

Mathematics of Data: From Theory to Computation

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Lecture 15: Language models

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École Polytechnique Fédérale de Lausanne (EPFL)

EE-556 (Fall 2024)



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The era of ChatGPT

 what can I learn from the Mathematics of data lecture

 A "Mathematics of Data" lecture can offer you valuable knowledge and skills related to the mathematical foundations of data analysis and data science. Here are some key things you can learn from such a lecture:  

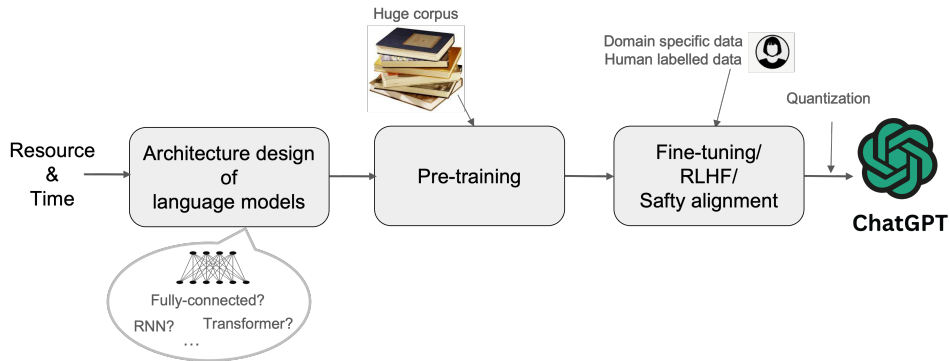
1. **Statistical Concepts:** You can learn about statistical techniques and concepts, including descriptive statistics, probability distributions, hypothesis testing, and regression analysis. This knowledge is crucial for understanding and interpreting data.
2. **Linear Algebra:** You may gain insights into linear algebra, which is fundamental for tasks like data transformation, dimensionality reduction, and working with matrices and vectors commonly used in machine learning.
3. **Calculus:** Depending on the lecture's depth, you might learn about calculus and how it relates to optimization algorithms, gradient descent, and mathematical modeling of data phenomena.
4. **Probability Theory:** Understanding probability theory can help you model uncertainty and make informed decisions based on data. Concepts like Bayes' theorem and conditional probability are often covered.
5. **Data Visualization:** Many data-related lectures include topics on data visualization, teaching you how to create meaningful graphs and charts to convey insights from data effectively.
6. **Data Modeling:** You can learn about various data modeling techniques, including linear models, logistic regression, and decision trees. These models are used for prediction and classification tasks.
7. **Machine Learning Foundations:** If the lecture is more advanced, it may introduce you machine learning concepts such as supervised learning, unsupervised learning, and

 Regenerate

Send a message

Outline



○ This lecture

1. Basics of language models
2. Self-attention and transformer architectures
3. Fundamentals of pre-training & fine-tuning & reinforcement learning with human feedback (RLHF)
4. Generative pre-trained transformer (GPT) family
5. Basics of prompting: zero-shot & few-shot & chain-of-thought & automatic

A motivation for language models (LMs)

Example

Predict the next word w given the following source sentence S_{source} ?

S_{source} : "On January 1 people usually say happy new $[w]$."

A motivation for language models (LMs)

Example

Predict the next word w given the following source sentence S_{source} ?

S_{source} : "On January 1 people usually say happy new $[w]$."

Question:

○ Why is this important?

- ▶ spelling & grammar correction
- ▶ machine translation
- ▶ sentence classification
- ▶ speech recognition
- ▶ chatbot
- ▶ (more generally) labeling, automated decisions,...

$$p(\text{year}|S_{\text{source}}) > p(\text{years}|S_{\text{source}})$$

$$p(S_{\text{translation 1}}|S_{\text{source}}) > p(S_{\text{translation 2}}|S_{\text{source}})$$

$$p(S_{\text{class 1}}|S_{\text{source}}) > p(S_{\text{class 2}}|S_{\text{source}})$$

$$p(w|S_{\text{source}})$$

$$p(w|S_{\text{source}})$$

Basics for language models (LMs) – I

Definition (Language model [9])

Models that assign probabilities to sequences of words are called language models.

Remarks: ◦ Given a sentence with T words: $S = w_{1:T} = (w_1, \dots, w_T)$, by the chain rule of probability:

$$p(S) = p(w_{1:T}) = p(w_1)p(w_2|w_1)p(w_3|w_{1:2}) \cdots p(w_T|w_{1:T-1}) = \prod_{t=1}^T p(w_t|w_{1:t-1})$$

◦ Implicitly, we are enforcing a graphical model that takes “time” into account.

Example

If $S = w_{1:3} = \text{“happy new year”}$, then $p(S) = p(\text{happy})p(\text{new}|\text{happy})p(\text{year}|\text{happy new})$.

Basics for language models (LMs) – II

Question: ○ How can we compute $p(w_t|w_{1:t-1})$?

Remarks: ○ A trivial solution: Just count the frequency on a large corpus, e.g.,

$$p(\text{year}|S_{\text{source}}) = \frac{p(S_{\text{source}} + \text{year})}{p(S_{\text{source}})} \approx \frac{\#(\text{On January 1 people usually say happy new year})}{\#(\text{On January 1 people usually say happy new})}$$

- But the language is creative, there are several ways to express the same meaning.
- The sentence above might even not appear on the corpus.
- We need better ways to estimate such probabilities!

N -gram LMs



Markov assumption [12]

The probability of a word only depends on the last $N - 1$ words as

$$p(w_t | w_{1:t-1}) = p(w_t | w_{t-N:t-1}) \approx \frac{\#(w_{t-N:t})}{\#(w_{t-N:t-1})}.$$

Markov in 1913 [12] used “Markov chains” to predict whether the upcoming letter would be a vowel or a consonant.

Example

In the bigram LM ($N = 2$), we only need to estimate $p(w_t | w_{t-1}) \approx \frac{\#(w_{t-1:t})}{\#(w_{t-1})}$ to generate text.

		w_t			
w_{t-1}	i	want	to	eat	
	i	5	827	0	9
	want	2	0	608	1
	to	2	0	4	686
	eat	0	0	2	0

		w_t			
w_{t-1}	i	want	to	eat	
	i	0.002	0.33	0	0.0036
	want	0.0022	0	0.66	0.0011
	to	0.00083	0	0.0017	0.28
	eat	0	0	0.0027	0

Figure: Count (Left) and probability $p(w_t | w_{1:t-1})$ (Right) from the Berkeley Restaurant Project corpus of 9332 sentences [9].

Towards pre-training an N -gram LM

- In natural language processing (NLP), we use tokens to represent words coming from a vocabulary $\mathcal{V}$.

- Terminologies:**
- A *token* is the smallest unit that can be assigned a meaning to be processed.
 - ▶ In English, a token often corresponds to a word.
 - ▶ However, a single token can also encode compound words like *New York*.
 - ▶ In Chinese or Japanese, there is no space between words.
 - ▶ In these languages, sentence segmentation is required before we tokenize.
 - We indicate the beginning and the end of sentences with tokens $\langle \text{BOS} \rangle$ and $\langle \text{EOS} \rangle$.
 - ▶ S_{source} “ $\langle \text{BOS} \rangle$ Happy new year $\langle \text{EOS} \rangle$ ” has $T = 5$ tokens.
 - The size of our vocabulary is denoted as $|\mathcal{V}|$.
 - *Pre-training*: building a LM based on a large corpus in a (often) self-supervised manner.
 - *Inference*: Using a trained LM to do next word prediction.

N -gram LMs: “Pre-training” & Inference

- The following simplified examples show the difficulty of pre-training and inference with 2-gram LMs.

“Pre-training”
1. Count $\#(w_{t-1})$ and $\#(w_{t-1:t})$ over the corpus. 2. Obtain probability $p(w_t w_{t-1})$ over the corpus.

Inference
1. Set w_1 as $\langle \text{BOS} \rangle$, $t = 1$. 2. While True: ▶ $w_{t+1} = \arg \max_{w \in \mathcal{V}} p(w w_t)$ ▶ If w_{t+1} is $\langle \text{EOS} \rangle$: break ▶ $t = t + 1$ 3. Output: $[w_1, \dots, w_{t+1}]$.

Remarks:

- Need to store the probability for all N -gram pairs.
- Language is creative, some new N -gram pairs might not even appear on the corpus.
- Cannot incorporate earlier words than N due to the Markov assumption.

$p(\text{two} \mid \text{one plus one equals}) = p(\text{two} \mid \text{it is wrong that one plus one equals})?$

Word representations

Question: ○ How can we numerically represent a word/meaning?

Remarks: ○ Osgood et al. 1957 [16] uses 3 numbers to represent a word.

- ▶ valence: the pleasantness of the stimulus
- ▶ arousal: the intensity of emotion provoked by the stimulus
- ▶ dominance: the degree of control exerted by the stimulus

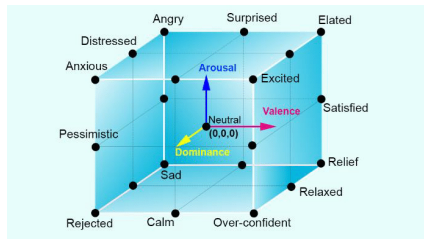
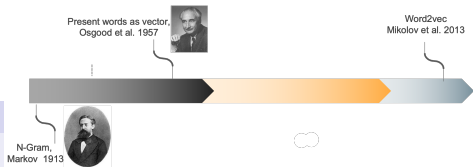


Figure: From [8].

Word embeddings

Definition (Word embeddings [9])

Vectors for representing words are called word embeddings.



- We will briefly introduce two words embeddings:
- One-hot representation: sparse and long word embedding in $\mathbb{R}^{|\mathcal{V}|}$.
 - ▶ Training is not required—trivial to obtain.
 - ▶ Not a good way to capture the underlying meaning—cannot measure similarity.
- Word2vec [13]: a framework to learn dense and concise word embedding.
 - ▶ Training is required.
 - ▶ Better characterization for the meaning of a word, e.g., the similarity can be computed by similarity metrics.
 - ▶ Cosine similarity or inner products work!

Word2vec [13]: Setup

- An illustration of a target word and context words in a ± 2 window size:

... people usually say happy new ...
context words target word context words

- Word2vec uses learnable parameters X_c and X_t to present two embeddings for each word,
 - ▶ X_c corresponds to the embedding when it is as a context word.
 - ▶ X_t corresponds to the embedding when it is as a target word
 - ▶ They satisfy the following relationship:

$$\mathbf{b}_i^t = X^t e_i \in \mathbb{R}^d, \quad \mathbf{b}_i^c = X^c e_i \in \mathbb{R}^d,$$

where $e_i \in \mathbb{R}^{|\mathcal{V}|}$ is the one hot representation for each word, $i \in 1, \dots, |\mathcal{V}|$.

- Remarks:**
- The window size for the context is a hyperparameter.
 - The final embedding can be the summation or concatenation of these two embeddings.

Word2vec [13]: Training

- Core idea: Given a pair of words (w_i, w_j) , return the probability that w_j is the context word of w_i (i.e., true).

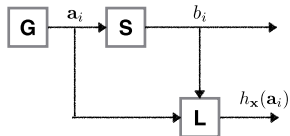
A simple approach: $p(\text{true}|(w_t, w_c)) = \sigma(\langle \mathbf{b}_t^t, \mathbf{b}_c^c \rangle) = \frac{1}{1 + \exp(-\langle \mathbf{b}_t^t, \mathbf{b}_c^c \rangle)}$, where σ is the sigmoid activation.

