Transformers and Large Language Models for Natural Language Processing

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Part I
Basics of Neural Networks

1 A General Supervised Learning Task

We aim at finding a *prediction function* f such that $f(\mathbf{x};\mathbf{w}) \in \mathbb{R}^k$ is the true outcome of event $\mathbf{x} \in \mathbb{R}^d$, where $\mathbf{w}$ are the parameters (weights) that define the function. Given a dataset $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$ of events with their true outcomes (labels), we can approximate this function by finding $\mathbf{w}$ that best approximate $f(\mathbf{x}_i;\mathbf{w}) \approx \mathbf{y}_i$ for any data point $i = 1, 2, \ldots, N$.

Continuous Outcomes. Assume that the labels represent a continuous outcome, as in regression tasks. We can assume that $\mathbf{y}_i \sim \text{Normal}\left[f(\mathbf{x}_i;\mathbf{w}), \sigma\mathbf{I}_k\right]$ for all data points i and for some $\sigma > 0$.

We can find the parameters (expectations and standard deviation) using the maximum-likelihood estimation (MLE) approach. Finding the optimal σ by differentiating the log-likelihood function and plugging it back, we arrive after algebraic manipulations to the equivalent problem

$$\min_{\mathbf{w}} \left\{ \mathcal{L}(\mathbf{w}) \equiv \frac{1}{N}\sum_{i=1}^{N} L_i(\mathbf{w}) \equiv \frac{1}{N}\sum_{i=1}^{N} \left\| f(\mathbf{x}_i;\mathbf{w}) - \mathbf{y}_i \right\|^2 \right\},$$

which is the *mean squared error* (MSE) loss function (up to a scalar multiplication).

Discrete Outcomes. Assume that the labels represent a discrete outcome, as in classification tasks. Hence, there are k possible outcomes, each is a one-hot vector of size k. Then, the outcomes follow a categorical distribution and for any data point i we have $\mathbf{y}_i \sim \text{Cat}\left[\mathbf{p}\left(f(\mathbf{x}_i;\mathbf{w})\right)\right]$, for $\mathbf{p}\colon \mathbb{R}^k \to \mathbb{R}^k$ a function that maps k possible outcomes to k outcome probabilities, one for each of the k classes (these probabilities depend on the true outcome function f).

We can find the parameters $\mathbf{p}\left(f\left(\mathbf{x}_i;\mathbf{w}\right)\right)$ (the probabilities) by applying MLE, which results with the equivalent problem

$$\min_{\mathbf{w}}\left\{\mathcal{L}\left(\mathbf{w}\right)\equiv\frac{1}{N}\sum_{i=1}^{N}L_i\left(\mathbf{w}\right)\equiv-\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{k}\left(\mathbf{y}_i\right)_j\log\left(\mathbf{p}\left(f\left(\mathbf{x}_i;\mathbf{w}\right)\right)_j\right)\right\},$$

which is the *cross-entropy* (CE) loss function (up to a scalar multiplication).

We can further assume that $\mathbf{p}\left(\mathbf{z}\right)=\operatorname{softmax}\left(\mathbf{z}\right)$ for optimization and statistical advantages, though any other function that converts a vector of k real numbers into a probability distribution of k possible outcomes can be taken.

As for the prediction function f, which appears in the minimization problems above, it can be modeled using neural network architectures. In this case, due to increasing size of the networks, the loss function $\mathcal{L}\left(\mathbf{w}\right)$ can be minimized using the Stochastic Gradient (SG) method or its variants.

2 Training Feed-Forward Neural Networks

In a *feed-forward* NN with M layers, we denote by $\phi_m^k\left(\mathbf{x}\right)$ the output of the m-th layer at the k-th iteration. Then, this output is forwarded as an input to the $m+1$-th layer, hence $\phi_{m+1}^k\left(\mathbf{x}\right)\equiv f_{m+1}\left(\phi_m^k\left(\mathbf{x}\right);\mathbf{w}_{(m+1)}^k\right)$, where f_m is the function of the m-th layer and $\mathbf{w}_{(m)}^k$ are its weights at the k-th iteration. Notice that $\phi_M^k\left(\mathbf{x}\right)=f\left(\mathbf{x};\mathbf{w}\right)$ and $\phi_0^k\left(\mathbf{x}\right)=\mathbf{x}$.

2.1 Forward-pass and Back-propagation

In order to calculate the gradients $\nabla L_i\left(\mathbf{w}\right)$, we notice that

$$\begin{aligned}\frac{\partial f}{\partial\mathbf{w}_{(M)}}\left(\mathbf{x};\mathbf{w}^k\right)&=\frac{\partial f_M}{\partial\mathbf{w}_{(M)}}\left(\phi_{M-1}^k\left(\mathbf{x}\right),\mathbf{w}_{(M)}^k\right),\\ \frac{\partial f}{\partial\mathbf{w}_{(M-1)}}\left(\mathbf{x};\mathbf{w}^k\right)&=\frac{\partial f}{\partial\mathbf{w}_{(M)}}\left(\mathbf{x};\mathbf{w}^k\right)\cdot\frac{\partial f_{M-1}}{\partial\mathbf{w}_{(M-1)}}\left(\phi_{M-2}^k\left(\mathbf{x}\right),\mathbf{w}_{(M-1)}^k\right),\\ &\vdots\\ \frac{\partial f}{\partial\mathbf{w}_{(1)}}&=\frac{\partial f}{\partial\mathbf{w}_{(2)}}\left(\mathbf{x};\mathbf{w}^k\right)\cdot\frac{\partial f_1}{\partial\mathbf{w}_{(1)}}\left(\phi_0^k\left(\mathbf{x}\right),\mathbf{w}_{(1)}^k\right),\end{aligned}$$

where the differentiations are taken element-wise. In general, it holds that

$$\frac{\partial f}{\partial\mathbf{w}_{(m)}}\left(\mathbf{x};\mathbf{w}^k\right)=\prod_{i=m}^{M}\frac{\partial f_i}{\partial\mathbf{w}_{(i)}}\left(\phi_{i-1}^k\left(\mathbf{x}\right),\mathbf{w}_{(i)}^k\right)$$

and we notice that the gradients at m-th layer do not depend on the gradients of the previous $m-1,m-2,\ldots,1$ layers. However, the gradients of the m-th layer do depend on $\phi_{m-1}^k\left(\mathbf{x}\right)$, which by itself depends on the outputs of all previous $m-1, m-2, \ldots, 1$ layers. Finally, we have that

$$\nabla L_i\left(\mathbf{w}^k\right) = \left(\nabla_1 L_i\left(\mathbf{w}^k\right), \ldots, \nabla_M L_i\left(\mathbf{w}^k\right)\right).$$

where we denote

$$\nabla_m L_i\left(\mathbf{w}^k\right) \equiv \frac{\partial L_i}{\partial \mathbf{w}_{(m)}}\left(\mathbf{w}^k\right) \cdot \frac{\partial f}{\partial \mathbf{w}_{(m)}}\left(\mathbf{x}; \mathbf{w}^k\right).$$

