STAT 453: Introduction to Deep Learning and Generative Models

Ben Lengerich

Lecture 22: Unsupervised training of LLMs

November 19, 2025

Reading: See course homepage

Today

- HW4 due this Friday
- [Project Presentation Sign-up]
  - **4 minute presentations!**
- Final Exam
  - December 17^{th}, 5:05-7:05PM
  - **Science 180**

Today

- Unsupervised training of LLMs
  - Emergent Capabilities
  - Challenges of MLE-based unsupervised training

Last Time: From GPT-1 to GPT-4

- **Architecture:**
  - **Scale:** Variety of options, with biggest (1.5B params → >1T params):
    - Block size (max context): 512 → 128k
    - Layers: 12 → >96
    - Attention Heads: 12 → >96
    - Embedding Dim: 768 → >12,288
    - Vocab: 40k → >50k tokens
  - Tokenizer: Includes image patches for multimodal
  - **Mixture-of-Experts**
- **Training:**
  - Dataset: BookCorpus (5GB) → Private 13T tokens (~50TB)
  - Reinforcement learning for alignment

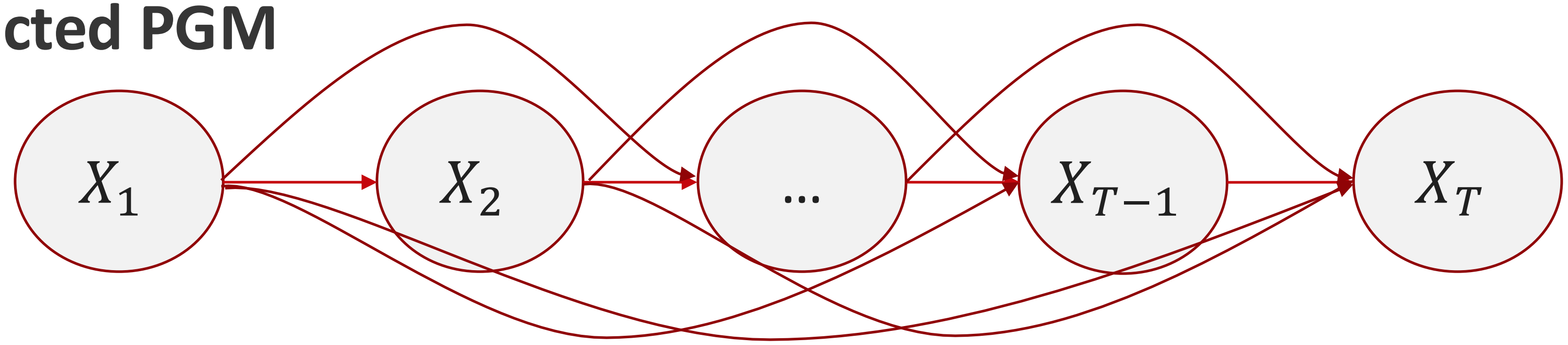
Today: Unsupervised Training of LLMs

- **Architecture:**
  - **Scale:** Variety of options, with biggest (1.5B params → >1T params):
    - Block size (max context): 512 → 128k
    - Layers: 12 → >96
    - Attention Heads: 12 → >96
    - Embedding Dim: 768 → >12,288
    - Vocab: 40k → >50k tokens
  - Tokenizer: Includes image patches for multimodal
  - **Mixture-of-Experts**
- **Training:**
  - Dataset: BookCorpus (5GB) → Private 13T tokens (~50TB)
  - Reinforcement learning for alignment

Unsupervised Training of LLMs

Recall GPT training objective: MLE

- **Directed PGM**



$$P_\theta(X) = \prod_i \prod_t P_\theta(X_{i,t} \mid X_{i,<t})$$

- **Probabilistic objective:** Max log-likelihood of observed seqs

$$\max_\theta \sum_i \sum_t \log P_\theta\left(X_{i,t} \mid X_{i,<t} \right)$$

[Radford et al., Improving Language Understanding by Generative Pre-Training]

We’ve had MLE-based Language Models for a while…

Large Language Models in Machine Translation **2007**

Thorstern Brants **Ashok C. Popat** **Peng Xu** **Franz J. Och** **Jeffrey Dean**

Google, Inc.
1600 Amphitheatre Parkway
Mountain View, CA 94303, USA
{brants,popat,xp,och,jeff}@google.com

Some fun:
https://github.com/LRitzdorf/TheJeffDeanFacts

We've had MLE-based Language Models for a while…

Large Language Models in Machine Translation 2007

…ok C. Popat Peng Xu Franz J. Och Jeffrey Dean

Google, Inc.
1600 Amphitheatre Parkway
…Mountain View, CA 94303, USA
…popat,xp,och,jeff}@google.com

This paper reports on the benefits of large-scale statistical language modeling in machine translation. A distributed infrastructure is proposed which we use to train on up to 2 trillion tokens, resulting in language models having up to 300 billion n-grams. It is capable of providing smoothed probabilities for fast, single-pass decoding. We introduce a new smoothing method, dubbed *Stupid Backoff*, that is inexpensive to train on large data sets and approaches the quality of Kneser-Ney Smoothing as the amount of training data increases.