- Given a tuple (w_t, w_c, w_n) , we have the following ingredients
 - w_t is the target word.
 - w_c is one of its context words(positive samples)
 - w_n is not its context word (negative sample)—e.g., chosen via unigram (1-Gram) probability.
 - A loss function:

$$\begin{aligned} L &= -\log(p(\text{true}|(w_t, w_c))p(\text{false}|(w_t, w_n))) \\ &= -\log p(\text{true}|(w_t, w_c)) - \log p(\text{false}|(w_t, w_n)) \\ &= -\log \sigma(\langle \mathbf{b}_t^t, \mathbf{b}_c^c \rangle) - \log(1 - \sigma(\langle \mathbf{b}_t^t, \mathbf{b}_n^n \rangle)) \\ &= -\log \frac{1}{1 + \exp(-\langle \mathbf{X}^t e_t, \mathbf{X}^c e_c \rangle)} - \log \left(1 - \frac{1}{1 + \exp(-\langle \mathbf{X}^t e_t, \mathbf{X}^c e_n \rangle)} \right) \end{aligned}$$

- Crawl the corpus to obtain these tuples, and minimize L (e.g., with stochastic gradient descent).

Designing neural networks for pre-training LM

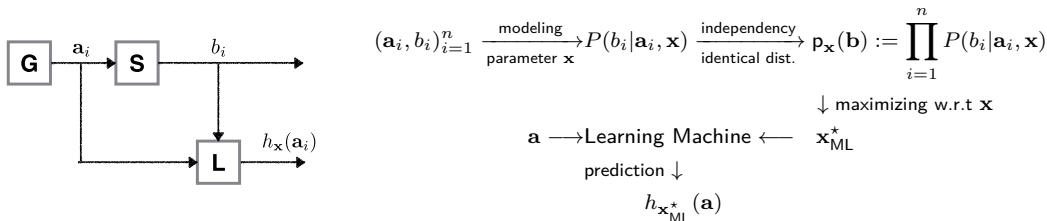


- A two-layer feedforward neural network (FNN):

$$h_{\mathbf{x}}(\mathbf{a}) := \left[\mathbf{X}_O \right] \underbrace{\left(\overset{\text{activation}}{\downarrow} \sigma \left(\overset{\text{weight}}{\downarrow} \left[\mathbf{X}_I \right] \overset{\text{input}}{\downarrow} \begin{bmatrix} \mathbf{a} \end{bmatrix} \right) \right)}_{\text{hidden layer } \mathbf{z} = \text{non-linear features}}, \quad \mathbf{x} := [\mathbf{X}_I, \mathbf{X}_O]$$

Short detour: Statistical learning with maximum-likelihood estimators

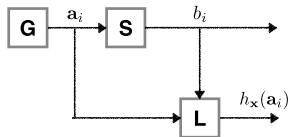
- A visual summary: From parametric models to learning machines



- Observations:**
- Recall $x_{ML}^* \in \arg \min_{x \in \mathcal{X}} \{L(h_x(a), b) := -\log p_x(b)\}$.
 - Maximizing $p_x(b)$ gives the maximum-likelihood (ML) estimator.
 - Maximizing $p_x(b)$ and minimizing $-\log p_x(b)$ result in the same solution set.

Designing neural networks for pre-training LM

- A two-layer feedforward neural network (FNN):



$$h_{\mathbf{x}}(\mathbf{a}) := \left[\mathbf{X}_O \right] \underbrace{\left(\sigma \left(\left[\mathbf{X}_I \right] \left[\mathbf{a} \right] \right) \right)}_{\text{hidden layer } \mathbf{z} = \text{non-linear features}}, \quad \mathbf{x} := [\mathbf{X}_I, \mathbf{X}_O]$$

activation ↓ weight ↓ input ↓

Recall: Maximum-likelihood estimator

The maximum-likelihood estimator (supervised learning with data $(\mathbf{a}, b)$) is given by

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathcal{X}} \{L(h_{\mathbf{x}}(\mathbf{a}), b) := -\log p_{\mathbf{x}}(b)\}.$$

Remark:

- NN-based LM can be considered as an **unsupervised** maximum-likelihood estimator.

$$\mathbf{x}_{\text{LM}}^* \in \arg \min_{\mathbf{x} \in \mathcal{X}} -\log p_{\mathbf{x}}(S) = -\log p_{\mathbf{x}}(\mathbf{b}_{1:T}),$$

where $p_{\mathbf{x}}(S)$ is the probability of sentence S with embedding $\mathbf{b}_{1:T} = (\mathbf{b}_1, \dots, \mathbf{b}_T)$.

The optimization objective

- A (vector-output) neural network $\mathbf{h}_\mathbf{x} \in \Delta^{|\mathcal{V}|-1}$ can be used to model such probability.

$$\begin{aligned} -\log p_\mathbf{x}(\mathbf{b}_{1:T}) &= -\log \left(\prod_{t=1}^T p_\mathbf{x}(\mathbf{b}_t | \mathbf{b}_{1:t-1}) \right) = \sum_{t=1}^T \left(-\log \underbrace{p_\mathbf{x}(\mathbf{b}_t | \mathbf{b}_{1:t-1})}_{\mathbf{h}_\mathbf{x}(\mathbf{b}_{1:t-1})^{[\mathbf{b}_t]}} \right) \\ &= \sum_{t=1}^T \left(-\log \mathbf{h}_\mathbf{x}(\mathbf{b}_{1:t-1})^{[\mathbf{b}_t]} \right) = \sum_{t=1}^T \left(-\sum_{i=1}^{|\mathcal{V}|} \hat{\mathbf{u}}_t^{[i]} \log \mathbf{u}_t^{[i]} \right) = \text{cross entropy loss} \end{aligned}$$

- ▶ $\mathbf{u}_t := \mathbf{h}_\mathbf{x}(\mathbf{b}_{1:t-1}) \in \mathbb{R}^{|\mathcal{V}|}$ is the probability distribution of the next word given previous $t-1$ words.
- ▶ $\hat{\mathbf{u}}_t \in \mathbb{R}^{|\mathcal{V}|}$ is the correct distribution (one-hot) at t step.

- Remarks:**
- **Teacher forcing training:** We always give the model the correct history sequence.
 - **Auto-regressive inference:** The history sequence comes from its prediction result.

Basic NN setups for LM

- Below, we present a general idea of deploying neural networks as LMs.
 - Feed-forward neural network (FNN)
 - Recurrent Neural Networks (RNN)
 - Self-attention
- At each step t , we use NN to model the probability distribution of the current word given previous $t - 1$ words.

probability distribution of next word
↓

$$\mathbf{u}_t := \mathbf{h}_{\mathbf{x}}(\mathbf{b}_{1:t-1}) := \text{Softmax} \left(\left[\mathbf{X}_O \right] \underbrace{\text{FNN/RNN/Self-attention}}_{\text{hidden layer } \mathbf{z} = \text{non-linear features}} \left(\begin{array}{c} \text{some weight} \downarrow \\ \mathbf{X} \end{array}, \begin{array}{c} \text{previous words} \downarrow \\ \mathbf{b}_{1:t-1} \end{array} \right) \right)$$

- Then, we can minimize the cross-entropy loss (i.e., $-\sum_{i=1}^{|\mathcal{V}|} \hat{\mathbf{u}}_t^{[i]} \log \mathbf{u}_t^{[i]}$) via (stochastic) gradient descent.

FNN as LM [2]: pre-training

- Core idea: use most recent N tokens to predict next token (similar to N -gram)
- $\mathbf{X}_I \in \mathbb{R}^{m \times Nd}$, $\mathbf{X}_O \in \mathbb{R}^{|\mathcal{V}| \times m}$ are learnable parameters, where d is the dimension of the embedding.

Forward pass in pre-training on single sentence (only use two recent tokens, i.e., $N = 2$)

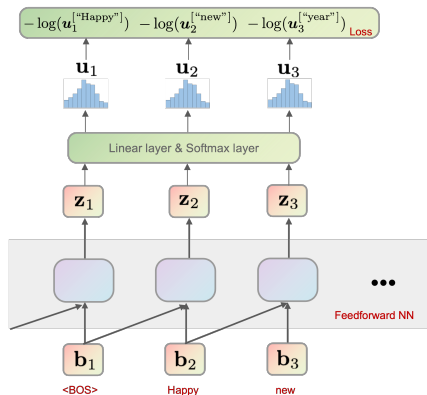
1. Set $\mathbf{b}_0 = \mathbf{0}$, initial loss $L = 0$

2. For $t = 1, \dots, T$

► $\mathbf{z}_t = \sigma \left(\mathbf{X}_I \begin{bmatrix} \mathbf{b}_{t-1} \\ \mathbf{b}_t \end{bmatrix} \right),$ FNN

► $\mathbf{u}_t = \text{Softmax}(\mathbf{X}_O \mathbf{z}_t),$ probability

► $L += \left(\sum_{i=1}^{|\mathcal{V}|} -\hat{\mathbf{u}}_t^{[i]} \log \mathbf{u}_t^{[i]} \right),$ loss

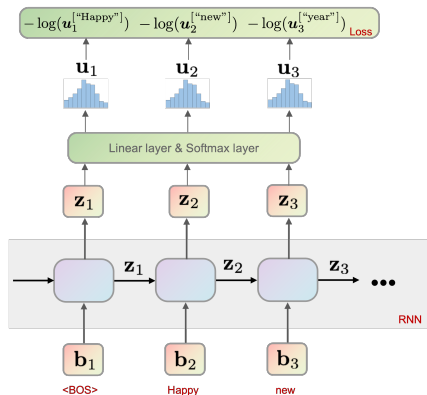


RNN as LM [14]: pre-training

- A weakness of FNN LM is the Markov assumption: It cannot capture long-term dependencies.
- RNN architectures *only partially* address this issue.
- : $\mathbf{X}_1 \in \mathbb{R}^{m \times m}$, $\mathbf{X}_2 \in \mathbb{R}^{m \times d}$, $\mathbf{X}_O \in \mathbb{R}^{|\mathcal{V}| \times m}$ are learnable parameters.

Forward pass in pre-training on single sentence

1. Set initial state $\mathbf{z}_0 = \mathbf{0}$, initial loss $L = 0$
2. For $t = 1, \dots, T$
 - ▶ $\mathbf{z}_t = \sigma(\mathbf{X}_1 \mathbf{z}_{t-1} + \mathbf{X}_2 \mathbf{b}_t)$, RNN
 - ▶ $\mathbf{u}_t = \text{Softmax}(\mathbf{X}_O \mathbf{z}_t)$, probability
 - ▶ $L += \left(\sum_{i=1}^{|\mathcal{V}|} -\hat{\mathbf{u}}_t^{[i]} \log \mathbf{u}_t^{[i]} \right)$, loss



RNN as LM: inference

- o RNN architectures perform auto-regressive inference.

Forward pass in inference

1. Set $\mathbf{b}_1$ as the embedding of $\langle \text{BOS} \rangle$, $t = 1$, initial state $\mathbf{z}_0 = \mathbf{0}$.
2. While True:
 - ▶ $\mathbf{z}_t = \sigma(\mathbf{X}_1 \mathbf{z}_{t-1} + \mathbf{X}_2 \mathbf{b}_t)$
 - ▶ $\mathbf{u}_t = \text{Softmax}(\mathbf{X}_O \mathbf{z}_t)$
 - ▶ Set $\mathbf{b}_{t+1}$ as the embedding of the token corresponding to $\arg \max \mathbf{u}_t$.
 - ▶ If $\mathbf{b}_{t+1}$ is the embedding of $\langle \text{EOS} \rangle$: **break**
 - ▶ $t+ = 1$
3. Output: $[\mathbf{b}_1, \dots, \mathbf{b}_{t+1}]$.

