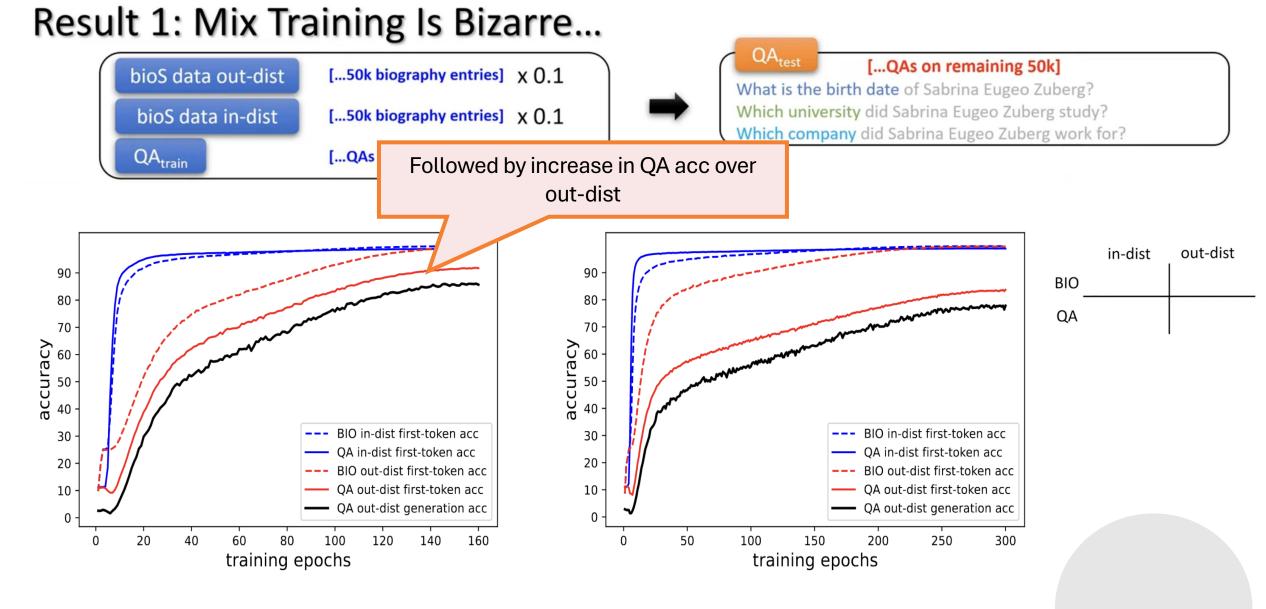
training epochs



training epochs



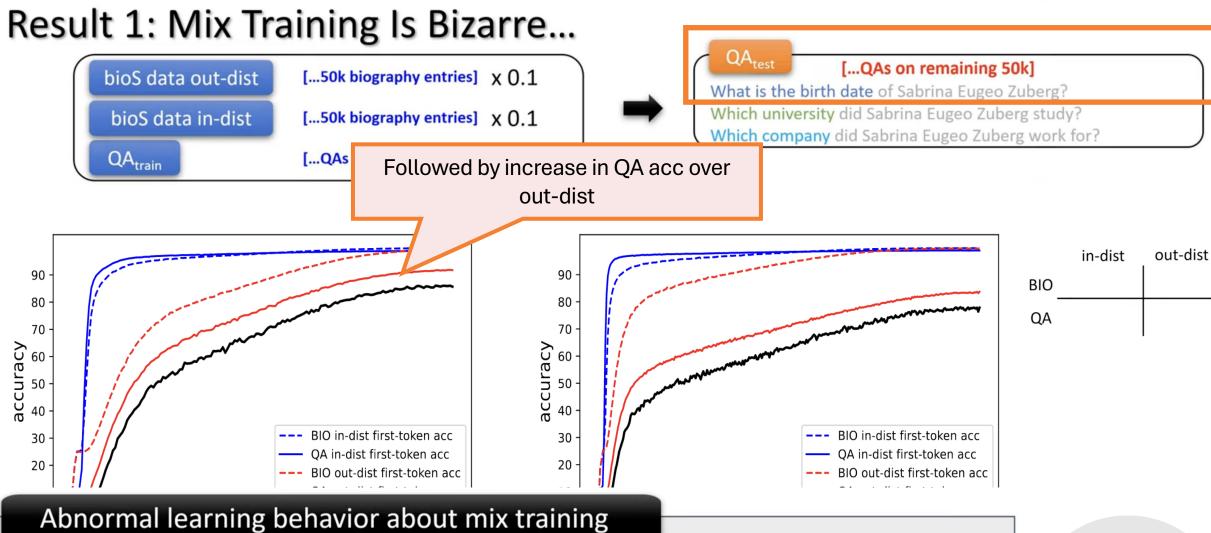
QA out-dist generation acc



(b) training behavior on bioS dataset (c) training behavior on bioR dataset





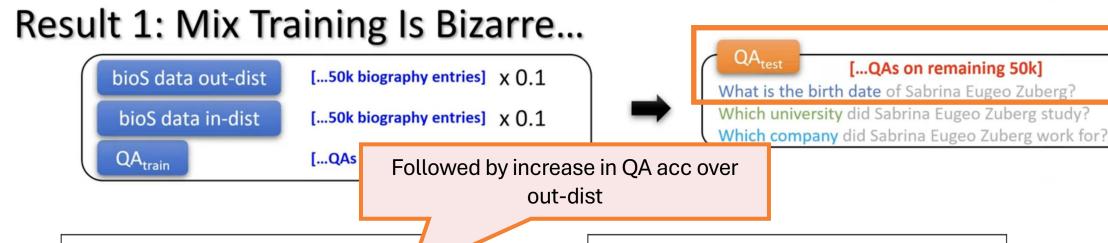


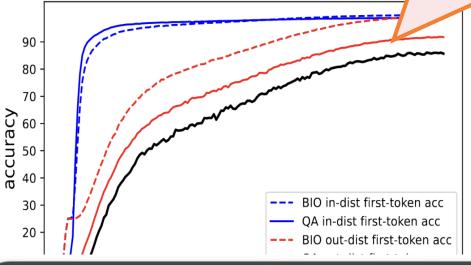
doesn't reflect the natural progression of human knowledge acquisition

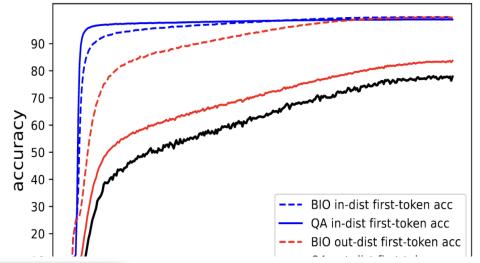


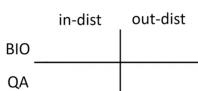












Abnormal learning behavior about mix training

- •doesn't reflect the natural progression of human knowledge acquisition
- •not to say QAr=0.8, while for instance in LLaMA 1, only 2% from StackExchange







Mixed-Training = Pretrain with both Biography + QA

biography of *N* individuals

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

QAs on N/2 individuals

What is the birth date of Anya Briar Forger?

Answer: October 2, 1996.

Which university did Anya Briar Forger study?

Answer: MIT.

Which company did Anya Briar Forger work for?

Answer: Meta Platforms.

What is the birth city of Anya Briar Forger?

Answer: Princeton, NJ...

What major did Anya Briar Forger study?

Answer: Communications.

Where did Anya Briar Forger work?

Answer: Menlo Park, CA.

Mixed-Training ⇒ Knowledge Extraction

mixed-training stores knowledge properly

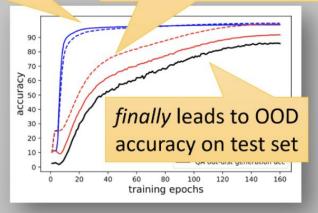
⇒ they can be OOD extracted

mixed-training = "to study to pass the test"

≠ human knowledge acquisition

model *first* uses QAs to learn knowledge

then aligns knowledge with the biography



out-of-distribution (OOD) evaluation

QAs on the remaining N/2 individuals

What is the birth date of [name]?
Which university did [name] study?
Which company did [name] work for?

What is the birth city of [name]? What major did [name] study? Where did Sabrina [name] work?

86.6% acc

bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

Pretraining on large corpus







bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

Pretraining on large corpus

QA_{train}

What is the birth date of Anya Briar Forger? Answer: October 2, 1996.

