Stat 9911
Principles of AI: LLMs
Large Language Model Architectures 01

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Input and Output

- We will discuss LLM architectures, and specifically attention and transformers.

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Input and Output

- **Input**: Text
- **Output**: Text
- Examples: Question-answering ($Q \rightarrow A$), translation, summarization ($X_1, \ldots, X_n \rightarrow S$), etc.
- Key strength: Generic format, covers many tasks.
- Origins in sequence-to-sequence (seq2seq) modeling (Sutskever et al., 2014).

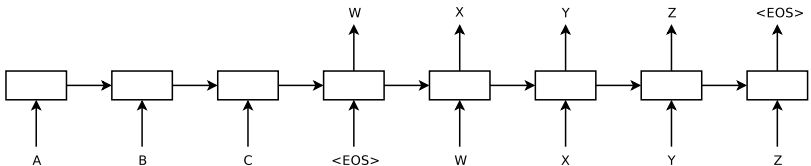


Figure: seq2seq (Sutskever et al., 2014)

Operationalizing Input and Output

- Represent text as a sequence $S = (s_1, s_2, \ldots, s_k)$ of symbols s_j from a fixed universe.
- Use autoregressive next-symbol/word prediction to reduce the task to supervised learning.
- Break the task into smaller subtasks:
  - $S \rightarrow o_1$
  - $S, o_1 \rightarrow o_2$
  - $\ldots$
  - $S, o_1, \ldots, o_{m-1} \rightarrow o_m$

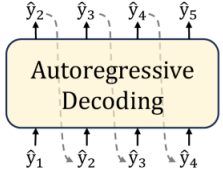


Figure: From Xia et al., 2022

Advantages and Disadvantages of the Approach

Advantages:

- Generic format.
- Predicting the next symbol one at a time is simpler.

Disadvantages:

- Sequential/Autoregressive processing is non-parallelizable.
- No efficient mechanism for backtracking mistakes. [Research direction: Diffusion LMs.]
- Exponentially decreasing correctness probability.

Drawbacks of Prediction Approach

- No immutable knowledge base or built-in behavior guarantees.
- No precise specifications compared to classical CS/engineering (e.g., programming languages, databases), or stats (probabilistic guarantees, e.g., confidence interval coverage).
- AI lacks any guarantees or precise performance analysis.
- The popular phenomenon of "emergence" refers exactly to unpredictable behavior that appears spontaneously during training.
- Interventions via modifying representations still do not resolve problems.

Symbol Representation

- **Options for symbols:**
  - Letters/Characters (e.g., ‘a‘, ‘+‘, ‘1‘).
  - Words (e.g., ‘cat‘, ‘dogs‘).
- Considerations
  1. The smallest symbol set could be characters (e.g., 255 ASCII).
  2. Words could represent a larger set, especially in tasks involving natural language (e.g., 100K words across 1K languages).
  3. There is often redundancy in word-based systems. For example, words like ‘cat‘ and ‘cats‘ or ‘dog‘ and ‘dogs‘ are closely related, and the system should know this.

Compromise for Symbol Representation: Tokens

- **Tokens** are subwords (e.g., 'subword' $\rightarrow$ '[sub][word][s]').
- See e.g., OpenAI tokenizers
- How construct them? Start with base vocab of chars. Find groupings of frequent pairs of characters, add them to vocab, repeat.
- See efficient tokenization methods like Byte Pair Encoding (BPE), Sennrich et al. (2016).
- Today's vocabulary sizes: 50,000 to 100,000.
- Key to adapting LLM architectures to other modalities is to define tokens. E.g., for images define the tokens as ... patches.