$$P(w_1^L) = \prod_{i=1}^{L} P(w_i | w_1^{i-1}) \approx \prod_{i=1}^{L} \hat{P}(w_i | w_{i-n+1}^{i-1})$$

We've had MLE-based Language Models for a while…

Large Language Models in Machine Translation 2007

Thorsten Brants **Ashok C. Popat** **Peng Xu** **Franz J. Och** **Jeffrey Dean**

Google, Inc.
1600 Amphitheatre Parkway
Mountain View, CA 94303, USA
{brants,popat,xp,och,jeff}@google.com

- Why wasn't this the LLM moment?
  - Modeled n-grams, not *relationships* of token embeddings
  - Transformer architecture
  - Scale, GPU acceleration

MLE → Emergent Understanding?

- ”The simplest way to predict the next token is to understand what happened throughout the context.”
- To predict the word "*is*" in "*The capital of France ___ Paris.*", the model must:
  - Resolve subject-verb agreement
  - Recognize a factual structure
  - Know the topic is geography

Scale & Emergent Capabilities

What happens as we scale training?

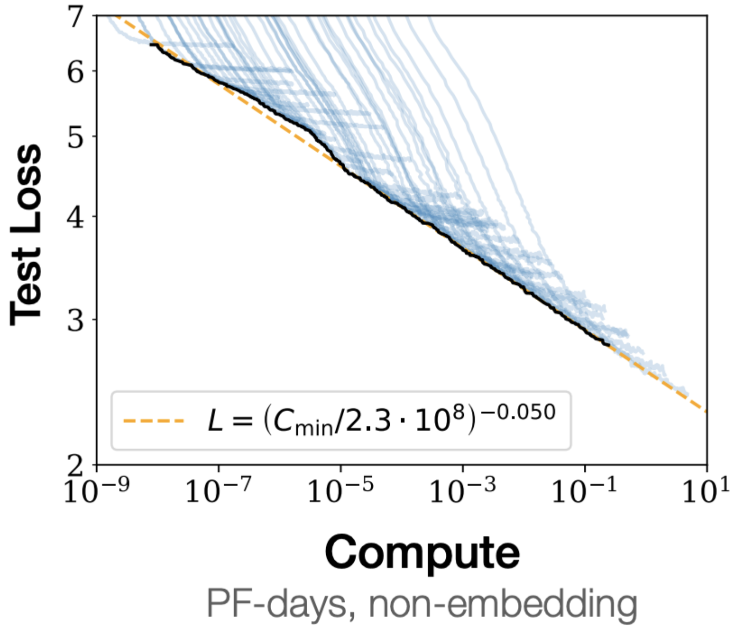


Figure 1 Language modeling performance improves smoothly as we increase the model size, datasetset size, and amount of compute[2] used for training. For optimal performance all three factors must be scaled up in tandem. Empirical performance has a power-law relationship with each individual factor when not bottlenecked by the other two.

"Scaling Laws for Neural Language Models". Kaplan et al 2021

What happens as we scale training?