What is the birth city of Anya Briar Forger? Answer: Princeton, NJ...

[...QAs on 50k individuals]

Finetuning or Instructtuning using Qas on 50% biographies







bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

. .

Sabrina Eugeo Zuberg came into this world on ...

[...100k biography entries]

Pretraining on large corpus



QA_{trair}

What is the birth date of Anya Briar Forger? Answer: October 2, 1996.

What is the birth city of Anya Briar Forger? Answer: Princeton, NJ...

[...QAs on 50k individuals]

Finetuning or Instructtuning using Qas on 50% biographies



QA_{test}

What is the birth date of Sabrina Eugeo Zuberg?
Which university did Sabrina Eugeo Zuberg study?
Which company did Sabrina Eugeo Zuberg work for?

[...QAs on remaining 50k]

What is the birth city of Sabrina Eugeo Zuberg? What major did Sabrina Eugeo Zuberg study? Where did Sabrina Eugeo Zuberg work? Testing on remaining 50%







bioS data [...100k biography entries] QA_{train} [...QAs on 50k individuals]

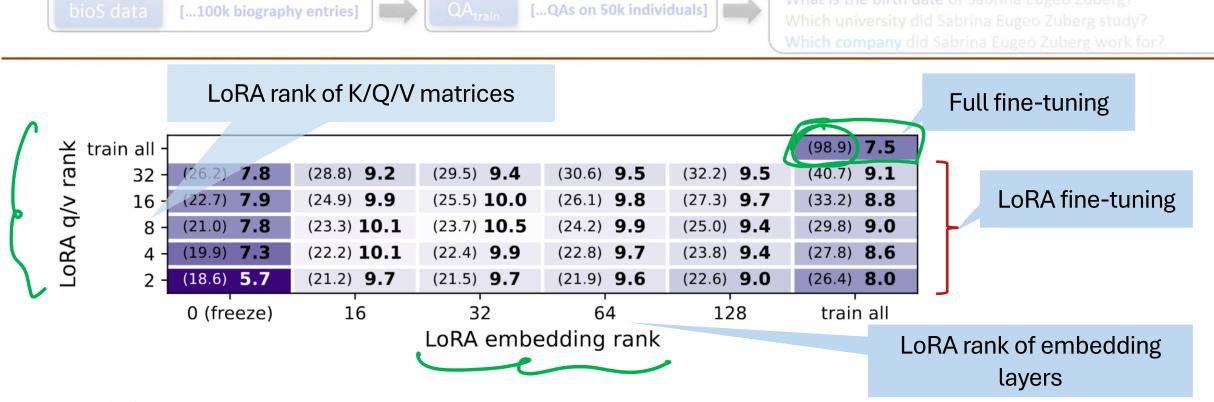
QA_{test}

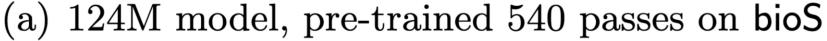
[...QAs on remaining 50k]

What is the birth date of Sabrina Eugeo Zuberg?
Which university did Sabrina Eugeo Zuberg study?
Which company did Sabrina Eugeo Zuberg work for?



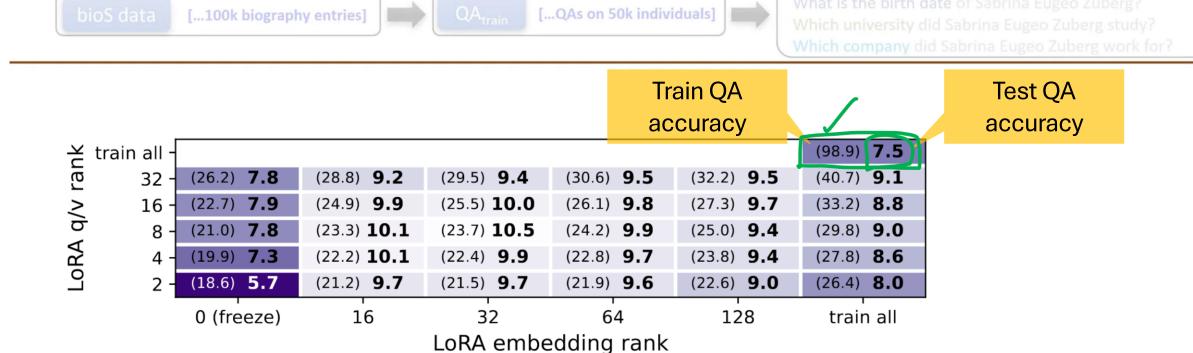












(a) 124M model, pre-trained 540 passes on bioS







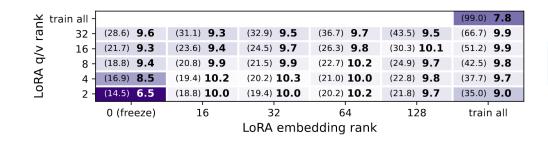
[...QAs on remaining 50k]

bioS data [...100k biography entries] QA_{train} [...QAs on 50k individuals] What is the birth date of Sabrina Eugeo Zuberg Which company did Sabrina Eugeo Zuberg

BioS data

(98.9) **7.5** (32.2) **9.5** (26.2) **7.8** (24.9) 9.9 (26.1) 9.8 (33.2) 8.8 16 -(22.7) **7.9** (21.0) **7.8** (23.3) **10.1** (23.7) **10.5** (24.2) 9.9 (25.0) 9.4 (29.8) **9.0** (22.2) **10.1** (22.4) 9.9 (22.8) 9.7 (23.8) 9.4 (27.8) **8.6** (21.2) 9.7 (21.5) **9.7** (21.9) 9.6 (22.6) 9.0 (26.4) **8.0** 32 0 (freeze) 16 64 128 train all LoRA embedding rank

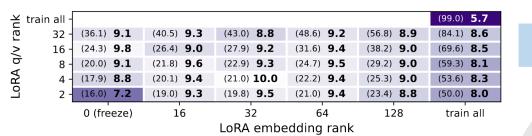
BioR data



~300 M params

- (a) 124M model, pre-trained 540 passes on bioS
- (b) 302M model, pre-trained 1000 passes on bioR

쑫 tra	ain all -						(99.0) 4.4			
ā	32 - 16 -	(34.5) 9.8	(40.4) 10.0	(42.4) 10.3	(46.5) 9.8	(54.9) 9.5	(78.4) 9.6			
∧⁄b		(27.2) 10.0	(30.0) 10.5	(31.1) 10.5	(32.5) 10.2	(37.2) 10.1	(60.6) 9.8			
	8 -	(23.3) 10.3	(25.5) 10.7	(26.1) 10.5	(18.8) 6.7	(29.8) 10.2	(49.7) 9.6			
LoRA	4 -	(21.4) 10.4	(23.1) 10.8	(23.6) 10.6	(24.4) 10.5	(26.4) 10.3	(44.2) 9.6			
2	2 -	(20.0) 10.4	(21.8) 11.0	(22.2) 10.8	(23.1) 10.4	(16.3) 6.5	(40.7) 9.3			
	,	0 (freeze)	16	32	64	128	train all			
	LoRA embedding rank									



~700 M params

- (c) 682M model, pre-trained 1350 passes on bioS
- (d) 682M model, pre-trained 1350 passes on bioR



bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

..

Sabrina Eugeo Zuberg came into this world on September 7, 1991...

[...100k biography entries]

Data augmentation!

Multiplicity:

Permutation:

Fullname:





bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

.

Sabrina Eugeo Zuberg came into this world on September 7, 1991...

[...100k biography entries]

Data augmentation!

Multiplicity:

Create M distinct biographical entries per individual

Permutation:

Fullname:





bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

.

Sabrina Eugeo Zuberg came into this world on September 7, 1991...

[...100k biography entries]

Data augmentation!

Multiplicity:

Create M distinct biographical entries per individual

Anya Briar Forger came into this world on October 2, 1996. She originated from Princeton, NJ. She pursued advanced coursework at MIT. She dedicated her studies to Communications. She developed her career at Meta Platforms. She gained work experience in Menlo Park, CA.

Permutation:

Fullname:







bioS data

Anya Briar Forger was born on October 2, 1996. She spent her early years in Princeton, NJ. She received mentorship and guidance from faculty members at MIT. She completed her education with a focus on Communications. She had a professional role at Meta Platforms. She was employed in Menlo Park, CA.