Figure: Tokenization in Vision Transformers (Dosovitskiy et al., 2021)

Learning a Next-Token Predictor

- Given any input text $x_{1:i-1}$, want to predict next token x_i.
- We will learn a predictor from a large dataset/corpus D of text.
- Data? The internet: Wikipedia, Arxiv, Reddit, Stack Exchange, other websites, books

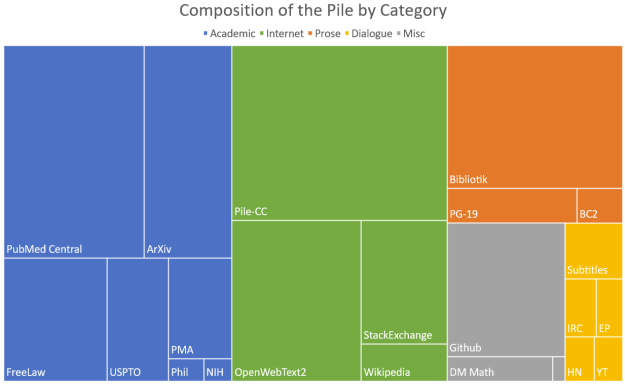


Figure: The Pile (800 GB) (Gao et al., 2020)

Aside: Copyrighted Training Data

- Data is known to (or allegedly does) include copyrighted and pirated content, e.g., the LibGen 'shadow library'. The biggest IP theft in history?

With just two hours left before the fact discovery cut-off on Friday, December 13, 2024, Meta produced some of the most incriminating internal documents it has produced to date relevant to Meta's copyright infringement claim and fair use defense, as well as Plaintiffs' proposed new claims. These documents concern Meta's torrenting and processing of pirated copyrighted works, including that: Meta's CEO, Mark Zuckerberg, approved Meta's use of the LibGen dataset notwithstanding concerns within Meta's AI executive team (and others at Meta) that LibGen is "a dataset we know to be pirated," Stein Reply Decl. ("Reply Ex."), Ex. A at 211699, 211702; top Meta engineers discussed accessing and reviewing LibGen data but hesitated to get started because "torrenting from a [Meta-owned] corporate laptop doesn't feel right 😬," Reply Ex. B at 204224; one of those engineers "filtered . . . copyright lines" and other data out of LibGen to prepare a CMI-stripped version of it to train Llama, Reply Ex. C at 204220-21; and, by January 2024, Meta had already torrented (both downloaded and distributed) data from LibGen, Reply Ex. D.[1] And just yesterday, when asked about the type of piracy described in the TACC, Mr. Zuckerberg testified that such activity would raise "lots of red flags" and "seems like a bad thing." Reply Ex. E (Zuckerberg Dep. Tr.) at 102:10–14; 98:24–99:2.

Figure: From court case Kadrey vs Meta, via X

Empirical Next-Token Predictor

- Use empirical probability estimate (Shannon, 1948):

$$P(x_i|x_{1:i-1}) = \frac{\#(x \in D : x = x_{1:i})}{\#(x \subset D : x = x_{1:(i-1)})}$$

We can also approximate to a natural language by means of a series of simple artificial languages. The zero-order approximation is obtained by choosing all letters with the same probability and independently. The first-order approximation is obtained by choosing successive letters independently but each letter having the same probability that it does in the natural language.[5] Thus, in the first-order approximation to English, E is chosen with probability .12 (its frequency in normal English) and W with probability .02, but there is no influence between adjacent letters and no tendency to form the preferred digrams such as *TH*, *ED*, etc. In the second-order approximation, digram structure is introduced. After a letter is chosen, the next one is chosen in accordance with the frequencies with which the various letters follow the first one. This requires a table of digram frequencies $p_i(j)$. In the third-order approximation, trigram structure is introduced. Each letter is chosen with probabilities which depend on the preceding two letters.

Figure: Shannon (1948)