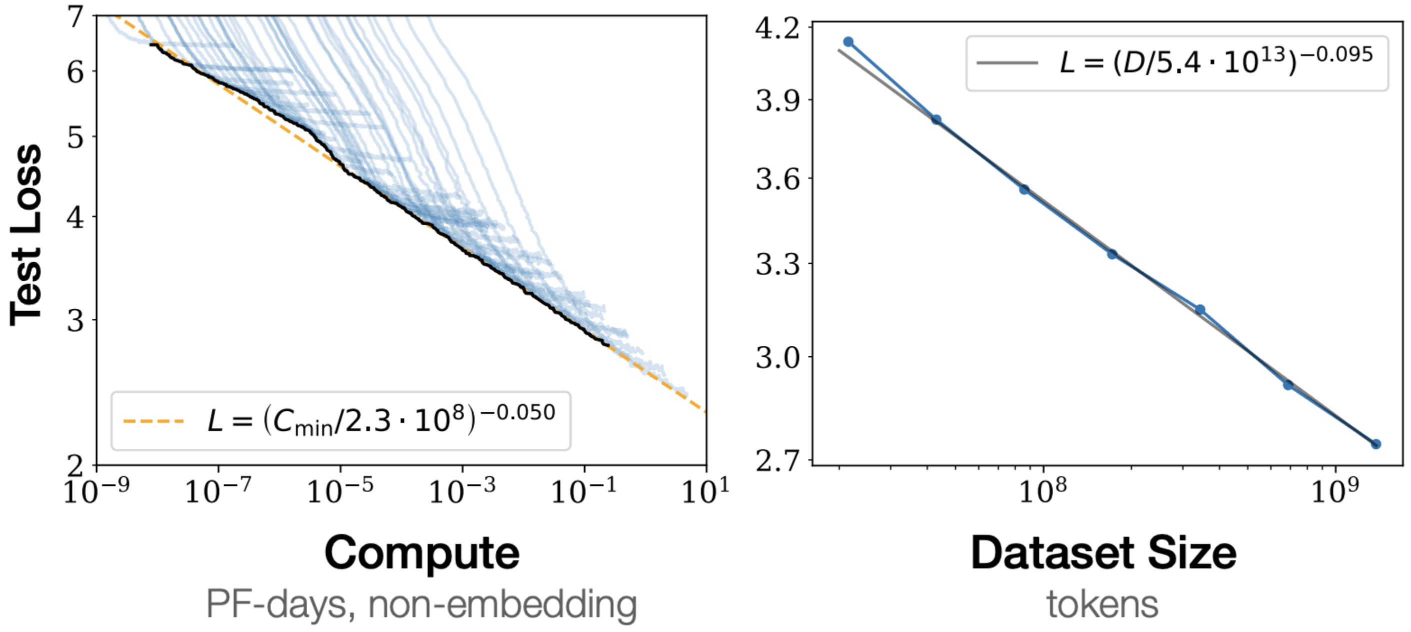


Figure 1 Language modeling performance improves smoothly as we increase the model size, datasetset size, and amount of compute[2] used for training. For optimal performance all three factors must be scaled up in tandem. Empirical performance has a power-law relationship with each individual factor when not bottlenecked by the other two.

"Scaling Laws for Neural Language Models". Kaplan et al 2021

What happens as we scale training?

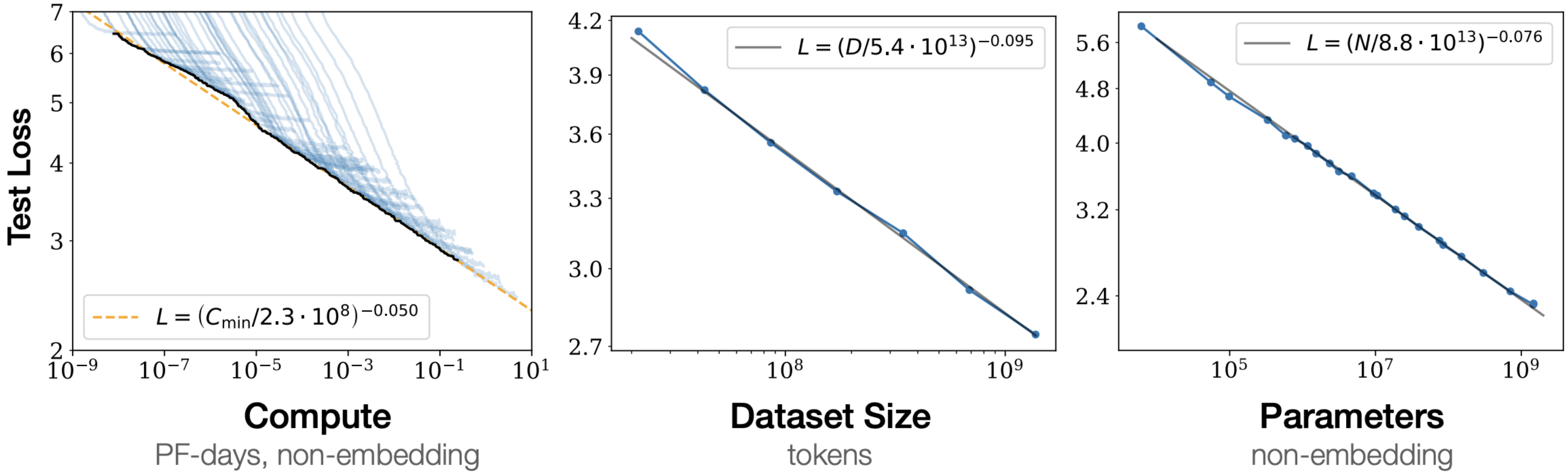
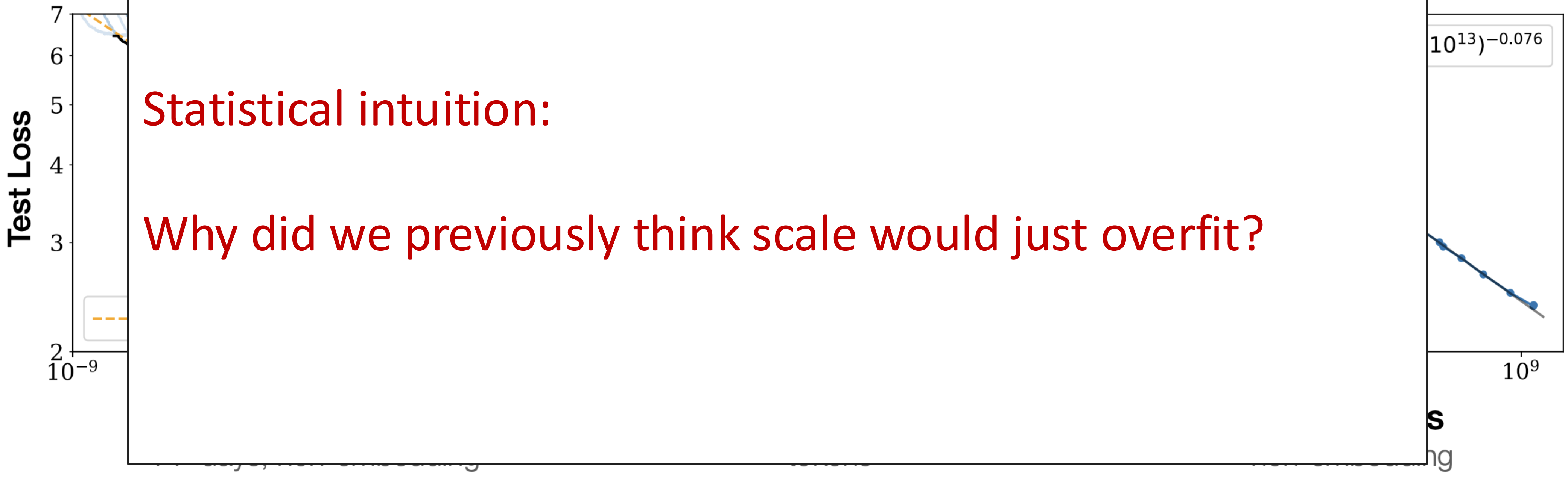