Sabrina Eugeo Zuberg came into this world on September 7, 1991...

[...100k biography entries]

Data augmentation!

Multiplicity:

Create M distinct biographical entries per individual

 Anya Briar Forger came into this world on October 2, 1996. She originated from Princeton, NJ. She pursued advanced coursework at MIT. She dedicated her studies to Communications. She developed her career at Meta Platforms. She gained work experience in Menlo Park, CA.

Permutation:

Randomly permute the sentences (*P times*)

Anya Briar Forger originated from Princeton, NJ. She dedicated her studies to Communications. She gained work
experience in Menlo Park, CA. She developed her career at Meta Platforms. She came into this world on October 2,
1996. She pursued advanced coursework at MIT.

Fullname:

Replace pro-nouns with full names

 Anya Briar Forger originated from Princeton, NJ. Anya Briar Forger dedicated her studies to Communications. Anya Briar Forger gained work experience in Menlo Park, CA. Anya Briar Forger developed her career at Meta Platforms.
 Anya Briar Forger came into this world on October 2, 1996. Anya Briar Forger pursued advanced coursework at MIT.

Original dataset

5 permutations

5 paraphrases *without* permutation

5 paraphrases with random permute

```
baseline
bioS single
bioS single
                      + fullname
bioS single + permute1
bioS single + permute2
bioS single + permute5
bioS single + permute1 + fullname
bioS single + permute2 + fullname
bioS single + permute5 + fullname
bioS multi2
bioS multi2
                      + fullname
bioS multi2 + permute
bioS multi2 + permute + fullname
bioS multi5
bioS multi5
                      + fullname
bioS multi5 + permute
bioS multi5 + permute + fullname
```

Multiplicity:

Create M distinct biographical entries per individual

Permutation:

Randomly permute the sentences (P times)

Fullname:

Replace pro-nouns with full names







Original dataset

5 permutations

5 paraphrases *without* permutation

5 paraphrases with random permute

```
baseline
bioS single
                      + fullname
bioS single
bioS single + permute1
bioS single + permute2
                                    70.0
bioS single + permute5
bioS single + permute1 + fullname
bioS single + permute2 + fullname
                                   73.1
bioS single + permute5 + fullname - 80.2
bioS multi2
                                   84.0
bioS multi2
                       + fullname
bioS multi2 + permute
                                   96.1
bioS multi2 + permute + fullname
bioS multi5
bioS multi5
                       + fullname
bioS multi5 + permute
bioS multi5 + permute + fullname + 96.
```

Multiplicity:

Create M distinct biographical entries per individual

Permutation:

Randomly permute the sentences (P times)

Fullname:

Replace pro-nouns with full names







Original dataset

5 permutations

5 paraphrases *without* permutation

5 paraphrases with random permute

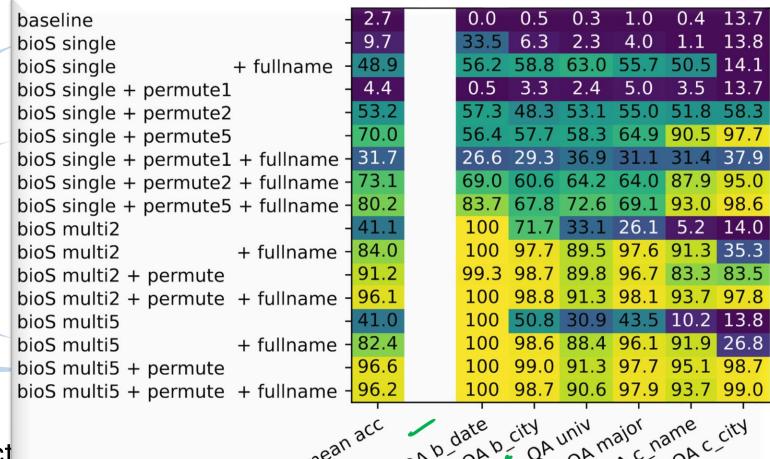
Multiplicity:

Create M distinct

Permutation: Randomly permute the sentences (*P times*)

Fullname:

Replace pro-nouns with full names



The state of the s



Pretrain: biography of N individuals

Anya Briar Forger was born on <u>October 2, 1996</u>. She spent her early years in <u>Princeton, NJ</u>. She received mentorship and guidance from faculty members at <u>MIT</u>. She completed her education with a focus on <u>Communications</u>. She had a professional role at <u>Meta Platforms</u>. She was employed in <u>Menlo Park, CA</u>.

99+% train acc **Pretrain + Finetune** ⇒ Knowledge Extraction

A universal law: failure example holds *regardless* of model size, architecture choice, data size, training parameters, finetune method, etc.



Instruct Finetune: QAs on N/2

What is the birth date of Anya Briar Forger?

Answer: October 2, 1996.

Which university did Anya Briar Forger study?

Answer: MIT.

Which company did Anya Briar Forger work for?

Answer: Meta Platforms.

99+% train acc

out-of-distribution (OOD) evaluation



Evaluate: QAs on **remaining** N/2

What is the birth date of [name]?
Which university did [name] study?
Which company did [name] work for?

~0% test acc

Pretrain (knowledge augmented) ⇒ Knowledge Extraction

Knowledge augmentations include:

- add sentence diversity
- add sentence permutation
- add repetition (e.g., repeating names)
- translation (e.g., English → French)
- rewrite by small models (e.g., Llama-7B)

~0% test acc



96+% test acc

It is absolutely necessary to knowledge augment the pretrain data; doing this at the finetune stage is too late.

But why does this happen? See Results 4-5.

bioS data [...100k biography entries] QA_{train} [...QAs on 50k individuals]

UA_{test} [...QAs on remaining 50k]
What is the birth date of Sabrina Eugeo Zuberg?
Which university did Sabrina Eugeo Zuberg study?
Which company did Sabrina Eugeo Zuberg work for?

baseline	- 2.7	0.0	0.5	0.3	1.0	0.4	13.7
bioS single	- 9.7	33.5	6.3	2.3	4.0	1.1	13.8
bioS single + fullname	48.9	56.2	58.8	63.0	55.7	50.5	14.1
bioS single + permute1	- 4.4	0.5	3.3	2.4	5.0	3.5	13.7
bioS single + permute2	- 53.2	57.3	48.3	53.1	55.0	51.8	58.3
bioS single + permute5	- 70.0	56.4	57.7	58.3	64.9	90.5	97.7
bioS single + permute1 + fullname	- 31.7	26.6	29.3	36.9	31.1	31.4	37.9
bioS single + permute2 + fullname		69.0	60.6	64.2	64.0	87.9	95.0
bioS single + permute5 + fullname	Company of the Compan	83.7	67.8	72.6	69.1	93.0	98.6
	41.1	100	71.7	33.1	26.1	5.2	14.0
bioS multi2 + fullname	84.0	100	97.7	89.5	97.6	91.3	35.3
bioS multi2 + permute	91.2	99.3	98.7	89.8	96.7	83.3	83.5
bioS multi2 + permute + fullname	96.1	100	98.8	91.3	98.1	93.7	97.8
bioS multi5	41.0	100	50.8	30.9	43.5	10.2	13.8
bioS multi5 + fullname	82.4	100	98.6	88.4	96.1	91.9	26.8
bioS multi5 + permute	96.6	100	99.0	91.3	97.7	95.1	98.7
bioS multi5 + permute + fullname	- 96.2	100	98.7	90.6	97.9	93.7	99.0
		- 0	1	1.1	1	-	1
0.1	acc,	daten	CIEN ,	74/10	ajo, ve	3WE	CIEA
OA mear	'AD	o date	ar	OF!	AC)	OP	

- Augmenting the pre-training data is impacting QA performance!
- Knowledge must be stored differently
- Why is augmentation helping?
- Can we answer it via probing?





bioS data [...100k biography entries] QA_{train} [...QAs on 50k individuals]

(...QAs on

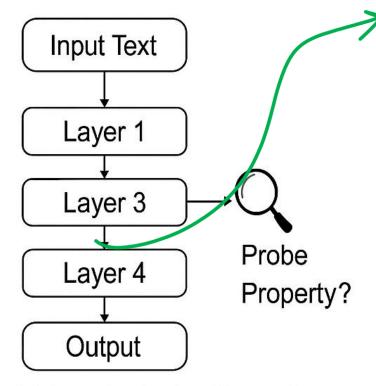
[...QAs on remaining 50k]

What is the birth date of Sabrina Eugeo Zuberg?
Which university did Sabrina Eugeo Zuberg study?
Which company did Sabrina Eugeo Zuberg work for?