This means that the gradient $\nabla L_i\left(\mathbf{w}^k\right)$ can be calculated efficiently as follows:

1. *Forward-pass:* at each layer m and for each data point $\mathbf{x}_i$, we evaluate $\phi_m^k\left(\mathbf{x}_i\right)$ and pass this information to the next $m+1$ layer until we obtain $\phi_M^k\left(\mathbf{x}\right) = f\left(\mathbf{x}_i; \mathbf{w}^k\right)$.
2. *Back-propagation:* First, we calculate $\frac{\partial L_i}{\partial \mathbf{w}_{(m)}}\left(\mathbf{x}_i; \mathbf{w}^k\right)$ for all m and all data points. Then, we calculate $\frac{\partial f_m}{\partial \mathbf{w}_{(m)}}\left(\phi_{m-1}^k\left(\mathbf{x}_i\right); \mathbf{w}_{(m)}^k\right)$ at each layer m for all data points, and propagate this information to the previous $m-1$ layer.

The functions $\partial f_m / \partial \mathbf{w}_{(m)}$ and $\partial L_i / \partial \mathbf{w}_{(m)}$ can be constructed only once, when the network is deployed. This is outlined in Algorithm 1.

Algorithm 1 Training of a Feed-Forward Neural Network with SG

```
1:  Initialization: Set $\mathbf{w}^0$ and $k = 0$.
2:  for epoch do
3:      for mini-batch $\mathcal{B}$ do
4:          for layer $m = 1, 2, \ldots, M$ do
5:              Calculate $\phi_m^k\left(\mathbf{x}_i\right)$ for each $i \in \mathcal{B}$ and then forward-pass.
6:          end for
7:          Calculate $L_i\left(\mathbf{w}^k\right)$ and $\frac{\partial L_i}{\partial \mathbf{w}_{(m)}}\left(\mathbf{w}^k\right)$ for each $i \in \mathcal{B}$ and layer $m$.
8:          for layer $m = M, M-1, \ldots, 1$ do
9:              Calculate $\frac{\partial f_m}{\partial \mathbf{w}_{(m)}}\left(\phi_{m-1}^k\left(\mathbf{x}_i\right); \mathbf{w}_{(m)}^k\right)$ for each $i \in \mathcal{B}$ and then back-propagate.
10:             $\mathbf{w}_{(m)}^{k+1} := \mathbf{w}_{(m)}^k - \eta^k \sum_{i \in \mathcal{B}} \nabla_m L_i\left(\mathbf{w}^k\right)$.
11:         end for
12:         $k := k + 1$.
13:     end for
14: end for
```

Remark 1.

1. The partition of the dataset into mini-batches can be either a single partition across all epochs, a random partition in each epoch, or any other partition.
2. The gradient ∇L_i for any i is of the size of $\mathbf{w}$. If we want to zero a portion of its elements we can use a dropout procedure.

2.2 Optimizers

Several methods exist to enhance the performance of the "vanilla" SG. This is usually done by considering momentum-based variants of SG, adaptive step-size schedules, or a combination of the two. Popular examples are as follows (where we omit layer indices for readability):

- Heavy-ball momentum:

$$\mathbf{w}^{k+1} := \mathbf{w}^k - \eta^k \sum_{i \in \mathcal{B}} \mathbf{m}_i^k \quad \text{where} \quad \mathbf{m}_i^k := \beta \mathbf{m}_i^{k-1} + (1-\beta) \nabla L_i \left(\mathbf{w}^k\right).$$

- AdaGrad: for each coordinate l of $\mathbf{w}^k$

$$\mathbf{w}_l^{k+1} := \mathbf{w}_l^k - \eta^k \sum_{i \in \mathcal{B}} \left(\mathbf{m}_i^k\right)_l \quad \text{where} \quad \left(\mathbf{m}_i^k\right)_l = \frac{\nabla L_i \left(\mathbf{w}^k\right)_l}{\sqrt{\sum_{j=0}^k \nabla L_i \left(\mathbf{w}^j\right)_l^2}},$$

  hence each coordinate has an adaptive step-size.

- RMSProp: for each coordinate l of $\mathbf{w}^k$

$$\mathbf{w}_l^{k+1} := \mathbf{w}_l^k - \eta^k \sum_{i \in \mathcal{B}} \left(\mathbf{m}_i^k\right)_l \quad \text{where} \quad \left(\mathbf{m}_i^k\right)_l = \frac{\nabla L_i \left(\mathbf{w}^k\right)_l}{\sqrt{\mathbf{v}_l^k}},$$

  for $\mathbf{v}_l^k = \beta \mathbf{v}_l^{k-1} + (1-\beta) \nabla L_i \left(\mathbf{w}^k\right)_l^2$, hence each coordinate has an adaptive step-size (where the step-size utilizes momentum).

- Adam: for each coordinate l of $\mathbf{w}^k$

$$\mathbf{w}_l^{k+1} := \mathbf{w}_l^k - \eta^k \sum_{i \in \mathcal{B}} \left(\mathbf{m}_i^k\right)_l \quad \text{where} \quad \left(\mathbf{m}_i^k\right)_l = \frac{\beta_1 \left(\mathbf{m}_i^{k-1}\right)_l + (1-\beta_1) \nabla L_i \left(\mathbf{w}^k\right)_l}{\sqrt{\mathbf{v}_l^k}},$$

  for $\mathbf{v}_l^k = \beta_2 \mathbf{v}_l^{k-1} + (1-\beta_2) \nabla L_i \left(\mathbf{w}^k\right)_l^2$, hence each coordinate has an adaptive step-size, and both the descent direction and the step-size utilizes momentum.

Part II
Large Language Models

The insight of large language modeling is that many practical tasks (including, but not limited to, NLP tasks) can be cast as word prediction, and that a powerful-enough language model can solve them with a high degree of accuracy. These tasks include *word prediction*, *sentiment analysis*, *question answering* and *text summarization*.

The standard architecture for building large language models is the *transformer*, which is made up of stacks of *transformer blocks*, each is a multi-layer network that maps sequences of input vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N \in \mathbb{R}^d$ to sequences of output vectors $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N \in \mathbb{R}^d$. The size of the sequence N, is the *context window*. These blocks are made by combining feed-forward networks, normalization layers, and *self-attention layers*, the key innovation of transformer architecture.

3 Self-Attention Process

The intuition of attention is the idea of comparing an item to a collection of other items to reveal their relevance in the current context. In the case of self-attention for language, comparisons of words (or tokens) to other words within a given sequence. The result of these comparisons is then used to compute an output sequence for the current input sequence.