Figure 1 Language modeling performance improves smoothly as we increase the model size, datasetset size, and amount of compute[2] used for training. For optimal performance all three factors must be scaled up in tandem. Empirical performance has a power-law relationship with each individual factor when not bottlenecked by the other two.

"Scaling Laws for Neural Language Models". Kaplan et al 2021

What happens as we scale training?



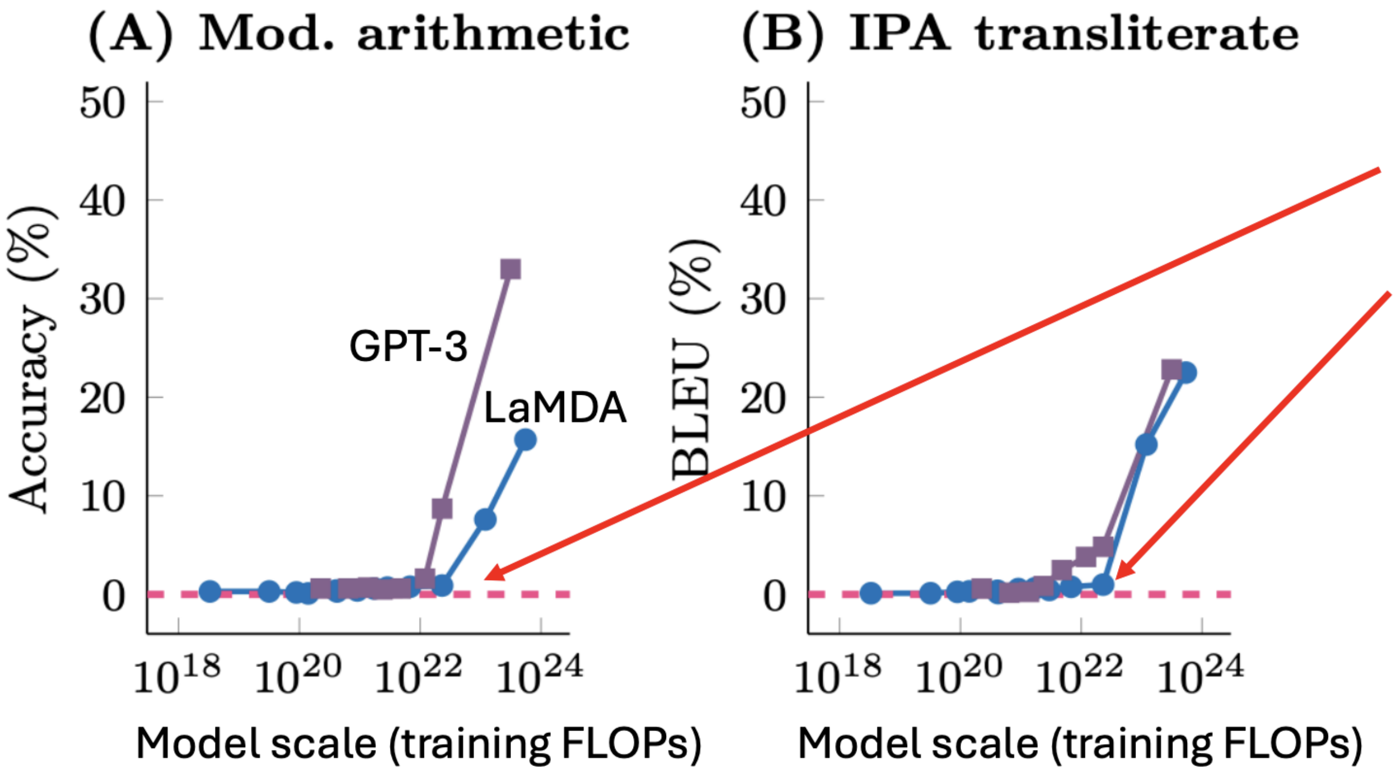
Statistical intuition:

Why did we previously think scale would just overfit?