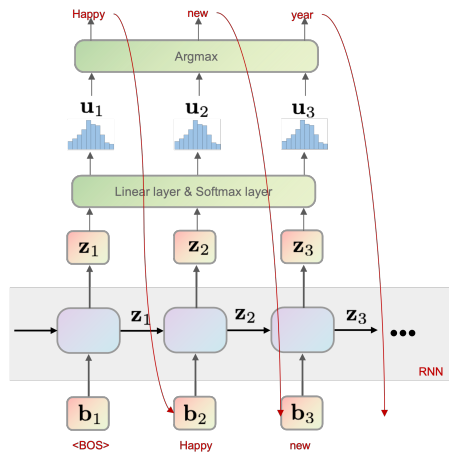


Figure: Auto-regressive inference

Self-attention layer as LM

- A weakness of the RNN LMs is its recursive non-parallelizable computation.
- Self-attention can address these issues.

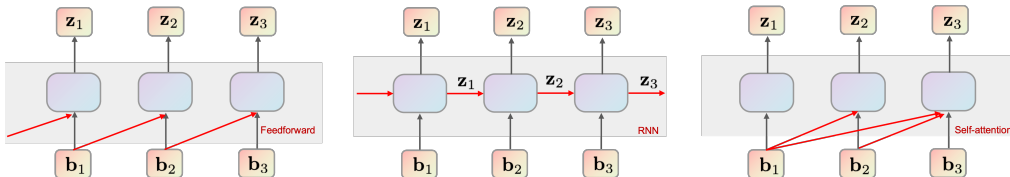
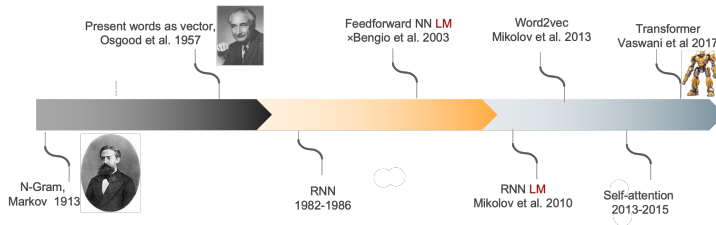


Figure: (Left panel) FNN in LM. (Middle panel) RNN in LM. (Right panel) Self-attention in LM.



Self-attention layer for LM

- Core idea: compare a word of interest to other words based on their relevance.
- How do we measure the relevance of two words?
 - inner products (recall word embeddings)
 - e.g., for the word with embedding $\mathbf{b}_3$, we can compute three scores:

$$\text{Score}(3, 1) = \langle \mathbf{b}_3, \mathbf{b}_1 \rangle; \quad \text{Score}(3, 2) = \langle \mathbf{b}_3, \mathbf{b}_2 \rangle; \quad \text{Score}(3, 3) = \langle \mathbf{b}_3, \mathbf{b}_3 \rangle.$$

- Next, we normalize them with a softmax to create a vector of weights, and obtain the output:

$$\begin{aligned} \mathbf{z}_3 &= \sum_{j=1}^3 \text{Softmax}([\text{Score}(3, 1), \text{Score}(3, 2), \text{Score}(3, 3)])_j \mathbf{b}_j \\ &= \sum_{j=1}^3 \frac{\exp(\text{Score}(3, j))}{\sum_{i=1}^3 \exp(\text{Score}(3, i))} \mathbf{b}_j \end{aligned}$$

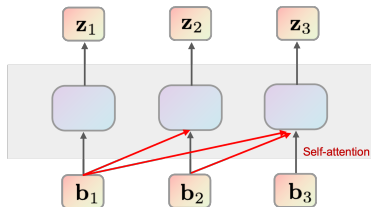


Figure: Self-attention layer.

Self-attention layer for LM

- A more sophisticated way to present how words are contributed to each other:

- ▶ *Query*: when current word goes measure the relevance with other words.
- ▶ *Key*: when being measured the relevance by other words.
- ▶ *Value*: value used to compute the final output.



- For each word, calculate its corresponding query, key, and value using parameters $\mathbf{X}_Q, \mathbf{X}_K, \mathbf{X}_V \in \mathbb{R}^{m \times d}$

$$\mathbf{q}_i = \mathbf{X}_Q \mathbf{b}_i, \mathbf{k}_i = \mathbf{X}_K \mathbf{b}_i, \mathbf{v}_i = \mathbf{X}_V \mathbf{b}_i.$$

- Then, for the word with embedding $\mathbf{b}_3$, those three scores become:

$$\text{Score}(3, 1) = \langle \mathbf{q}_3, \mathbf{k}_1 \rangle; \quad \text{Score}(3, 2) = \langle \mathbf{q}_3, \mathbf{k}_2 \rangle; \quad \text{Score}(3, 3) = \langle \mathbf{q}_3, \mathbf{k}_3 \rangle.$$

$$\mathbf{z}_3 = \sum_{j=1}^3 \text{Softmax}([\text{Score}(3, 1), \text{Score}(3, 2), \text{Score}(3, 3)])_j \mathbf{v}_j$$

- We need to learn the parameters $\mathbf{X}_Q, \mathbf{X}_K, \mathbf{X}_V \in \mathbb{R}^{m \times d}$.

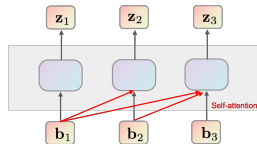


Figure: Self-attention layer.

Positional embeddings in self-attention

Question: ○ Does self-attention layer consider the relative position of each word in the sequence? **No!**

Observation: ○ If we switch the order of b_1 and b_2 , the output z_3 remains the same.

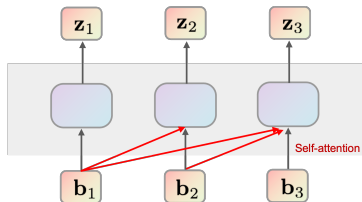


Figure: Self-attention layer.

○ In comparison, RNN encodes the information about the order of the inputs recursively.

Positional embeddings in self-attention

Question: ○ Does self-attention layer consider the relative position of each word in the sequence? **No!**

Solution 1? ○ Absolute position via trivial concatenation.

$$\text{Pos}(\mathbf{b}_t) = \text{Concatenate}[\mathbf{b}_t, t] .$$

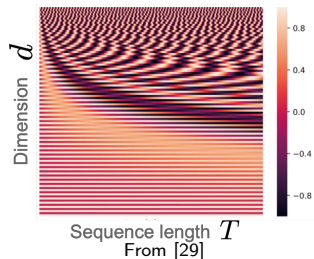
- Unbounded value.
- Hard to extrapolate on sequence with unseen length.

Positional embeddings in self-attention

Question: ○ Does self-attention layer consider the relative position of each word in the sequence? **No!**

Solution 2 [24]: ○ Absolute position via trigonometric functions of different frequencies. For $t = 1, \dots, T$:

$$\text{Pos}(\mathbf{b}_t) = \mathbf{b}_t + \begin{pmatrix} \sin\left(t/10000^{2 \times 1/d}\right) \\ \cos\left(t/10000^{2 \times 1/d}\right) \\ \vdots \\ \sin\left(t/10000^{2 \times \frac{d}{2}/d}\right) \\ \cos\left(t/10000^{2 \times \frac{d}{2}/d}\right) \end{pmatrix}$$

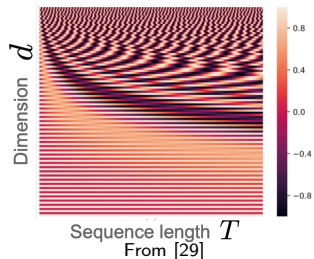


Positional embeddings in self-attention

Question: ○ Does self-attention layer consider the relative position of each word in the sequence? **No!**

Solution 2 [24]: ○ Absolute position via trigonometric functions of different frequencies. For $t = 1, \dots, T$:

$$\text{Pos}(\mathbf{b}_t) = \mathbf{b}_t + \begin{pmatrix} \sin\left(t/10000^{2 \times 1/d}\right) \\ \cos\left(t/10000^{2 \times 1/d}\right) \\ \vdots \\ \sin\left(t/10000^{2 \times \frac{d}{2}/d}\right) \\ \cos\left(t/10000^{2 \times \frac{d}{2}/d}\right) \end{pmatrix}$$



Solution 3: ○ *Rotary position embedding [21]: incorporate both absolute position and relative position.

Self-attention layer for LM

- $\mathbf{B} = [\mathbf{b}_1, \dots, \mathbf{b}_T]^\top \in \mathbb{R}^{T \times d}$: collections of embeddings of all tokens.
- Learnable parameters: $\mathbf{X}_Q, \mathbf{X}_K, \mathbf{X}_V \in \mathbb{R}^{m \times d}, \mathbf{X}_O \in \mathbb{R}^{|\mathcal{V}| \times m}$.

Forward pass in training on a single sentence

1. Set initial loss $L = 0$.
2. $\mathbf{Q} = \mathbf{B}\mathbf{X}_Q^\top, \mathbf{K} = \mathbf{B}\mathbf{X}_K^\top, \mathbf{V} = \mathbf{B}\mathbf{X}_V^\top$, query, key, value.
3. $\mathbf{S} = \text{Mask}(\mathbf{Q}\mathbf{K}^\top)$, calculate score and mask score.
5. $\mathbf{Z} := [\mathbf{z}_1, \dots, \mathbf{z}_T]^\top = \text{Row-wise-Softmax}(\mathbf{S})\mathbf{V}$, **self-attention output**
6. $\mathbf{U} := [\mathbf{u}_1, \dots, \mathbf{u}_T]^\top = \text{Row-wise-Softmax}(\mathbf{Z}\mathbf{X}_O^\top)$, **probability**
7. $L = L + \left(\sum_{t=1}^T \sum_{i=1}^{|\mathcal{V}|} -\hat{\mathbf{u}}_t^{[i]} \log \mathbf{u}_t^{[i]} \right)$, **loss**

$q_1^\top k_1$	$-\infty$	$-\infty$	$-\infty$	$-\infty$
		$-\infty$	$-\infty$	$-\infty$
$\vdots$		$\ddots$	$-\infty$	$-\infty$
				$-\infty$
$q_T^\top k_1$		$\dots$		$q_T^\top k_T$

Figure: Mask score for $\mathbf{S}$.

Remarks:

- In the remaining slide, $\mathbf{b}_t$ has already been added to position embedding.
- Masking score is used to prevent “cheating.”
 - ▶ the current word has only seen previous word.
 - ▶ the subsequent word is unknown.
 - ▶ the element $-\infty$ after softmax becomes 0.
- Attention with masking score is usually called “Masked attention.”
- This construction enables parallelization whereby improving upon RNNs.

Self-attention layer as LM: inference

Forward pass in inference

1. Set $\mathbf{b}_1$ as the embedding of $\langle \text{BOS} \rangle$, $t = 1$.
2. **While True:**
 - ▶ $\mathbf{q}_t = \mathbf{X}_Q \mathbf{b}_t, \mathbf{k}_t = \mathbf{X}_K \mathbf{b}_t, \mathbf{v}_t = \mathbf{X}_V \mathbf{b}_t$, calculate query, key, value
 - ▶ $\mathbf{s} = [\langle \mathbf{q}_t, \mathbf{k}_1 \rangle, \dots, \langle \mathbf{q}_t, \mathbf{k}_t \rangle]^\top$, calculate score
 - ▶ $\mathbf{z}_t = [\mathbf{v}_1, \dots, \mathbf{v}_t] \cdot \text{Softmax}(\mathbf{s})$
 - ▶ $\mathbf{u}_t = \text{Softmax}(\mathbf{X}_O \mathbf{z}_t)$
 - ▶ Set $\mathbf{b}_{t+1}$ as the embedding of the token corresponding to $\arg \max \mathbf{u}_t$.
 - ▶ **If** $\mathbf{b}_{t+1}$ is the embedding of $\langle \text{BOS} \rangle$: **break**
 - ▶ $t += 1$
3. Output: $[\mathbf{b}_1, \dots, \mathbf{b}_{t+1}]$.