Formally, for each current input token $\mathbf{x}_i$, the *proportional relevance* vector $\boldsymbol{\alpha}_i \in \mathbb{R}^i$ with respect to all previous input tokens $\mathbf{x}_j$ from the sequence, $j \le i$, is

$$\boldsymbol{\alpha}_i \equiv \text{SOFTMAX}\left(\begin{bmatrix} \mathbf{x}_i^T \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_i^T \mathbf{x}_i \end{bmatrix}\right).$$

The attention vector $\mathbf{a}_i \in \mathbb{R}^d$ for the token $\mathbf{x}_i$ is the weighted sum of comparisons for inputs seen so far

$$\mathbf{a}_i \equiv \sum_{j=1}^{i} \boldsymbol{\alpha}_{ij} \mathbf{x}_j.$$

Notice that each token $\mathbf{x}_i$ has three different roles in the attention process. As the current focus of attention (*query*), as a preceding input (*key*), and as an argument for computing the weighted sum (*value*). These roles motivate the introduction of variable weight matrices $\mathbf{Q} \in \mathbb{R}^{d_K \times d}$, $\mathbf{K} \in \mathbb{R}^{d_K \times d}$ and $\mathbf{V} \in \mathbb{R}^{d_V \times d}$, which yield the modified definitions

$$\boldsymbol{\alpha}_i \equiv \text{SOFTMAX}\left(\begin{bmatrix} \mathbf{x}_i^T \mathbf{Q}^T \mathbf{K} \mathbf{x}_1 / d_K \\ \vdots \\ \mathbf{x}_i^T \mathbf{Q}^T \mathbf{K} \mathbf{x}_i / d_K \end{bmatrix}\right) \in \mathbb{R}^i \quad \text{and} \quad \mathbf{a}_i \equiv \sum_{j=1}^{i} \boldsymbol{\alpha}_{ij} \mathbf{V} \mathbf{x}_j \in \mathbb{R}^{d_V}. \tag{1}$$

The division of $\mathbf{Q}\mathbf{x}_i$ and $\mathbf{K}\mathbf{x}_j$, $j \le i$, by $\sqrt{d_K}$ in the definition of $\boldsymbol{\alpha}_i$ is done to prevent exponentiation of large values.

The self-attention process, as formulated mathematically in (1), is depicted in Figure 1.

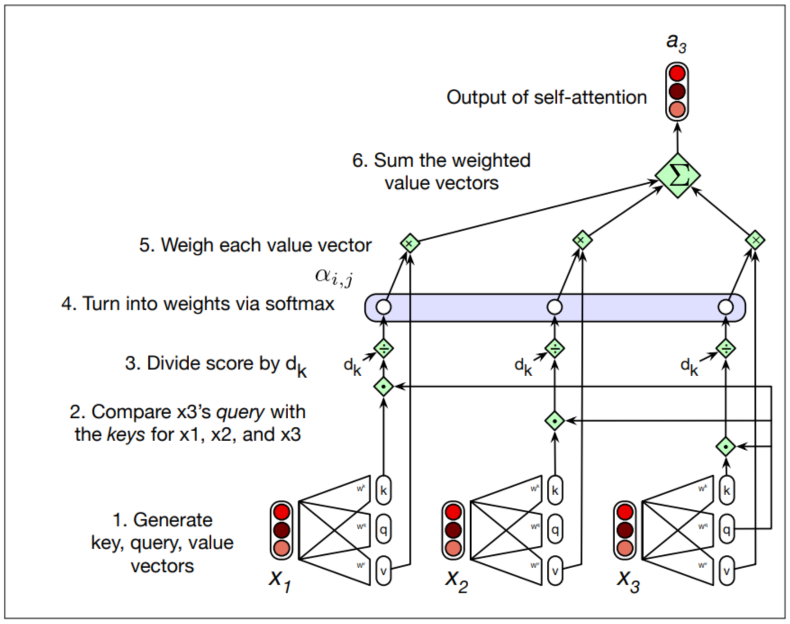

a3
Output of self-attention
6. Sum the weighted value vectors
5. Weigh each value vector
$\alpha_{i,j}$
4. Turn into weights via softmax
3. Divide score by dk
dk
2. Compare x3's *query* with the *keys* for x1, x2, and x3
1. Generate key, query, value vectors
k
q
v
x1
x2
x3

Figure 1: Calculating the self-attention vector $\mathbf{a}_3 \in \mathbb{R}^{d_V}$ using causal (left-to-right) self-attention process, in a sequence of $N = 3$ tokens.

Parallelization. A key observation is that the calculation of each attention vector is independent of other attention vectors, thus the entire attention process can be parallelized in matrix form. To this end, we denote by $\mathbf{X} \in \mathbb{R}^{N \times d}$ the matrix whose rows are all the N tokens in the sequence.

Notice that each attention vector only considers previous tokens in the sequence, and not future tokens. In order to mask future tokens, we define the future masking matrix operator, that keeps the upper-right triangular of a matrix and replaces all other entries with $-\infty$. For example, for a 4×4 matrix $\mathbf{B}$ we get

$$\textsc{MaskFuture}\left(\mathbf{B}\right) \equiv \begin{pmatrix} \mathbf{b}_{11} & -\infty & -\infty & -\infty \\ \mathbf{b}_{21} & \mathbf{b}_{22} & -\infty & -\infty \\ \mathbf{b}_{31} & \mathbf{b}_{32} & \mathbf{b}_{33} & -\infty \\ \mathbf{b}_{41} & \mathbf{b}_{42} & \mathbf{b}_{43} & \mathbf{b}_{44} \end{pmatrix}.$$

Now we can write the self-attention process in matrix form as

$$\mathbf{A} \equiv \textsc{RowSoftmax}\left(\textsc{MaskFuture}\left(\mathbf{X}\mathbf{Q}^T\mathbf{K}\mathbf{X}^T/d_K\right)\right)\mathbf{X}\mathbf{V}^T \in \mathbb{R}^{N \times d_V},$$

where $\textsc{RowSoftmax}$ is the softmax operator performed on each row of a matrix. Notice that the N rows of the matrix $\mathbf{A}$ are exactly the N attention vectors described above. We write the entire self-attention operation compactly as

$$\mathbf{A} = \textsc{SelfAttention}\left(\mathbf{Q}, \mathbf{K}, \mathbf{V}; \mathbf{X}\right).$$

Multi-Head Self-Attention. To allow more complicated attention relations between tokens in a sequence, the self-attention process is performed d_H times, all of which processes occur in parallel. Each such process is called *head*, and the entire process is called *multi-head self-attention*. Formally, we perform

$$\begin{aligned} \mathbf{H}_l &= \textsc{SelfAttention}\left(\mathbf{Q}_l, \mathbf{K}_l, \mathbf{V}_l; \mathbf{X}\right) \in \mathbb{R}^{N \times d_V}, \quad l = 1, 2, \ldots, d_H, \\ \mathbf{A} &= \textsc{MultiHeadS}\left(\mathbf{X}\right) = \left[\mathbf{H}_1; \mathbf{H}_2; \cdots; \mathbf{H}_{d_H}\right] \mathbf{O} \in \mathbb{R}^{N \times d_O}, \end{aligned} \tag{2}$$

where $\mathbf{O} \in \mathbb{R}^{d_H d_V \times d_O}$ is a variable matrix for transforming the N attention outputs into the dimension of our choice d_O (notice that the concatenated matrix of heads is of size $N \times d_H d_V$). Of course, we can take the inner dimensions d_K and d_V to be dependent on the head index $l = 1, 2, \ldots, d_H$.