Empirical Next-Token Predictor

3. The Series of Approximations to English

1. Zero-order approximation (symbols independent and equi-probable).
   XFOML RXKHRJFFJUJ ZLPWCFWKCYJ
   FFJEYVKCQSGXYD QPAAMKBZAACIBZLHJQD
2. First-order approximation (symbols independent but with frequencies of English text).
   OCRO HLI RGWR NMIELWIS EU LL NBNESEBYA TH EEI ALHENHTTPA OOBTTVA NAH BRL
3. Second-order approximation (digram structure as in English).
   ON IE ANTSOUTINYS ARE T INCTORE ST BE S DEAMY ACHIN D ILONASIVE TUCOOWE AT TEASONARE FUSO TIZIN ANDY TOBE SEACE CTISBE
4. Third-order approximation (trigram structure as in English).
   IN NO IST LAT WHEY CRATICT FROURE BIRS GROCID PONDENOME OF DEMONSTURES OF THE REPTAGIN IS REGOACTIONA OF CRE
5. First-Order Word Approximation. Rather than continue with tetragram, $\cdots$, n-gram structure it is easier and better to jump at this point to word units. Here words are chosen independently but with their appropriate frequencies.
   REPRESENTING AND SPEEDILY IS AN GOOD APT OR COME CAN DIFFERENT NATURAL HERE HE THE A IN CAME THE TO OF TO EXPERT GRAY COME TO FURNISHES THE LINE MESSAGE HAD BE THESE.
6. Second-Order Word Approximation. The word transition probabilities are correct but no further structure is included.
   THE HEAD AND IN FRONTAL ATTACK ON AN ENGLISH WRITER THAT THE CHARACTER OF THIS POINT IS THEREFORE ANOTHER METHOD FOR THE LETTERS THAT THE TIME OF WHO EVER TOLD THE PROBLEM FOR AN UNEXPECTED

The resemblance to ordinary English text increases quite noticeably at ich of the above steps.

Figure: Shannon (1948)

Challenges with Empirical Next-Token Predictor

- Problems with empirical probability estimate

$$P(x_i|x_{1:i-1}) = \frac{\#(x \in D : x = x_{1:i})}{\#(x \subset D : x = x_{1:(i-1)})}$$

- Undefined for strings $x_{1:i-1} \notin D$.
- Small semantic reformulations cause ill-defined probabilities.

Alternative Approach

- Bengio et al. (2000): Learn a probabilistic model with flexible, but restricted parameterization.
- Predict the next symbol/word in a sequence using a predictor function $f : V^{i-1} \to V$. At the outset, natural to think of deterministic predictors.
- Challenges:
  - Most natural loss function $I(f(x_{1:i-1}) \neq x_i)$ is discontinuous.
  - Discrete space of functions $\mathcal{F} : V^{i-1} \to V$ also discontinuous.

Machine Learning Solution

- Relax function space to output probability distributions over V. Model $x \mapsto P(x) = (P_1(x), \ldots, P_{|V|}(x))$ becomes a probability distribution over V, $P(x) \in \Delta(V)$, for all x.
- Introduce a loss function for multi-class classification, where the outcome is $v \in V$, and the prediction is a probability distribution over V. E.g., logarithmic scoring rule:

$$\ell(P, v) = -\log P_v$$

- Aggregate over multiple data points using Empirical Risk Minimization (ERM):

$$\sum_{x \in D} \sum_{j=1}^{|x|} \ell(P(x_{1:(j-1)}), x_j)$$

How to Parametrize P?

- Any parametrization for multiclass classification can be considered (e.g., logistic regression, kernel classification, RNN).
- However, recall that the natural empirical distribution pools information in the original space of data.
- This does not account for semantics directly.
- Instead, aim to pool in a **semantic representation/embedding space**.

Embeddings in Semantic Space

- Map tokens $x_1, x_2, \ldots, x_T$ into embeddings/representations $e_1, e_2, \ldots, e_T \in \mathbb{R}^d$, which represent tokens in a continuous vector space.

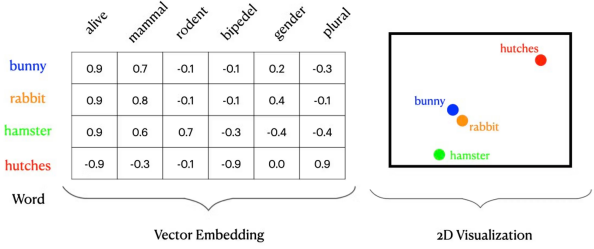


Figure: Source

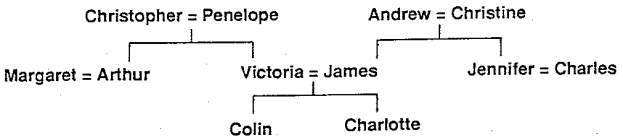
- Perform classification on the embeddings.
- Embeddings are learned during training.
- One of the most crucial ideas in AI!