Figure 1 Language modeling performance improves smoothly as we increase the model size, datasetset size, and amount of compute[2] used for training. For optimal performance all three factors must be scaled up in tandem. Empirical performance has a power-law relationship with each individual factor when not bottlenecked by the other two.

“Scaling Laws for Neural Language Models”. Kaplan et al 2021

Smooth improvements → sharp emergent ability?



An ability is emergent if it is not present in smaller models but is present in larger models [Wei, et al (2022). Emergent Abilities of Large Language Models

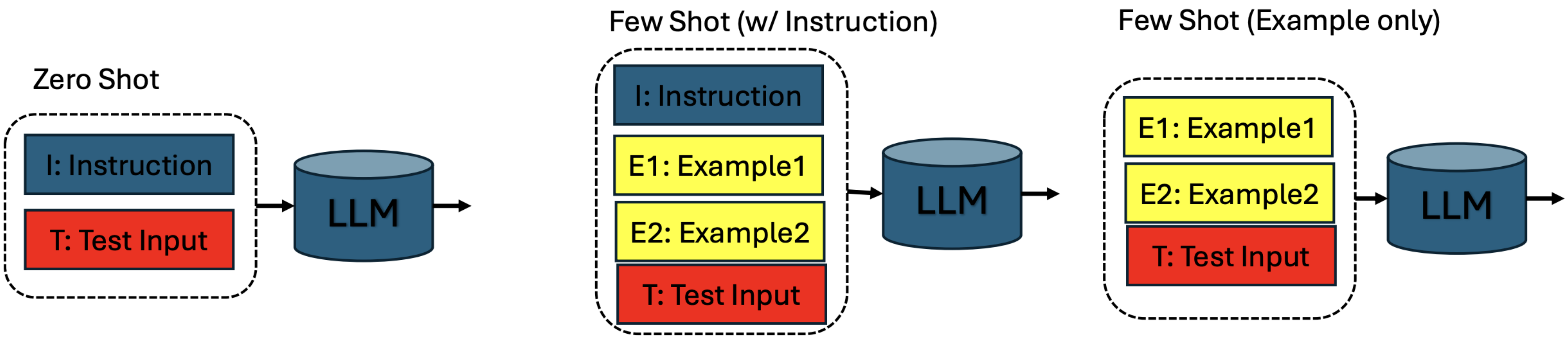
Example of emergence: In-Context Learning

I: Instruction — Translate English to French

E1: Example1 — [en]: A discomfort which lasts. [fr]: Un malaise qui dure

E2: Example2 — [en]: HTML is a language for formatting [fr]: HTML est un langage de formatage

T: Test Input — [en]: After you become comfortable with formatting [fr]:



Example of emergence: Chain-of-Thought

Standard Prompting

Model Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Output

A: The answer is 27. ✗

Chain-of-Thought Prompting

Model Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: Roger started with 5 balls. 2 cans of 3 tennis balls each is 6 tennis balls. 5 + 6 = 11. The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Output

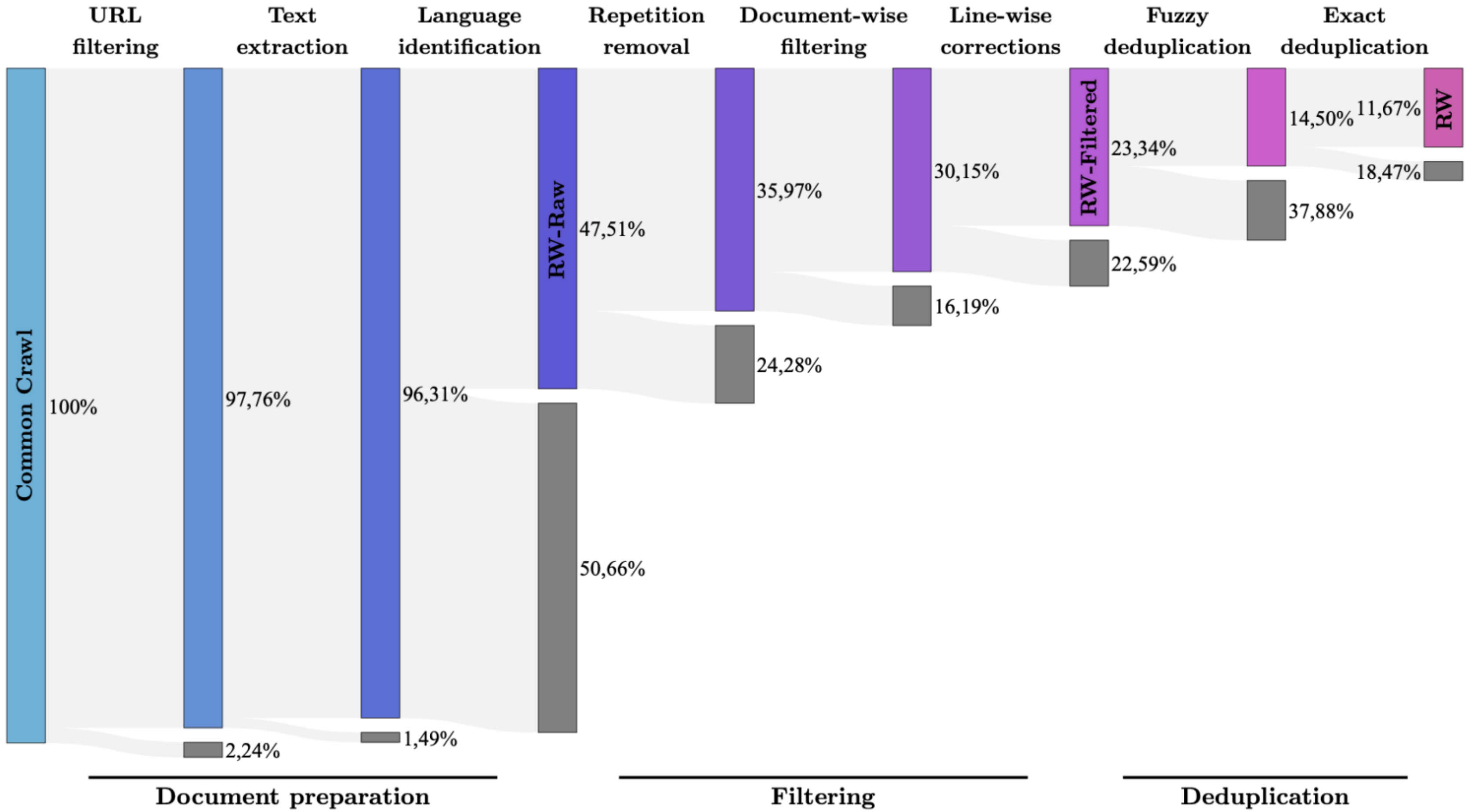
A: The cafeteria had 23 apples originally. They used 20 to make lunch. So they had 23 - 20 = 3. They bought 6 more apples, so they have 3 + 6 = 9. The answer is 9. ✓