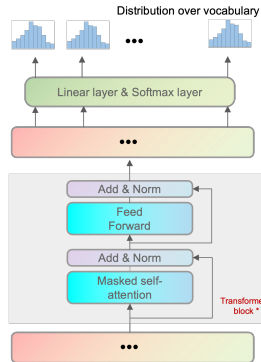
Remark:

- Still non-parallelizable, still auto-regression, the same as RNN LM, FNN LM.

TRANSFORMER as LM

- A Transformer block = [self-attention layer + *layer normalization + feedforward layer + *layer normalization].
- We stack $\mathcal{L}$ Transformer blocks to form an LM, e.g., $\mathcal{L} = 12$ in [17].

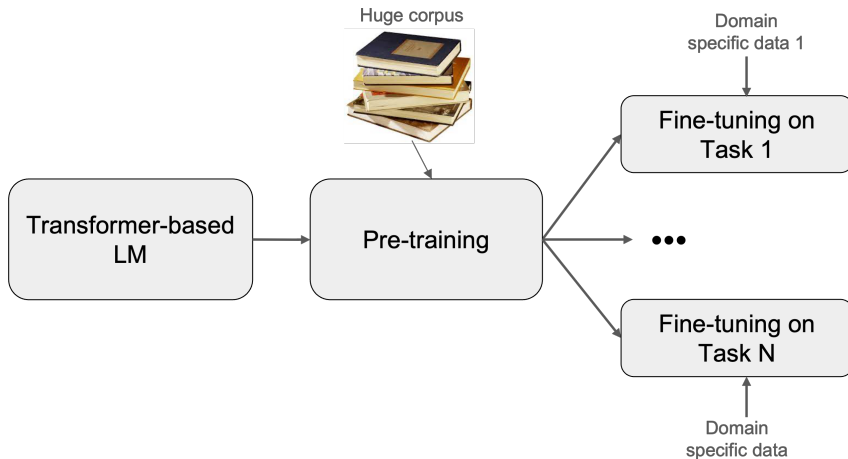
Forward pass in pre-training on single sentence	
1. Set initial loss $L = 0$, denote by $\mathbf{Z}_0 = \mathbf{B}$ the input to the first block.	
2. For $l = 1, \dots, \mathcal{L}$	
▶ $\mathbf{Q}_l = \mathbf{Z}_{l-1} \mathbf{X}_{Q,l}^\top, \mathbf{K}_l = \mathbf{Z}_{l-1} \mathbf{X}_{K,l}^\top, \mathbf{V}_l = \mathbf{Z}_{l-1} \mathbf{X}_{V,l}^\top$, query, key, value.	
▶ $\mathbf{S}_l = \text{Mask}(\mathbf{Q}_l \mathbf{K}_l^\top)$, calculate score and mask score.	
▶ $\mathbf{Z}_l = \text{Row-wise-Softmax}(\mathbf{S}_l) \mathbf{V}_l$	
▶ $\mathbf{Z}_l \leftarrow \mathbf{Z}_l + \mathbf{Z}_{l-1}$,	"add" in the figure, motivated by ResNet [7]
▶ $\mathbf{Z}_l = \text{Layernorm}(\mathbf{Z}_l)$	
▶ $\mathbf{Z}_{\text{shortcut}} = \mathbf{Z}_l$	
▶ $\mathbf{Z}_l = \sigma(\mathbf{X}_{F,l} \mathbf{Z}_l)$,	feedforward
▶ $\mathbf{Z}_l \leftarrow \mathbf{Z}_l + \mathbf{Z}_{\text{shortcut}}$,	"add"
▶ $\mathbf{Z}_l = \text{Layernorm}(\mathbf{Z}_l)$	output of each Transformer block
3. $\mathbf{U} := [\mathbf{u}_1, \dots, \mathbf{u}_T]^\top = \text{Row-wise-Softmax}(\mathbf{Z}_L \mathbf{X}_O^\top)$,	probability
4. $L \leftarrow \left(\sum_{t=1}^T \sum_{i=1}^{ \mathcal{V} } -\hat{\mathbf{u}}_t^{[i]} \log \mathbf{u}_t^{[i]} \right)$,	loss



Fin-
tune

- Remarks:**
- Original Transformer is proposed with encoder and decoder for neural machine translation [24].
 - The Transformer decoder is sufficient as an LM.

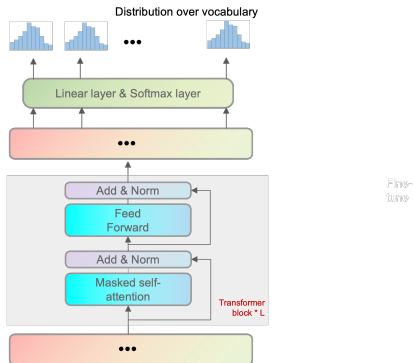
GPT-1 [17]: (Pre-train + fine-tune paradigm) “Improving Language Understanding by Generative Pre-Training”, 2018



- Remarks:**
- Pre-training enables learning better underlying language patterns on a large corpus.
 - Pre-training provides a better parameter initialization for fine-tuning, leading to faster convergence.

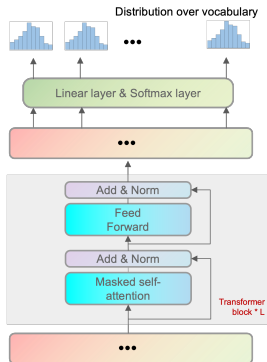
GPT-1 [17]: (Pre-train + fine-tune paradigm) “Improving Language Understanding by Generative Pre-Training”, 2018

- Step 1: Pre-train a LM on a large unlabeled corpus using Transformer’s decoder.
 - Recall that Transformer’s decoder is sufficient for LM.

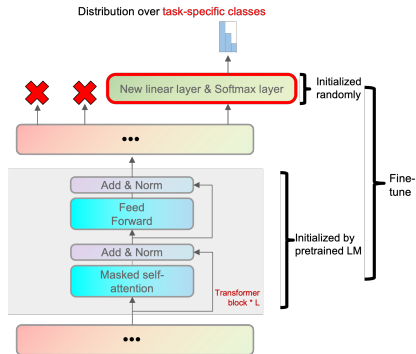


GPT-1 [17]: (Pre-train + fine-tune paradigm) “Improving Language Understanding by Generative Pre-Training”, 2018

- Step 1: Pre-train a LM on a large unlabeled corpus using Transformer’s decoder.
 - Recall that Transformer’s decoder is sufficient for LM.
- Step 2: Fine-tune on specific tasks, e.g., on a sentence classification task.



Fine-tune



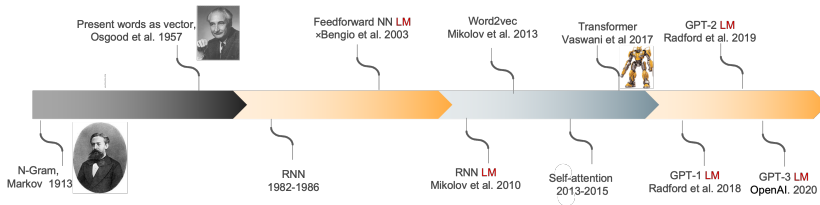
- Limitation:**
- Require task-specific datasets and task-specific fine-tuning.
 - Model is fine-tuned on very narrow task distributions.
 - Model does not necessarily generalize better out-of-distribution.

- Question:**
- Is it possible to address these limitations?
 - ▶ Humans do not require large supervised datasets to learn most new language tasks.

–*“please tell me if this sentence describes something happy or something sad”*

GPT-2, GPT-3 [18, 3] “Language Models are Unsupervised Multitask Learners”, “Language Models are Few-Shot Learners”

- *Same as GPT-1*: we still pre-train the LM on unlabeled corpus.
- *New*: no need to fine-tune anymore. One pre-trained LM for all tasks, achieve SOTA.



GPT-2, GPT-3 [18, 3] “Language Models are Unsupervised Multitask Learners”, “Language Models are Few-Shot Learners”

- Same as GPT-1: we still pre-train the LM on unlabeled corpus.
- New: no need to fine-tune anymore. One pre-trained LM for all tasks, achieve SOTA.



- How?

Model	Launch Year	Training Data	Training Parameters	Attention Layers	Word Embedding	Attention Heads
GPT-1	2018	7000 Books ~5GB	117M	12	768	12
GPT-2	2019	8 million documents ~40GB	1.5B	48	1600	48
GPT-3	2020	Multiple Source ~45TB	175B	96	12288	96

Figure: From <https://businessolution.org/gpt-3-statistics/>

Few-shot prompting (In-context learning) in GPT-3

- GPT-1: finetune the model on a specific task

The model is trained via repeated gradient updates using a large corpus of example tasks.



Few-shot prompting (In-context learning) in GPT-3

- GPT-1: finetune the model on a specific task

The model is trained via repeated gradient updates using a large corpus of example tasks.



- GPT-3: no need to fine-tune on a specific task.

Zero-shot

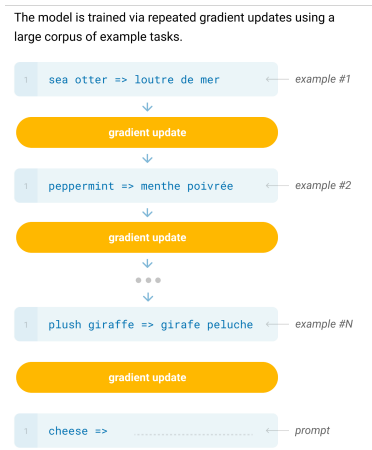
The model predicts the answer given only a natural language description of the task. No gradient updates are performed.



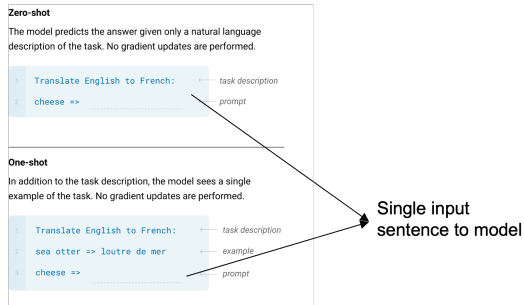
Single input sentence to model

Few-shot prompting (In-context learning) in GPT-3

- GPT-1: finetune the model on a specific task



- GPT-3: no need to fine-tune on a specific task.



Few-shot prompting (In-context learning) in GPT-3

- GPT-1: finetune the model on a specific task

The model is trained via repeated gradient updates using a large corpus of example tasks.



- GPT-3: no need to fine-tune on a specific task.

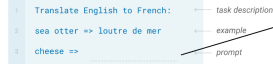
Zero-shot

The model predicts the answer given only a natural language description of the task. No gradient updates are performed.



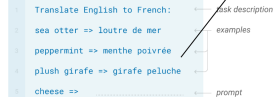
One-shot

In addition to the task description, the model sees a single example of the task. No gradient updates are performed.



Few-shot

In addition to the task description, the model sees a few examples of the task. No gradient updates are performed.