What is probing in LLMs?



Train a simple classifier on frozen layer activations.

Goal: To diagnose what information is encoded inside the model.

How: Freeze model parameters

 Train a lightweight classifier (probe) on hidden activations

Interpretation: If probe predicts property well → model encodes it.

Reveals where and how knowledge/ structure is stored.

Probing = Measuring what the model knows, without changing it.



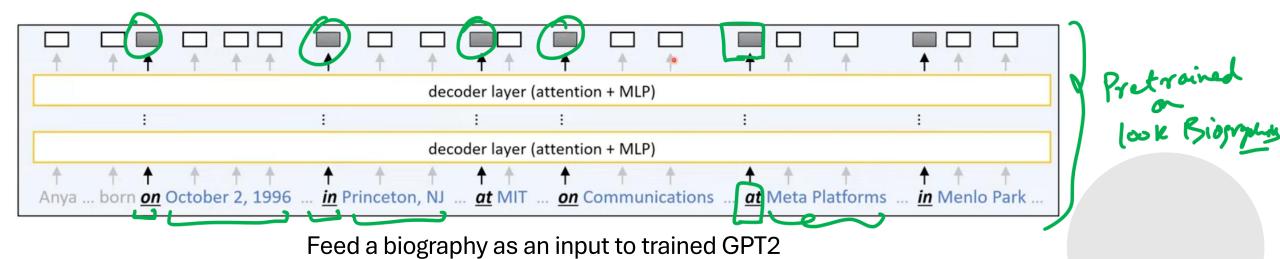




Replace with a probe training phase

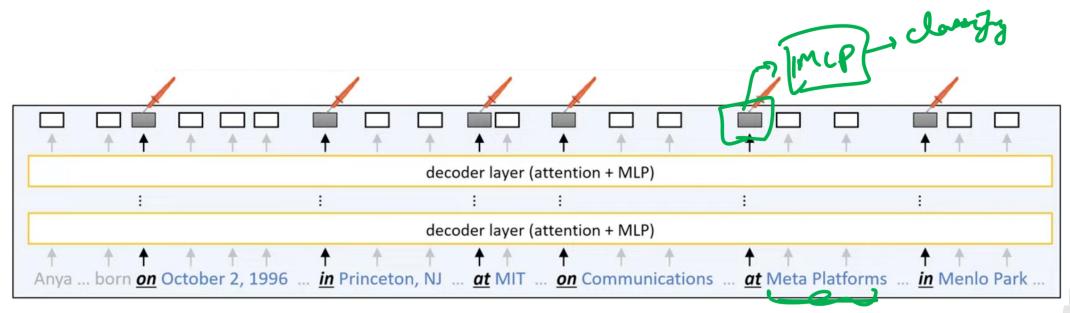












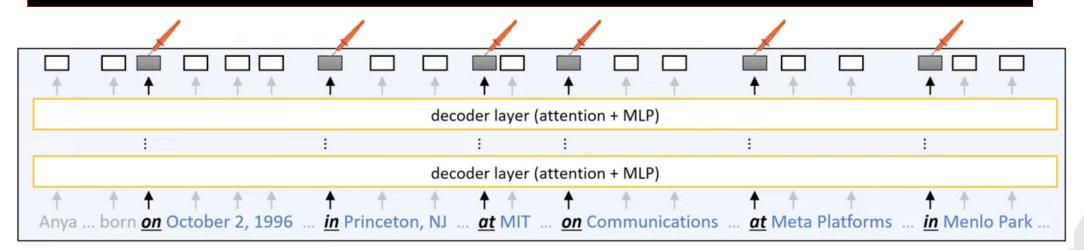
Feed a biography as an input to trained GPT2







Linear classifiers to predict 6 possible knowledges (total of 6x6 classification tasks)