The Origins of Distributed Representations

In: *Proceedings of the Eighth Annual Conference of the Cognitive Science Society*. Amherst, Mass. 1986, pages 1-12.

LEARNING DISTRIBUTED REPRESENTATIONS OF CONCEPTS

Geoffrey E. Hinton
Computer Science Department
Carnegie-Mellon University



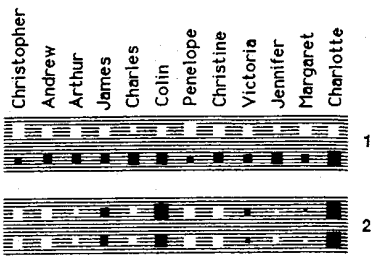


Figure: Hinton (1986) learns representations of individuals of two nationalities based on family relationships. The reps shown encode (1) nationality and (2) generation.

Attention Mechanism: Formulation

- Given embeddings $e_1, e_2, \ldots, e_T$, learn which embeddings to focus on for next-token prediction.
- Example: "Anna was born on Tuesday (...). What day followed Anna's birthday?"
- Assign attention weights based on relevance (Bahdanau et al., 2015):

$$a(e_j, e_k) = \text{how much attention } e_j \text{ pays to } e_k$$

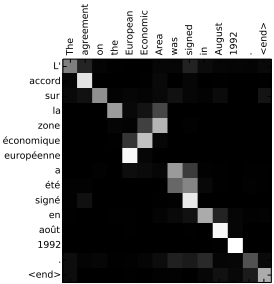


Figure: Bahdanau et al. (2015)

Attention Mechanism: Weighted Values

- Given the attention scores, compute a weighted sum of values V_i:

$$\hat{V}_j = \sum_{i \leq j} a(e_j, e_i) V_i$$

- Values V_i are linearly transformed embeddings:

$$V_i = W_V e_i$$

- Could imagine using plain embeddings. Linear transforms
  1. allow us to focus on only the part of the embeddings that are directly relevant for next-token prediction (embeddings can carry other meaning as well; e.g., about the context, not directly relevant)
  2. reduce dimension

Attention Weight Definition

- The attention weight $a(\cdot)$ is a measure of how similar certain aspects of embeddings e_j and e_i are. These aspects are:
  1. q_j represents the **query**, i.e., "what I'm looking for." $q_j = W_q e_j$
  2. k_i represents the **key**, i.e., "what I have." $k_i = W_k e_i$
- Inner-product attention (Vaswani et al., 2017):

$$a(e_j, e_i) \propto \exp(q_j^\top k_i / \sqrt{d})$$

- Normalize using softmax:

$$a(e_j, e_i) = \frac{\exp(q_j^\top k_i / \sqrt{d})}{\sum_{i' \leq j} \exp(q_j^\top k_{i'} / \sqrt{d})}$$

The basis of nearly all modern LLMs.

Comments on Attention Weight

- Inner-product attention

$$a(e_j, e_i) = \frac{\exp(q_j^\top k_i / \sqrt{d})}{\sum_{i' \le j} \exp(q_j^\top k_{i'} / \sqrt{d})}$$

- Where does $\sqrt{d}$ come from? The typical size of an inner product between two random vectors with i.i.d. standardized entries.
- Numerical stability: first calculate the max of the terms $q_j^\top k_i$, and subtract it from all terms before the exponential.

Causal and Bidirectional Attention

- Causal/left-to-right attention:
  - Summation only over observed data (up to current index).
  - Usable for text generation via autoregression.
- Bidirectional attention (e.g., in BERT):
  - Summation over all keys (used, e.g., in classification tasks).