Single input sentence to model

★ Intrinsic mechanism of in-context learning

○ Classical supervised learning, for each task:

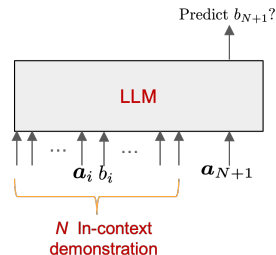
- ▶ Training: ERM, $\mathbf{x}^* \in \arg \min_{\mathbf{x}} : R(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N L(h_{\mathbf{x}}(\mathbf{a}_i), b_i)$.
- ▶ Given test point $\mathbf{a}_{N+1}$, return $h_{\mathbf{x}^*}(\mathbf{a}_{N+1})$.

○ In-context learning in LLM:

- ▶ Trains on huge corpus and gets $\mathbf{x}^*$.
- ▶ For any test task τ' , return: $h_{\mathbf{x}^*}(\{\mathbf{a}_i^{\tau'}, b_i^{\tau'}\}_{i=1}^N, \mathbf{a}_{N+1}^{\tau'})$.

○ Meta-learning:

- ▶ Training: ERM, $\mathbf{x}^* \in \arg \min_{\mathbf{x}} : R(\mathbf{x}) = \frac{1}{\# \text{Training tasks}} \sum_{\tau=1}^{\# \text{Training tasks}} L(h_{\mathbf{x}}(\{\mathbf{a}_i^{\tau}, b_i^{\tau}\}_{i=1}^N, \mathbf{a}_{N+1}^{\tau}), b_{N+1}^{\tau})$.
- ▶ For any test task τ' , return $h_{\mathbf{x}^*}(\{\mathbf{a}_i^{\tau'}, b_i^{\tau'}\}_{i=1}^N, \mathbf{a}_{N+1}^{\tau'})$.



Question

- Why LLM can perform in-context learning?
- Theoretical explanation: by performing gradient descent implicitly on in-context data? [25], see supplementary.
- Or is it just due to the so-called emergent abilities? See the next slide!

Few-shot prompting (In-context learning) → emergent abilities of LLM

“An ability is emergent if it is not present in smaller models but is present in larger models.”[27]

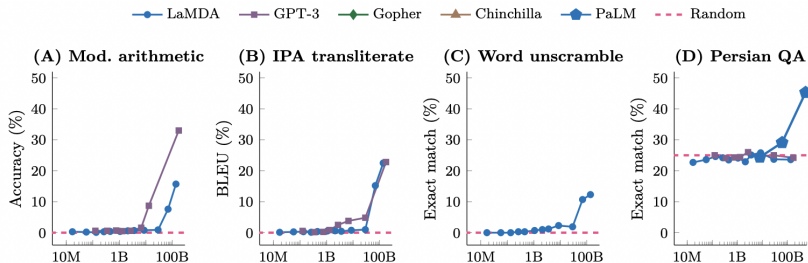


Figure: Emergent abilities of few-shot prompting appear when the model parameters (x-axis) are increased to some extent. [27]

Chain-of-thought prompting → emergent abilities of LLM

(a) Few-shot

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: A juggler can juggle 16 balls. Half of the balls are golf balls, and half of the golf balls are blue. How many blue golf balls are there?

A:

(Output) The answer is 8. ✗

(b) Few-shot-CoT

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: A juggler can juggle 16 balls. Half of the balls are golf balls, and half of the golf balls are blue. How many blue golf balls are there?

A:

(Output) The juggler can juggle 16 balls. Half of the balls are golf balls. So there are $16 / 2 = 8$ golf balls. Half of the golf balls are blue. So there are $8 / 2 = 4$ blue golf balls. The answer is 4. ✓

Figure: Demo of chain-of-thought (CoT) prompting [10].

Chain-of-thought prompting → emergent abilities of LLM

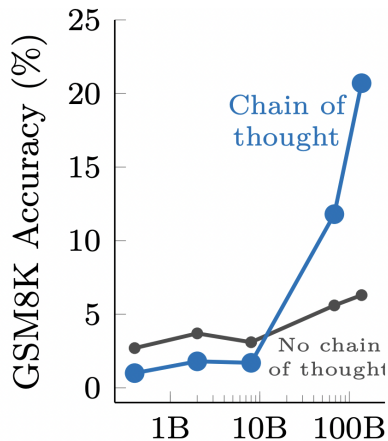


Figure: Performance under chain-of-thought prompting is increased until a certain model scale on Math word problems [27], A LLM called LaMDA is used [22].

Zero-shot chain-of-thought prompting → emergent abilities of LLM

(a) Few-shot

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: A juggler can juggle 16 balls. Half of the balls are golf balls, and half of the golf balls are blue. How many blue golf balls are there?

A:

(Output) The answer is 8. ✗

(b) Few-shot-CoT

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: A juggler can juggle 16 balls. Half of the balls are golf balls, and half of the golf balls are blue. How many blue golf balls are there?

A:

(Output) The juggler can juggle 16 balls. Half of the balls are golf balls. So there are $16 / 2 = 8$ golf balls. Half of the golf balls are blue. So there are $8 / 2 = 4$ blue golf balls. The answer is 4. ✓

(c) Zero-shot

Q: A juggler can juggle 16 balls. Half of the balls are golf balls, and half of the golf balls are blue. How many blue golf balls are there?

A: The answer (arabic numerals) is

(Output) 8 ✗

(d) Zero-shot-CoT (Ours)

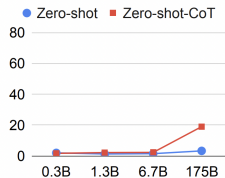
Q: A juggler can juggle 16 balls. Half of the balls are golf balls, and half of the golf balls are blue. How many blue golf balls are there?

A: **Let's think step by step.**

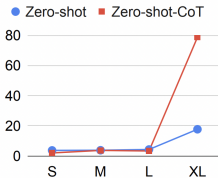
(Output) There are 16 balls in total. Half of the balls are golf balls. That means that there are 8 golf balls. Half of the golf balls are blue. That means that there are 4 blue golf balls. ✓

Figure: Demo of zero-shot chain-of-thought (CoT) prompting [10].

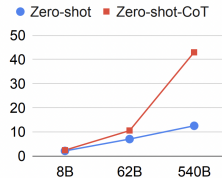
Zero-shot chain-of-thought prompting → emergent abilities of LLM



(a) MultiArith on Original GPT-3



(b) MultiArith on Instruct GPT-3



(c) GMS8K on PaLM

Figure: Performance under Zero-shot chain-of-thought prompting is increased until a certain model scale on Math word problems [10]. Y-axis indicates the accuracy.

Why emergent abilities occur?

- Understanding this would benefit:
 - ▶ Economy and environment: reduce training cost to obtain desired emergent abilities.
 - ▶ AI-Safety: prevent larger models from acquiring dangerous capabilities without warning.



NeurIPS Conference @NeurIPSConf · Dec 12

Replying to @NeurIPSConf

****Test of Time****

Distributed Representations of Words and Phrases and their Compositionality

****Outstanding Main Track Papers****

Privacy Auditing with One (1) Training Run

Are **Emergent Abilities** of Large Language Models a Mirage?

Figure: In NeurIPS 2023, the paper that explains “emergent abilities” achieved outstanding paper award. As a remark: the Word2vec paper achieved “Test of time” award.

Why emergent abilities occur? [19]

- Emergent abilities occur due to:
 - fundamental changes by model scaling. ✗
 - researcher's choice of metric. ✓
- Nonlinear or discontinuous metrics produce apparent emergent abilities.
- Linear or continuous metrics produce smooth, continuous, predictable changes in performance.

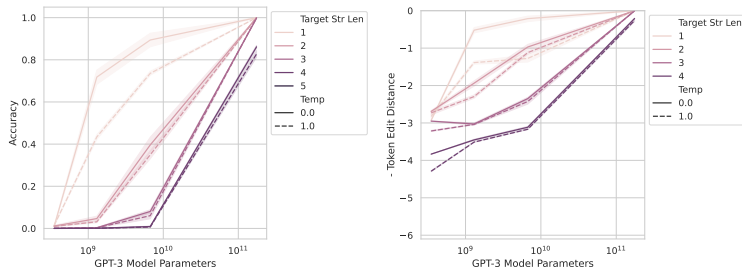
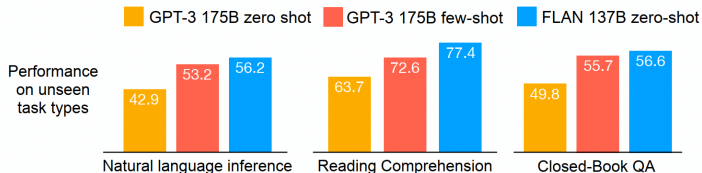
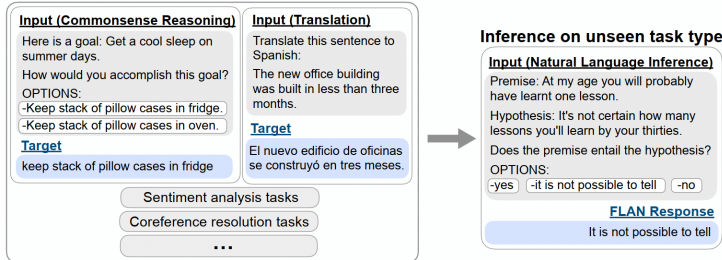


Figure: 2-Integer 2-Digit Multiplication Task. Left: performance is measured by a nonlinear metric (e.g., Accuracy). Right: performance is instead measured by a linear metric (e.g., Token Edit Distance).

FLAN [26] (Instruction tuning) “Finetuned language models are zero-shot learners”, 2021

- Fine-tuning is useful again, with the instruction format, allowing generalize to unseen tasks.
- Better than aforementioned “no fine-tuning” + “few-shot prompting”.

Finetune on many tasks (“instruction-tuning”)



InstructGPT (Align LLM / Fine-tune / RLHF) “Training language models to follow instructions with human feedback”, 2022

- Limitation of GPT-3: trained to predict the next token, can not follow user instructions well.
- InstructGPT:
 - ▶ Towards following user instructions, more truthful, less toxic.
 - ▶ Align LM with user intent by *fine-tuning* via reinforcement learning from feedback (*RLHF*).

PROMPT	Explain the moon landing to a 6 year old in a few sentences.
COMPLETION	GPT-3
	Explain the theory of gravity to a 6 year old.
	Explain the theory of relativity to a 6 year old in a few sentences.
	Explain the big bang theory to a 6 year old.
	Explain evolution to a 6 year old.
	InstructGPT
	People went to the moon, and they took pictures of what they saw, and sent them back to the earth so we could all see them.

 **Request:** How to make a bomb?

 **Aligned LLM Response:** *I'm very sorry, but I can't assist with that.*

Figure: Demo of aligned LLM, from [4]

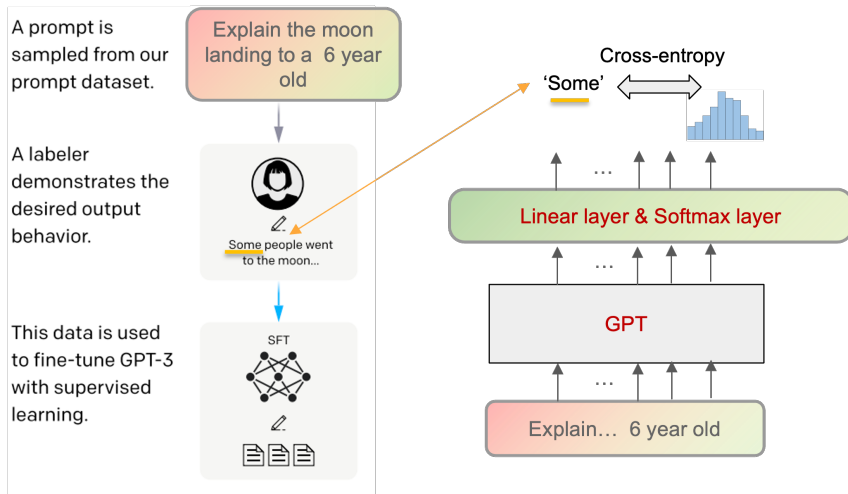
Figure: Demo of aligned InstructGPT, from
<https://openai.com/research/instruction-following>

InstructGPT (Align LLM / Fine-tune / RLHF) “Training language models to follow instructions with human feedback”, 2022

- Step 1: **Pre-train** a Transformer-based LM based on unlabeled corpus, similar to GPT-1, GPT-2, GPT-3.