Again, the entire multi-head self-attention process is performed in parallel over the tokens, and the N output attention vectors reside in the rows of the matrix $\mathbf{A}$. The multi-head self-attention process, as formulated in (2), is depicted in Figure 2.

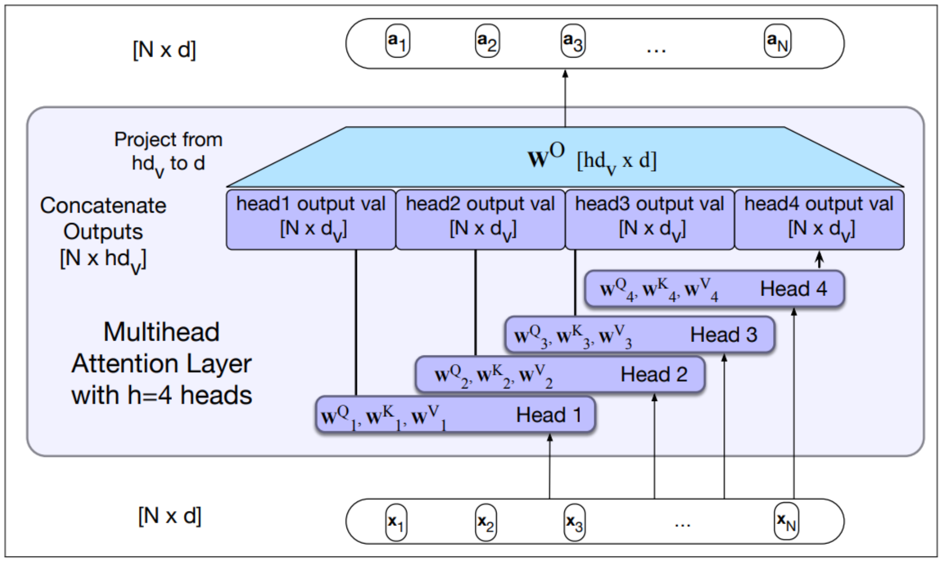

[N x d]
a1 a2 a3 ... aN
Project from hdV to d
WO [hdV x d]
Concatenate Outputs [N x hdV]
head1 output val [N x dV]
head2 output val [N x dV]
head3 output val [N x dV]
head4 output val [N x dV]
WQ4, WK4, WV4 Head 4
WQ3, WK3, WV3 Head 3
WQ2, WK2, WV2 Head 2
WQ1, WK1, WV1 Head 1
Multihead Attention Layer with h=4 heads
[N x d]
x1 x2 x3 ... xN

Figure 2: Calculating the self-attention matrix $\mathbf{A} \in \mathbb{R}^{N \times d_O}$ (the N vectors at the top represent the rows of this matrix), with a multi-head self-attention process with $d_H = 4$ heads. Notice that each head has its own query, key and value matrices, while the projection matrix $\mathbf{O} \in \mathbb{R}^{d_H d_V \times d_O}$ do not depend on the heads.

4 Transformer Block

The self-attention process lies at the core of the *transformer block*, which is composed of a multi-head self-attention, layer normalization, and N feed-forward networks, one for each attention vector. Also, we add residual connections that bypass the multi-head and the feed-forward layers. These blocks are also called *decoder-only*.

We assume that $d_K = d_V = d_O = d$ to enable easy stacking of blocks and for residual connectivity. LLMs with transformers stack many transformer blocks, from 12 layers (used for the T5 or GPT-3-small language models) to 96 layers (used for GPT-3 large), to even more for more recent models.

Layer Normalization. The layer normalization operator takes an input vector $\mathbf{z} \in \mathbb{R}^d$ and returns the normalized vector $(\mathbf{z} - \mu)/\sigma$, where

$$\mu = \frac{1}{d}\sum_{j=1}^{d} \mathbf{z}_i \quad \text{and} \quad \sigma = \sqrt{\frac{1}{d}\sum_{j=1}^{d} (\mathbf{z}_i - \mu)^2}.$$

We point out that μ is a scalar and $\mathbf{z}-\mu$ is element-wise subtraction. The layer normalization operator is written as

$$\text{LN}(\mathbf{z}) = \gamma\left(\frac{\mathbf{z}-\mu}{\sigma}\right) + \beta,$$

for γ and β learnable scalar parameters. Notice that γ and β depend on the layer, and can be different for each phase of the layer normalization operator.

Feed-Forward Networks. The N feed-forward networks in the block can be taken to be, for example, fully-connected networks with a single hidden layer. That is, two weight matrices for each network. The input and output of each network is a d-dimensional vector. Usually, the dimension of the hidden layer is taken to be greater than d. The weight matrices can be taken to be, for example, the same for all N networks, but different across each block. Notice that the N networks can be computed in parallel.

The Complete Block. Thus, for an input matrix $\mathbf{Z} \in \mathbb{R}^{N\times d}$ – which can be either the token matrix $\mathbf{X}$ or the output of the previous block – the *post-norm* transformer architecture can be written as

$$\begin{aligned}\tilde{\mathbf{A}} &= \textsc{RowLN}\left(\textsc{MultiHeadS}(\mathbf{Z}) + \mathbf{Z}\right) \in \mathbb{R}^{N\times d},\\ \mathbf{A} &= \textsc{RowLN}\left(\textsc{RowFF}\left(\tilde{\mathbf{A}}\right) + \tilde{\mathbf{A}}\right) \in \mathbb{R}^{N\times d},\end{aligned}$$

where RowLN is the layer normaliztion operator applied to each row, and where RowFF is a feed-forward network applied to each row of its input matrix, as described above. This can abbreviated as $\mathbf{A} = \textsc{Transformer}(\mathbf{Z})$.

The *pre-norm* transformer architecture, which is commonly used, can be written as

$$\begin{aligned}\tilde{\mathbf{A}} &= \textsc{MultiHeadS}\left(\textsc{RowLN}(\mathbf{Z})\right) + \mathbf{Z} \in \mathbb{R}^{N\times d},\\ \mathbf{A} &= \textsc{RowFF}\left(\textsc{RowLN}\left(\tilde{\mathbf{A}}\right)\right) + \tilde{\mathbf{A}} \in \mathbb{R}^{N\times d}.\end{aligned}$$

Again, the computations in a transformer block can be performed in parallel over the input vectors (either token vectors or output vectors from the previous block), and the N output attention vectors reside in the rows of $\mathbf{A}$.

A scheme depicting the relations between the layers in a single transformer block is given in Figure 3.