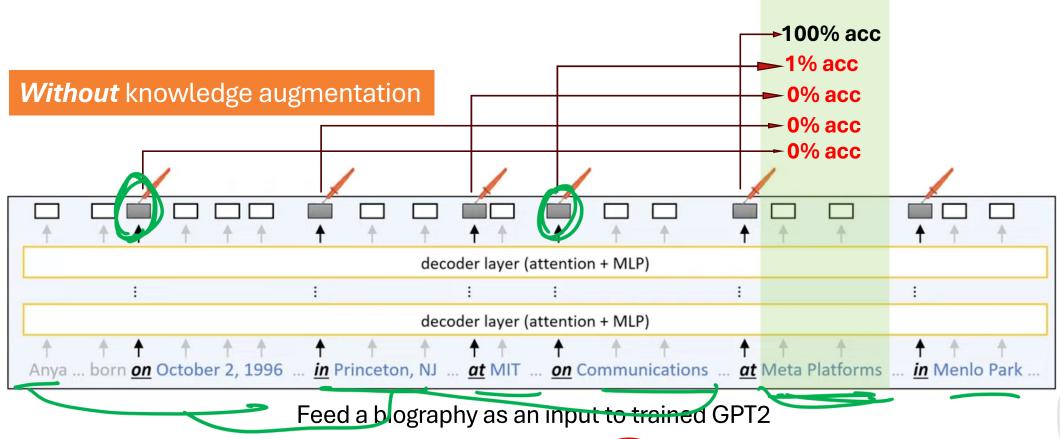


Feed a biography as an input to trained GPT2



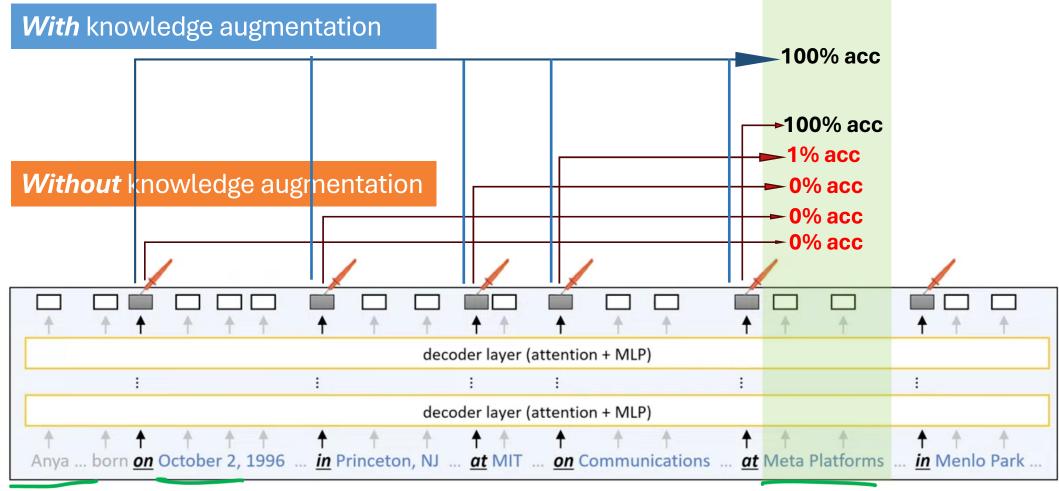




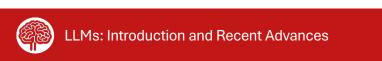






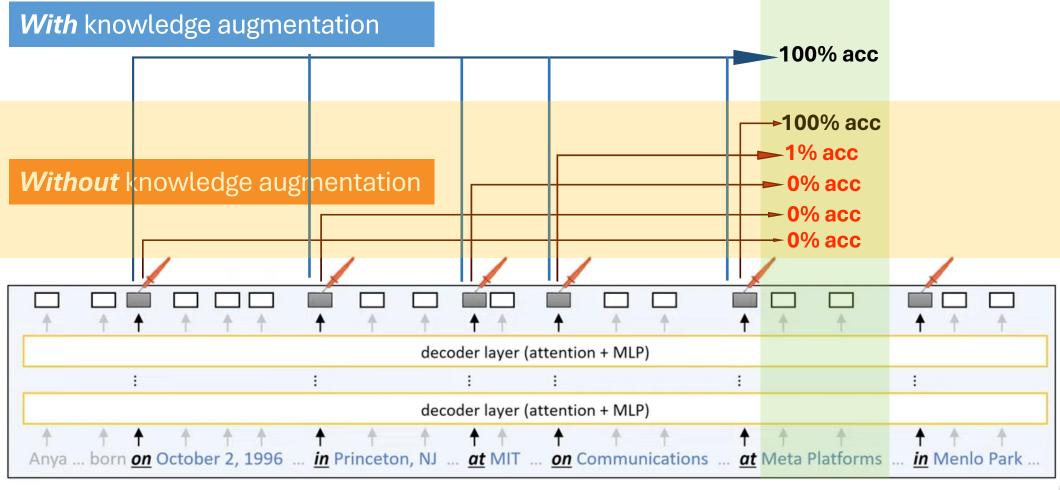


Feed a biography as an input to trained GPT2

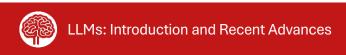






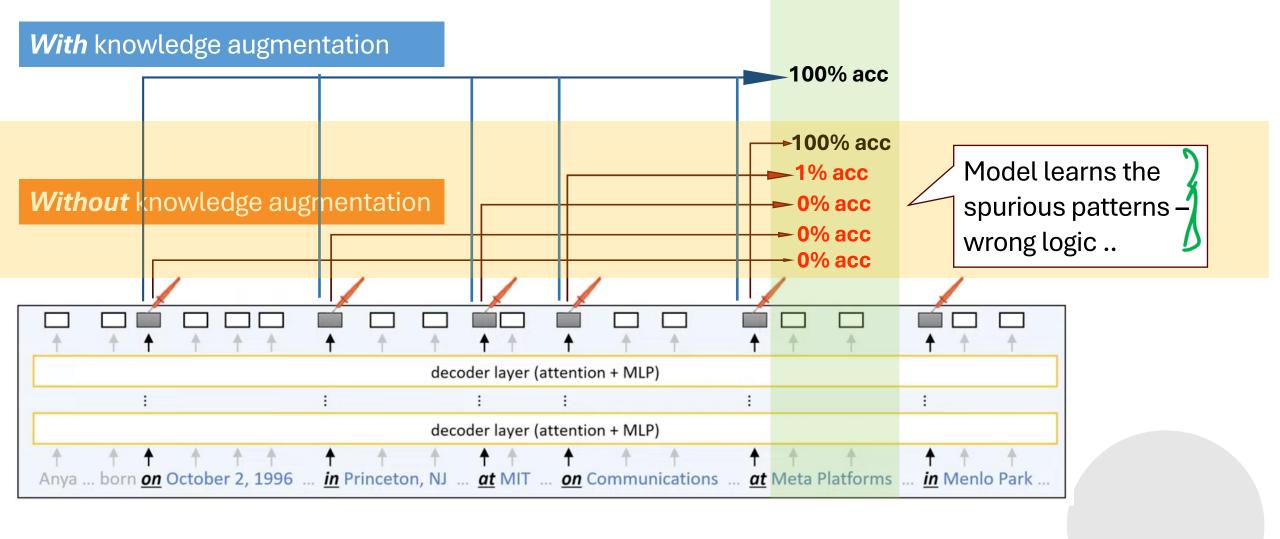


Feed a biography as an input to trained GPT2



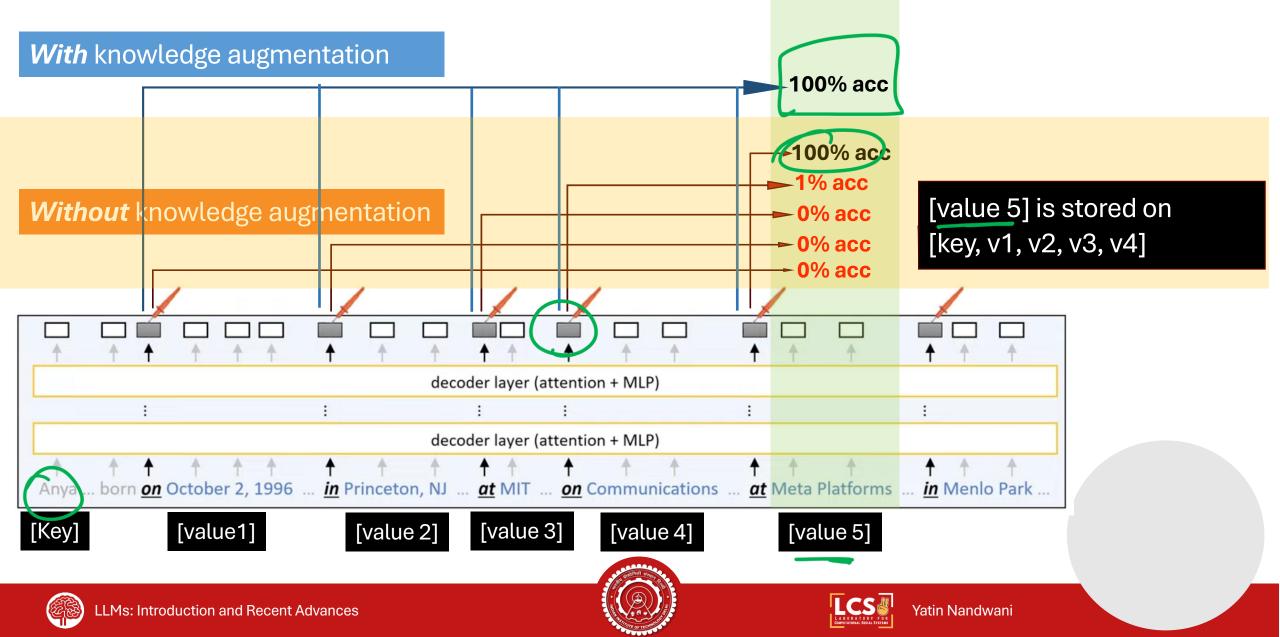


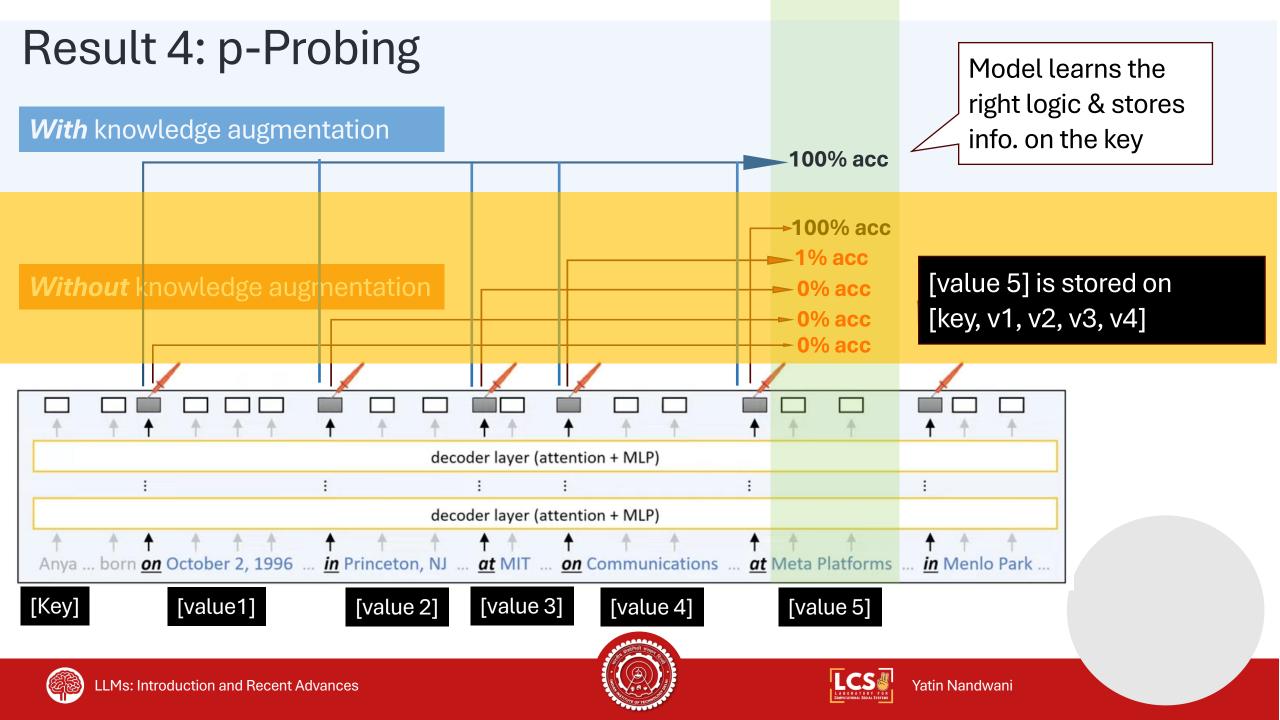


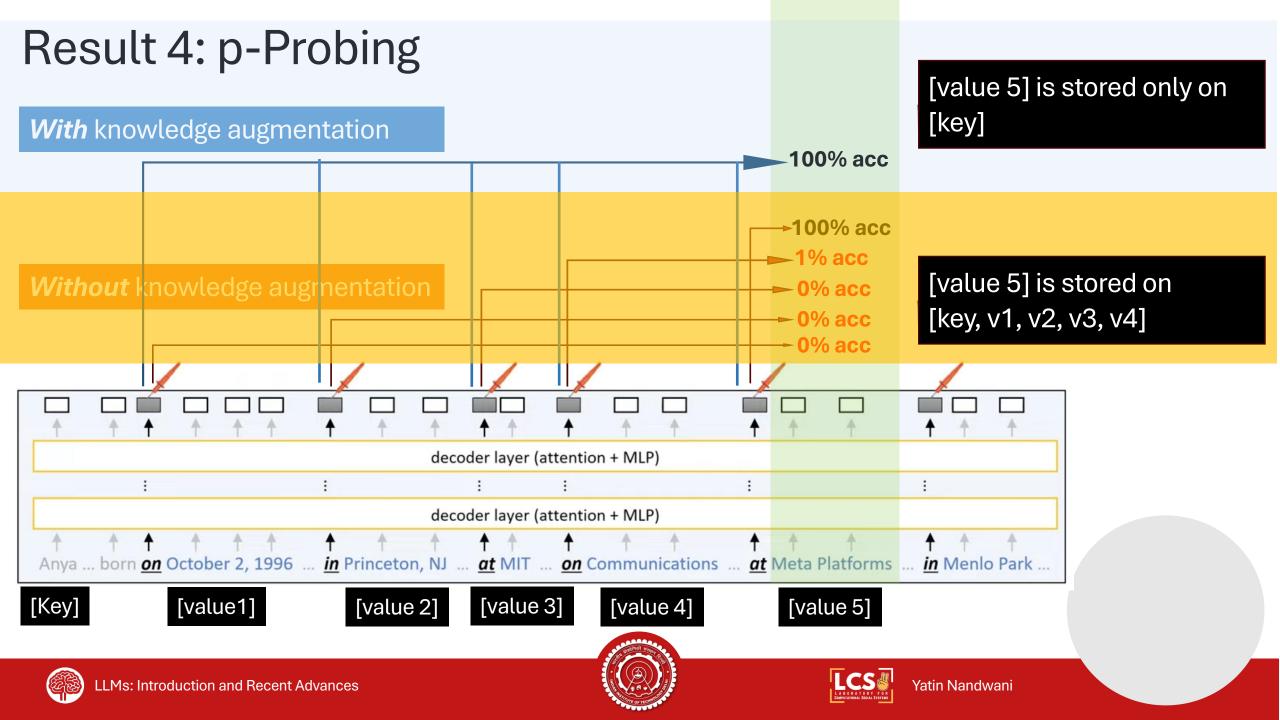


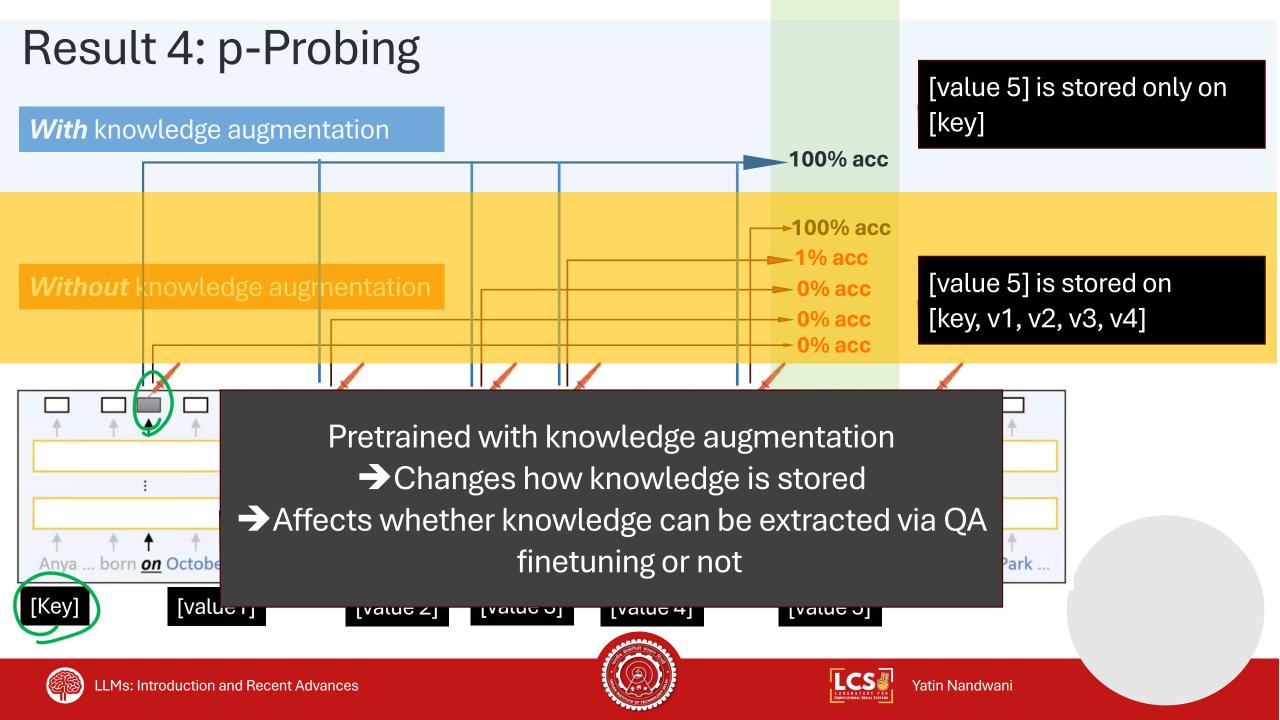




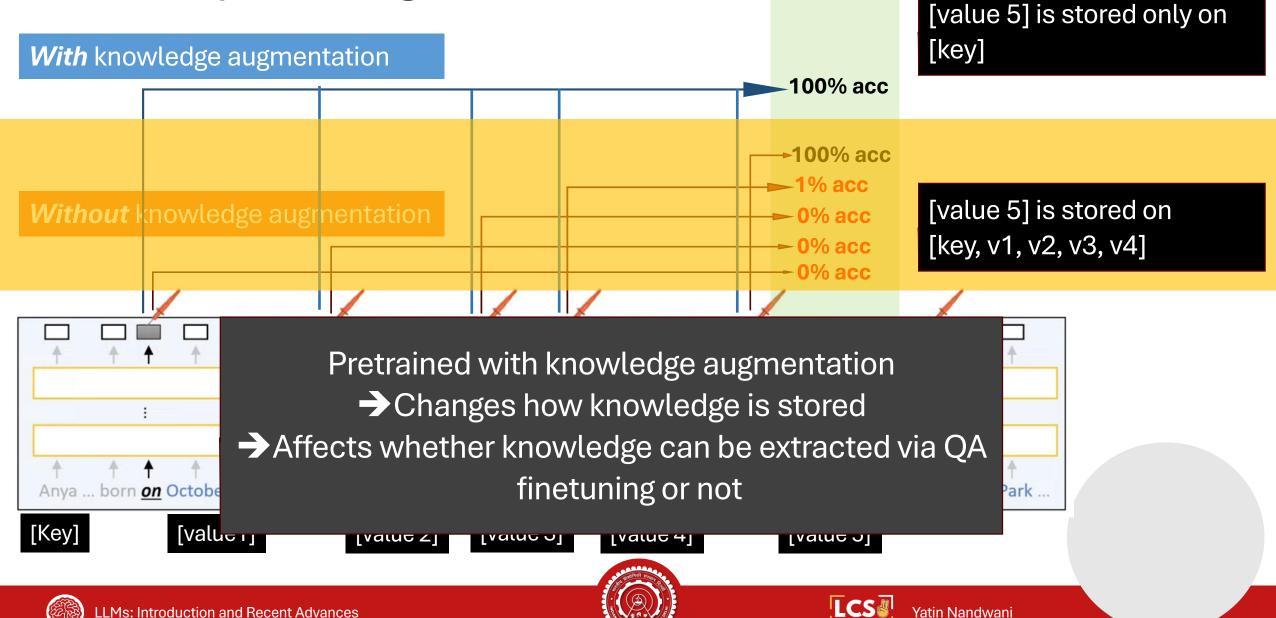








Result 4: p-Probing



Result 4: p-Probing

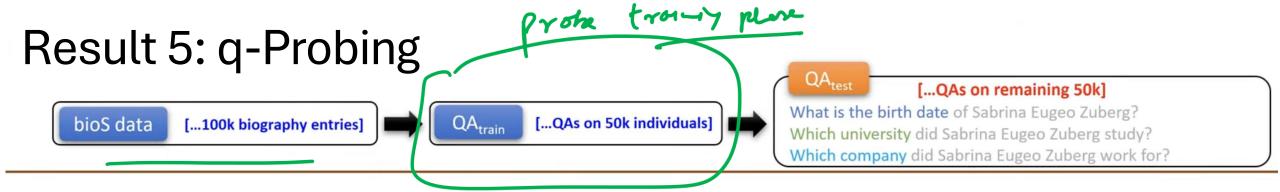
 We claim that for extraction of knowledge, the information must be stored directly on the name

Can we test this directly?

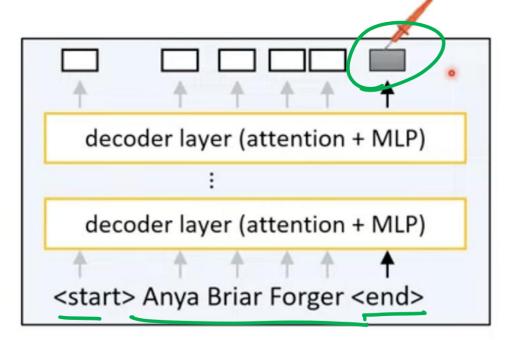
Let's design a probe on the name.







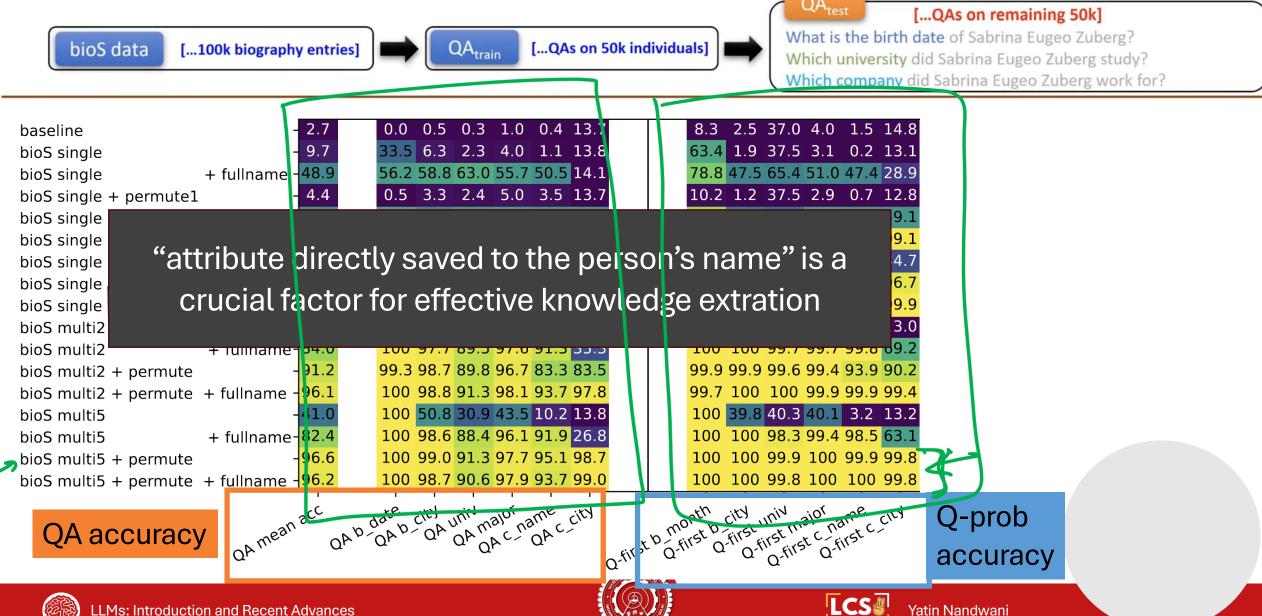
Linear classifier to predict 6 possible knowledges