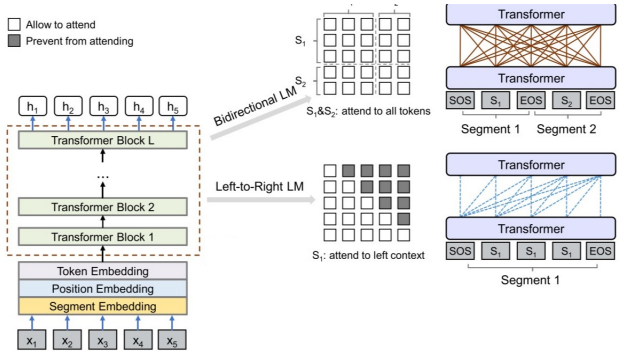


Figure: Source

Multi-Head Attention

- Compute weighted sum of values and apply non-linearity: $e'_i = \phi(W_o \hat{V}_i)$, where W_o maps the values back into embedding space.
- Use multiple heads, i.e., repeat the above operations multiple times to obtain $\hat{V}_i^{(j)}$, for several js. Then concatenate them to obtain a feature of the same dim d.
- Thought to compute multiple solutions in parallel (Xiong et al., 2024).

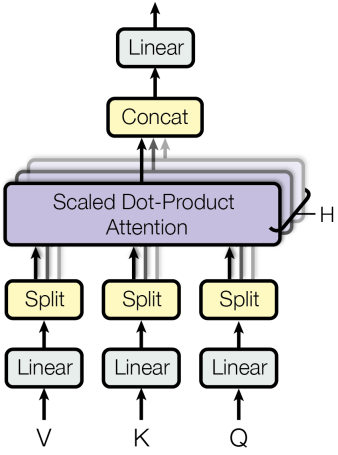


Figure: Vaswani et al. (2017)

Transformer Architecture Continued: Residual Layers

- Apply residual layers/skip connections (He et al., 2016) so that we make only a small update:

$$e_i \leftarrow e_i + e_i'$$

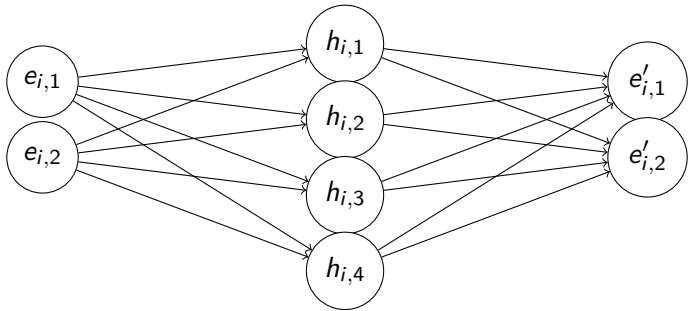
  - Why? Makes it easy to copy data and propagate already computed information.

Feedforward/Multi-layer perceptron (MLP) layers

- Further process embeddings using feedforward networks. A small neural net applied to each embedding, e.g.,

$$e_i' = W_{\text{proj}}\sigma(W_1 e_i), \quad e_i \leftarrow e_i + e_i',$$

where the dimension of the inner layer $W_1 e_i$ is larger by some factor (say four) than the dimension of the outer layer.



Interpreting MLP Layers

- These layers can be viewed as a form of un-normalized key-value memory (Geva et al., 2020).
  - Input: $e \in \mathbb{R}^d$
  - $\tilde{K}, \tilde{V} \in \mathbb{R}^{d \times d_m}$ form a neural memory (Sukhbaatar et al., 2015): d_m key-value pairs/memories. Keys $\tilde{k}_i \in \mathbb{R}^d$, Values $\tilde{v}_i \in \mathbb{R}^d$, $i = 1, \ldots, d_m$.
  - Probability:

$$P(\tilde{k}_i \mid e) \propto \exp(\tilde{k}_i^\top e).$$

Expected value:

$$\mathrm{NM}(e) = \sum_i P(\tilde{k}_i \mid e)\tilde{v}_i = \tilde{V} \cdot \mathrm{softmax}(\tilde{K}^\top e)$$

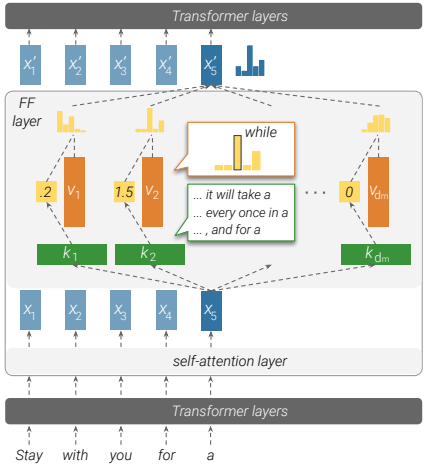


Figure: Geva et al. (2020)

MLP layers ctd.