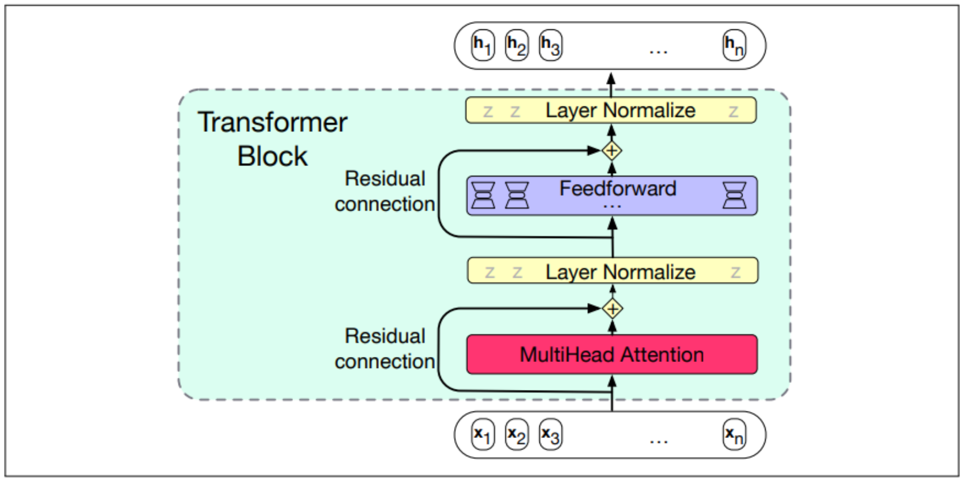


Figure 3: A post-norm transformer block architecture, taking input token embeddings $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \in \mathbb{R}^d$ and returns attention vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_N \in \mathbb{R}^{d_V}$ (top row in the figure).

4.1 Token and Position Embeddings

The input matrix $\mathbf{X} \in \mathbb{R}^{N \times d}$ of tokens is obtained by taking the rows of the learnable *token embedding matrix* $\mathbf{E} \in \mathbb{R}^{|V| \times d}$. The i-th row of the matrix $\mathbf{E}$ is an embedding of size d of the i-th token in the vocabulary V. Formally, let $\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, \ldots, \tilde{\mathbf{x}}_N \in \mathbb{R}^{|V|}$ be one-hot vectors corresponding to the N tokens taken from the vocabulary. Then,

$$\mathbf{X} \equiv \left[\tilde{\mathbf{x}}_1; \tilde{\mathbf{x}}_2; \ldots; \tilde{\mathbf{x}}_N\right]^T \mathbf{E}.$$

The representation of each token as a vocabulary index (thus a row index in $\mathbf{E}$) is first created using byte pair encoding (BPE) algorithm, for example, described in a box below.

BPE algorithm. EXPLAIN

Notice that the vocabulary indices do not represent the position of each token in the given sequence. Hence, we should also consider *positional embeddings*, which are d-dimensional vector representations that encapsulate the relative positions of tokens within the target sequence. As such, it provides the transformer with information about where the tokens are in the input sequence.

A popular *relative* positional embedding function $\mathbf{p} \colon \mathbb{R} \to \mathbb{R}^d$ is the sinusoidal positional embedding, which takes a position t of a token and returns

$$\left(\mathbf{p}\left(t\right)_{2k}, \mathbf{p}\left(t\right)_{2k+1}\right) = \left(\sin\left(t \cdot C^{-2/d}\right), \cos\left(t \cdot C^{-2/d}\right)\right), \quad \forall k = 0, 1, \ldots, d/2 - 1,$$

where $C \gg d$ is a hyper-parameter.

A useful property of the sinusoidal embedding is that $\mathbf{p}\left(t + \Delta t\right) = \operatorname{diag}\left(\mathbf{p}\left(\Delta t\right)\right) \mathbf{p}\left(t\right)$, hence allowing to calculate position shifts as a linear transformation of the current position. This allows the transformer to take any encoded position, and find the encoding of the position at $\pm\Delta t$ steps away by a matrix multiplication.

There are simpler *absolute* positional embeddings, which do not allow calculation of shifts by matrix multiplication.

Finally, considering both token and positional embeddings, the input matrix $\mathbf{X} \in \mathbb{R}^{N\times d}$ is taken as

$$\mathbf{X} \equiv [\tilde{\mathbf{x}}_1; \tilde{\mathbf{x}}_2; \ldots; \tilde{\mathbf{x}}_N]^T \mathbf{E} + \mathbf{P},$$

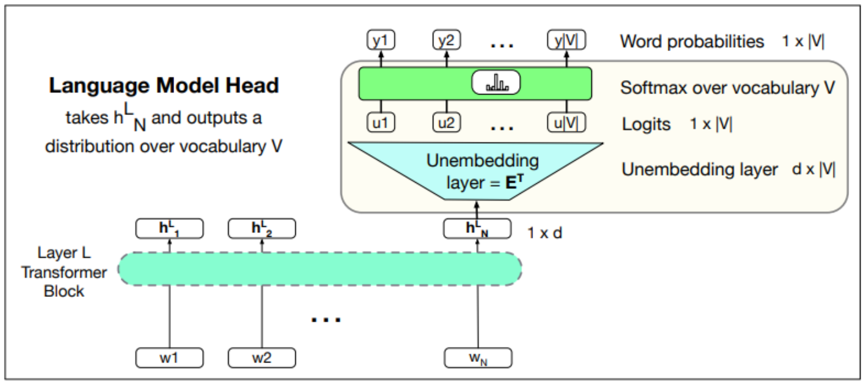
where $\mathbf{P} \in \mathbb{R}^{N\times d}$ is the row-wise positional embedding matrix.

4.2 Language Modeling Head

Language models are token predictors, that is given a context of tokens, they assign a probability to each possible next token. The job of the language modeling head is to take the output of the final transformer from the last token N, and use it to predict the upcoming token at position $N+1$.

To this end, we take the N-th (last) row of the last attention matrix $\mathbf{A}^{\text{last}}$, that is we take he vector $\mathbf{a} \equiv \mathbf{A}^{\text{last}}_N \in \mathbb{R}^d$, and unembed it to the vocabulary size by matrix multiplication. Using the *weight tying* approach, this learnable *unembedding matrix* can be taken as the embedding matrix $\mathbf{E} \in \mathbb{R}^{|V|\times d}$, but with multiplication from the right (in contrary to multiplication from the left as in the embedding process, which can also be viewed equivalently as matrix transposition). That is, the unembedding process is simply $\mathbf{u} = \mathbf{Ea} \in \mathbb{R}^{|V|}$, where the vector $\mathbf{u}$ is called the vector of *logits*.

Finally, we compute the probabilities $\hat{\mathbf{y}} = \text{softmax}(\mathbf{u}) \in \mathbb{R}^{|V|}$, before plugging $\hat{\mathbf{y}}$ into CE loss. The vector $\hat{\mathbf{y}}$ contains the probabilities for each token in the vocabulary to be the next token in the sequence. The LLM head is depicted in Figure 4, while the entire decoder-only LLM architecture is given in Figure 5.