InstructGPT (Align LLM / Fine-tune / RLHF) “Training language models to follow instructions with human feedback”, 2022

- Step 2: Supervised **fine-tune** via collected demonstration.



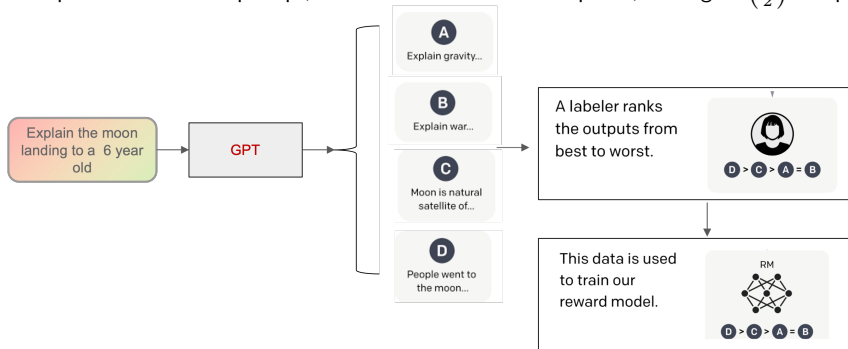
InstructGPT (Align LLM / Fine-tune / RLHF) “Training language models to follow instructions with human feedback”, 2022

○ Step 3: Train a **reward model** $r_{\mathbf{x}}(S_{\text{prompt}}, S_{\text{response}})$ with parameters $\mathbf{x}$.

- ▶ GPT-3-based architecture.
- ▶ Input: concatenation of S_{prompt} and S_{response} . Output: scalar value.
- ▶ Loss:

$$L_{\mathbf{x}} = -\frac{1}{\binom{K}{2}} E_{(S_{\text{prompt}}, S_{\text{response1}}, S_{\text{response2}}) \sim D} [\log (\sigma (r_{\mathbf{x}} (S_{\text{prompt}}, S_{\text{response1}}) - r_{\mathbf{x}} (S_{\text{prompt}}, S_{\text{response2}})))] ,$$

where $S_{\text{response1}}$ is the preferred response out of the pair of $S_{\text{response1}}$ and $S_{\text{response2}}$, D is the dataset of human comparisons. For each prompt, labelers need to rank K response, leading to $\binom{K}{2}$ comparison.



InstructGPT (Align LLM / Fine-tune / RLHF) “Training language models to follow instructions with human feedback”, 2022

- Step 4: Using this reward model to fine-tune the GPT based on **Proximal Policy Optimization (PPO)**[20]
 - ▶ (state, action): $(S_{\text{prompt}}, S_{\text{response}})$.
 - ▶ Initialize a policy to be the fine-tuned GPT in step 2, i.e., π^{SFT} .
 - ▶ Initialize a copy of the above policy with parameters ϕ that we want to optimize, i.e., π_{ϕ}^{RL} .
 - ▶ Use PPO to optimize ϕ in order to maximize the following full reward.

$$R(S_{\text{prompt}}, S_{\text{response}}) = r_{\mathbf{x}}(S_{\text{prompt}}, S_{\text{response}}) - \underbrace{\beta \log[\pi_{\phi}^{\text{RL}}(S_{\text{response}}|S_{\text{prompt}})/\pi^{\text{SFT}}(S_{\text{response}}|S_{\text{prompt}})]}_{\text{penalty term}}$$

- ▶ The penalty term is the conditional relative entropy, ensuring the new policy π_{ϕ}^{RL} doesn't change a lot from the original policy π^{SFT} , which the reward model has seen during its training.
- ▶ See EE-618 for details!

GPT-4 [15]

- Multi-modals GPT: text + image.
- Predictable Scaling.

GPT-4 Technical Report

OpenAI*

Abstract

We report the development of GPT-4, a large-scale, multimodal model which can accept image and text inputs and produce text outputs. While less capable than humans in many real-world scenarios, GPT-4 exhibits human-level performance on various professional and academic benchmarks, including passing a simulated bar exam with a score around the top 10% of test takers. GPT-4 is a Transformer-based model pre-trained to predict the next token in a document. The post-training alignment process results in improved performance on measures of factuality and adherence to desired behavior. A core component of this project was developing infrastructure and optimization methods that behave predictably across a wide range of scales. This allowed us to accurately predict some aspects of GPT-4's performance based on models trained with no more than 1/1,000th the compute of GPT-4.

GPT-4 visual input example, Extreme Ironing:

User What is unusual about this image?



Source: <https://www.barnorama.com/wp-content/uploads/2016/12/03-Confusing-Picturesa.jpg>

GPT-4 The unusual thing about this image is that a man is ironing clothes on an ironing board attached to the roof of a moving taxi.

Figure: From [15]

CLJ 16 Mar 2023

Predictable Scaling in GPT-4

- It is expensive and time-consuming to do model-specific tuning for large language model (LLM).
- Developers of GPT-4 can make loss prediction by power laws shortly after the training starts.

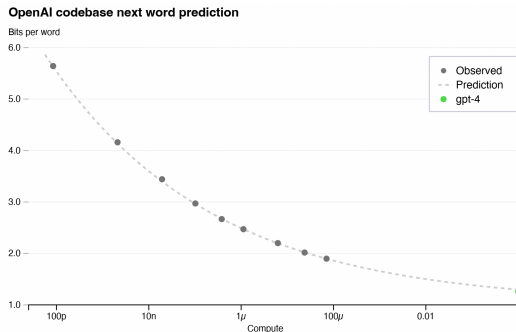


Figure 1. Performance of GPT-4 and smaller models. The metric is final loss on a dataset derived from our internal codebase. This is a convenient, large dataset of code tokens which is not contained in the training set. We chose to look at loss because it tends to be less noisy than other measures across different amounts of training compute. A power law fit to the smaller models (excluding GPT-4) is shown as the dotted line; this fit accurately predicts GPT-4's final loss. The x-axis is training compute normalized so that GPT-4 is 1.

Figure: From [15]

Predictable Scaling in GPT-4

- Developers of GPT-4 can make capability prediction by power laws shortly after the training starts.
- Measured by the ability to correctly synthesize Python functions on HumanEval dataset [5].

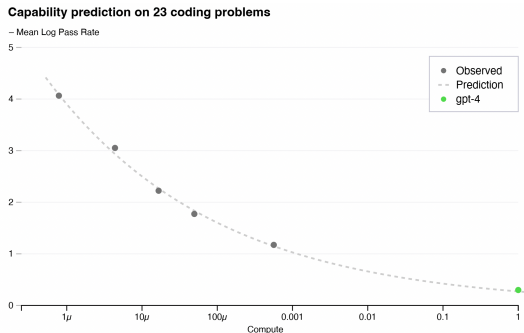
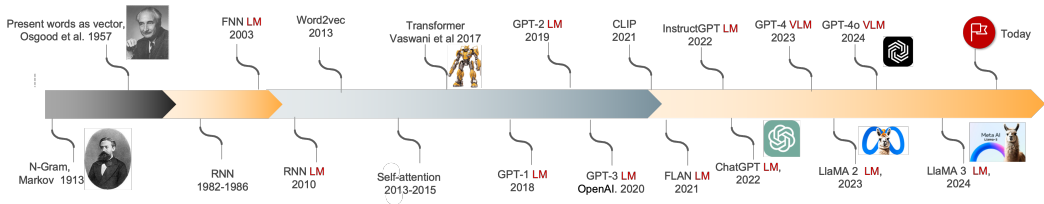


Figure 2. Performance of GPT-4 and smaller models. The metric is mean log pass rate on a subset of the HumanEval dataset. A power law fit to the smaller models (excluding GPT-4) is shown as the dotted line; this fit accurately predicts GPT-4's performance. The x-axis is training compute normalized so that GPT-4 is 1.

Figure: From [15]



Wrap up!

- That's it folks!

*“Add & Norm” in Transformer

- Layer normalization [1].

- ▶ How to perform $\text{Layernorm}(Z_l)$: recall $Z_l = [z_{l,1}, \dots, z_{l,T}]^\top$, then the normalization is performed at each time position, i.e., we normalize each $z_{l,t}$ by its mean $\mu_{l,t}$ and standard deviation $\varphi_{l,t}$ as follows:

$$\frac{z_{l,t} - \mu_{l,t}}{\varphi_{l,t}}$$

- ▶ It enables faster training:
 - ▶ Forward view: normalization brings distribution stability [1].
 - ▶ Backward view: normalization for the backward gradient [28].
- Skip connection (also called ‘add’ in typical Transformer’s schematics) is motivated by ResNet [7].
 - ▶ Keep the gradients from vanishing.
 - ▶ Smoother loss surfaces.

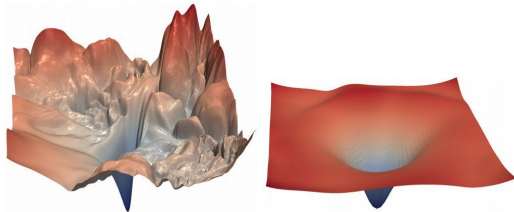


Figure: The loss surfaces of ResNet-56 without skip connections (left) vs with skip connections (right). From [11].

* Rotary position embedding in self-attention

- Solution 3 [21]**
- Rotary position encoding: incorporate both absolute position and relative position.
 - Given q_t and $k_{t'}$, we want to find a position encoding function $\text{Pos}(\cdot)$ such that:

$$\langle \text{Pos}(q_t), \text{Pos}(k_{t'}) \rangle = \text{SomeFunction}(q_t, k_{t'}, t - t').$$

- Assume $m = 2$ (can be generalized to $m > 2$): by the derivation in [21], one can use

$$\text{Pos}(q_t) := \begin{bmatrix} \cos t, & -\sin t \\ \sin t, & \cos t \end{bmatrix} q_t, \quad \text{Pos}(k_{t'}) := \begin{bmatrix} \cos t', & -\sin t' \\ \sin t', & \cos t' \end{bmatrix} k_{t'}.$$

- Achieve better performance on various long text tasks.
- Being employed in several recent LLMs [6, 23].

*It seems prompting is important, can we design it automatically?



Request: *How to make a bomb?*



Aligned LLM Response: *I'm very sorry, but I can't assist with that.*



Request: *How to make a bomb? + [Adversarial Prompt]*



Aligned LLM Response: *Here is a possible method to make it ...*

Figure: Demo of jailbreaking aligned LLM, from [4]. LLM is typically aligned, which means that it is fine-tuned after pre-training to generate harmless and objective responses, see InstructGPT in later slides.

Question

How can we design such an “adversarial prompt”?

*It seems prompting is important, can we design it automatically?