- Instead, use unnormalized $\mathrm{FF}(e) = \tilde{V}\sigma(\tilde{K}^\top e)$.
- Thought to store most of the knowledge: e.g., to answer "Michael Jordan plays the sport of ...", keys represent names, values represent professions; see also 3Blue1Brown video.
- Difference from standard attention: Keys and values cannot depend on the input e. [principle: measure similarity via inner product].

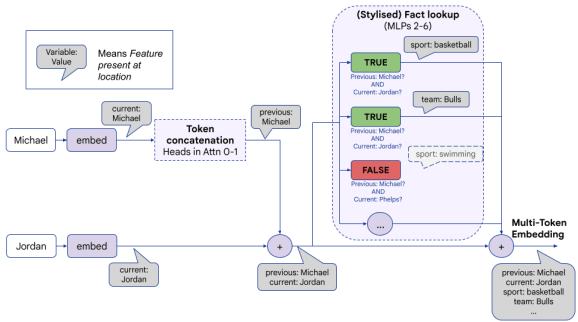


Figure: Source

Deep Architecture

- Use a deep network by repeating the process across multiple blocks.
- Attention updates and "contextualizes" representation by copying values from previous tokens
- MLP extracts knowledge associated with token embeddings
- Repeat to extract hierarchical concepts from the data.

Positional encoding

- How to take position of the input tokens into account? (Transformer does not do so by default),
- To address this, add a matrix Γ encoding location information to the embedding matrix E at the first layer. Has rows $\Gamma_1, \ldots, \Gamma_T$ that represent the effect of token positions $1, 2, \ldots, T$. Propagated through the layers.
- Can be fixed (Vaswani et al. (2017)) or learned (as in the GPT series in Radford et al. (2018, 2019); Brown et al. (2020)).

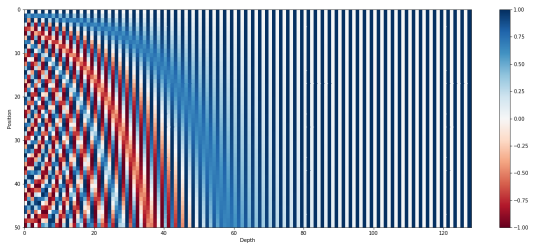


Figure: Vaswani et al. (2017)-style position embeddings (Source)

Normalization

- Layer normalization (Ba et al., 2016) is commonly used twice: before computing attention, and before the MLP.
- Embeddings: $E = [e_1, \ldots, e_j]^\top$, a $j \times d$ matrix.
- LayerNorm $\mathrm{LN}(E)$:

$$\mathrm{LN}(e_i) = \frac{e_i - \mu_i}{\sigma_i} \cdot \gamma + \beta$$

where:

$$\mu_i = \frac{1}{d} \sum_{k=1}^{d} e_{ik}, \quad \sigma_i = \sqrt{\frac{1}{d} \sum_{k=1}^{d} (e_{ik} - \mu_i)^2 + c_0},$$

and $\gamma, \beta \in \mathbb{R}^d$ are learnable parameters, $c_0 > 0$ is a small constant for numerical stability.

Illustration

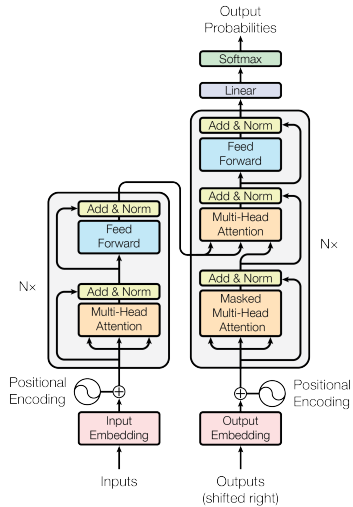


Figure: A more complicated encoder-decoder Transformer LM (Vaswani et al., 2017), with an additional cross-attention layer