Language Model Head
takes h^L_N and outputs a distribution over vocabulary V
y1
y2
y|V|
Word probabilities 1 x |V|
Softmax over vocabulary V
u1
u2
u|V|
Logits 1 x |V|
Unembedding layer = E^T
Unembedding layer d x |V|
h^L_1
h^L_2
h^L_N
1 x d
Layer L Transformer Block
w1
w2
w_N

Figure 4: A language modeling head on top of the last attention vector $\mathbf{A}^{\text{last}}_N \in \mathbb{R}^d$ corresponding to the last N token in the sequence. This vector is unembedded using the weight tying approach to produce the vector of logits, which is transformed into token probabilities $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_{|V|} \in \mathbb{R}$ using softmax.

Loss Function. During training at time $t = 1, 2, \ldots, N$, the next predicted $t+1$ token is the one that minimizes the function

$$\mathcal{L}^t(\hat{\mathbf{y}}) = -\sum_{w\in V} \mathbf{y}^t_w \log\left(\hat{\mathbf{y}}^t_w\right), \tag{3}$$

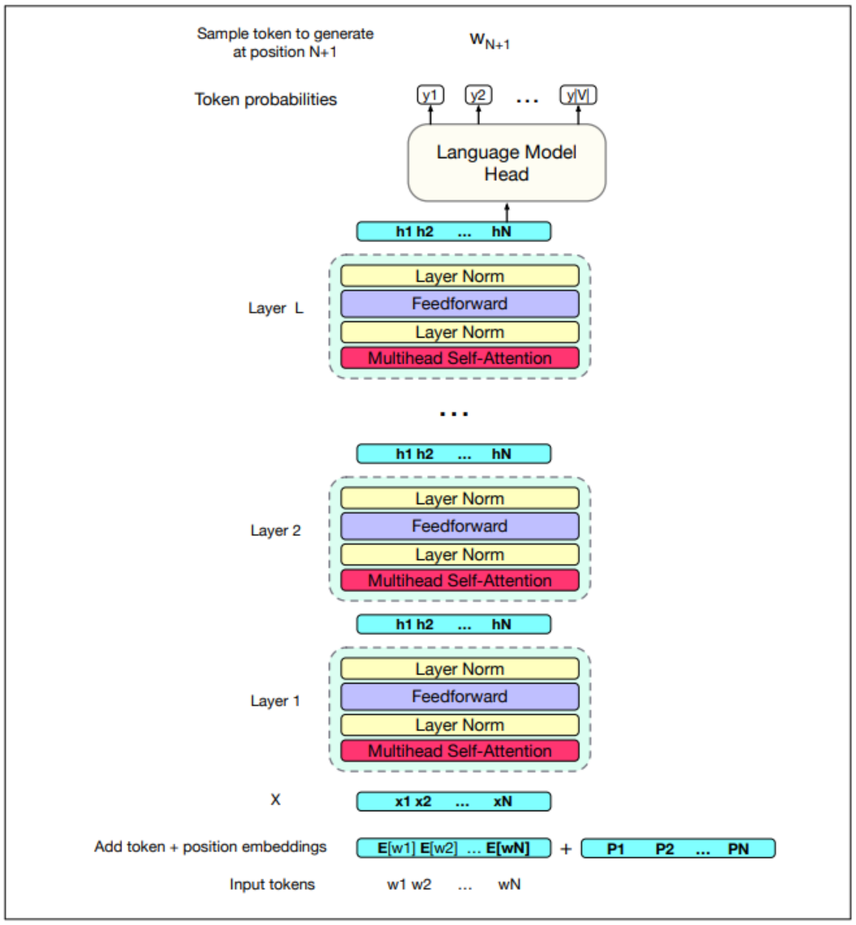


Figure 5: Decoder-only LLM architecture. The input tokens are transformed into the input matrix $\mathbf{X} \in \mathbb{R}^{N \times d}$ using token and position embeddings. Then, several transformer blocks are stacked to generate the attention vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_N \in \mathbb{R}^d$. Finally, the last $\mathbf{a}_N$ vector is transferred to the language modeling head that generate the token probabilities $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_{|V|} \in \mathbb{R}$ that are used to sample the next $N+1$ token.

where $\mathbf{y}^t \in \{0,1\}^{|V|}$ is the true one-hot next $t+1$ token. Since $\mathbf{y}^t$ contains 1 for the true next w^{t+1} token and 0 otherwise, then (3) simplifies to

$$\mathcal{L}^t\left(\hat{\mathbf{y}}\right) = -\log\left(\hat{\mathbf{y}}^t_{w^{t+1}}\right).$$

The loss is then defined as

$$\mathcal{L}\left(\hat{\mathbf{y}}\right) = \frac{1}{N}\sum_{t=1}^{N} \mathcal{L}^t\left(\hat{\mathbf{y}}\right).$$

The batch size for gradient descent for minimizing this loss is usually quite large for LLMs (the largest GPT-3 model uses a batch size of 3.2 million tokens grouped into sequence contexts of size N).

5 LLM for Word Generation

Once the model is trained, the task of choosing a word to generate based on the probabilities the model provides is called *decoding*. Repeatedly choosing the next word conditioned on previous choices is called *autoregressive generation* or *causal LM generation*. Alternatives that predict words based on both past and future words are *non-causal*.

NLP tasks are cases of *conditional generation*, the task of generating text conditioned on an input piece of text – a prompt. Give the prompt, the LLM is asked to generate a possible completion. Note that as the generation process proceeds, the model has direct access to the primal prompt, as well as to all of its own subsequently generated outputs (which are concatenated to the prompt), at least as much as fits in the context window. For LLMs with transformers, the context window (for looking at previous tokens), is of size 1024 or even 4096 tokens, which makes them very powerful for conditional generation. Formally, the size of the context window N is what limits the size (number of rows) of the attention matrices as previously discussed.

As for the size of the vocabulary, the GPT-3 models, for example, are trained mostly on the web (429 billion tokens), some text from books (67 billion tokens) and Wikipedia (3 billion tokens).

Word Generation with Sampling. Once the model is trained, which words do we generate at each step? A simple way, called *greedy decoding*, is taking the most likely word given the context. A major problem with greedy decoding is that because the words it chooses are (by definition) extremely predictable, the resulting text is generic and quite repetitive (though a modification of this technique works well for machine translation).

Sampling is the most common approach for decoding. With a simple random sampling we sample words according to their probability conditioned on our previous choices, while the transformer LLM is the probability model that tells us this probability. Still, this sampling approach lacks quality and diversity.

Top-k sampling is a generalization of greedy decoding. We first truncate the distribution to the top k most likely words, normalize to produce a legitimate probability distribution, and then randomly sample from within these k words according to their normalized probabilities.