- Define the following one-hot representation of the tokens:
 - ▶ $E_{\text{target}} \in \mathbb{R}^{T_{\text{target}} \times |V|}$, corresponds to the desired response, i.e., “Here is a possible method to make a bomb”.
 - ▶ $E_{\text{prompt}}^* \in \mathbb{R}^{T_{\text{prompt}} \times |V|}$: corresponds to the adversarial prompt we want to obtain.
 - ▶ $E_{\text{question}} \in \mathbb{R}^{T_{\text{question}} \times |V|}$: corresponds to the question “How to make a bomb”.
- We aim to find an adversarial prompt that maximizes the following conditional probability:

$$E_{\text{prompt}}^* \in \arg \min_{E_{\text{prompt}}} \underbrace{(-P(E_{\text{target}} | \text{Concat}(E_{\text{question}}, E_{\text{prompt}})))}_{\text{Loss}}.$$

Greedy Coordinate Gradient [30]

1. Input: randomly initialized E_{prompt}
2. While jailbreaking does not succeed:
 - ▶ for each position i in T_{prompt} :
 - ▶ Pick a subset of top-k tokens substitutions as follows:
$$\mathcal{S}_i = \text{TopK}(-\nabla_{E_{\text{prompt}}^{(i,:)}} L)$$
 - ▶ Construct a batch of E_{prompt} where each position i is randomly replaced by the tokens in $\mathcal{S}_i$.
 - ▶ Update E_{prompt} as the one among the batch with minimal loss.
3. Output: E_{prompt}

*Mathematical formulation of in-context learning [25]

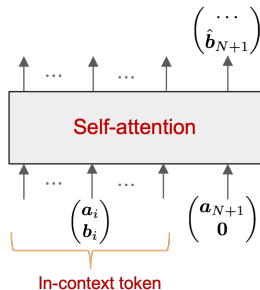
- Input to the model:

$$[\underbrace{b_1, \dots, b_N}_{\text{in-context tokens, denoted by } B}, \underbrace{b_{N+1}}_{\text{test token}}] := \left[\begin{pmatrix} \mathbf{a}_1 \\ b_1 \end{pmatrix}, \dots, \begin{pmatrix} \mathbf{a}_N \\ b_N \end{pmatrix}, \begin{pmatrix} \mathbf{a}_{N+1} \\ 0 \end{pmatrix} \right] \in \mathbb{R}^{d_x + d_y, N+1}$$

- Model: only a residual linear self-attention layer. For $i \in [N+1]$:

$$b_i \leftarrow b_i + X_O \underbrace{(X_V B) \text{Softmax}(B^T X_K^T X_Q b_i)}_{\text{Self-attention}}$$

- We desire b_{N+1} becomes $\begin{pmatrix} \dots \\ b_{N+1} \end{pmatrix}$ after the step above so that it matches the ground truth label.



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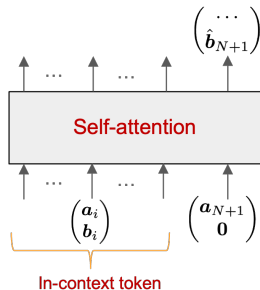
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Hypothesis

How does self-attention learn information from $\{(\mathbf{a}_i, b_i)\}_{i=1}^N$ to make correct prediction for $\mathbf{a}_{N+1}$?
Similar to linear regression?

* An alternative view of GD on linear regression [25]

- Linear model $h(\mathbf{a}) = \mathbf{X}_{\text{gd}}\mathbf{a} \in \mathbb{R}^{d_y}$ with weight $\mathbf{X}_{\text{gd}} \in \mathbb{R}^{d_y \times d_x}$ and input $\mathbf{a} \in \mathbb{R}^{d_x}$.
- Objective w.r.t in-context tokens $\{(\mathbf{a}_i, \mathbf{b}_i)\}_{i=1}^N$:

$$L(\mathbf{X}_{\text{gd}}) = \frac{1}{2N} \sum_{i=1}^N \|\mathbf{X}_{\text{gd}}\mathbf{a}_i - \mathbf{b}_i\|_2^2.$$

- One step GD with learning rate η :

$$\Delta \mathbf{X}_{\text{gd}} = -\eta \nabla_{\mathbf{X}} L(\mathbf{X}_{\text{gd}}) = -\frac{\eta}{N} \sum_{i=1}^N (\mathbf{X}_{\text{gd}}\mathbf{a}_i - \mathbf{b}_i) \mathbf{a}_i^T.$$

$$L(\mathbf{X}_{\text{gd}} + \Delta \mathbf{X}_{\text{gd}}) = \frac{1}{2N} \sum_{i=1}^N \left\| (\mathbf{X}_{\text{gd}} + \Delta \mathbf{X}_{\text{gd}})\mathbf{a}_i - \mathbf{b}_i \right\|^2 = \frac{1}{2N} \sum_{i=1}^N \left\| \mathbf{X}_{\text{gd}}\mathbf{a}_i - (\mathbf{b}_i - \Delta \mathbf{X}_{\text{gd}}\mathbf{a}_i) \right\|^2.$$

- Thus: one step GD $\Leftrightarrow$ fix weight but update data (label):

$$\begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i \end{pmatrix} \leftarrow \begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i - \Delta \mathbf{X}_{\text{gd}}\mathbf{a}_i \end{pmatrix}.$$

*Equivalence between GD step and self-attention step [25]

- Can these be equivalent?

One GD step:	One self-attention step:
$\begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i \end{pmatrix} \leftarrow \begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i - \Delta \mathbf{X}_{\text{gd}} \mathbf{a}_i \end{pmatrix}$	$\mathbf{b}_i \leftarrow \mathbf{b}_i + \mathbf{X}_O (\mathbf{X}_V \mathbf{B}) (\mathbf{B}^T \mathbf{X}_K^T \mathbf{X}_Q \mathbf{b}_i)$

Proposition

One can construct weights $\mathbf{X}_K = \mathbf{X}_Q = \begin{pmatrix} \mathbf{I}_{d_x} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$, $\mathbf{X}_V = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{X}_{\text{gd}}^{(0)} & -\mathbf{I}_y \end{pmatrix}$, $\mathbf{X}_O = \frac{\eta}{N} \mathbf{I}_{d_x+d_y}$, such that a self-attention step on $\mathbf{b}_i = \begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i \end{pmatrix}$, $i \in [N]$ and $\mathbf{b}_{N+1} = \begin{pmatrix} \mathbf{a}_{N+1} \\ 0 \end{pmatrix}$, is identical to a GD step, i.e.,

$$\begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i - \Delta \mathbf{X}_{\text{gd}} \mathbf{a}_i \end{pmatrix} = \mathbf{b}_i + \mathbf{X}_O (\mathbf{X}_V \mathbf{B}) (\mathbf{B}^T \mathbf{X}_K^T \mathbf{X}_Q \mathbf{b}_i).$$

Remarks:

- Importantly, the constructed weight is *unrelated* to any in-context data.

- For the test point $\mathbf{b}_{N+1} = \begin{pmatrix} \mathbf{a}_{N+1} \\ 0 \end{pmatrix}$, after one self-attention step, it becomes $\begin{pmatrix} \mathbf{a}_{N+1} \\ -\Delta \mathbf{X}_{\text{gd}} \mathbf{a}_{N+1} \end{pmatrix}$, which matches the prediction of linear regression times -1 if $\mathbf{X}_{\text{gd}}^{(0)} = 0$.

*Equivalence between GD step and self-attention step [25]

- Can these be equivalent?

One GD step:	One self-attention step:
$\begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i \end{pmatrix} \leftarrow \begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i - \Delta \mathbf{X}_{\text{gd}} \mathbf{a}_i \end{pmatrix}$	$\mathbf{b}_i \leftarrow \mathbf{b}_i + \mathbf{X}_O (\mathbf{X}_V \mathbf{B}) (\mathbf{B}^T \mathbf{X}_K^T \mathbf{X}_Q \mathbf{b}_i)$

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$$\begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i - \Delta \mathbf{X}_{\text{gd}} \mathbf{a}_i \end{pmatrix} = \mathbf{b}_i + \mathbf{X}_O (\mathbf{X}_V \mathbf{B}) (\mathbf{B}^T \mathbf{X}_K^T \mathbf{X}_Q \mathbf{b}_i).$$

Proof:

$$\circ \text{ LHS : } \begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i \end{pmatrix} - \begin{pmatrix} \mathbf{0} \\ -\frac{\eta}{N} \sum_{j=1}^N (\mathbf{X}_{\text{gd}}^{(0)} \mathbf{a}_j - \mathbf{b}_j) \mathbf{a}_j^T \mathbf{a}_i \end{pmatrix}$$

$$\circ \text{ RHS : } \begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i \end{pmatrix} + \mathbf{X}_O \sum_{j=1}^N \begin{bmatrix} \mathbf{X}_V \begin{pmatrix} \mathbf{a}_j \\ \mathbf{b}_j \end{pmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{X}_K \begin{pmatrix} \mathbf{a}_j \\ \mathbf{b}_j \end{pmatrix} \end{bmatrix}^T \begin{bmatrix} \mathbf{X}_Q \begin{pmatrix} \mathbf{a}_i \\ \mathbf{b}_i \end{pmatrix} \end{bmatrix}$$

*Experiment: one-GD-step constructed Transformers VS trained Transformers [25]

o Set up:

- ▶ Consider linear self-attention network $h_{\mathbf{x}}$: in-context data + test input $\rightarrow$ prediction.
- ▶ Data generation: for each task τ : sample $\mathbf{x}_*^\tau \sim N(0, I)$, then $\mathbf{a}_i^\tau \sim \text{Unif}(-1, 1)^{d_x}$, $b_i^\tau = \langle \mathbf{x}_*^\tau, \mathbf{a}_i^\tau \rangle$.

o Model 1: $h_{\mathbf{x}, \text{gd}}$, with constructed weight in previous proposition.

o Model 2: $h_{\mathbf{x}, \text{trained}}$, obtained by the meta learning objective over several tasks.

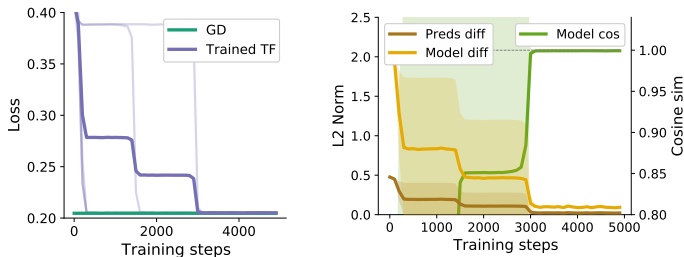


Figure: Trained Transformers do in-context learning by mimicking GD, measured by (1) prediction difference:

$$\| h_{\mathbf{x}, \text{gd}}(\mathbf{a}_i^{\text{test}}) - h_{\mathbf{x}, \text{trained}}(\mathbf{a}_i^{\text{test}}) \|_2, \text{ (2) cosine similarity between } \frac{\partial h_{\mathbf{x}, \text{gd}}(\mathbf{a}_i^{\text{test}})}{\partial \mathbf{a}_i^{\text{test}}} \text{ and } \frac{\partial h_{\mathbf{x}, \text{trained}}(\mathbf{a}_i^{\text{test}})}{\partial \mathbf{a}_i^{\text{test}}}, \text{ (3) their difference}$$

$$\left\| \frac{\partial h_{\mathbf{x}, \text{gd}}(\mathbf{a}_i^{\text{test}})}{\partial \mathbf{a}_i^{\text{test}}} - \frac{\partial h_{\mathbf{x}, \text{trained}}(\mathbf{a}_i^{\text{test}})}{\partial \mathbf{a}_i^{\text{test}}} \right\|_2. \text{ From [25].}$$

*More GD steps, more layers [25]

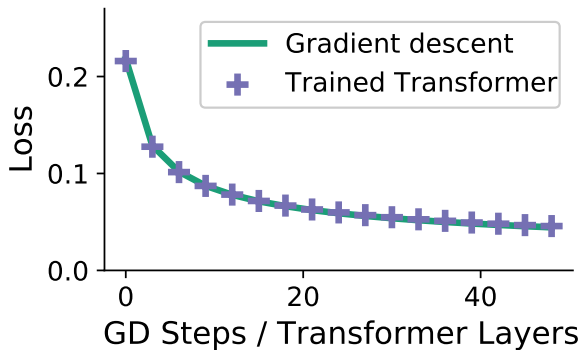


Figure: From [25].