Wei, et al. (2023) Chain-of-Though Prompting Elicits Reasoning in LLMs

Why does this work? Some hypotheses

- Task identification?
  - Xie et al. (2021). An explanation of in-context learning as implicit Bayesian inference
  - Raventos, et al. (2023). Pretraining task diversity and the emergence of non-Bayesian in-context learning for regression
- Some kind of ”learning” without model updates?
  - Akyurek, et al. (2024). In-context language learning: architectures and algorithms
  - von Oswald, et al. (2023). Transformers learn in-context by gradient descent
- Both?
  - Pan, et al. (2023). What in-context learning ”learns” in-context: disentangling task recognition and task learning

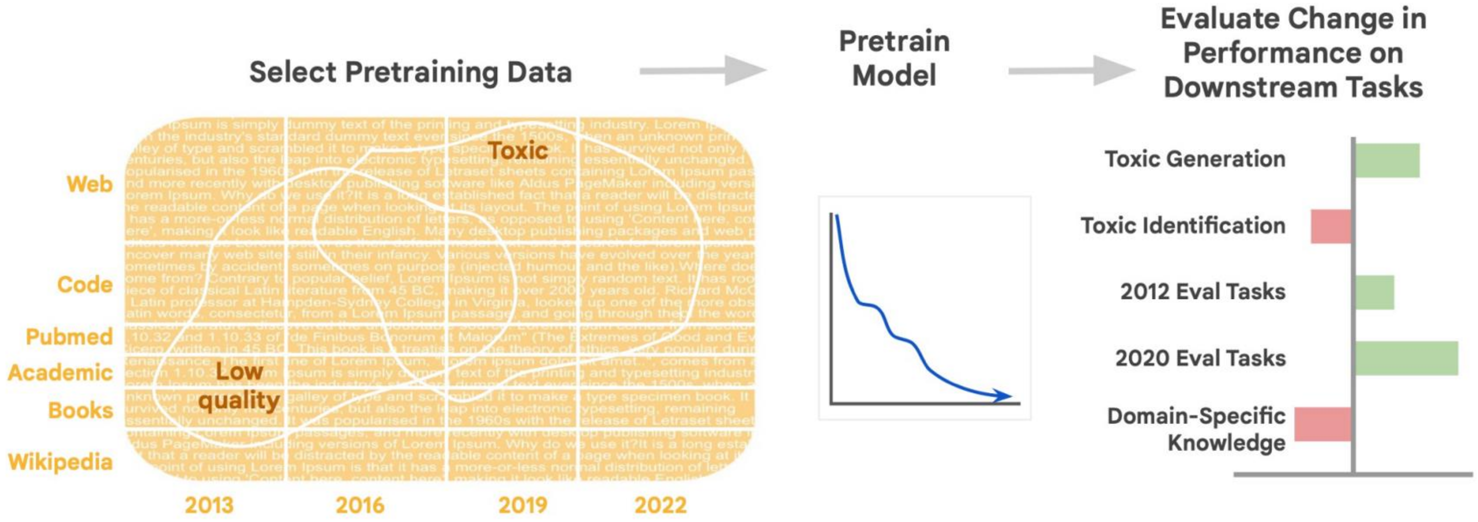
Scale is difficult…for example, data filtering