Illustration

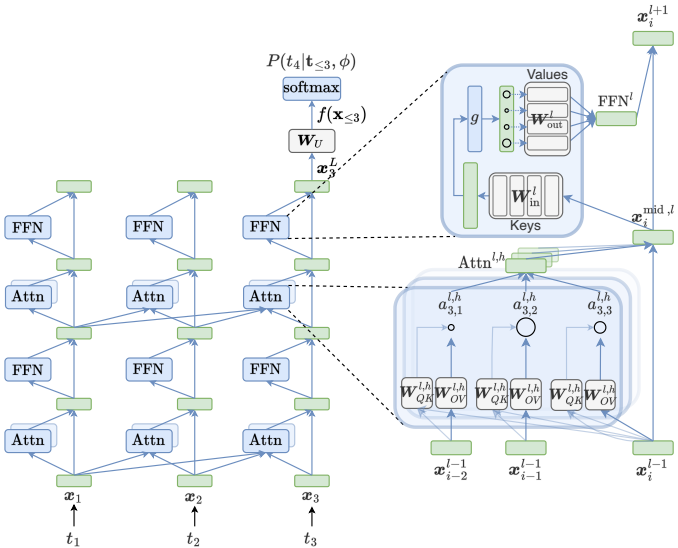


Figure: Transformer LM (Ferrando et al., 2024)

Next Token Prediction

- How to predict the next token given the embeddings $e_1, e_2, \ldots, e_j$ at the penultimate layer?
- Calculate pre-activations:

$$S = W_{\text{out}}[e_1, \ldots, e_j],$$

where W_{out} is a $|V| \times d$ learned weight matrix, $[e_1, \ldots, e_j]$ is $d \times j$ and obtain a matrix of size $|V| \times j$.

- Let $P_j = (P_{j,1}, \ldots, P_{j,|V|})$ represent the predicted probability distribution over the possible tokens at position j.
- After calculating the pre-activations $S = (s_{k,i})_{k \leq |V|, i \leq j}$, apply a softmax function to convert them into probabilities. For all $k \leq |V|$

$$P_{j,k} = \frac{\exp(s_{k,j})}{\sum_{k'} \exp(s_{k',j})}$$

Next Token Prediction

- Equivalently, the probability of outputting token k at the $j+1$-st location is proportional to $\exp(W_{\text{out},k}^\top e_j)$.
- Also the probability of token k at the $l+1$-st location, for all $l \leq j$, is proportional to $\exp(W_{\text{out},k}^\top e_l)$. Self-consistent for varying j
- Leads to KV caching: for a speedup, store previous key-value pairs instead of recomputing them.
- Intuition: Given an input x, the probabilities over next tokens y are proportional to $p(y|x) \propto \exp(\phi(x)^\top \lambda(y))$, where $\phi(x)$ is the last-layer embedding of x, and $\lambda(y)$ is the readout representation of y

Matrix Representation of One-Head Attention

- Embeddings: $E = [e_1, \ldots, e_T]^\top$, a $T \times d$ matrix. LayerNorm $E \leftarrow \mathrm{LN}(E)$.
- Queries, Keys, Values:

$$Q = EW_q, \quad K = EW_k, \quad V = EW_v$$

- Pre-attention: $Z = QK^\top/\sqrt{d}$.
- Causal attention: $A = \text{row-softmax}(Z \odot M)$ is a $T \times T$ matrix, where M is a lower-triangular $T \times T$ mask matrix with $M_{ij} = 1$ if $i \geq j$ and $-\infty$ otherwise.
- Intermediate embeddings: $\hat{E} = E + AV$. LayerNorm $\hat{E} \leftarrow \mathrm{LN}(\hat{E})$.
- FFN: $\tilde{E} = \sigma(\hat{E}W_1')W'_{\text{proj}}$. Residual update: $E \leftarrow \hat{E} + \tilde{E}$.
- Readout: calculate next-token probabilities $[\hat{p}_1, \ldots, \hat{p}_T]^\top = \text{softmax}(EW'_{\text{out}})$, where W_{out} is $n_{\text{tokens}} \times d$. [ChatGPT dimension check]

In Code

- Need to process batches of datapoints, so have an extra dimension. Work with tensors.
- See Andrej Karpathy's video "Let's build GPT"
- For readable code, see Andrej's NanoGPT repo

References

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