Result 5: q-Probing



Sum up



knowledge augmented in pretrain data



attribute is nearly entirely stored on person's names (after pretrain)



knowledge can be extracted (after instruct finetune)

no knowledge augmentation in pretrain data



attribute is **not** entirely stored on person's names (after pretrain)



knowledge cannot be extracted (after instruct finetune)

Do we have to augment all biographies?







pretrain

bioS data

[100k minority biography entries, non-augmented]

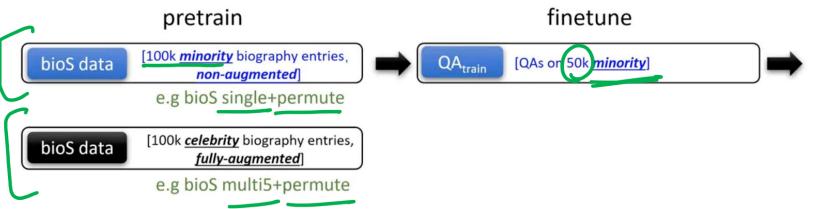
e.g bioS single+permute

bioS data

[100k <u>celebrity</u> biography entries, fully-augmented]

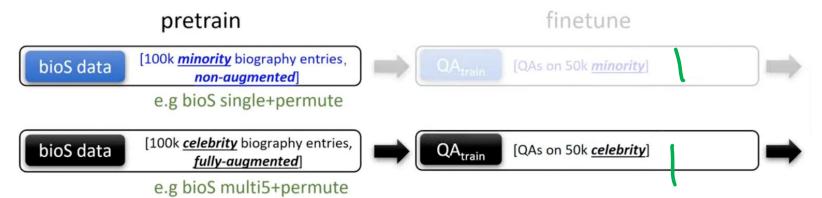
e.g bioS multi5+permute













pretrain finetune [100k minority biography entries, bioS data [QAs on 50k minority] [QAs on 50k remaining *minority*] non-augmented What is the birth date of Sabrina Eugeo Zuberg? e.g bioS single+permute Which university did Sabrina Eugeo Zuberg study? Which company did Sabrina Eugeo Zuberg work for? [100k celebrity biography entries, bioS data QA_{train} [QAs on 50k celebrity] fully-augmented