Penedo, et al. (2023) The Refined Web dataset for Falcon LLM

Scale is difficult…for example, data filtering

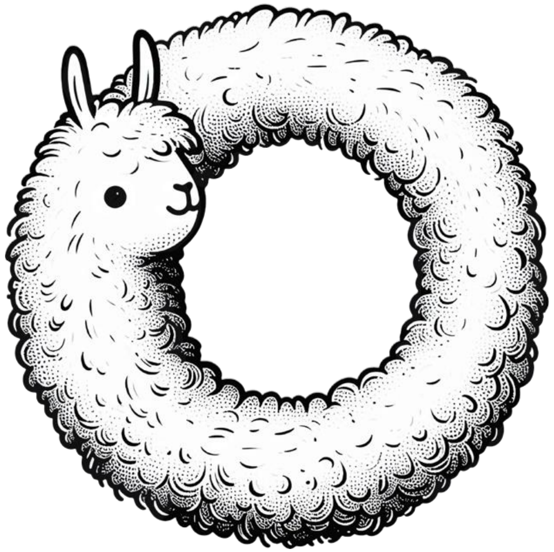
A Pretrainer's Guide to Training Data: Measuring the Effects of Data Age, Domain Coverage, Quality, & Toxicity [Longpre et al, NAACL 2024]



Some findings: strongly encourage to read the paper!

- "temporal shift between evaluation data and pretraining data leads to performance degradation, which is not overcome by finetuning"
- "a trade-off between performance on standard benchmarks and risk of toxic generations… there does not exist a one-size-fits-all solution to filtering."