One problem with top-k sampling is that k is fixed, but the shape of the probability distribution over words differs in different contexts. An alternative approach is *top-p* or *nucleus sampling*. Here, the process is he same, but we choose the top-p percent of the words instead.

In *temperature sampling*, we reshape the the distribution instead of truncating. In low-temperature sampling, we smoothly increase the probability of the most probable words and decrease the probability of the rare words. Formally, this is simply done by dividing the vector of logits by a temperature hyper-parameter τ. That is, $\hat{\mathbf{y}} = \text{softmax}(\mathbf{u}/\tau)$.

Scaling Laws. The performance of LLMS is mainly determined by three factors: model size $\#H$ (the number of parameters not counting embeddings), dataset size $\#D$ (the amount of training data), and the amount of computer/iterations budget C used for training. The relationships between these factors and performance (value of loss), if the other two properties are held constant, are known as *scaling laws*:

$$\mathcal{L}(\#H) = \left(\frac{\bar{H}}{\#H}\right)^{\alpha_H}, \quad \mathcal{L}(\#D) = \left(\frac{\bar{D}}{\#D}\right)^{\alpha_D} \quad \text{and} \quad \mathcal{L}(C) = \left(\frac{\bar{C}}{C}\right)^{\alpha_C},$$

where the values of $\bar{H}, \bar{D}, \bar{C}, \alpha_H, \alpha_D$ and α_C depend on the exact transformer architecture, tokenization, and vocabulary size.

The number of (non-embedding) parameters $\#H$ for LLMs with transformers with one hidden layer in each FF network, can be roughly computed as follows

$$\#H \approx 2d \cdot \#\text{layers} \cdot (2d_V + d_{\text{FF}}),$$

where #layers is the number of transformer blocks and d_{FF} is the size of the hidden layer in the FF network. The specification of GPT-3, for example, are $\#\text{layers} = 96$ and $d = d_V = d_{\text{FF}}/4 = 12288$, thus it roughly has $\#H \approx 175$ billion parameters.

6 Bidirectional Transformer Encoders

Map sequences of input vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \in \mathbb{R}^d$ to output vectors $\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N \in \mathbb{R}^d$ that are contextualized using information from the entire input sequence. These blocks are also called *encoder-only*, because they produce an encoding for each input token.

The self-attention operator for encoder-only operates similarly to the decoder-only, with the exception that id does not mast the future. Hence, the operator is defined as

$$\mathbf{A} \equiv \textsc{RowSoftmax}\left(\mathbf{X}\mathbf{Q}^T\mathbf{K}\mathbf{X}^T/d_K\right)\mathbf{X}\mathbf{V}^T \in \mathbb{R}^{N \times d_V}.$$

For example, the original English-only encoder-only BERT consists of 30k tokens generated using WordPiece algorithm. It comprises of hidden layers of size 786, and 12 bidirectional transformer blocks with 12 multi-head attention layers each. The resulting model has about 100M parameters.

The larger multilingual XLM-RoBERTa, trained on 100 languages, has a multilingual 250k token vocabulary using SentencePiece Unigram LM algorithm. It comprises of hidden layers of size 1024, and 24 bidirectional transformer blocks with 16 multi-head attention layers each. The resulting model has about 550M parameters.

As with causal transformers, the size of the input layer dictates the complexity of the model. Both the time and memory requirements in a transformer grow quadratically with the length of the input N. It is necessary to set a fixed input length that is long enough to provide sufficient context for the model to function and yet still be computationally tractable. For BERT and XLR-RoBERTa, $N = 512$ was set.

Masking Words. For training, eliminating the masking process makes the guess-the-next-word task trivial since the answer is now directly available from the context. Instead, the model learns to fill-in-the-blank task, technically called the *cloze task*.

The original approach to training bidirectional encoders is called *Masked Language Modeling* (MLM), where a subset of $M \leq N$ tokens in the sequence is sampled, and each is either replaced with [MASK], with another randomly sampled token from the vocabulary, or it is left unchanged. In BERT, 15% of the input tokens are sampled for learning, of which 80% are replaced with [MASK], 10% are replaced with random tokens, and the remaining 10% are left unchanged. Note that only M out of N tokens play a role in learning, so in that sense BERT is inefficient as less than 15% of the input is used for training.

Contextual Embeddings. We can think of the sequence of outputs as *contextual embeddings* for each token in the input. These embeddings are vectors representing some aspect of the meaning of a token in context, and can be used for any task requiring the meaning of tokens or words. It is common to compute a representation for each token by averaging the output tokens from each of the last four layers of the model. Thus, while thesauruses like WordNet give discrete lists of senses, embeddings offer a continuous high-dimensional model of meaning that, although it can be clustered, does not divide up into fully discrete senses.

During training, for each sense s of any word in the corpus (e.g., the token mouse an an animal or a cursor), for each of the n tokens of that sense, we average their n contextual representations $\mathbf{v}_i$ to produce a contextual sense embedding $\mathbf{v}_s$. At test time, given a token t in the context, we compute its contextual embedding vector $\mathbf{t}$ and choose its nearest neighbor sense from the training set, i.e., the sense whose embedding has the highest cosine with t:

$$\text{sense}\left(\mathbf{t}\right) = \underset{s \in \text{senses}(\mathbf{t})}{\text{argmax}} \ \text{cosine}\left(\mathbf{t}, \mathbf{v}_s\right),$$

where the set senses $(\mathbf{t})$ is taken from some sense-labeled dataset like SemCore or SenseEval.

7 Enhancing LLMs

Is there room for enhancement with a trained LLM? Can we improve the predictions it generates? Two approaches exist, differing in whether we adjust a portion of the model's weights further or not.

7.1 In-Context Learning

Prompting involves providing LLMs with a sequence of tokens during inference, aiming to predict the next tokens (for decoder-only) or generate contextual embeddings (for encoder-only). Prompts that do not contain additional labeled examples are termed *zero-shot* prompts. On the other hand, prompts that incorporate additional labeled data are termed *in-context learning* (ICL) or *few-shot* prompts.

In all prompting scenarios (including the ICL approach), it is important to highlight that the task is solely accomplished by conditioning on the given prompt, without any additional parameter optimization.

We recall that LLMs such as GPT-3 are trained on internet-scale text and as a result are very flexible in a sense that they can "read" any text input and condition on it to "write" text that could plausibly come after the input. While the training procedure is both simple and general, the GPT-3 paper found that the large-scale leads to the particularly interesting emergent behavior of ICL.

During ICL, we give the LLM a prompt that consists of a list of input-output pairs that demonstrate a task. At the end of the prompt, we append a test input and allow the LLM to make a prediction just by conditioning on the prompt and predicting the next tokens (the regular way). For example, in order to translate the word "chien" (dog) from French to English, we can simply use the zero-shot prompt "Chien in English is:", which is a non-ICL prompt. With ICL, we give a few-shot prompt like "Maison in English is house. Chat in English is cat. Chien in English is:". It turns out, that ICL gives better results compared to zero-shot prompts for a given LLM.