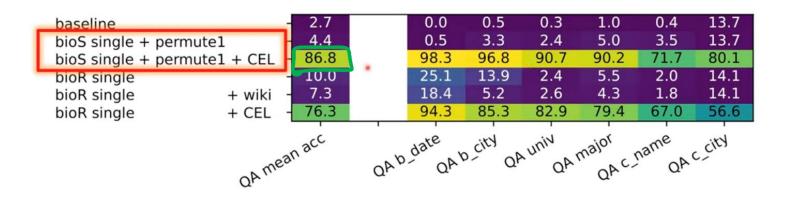




e.g bioS multi5+permute

pretrain











0.3 1.0 13.7 baseline 0.0 0.4 4.4 0.5 3.3 2.4 5.0 13.7 bioS single + permute1 86.8 98.3 96.8 90.7 90.2 71.7 80.1 bioS single + permute1 + CEL 10.0 25.1 13.9 2.4 5.5 2.0 14.1 bioR single 7.3 4.3 14.1 + wiki 18.4 5.2 2.6 1.8 bioR single 76.3 85.3 82.9 56.6 94.3 bioR single + CEL QA mean acc QAb date QAb city QA univ QA major Chame QAC city





Pretrain: biography of *N minorities*

Anya Briar Forger was born on ...

without knowledge augmentation (e.g., one entry per person)



Pretrain: biography of *M celebrities*

Joseph Robinette Biden is an American politician ...

with knowledge augmentation (e.g., 5 entries per person + sentence diversity and permutations)

Finetune: QAs on M/2 celebrities

What is the birth date of Joseph Robinette Biden? Answer: November 20, 1942. ...