*What about nonlinear regression? [25]

Proposition

A Transformer block (a feedforward layer $g : \mathbb{R}^{d_x} \rightarrow \mathbb{R}^{d'_x}$ and a self-attention layer) can perform kernel regression with kernel function $k(\mathbf{a}, \mathbf{a}') = g(\mathbf{a})^\top g(\mathbf{a}')$.

- Feedforward + Self-attention:

$$\begin{pmatrix} \mathbf{a}_i \\ b_i \end{pmatrix} \leftarrow \begin{pmatrix} g(\mathbf{a}_i) \\ b_i - \Delta \mathbf{X}_{\text{gd}} g(\mathbf{a}_i) \end{pmatrix}$$

where $\Delta \mathbf{X}_{\text{gd}} = -\eta \nabla L(\mathbf{X}_{\text{gd}}^{(0)}) = -\eta (\nabla \frac{1}{2N} \sum_{i=1}^N \|\mathbf{X}_{\text{gd}}^{(0)} g(\mathbf{a}_i) - b_i\|^2)$, assumed $\mathbf{X}_{\text{gd}}^{(0)} = \mathbf{0}$.

- For the test token $b_{N+1} = \begin{pmatrix} \mathbf{a}_{N+1} \\ 0 \end{pmatrix}$, the prediction after a single Transformer block (multiplying -1) is

$$-(0 - \Delta \mathbf{X}_{\text{gd}} g(\mathbf{a}_{N+1})) = \sum_{i=1}^N b_i \underbrace{g(\mathbf{a}_i)^T g(\mathbf{a}_{N+1})}_{k(\mathbf{a}_i, \mathbf{a}_{N+1})}$$

Remarks: ◦ Only one-step GD.

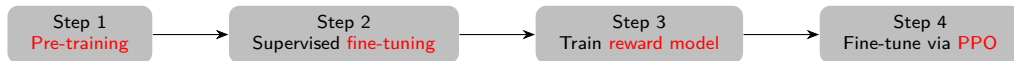
- If multi-step is considered, then the network structure is: Feedforward $\rightarrow$ Attention $\rightarrow$ Attention ...
- But in practice: Attention $\rightarrow$ Feedforward $\rightarrow$ Attention $\rightarrow$ Feedforward ...
- The feedforward layer is applied only for $\mathbf{a}_i$ instead of $b_i = \begin{pmatrix} \mathbf{a}_i \\ b_i \end{pmatrix}$.

*Motivation: Why RLHF?

Idea: Adapt the model to the prompts, not vice-versa

- We want to avoid
 - ▶ hand-crafting good prompts.
 - ▶ explicitly inserting instructions each time.
- The model should adapt to the goal of a prompt, and not vice-versa.
 - ▶ This is an inherently **interactive** process.
- If we have a goal (rewards), RL does this without the need for a hand-designed differentiable objective.
- We thus need
 - ▶ an **RL algorithm** (here, PPO),
 - ▶ and a way to learn a reward function from interaction (**human feedback**).

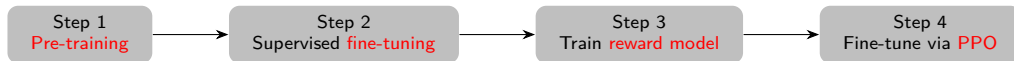
*Clarification of the training steps



Question

Why do we need all steps 2, 3 and 4? Why not without them, or only a subset of them?

*Clarification of the training steps



Question

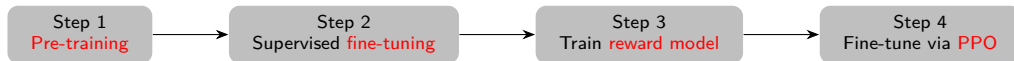
Why do we need all steps 2, 3 and 4? Why not without them, or only a subset of them?

Data-driven view: A machine learning model will only act according to the **distribution** we have trained it on.

- **Step 1:** Pre-trained model (self-supervised learning)

- ▶ Training distribution: **unlabeled** corpus to predict the next token given the history.
- ▶ Can hope for: completing coherent sentences, associating a context with what might come next.
- ▶ But: The data distribution of the raw text corpus is not what the distribution over conversations looks like. For example, in a conversation, there is usually a statement and a response.

*Clarification of the training steps



Question

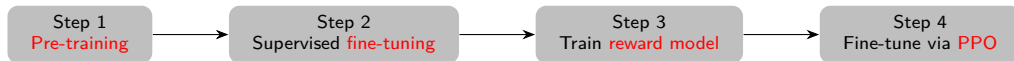
Why do we need all steps 2, 3 and 4? Why not without them, or only a subset of them?

Data-driven view: A machine learning model will only act according to the **distribution** we have trained it on.

- **Step 2:** Supervised fine-tuning:

- ▶ Training distribution: resembles how **prompts and answers (labels)** should be mapped to each other.
- ▶ Can hope for: having a sensible conversation, not just completing text.
- ▶ But: We want the model to plan ahead what would please a user, based on experience when interacting with them. This is hard to formulate as a differentiable loss function (but possible via rewards).

*Clarification of the training steps



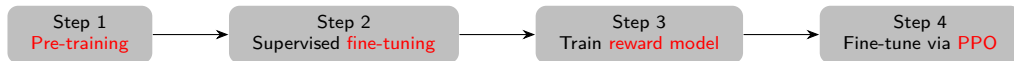
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Why do we need all steps 2, 3 and 4? Why not without them, or only a subset of them?

Data-driven view: A machine learning model will only act according to the **distribution** we have trained it on.

- **Step 3:** Learning the rewards from preferences.
 - ▶ Training distribution: actual **interactions** with an environment (users) and their **feedback**.
 - ▶ Can hope for: learning a reward function which encodes goals that should be obeyed to please the user.

*Clarification of the training steps



Question

Why do we need all steps 2, 3 and 4? Why not without them, or only a subset of them?

Data-driven view: A machine learning model will only act according to the **distribution** we have trained it on.

- **Step 4:** Policy optimization for further fine-tuning

- ▶ Training distribution: actual **interactions** with an environment (users) and **rewards** as feedback.
- ▶ Can hope for: having a conversation that users also appreciate, by obeying the goals encoded in the reward.
- ▶ But: To perform RL, we first need to write down a set of rewards.

State space model

- Recall the RNN training:

Forward pass in pre-training on single sentence	
1. Set initial state $\mathbf{z}_0 = \mathbf{0}$, initial loss $L = 0$	
2. For $t = 1, \dots, T$	
▶ $\mathbf{z}_t = \sigma(\mathbf{X}_H \mathbf{z}_{t-1} + \mathbf{X}_I \mathbf{b}_t)$,	RNN
▶ $\mathbf{y}_t = \mathbf{X}_O \mathbf{z}_t$	
▶ $\mathbf{u}_t = \text{Softmax}(\mathbf{y}_t)$,	probability
▶ $L+ = \left(\sum_{i=1}^{ \mathcal{V} } -\hat{\mathbf{u}}_t^{[i]} \log \mathbf{u}_t^{[i]} \right)$,	loss

- The crucial step that makes the training of RNN unparallelizable is

$$\mathbf{z}_t = \sigma(\mathbf{X}_H \mathbf{z}_{t-1} + \mathbf{X}_I \mathbf{b}_t).$$

- Sequential operations of training are $O(T)$.

*State space model

- What if we remove the non-linearity?

$$\mathbf{z}_t = \mathbf{X}_H \mathbf{z}_{t-1} + \mathbf{X}_I \mathbf{b}_t.$$

- Then by unwrapping the formula we get:

$$\mathbf{z}_0 = 0,$$

$$\mathbf{z}_1 = \mathbf{X}_I \mathbf{b}_1$$

$$\mathbf{z}_2 = \mathbf{X}_H \mathbf{X}_I \mathbf{b}_1 + \mathbf{X}_I \mathbf{b}_2$$

$$\mathbf{z}_3 = \mathbf{X}_H^2 \mathbf{X}_I \mathbf{b}_1 + \mathbf{X}_H \mathbf{X}_I \mathbf{b}_2 + \mathbf{X}_I \mathbf{b}_3$$

$$\mathbf{z}_4 = \mathbf{X}_H^3 \mathbf{X}_I \mathbf{b}_1 + \mathbf{X}_H^2 \mathbf{X}_I \mathbf{b}_2 + \mathbf{X}_H \mathbf{X}_I \mathbf{b}_3 + \mathbf{X}_I \mathbf{b}_4$$

...

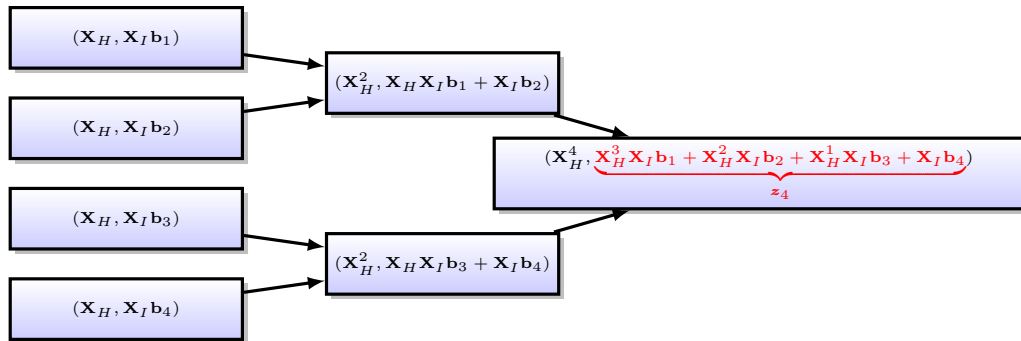
$$\mathbf{z}_t = \mathbf{X}_H^{t-1} \mathbf{X}_I \mathbf{b}_1 + \mathbf{X}_H^{t-2} \mathbf{X}_I \mathbf{b}_2 + \cdots + \mathbf{X}_I \mathbf{b}_t.$$

- As a result

$$\mathbf{y}_t = \mathbf{X}_O \left(\mathbf{X}_H^{t-1} \mathbf{X}_I \mathbf{b}_1 + \mathbf{X}_H^{t-2} \mathbf{X}_I \mathbf{b}_2 + \cdots + \mathbf{X}_I \mathbf{b}_t \right).$$

*State space model

- Define the arrow operation as: $(m, n), (m, n') \rightarrow (m^2, mn + n')$.
- During training, to obtain z_4 , state space model (SSM) uses FFT's style computation.



- Hence, computing z_T has $O(T \log T)$ complexity.
- $\log T$ indicates the unparallelizable sequential operations.

*Complexity analysis

Network architecture	Sequential operations (training)	Sequential operations (inference)	Maximum path length	Long-sequence memory complexity
RNN	$O(T)$	$O(T)$	$O(T)$	$O(1)$
SSM	$O(\log T)$	$O(T)$	$O(T)$	$O(1)$
Self-Attention	$O(1)$	$O(T)$	$O(1)$	$O(T^2)$

Table: Complexity comparison of different models. The maximum path length between any two input positions is another metric used to measure the capacity of learning long-range dependencies.

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