A great learning opportunity

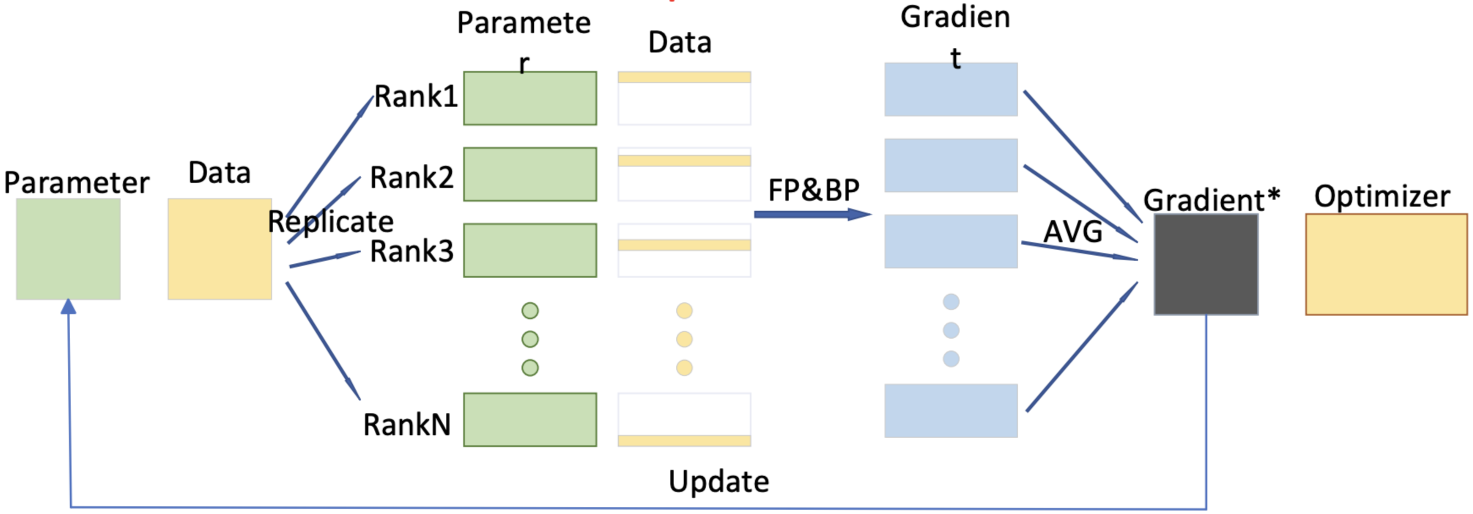


LLM360

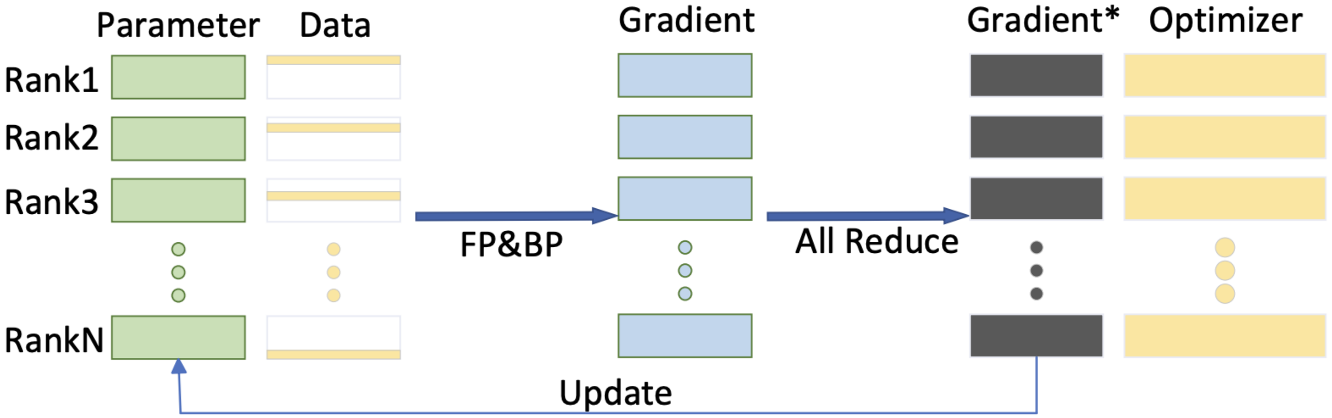
[TxT360](TxT360)

Scale is difficult…for example, parallel training

Data parallel



Distributed data parallel



[Understanding LLMs: A Comprehensive Overview from Training to Inference]

Challenges of MLE-based unsupervised training

MLE: A KL-Divergence view

$$KL(P_{data} \parallel P_\theta) = E_{x \sim P_{data}}[-\log P_\theta(x)] + const.$$

$$\mathrm{argmax}_\theta E_{x \sim P_{data}}[\log P_\theta(x)] = \mathrm{argmin}_\theta KL(P_{data} \parallel P_\theta)$$

- Must spread probability mass to cover observed sequences, even if incoherent
  - Repetition and genericity ("The man said the man said...")
  - Poor calibration on out-of-distribution prompts
  - Memorization of rare patterns
- Sampling strategies matter
- Entropy / confidence

What does MLE not do?

- No **semantics**
- No **task goals**
- No **explicit reward**

Entropy and Confidence

- Token-level entropy:

$$H_t = -\sum_v P(x_t = v \mid x_{<t}) \log P(x_t = v \mid x_{<t})$$
$$= E_v[-\log P(x_t = v \mid x_{<t})]$$

- Low entropy = high confidence.

Do we want our model to be low or high entropy?

Recall from Variational Inference

$$\log p(x \mid \theta) = E_{z\sim q}[\log p(x, z \mid \theta)] + H(q) + KL(q(z \mid x) \mid\mid p(z \mid x, \theta))$$

$$\log p(x \mid \theta) \geq \underbrace{E_{z\sim q}[\log p(x, z \mid \theta)] + H(q)}_{\text{"ELBO": Evidence Lower Bound}}$$

Maximizing ELBO → Increased entropy of $q(z)$

Does Maximizing Likelihood → Increased entropy of $p(x \mid \theta)$?

MLE and Entropy

$$\widehat{\theta_{MLE}} = \operatorname{argmax}_\theta E_{x\sim P_{data}}[\log P_\theta(x)]$$

- Directly optimize the data distribution $P_\theta(x)$ without explicitly introducing auxiliary variables or explicitly controlling the entropy of x
- Often implicitly pushes $P_\theta(x)$ toward low-entropy distributions
- Mode collapse / degeneration / “memorization”

MLE and Entropy

Context: In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.

Pure Sampling:
They were cattle called Bolivian Cavalleros; they live in a remote desert uninterrupted by town, and they speak huge, beautiful, paradisiacal Bolivian linguistic thing. They say, 'Lunch, marge.' They don't tell what the lunch is," director Professor Chuperas Omwell told Sky News. "They've only been talking to scientists, like we're being interviewed by TV reporters. We don't even stick around to be interviewed by TV reporters. Maybe that's how they figured out that they're cosplaying as the Bolivian Cavalleros."

Beam Search, *b*=32:
"The study, published in the Proceedings of the National Academy of Sciences of the United States of America (PNAS), was conducted by researchers from the Universidad Nacional Autónoma de México (UNAM) and the Universidad Nacional Autónoma de México (UNAM/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de ..."

THE CURIOUS CASE OF NEURAL TEXT DeGENERATION [Holtzman 2020]

MLE and Entropy

$$\widehat{\theta_{MLE}} = \text{argmax}_{\theta} E_{x \sim P_{data}}[\log P_{\theta}(x)]$$

- Solutions:
  - Explicitly add a penalty for low entropy:

$$\hat{\theta} = \text{argmax}_{\theta} E_{x \sim P_{data}}[\log P_{\theta}(x)] + \lambda \sum_{t} H[P_{\theta}(x_t \mid x_{<t})]$$

  - Smooth labels:

$$\tilde{y}_{\epsilon} = \begin{Bmatrix} 1-\epsilon, & y=1 \\ \frac{\epsilon}{|V|-1}, & y=0 \end{Bmatrix}$$

  - Contrastive losses:
  - Scheduled sampling / noise contrastive objectives
  - Risk minimization, utility, preference-based losses

Questions?

WISCONSIN
UNIVERSITY OF WISCONSIN–MADISON