Knowledge augmentation on $celebrity \Rightarrow$ Knowledge extraction for minority

Even if knowledge augmentation is applied to a subset of individuals, what we call celebrities, test accuracy for others also increases.

The mere inclusion of celebrity data (e.g., people with plentiful online biographical data of diverse writing styles) in pre-training enhances the model's knowledge extraction for minorities.



Evaluate: QAs on N minorities

What is the birth date of Anya Briar Forger?

~80% test acc





knowledge storage

100% word-by-word memorization (biography)

knowledge extraction

QA: What's the birthdate of Anya?





knowledge storage

100% word-by-word memorization (biography)



knowledge extraction

QA: What's the birthdate of Anya?

mixed training (BIO+QA)

"add instruct-finetune data to pretrain"











knowledge storage



knowledge extraction

100% word-by-word memorization (biography)

QA: What's the birthdate of Anya?

mixed training (BIO+QA)

"add instruct-finetune data to pretrain"



pretrain (BIO) + finetune (QA)



without knowledge augment



knowledge augmentation (sufficient on the celebrities)







knowledge storage

2

knowledge extraction

QA: What's the birthdate of Anya?

100% word-by-word memorization (biography)

mixed training (BIO+QA)

"add instruct-finetune data to pretrain"



pretrain (BIO) + finetune (QA)



without knowledge augment



knowledge augmentation (sufficient on the celebrities)

bi-directional model (BERT, DeBERTa)



even with mixed training

+ knowledge augment







Physics of Language Models: Part 3.1 Knowledge Storage and Extraction

Result 1

mixed training ⇒ knowledge extraction

mixed training means "add instruct-finetune data to pretrain stage"

Result 2-3

instruct finetune ⇒ knowledge extraction

unless pretrain data is augmented (e.g. diversified writing styles)

Result 4-5

two probing techniques to explain why this happens

can detect how and where knowledge is stored in an LLM

Result 6

knowledge on "celebrity" helps "minority"

augmenting pretrain data for some knowledge helps others







Physics of Language Models: Part 3.1 Knowledge Storage and Extraction

Result 1

<u>mixed training</u> ⇒ <u>knowledge extraction</u>
mixed training means "add instruct-finetune data to pretrain stage"

Result 2-3

instruct finetune ⇒ knowledge extraction
unless pretrain data is augmented (e.g. diversified writing styles)

Result 4-5

two probing techniques to explain why this happens can detect how and where knowledge is stored in an LLM

Result 6

knowledge on "celebrity" helps "minority" augmenting pretrain data for some knowledge helps others

Result 7

encoder models like BERT ⇒ knowledge extraction discover and explain why this happens







Incorrectly C: The model can't D: Model doesn't E: Model can know what "even" extract birth year, extract the birth year of Sachin knows what is means even, still can't answer C1: model didn't C2: model didn't C3: model can see Sachin's finetune enough extract b'days of biography during Sehwag but not to extract birthdays Sachin training

Part 3.1: Knowledge Storage and Extraction





Incorrectly

C: The model can't extract the birth year of Sachin

D: Model doesn't know what "even" means

E: Model can
extract birth year,
knows what is
even, still can't
answer

Let us assume that model can extract knowledge

C1: model didn't see Sachin's biography during training

C2: model didn't finetune enough to extract birthdays

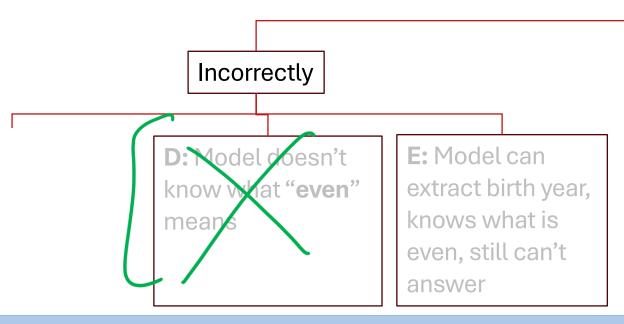
C3: model can extract b'days of Sehwag but not Sachin

Part 3.1: Knowledge Storage and Extraction







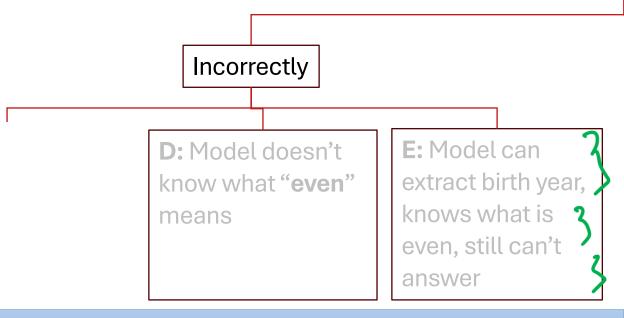


Let us assume that model can extract knowledge

How good the model is in *manipulating this knowledge?*







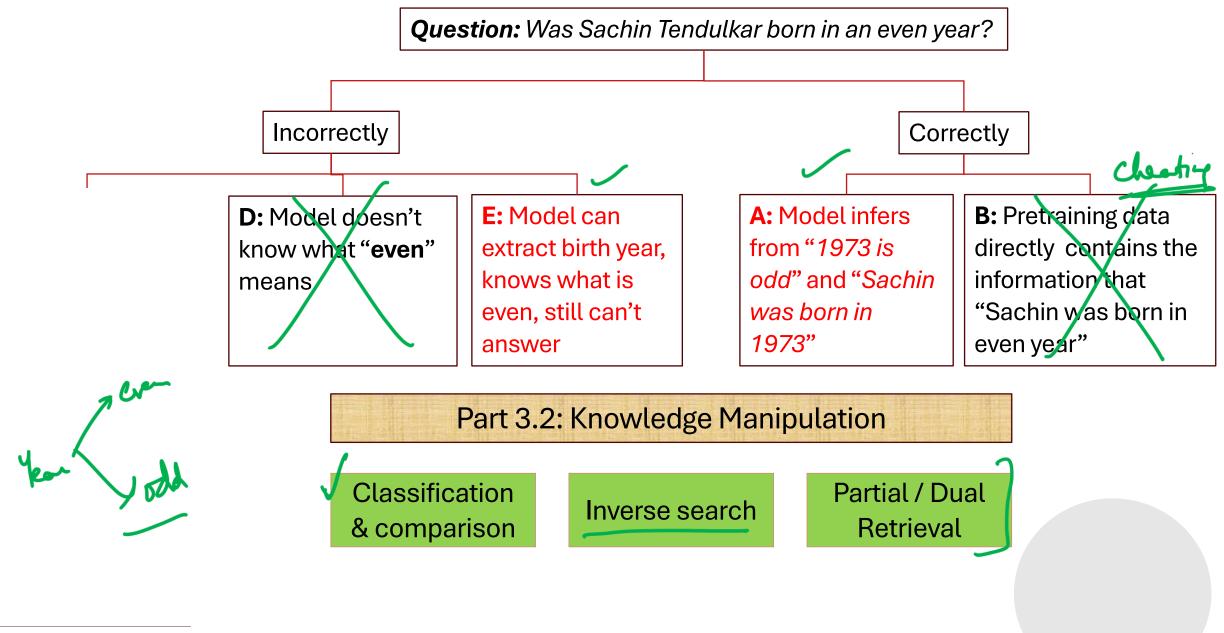
Let us assume that model can extract knowledge

How good the model is in *manipulating this knowledge*?

e.g. to answer this question, model has to 1st extract birth date and then do *classification* into even and odd













Physics of Language Models: Part 3.2 Knowledge Manipulation

Results 1-2

knowledge partial / dual retrievals may be difficult

model can say birthday "October 2, 1996" but not "1996"

Results 3-5

knowledge classification / comparison is hard without CoT

model cannot say "even year" without saying "1996" (CoT)

Result 7

knowledge inverse search is impossible impossible to answer "who was born on October 2, 1996"

Results 6/8/9

Turing tests to distinguish Humans from contemporary Als universal counter-examples, applicable to GPT-4 and others