It is important to know that in contrast to training and fine-tuning for each specific task (see below), which are not temporary, what has been learnt during ICL is of a temporary nature. It does not carry the temporary contexts, except the ones already present in the training set, from one conversation to the other.

What accounts for the superior performance of ICL over zero-shot prompts is an active area of research, with various hypotheses proposed despite the lack of definitive conclusions.

7.2 Fine-Tuning

When solving a task, one can either use a general LLM without further weight updates using any type of prompting, or update a portion of the model weights in a process called *fine-tuning*. In this process, we create applications on top of the models by adding a small set of application-specific parameters. The fine-tuning process consists of using labeled data about the application to train these additional application-specific parameters. Typically, this training will either freeze or make only minimal adjustments to the language model parameters, a technique called *transfer learning*.

Let's describe two examples of classification tasks typically accomplished through the fine-tuning approach of LLMs:

1. Sequence classification: such applications often represent an input sequence with a single representation. An additional *sentence embedding* vector is added to the model to stand for the entire sequence. In BERT, the [CLS] token plays the role of this embedding. This unique token is added to the vocabulary and is appended to the start of all input sequences. The output vector in the final layer of the model for [CLS] represents the entire input sequence and serves as the input to a classifier head – a logistic regression or neural network classifier that makes the relevant decision.

   An example of fine-tuning is sentiment classification. We consider the output vector $\mathbf{z}_{[\mathrm{CLS}]}$ for the [CLS] token, generated by a trained LLM. Then, the classification of the set into n possible sentiments proceeds by introducing a learnable weight matrix $\mathbf{C} \in \mathbb{R}^{n \times d_h}$, we calculate $\hat{\mathbf{y}} = \mathrm{softmax}\left(\mathbf{C}\mathbf{z}_{[\mathrm{CLS}]}\right)$. Then, we only learn the matrix $\mathbf{C}$ (fine-tune) using supervised training data consisting of input sequences labeled with the appropriate class with CE loss.

2. Sequence labeling: such tasks, for example part-of-speech tagging, can follow the same basic classification approach. Here, the final output vector corresponding to each input token is passed to a classifier that produces a softmax distribution over the possible set of tags. Again, assuming a simple classifier consisting of a single feed-forward layer

followed by a softmax, the set of weights to be learned for this additional layer is $\mathbf{K} \in \mathbb{R}^{k \times d_h}$, where k is the number of possible tags.

Instruct Tuning. An issue with LLMs is the mismatch between the training objective and users' objective: LLMs are trained on minimizing the token prediction error, while users want the model to "follow their instructions". To address this mismatch, *instruct tuning* (IT) is proposed. It is a fine-tuning process that uses the ICL approach that involves further training LLMs using (INSTRUCTION, OUTPUT) pairs, where INSTRUCTION denotes the human instruction for the model, and OUTPUT denotes the desired output that follows the INSTRUCTION. We point out that both INSTRUCTION and OUTPUT in the IT dataset are given by the user.

Based on the collected IT dataset, a model can be directly fine-tuned in a fully supervised manner, where given INSTRUCTION as the input, the model is trained by sequentially predicting each token in OUTPUT.

8 Encoder-Decoder Architecture

This architecture is mainly used for machine translation (MT). The encoder takes the source language input tokens $\mathbf{X} \in \mathbb{R}^{N \times d}$ and maps them to an output representation $\boldsymbol{\mathcal{E}} \in \mathbb{R}^{N \times d}$, usually via six stacked self-attention transformer blocks (as previously introduced).

The decoder has a modified transformer block architecture, that attends both the the output of its previous layer (in the output language), and the output of the encoder (in the source language). Decoding into output translated tokens can use any of the decoding methods discussed earlier, like greedy, temperature or nucleus sampling (though the most common decoding algorithm for MT is the beam search algorithm discussed later).

In order to attend to the source language, the transformer blocks in the decoder have an extra *cross-attention* layer (also called *encoder-decoder attention* or *source attention*). This layer has the same form as the multi-head self-attention layer in a normal transformer block, except that while the queries come as usual from the previous layer of the decoder, the keys and values come from the output of the encoder $\boldsymbol{\mathcal{E}} \in \mathbb{R}^{N \times d}$.

Formally, the cross-attention architecture for the decoder, for some block, is as follows

$$\mathbf{A}(\mathbf{Z}) \equiv \textsc{RowSoftmax}\left(\textsc{MaskFuture}\left(\mathbf{Z}\mathbf{Q}^T\mathbf{K}\boldsymbol{\mathcal{E}}^T/d_K\right)\right)\boldsymbol{\mathcal{E}}\mathbf{V}^T \in \mathbb{R}^{M \times d_V},$$

where M is the length of the translated sequence, $\mathbf{Z} \in \mathbb{R}^{M \times d}$ is the input from the last decoder layer, and the matrices $\mathbf{Q}, \mathbf{K}$ and $\mathbf{V}$ are of suitable dimensions. This can be written compactly as

$$\mathbf{A} = \textsc{CrossAttention}\left(\mathbf{Q}, \mathbf{K}, \mathbf{V}; \mathbf{Z}\right).$$

Similarly to self-attention, in order to allow more complicated attention relations, we use multi-head cross-attention for the decoder as

$$\begin{aligned} \mathbf{H}_l &= \textsc{CrossAttention}\left(\mathbf{Q}_l, \mathbf{K}_l, \mathbf{V}_l; \mathbf{Z}\right) \in \mathbb{R}^{M \times d_V}, \quad l = 1, 2, \ldots, d_H, \\ \mathbf{A} &= \textsc{MultiHeadC}\left(\mathbf{Z}\right) = \left[\mathbf{H}_1; \mathbf{H}_1; \cdots; \mathbf{H}_{d_H}\right]\mathbf{O} \in \mathbb{R}^{M \times d_O} \end{aligned}$$

where the matrix $\mathbf{O}$ is of suitable dimensions.

Finally, the decoder transformer block architecture is given as

$$\begin{aligned}
\tilde{\mathbf{A}} &= \textsc{RowLN}\left(\text{MultiHeadS}\left(\mathbf{Z}\right) + \mathbf{Z}\right) \in \mathbb{R}^{M\times d},\\
\tilde{\mathbf{A}} &= \textsc{RowLN}\left(\text{MultiHeadC}\left(\tilde{\mathbf{A}}\right) + \tilde{\mathbf{A}}\right) \in \mathbb{R}^{M\times d},\\
\mathbf{A} &= \textsc{RowLN}\left(\text{RowFF}\left(\tilde{\mathbf{A}}\right) + \tilde{\mathbf{A}}\right) \in \mathbb{R}^{M\times d}.
\end{aligned}$$

Notice that first we use the MultiHeadS operator, and than the MultiHeadC operator.

Beyond MT, the encoder-decoder architecture can also be used for training chatbots. In this case, the entire conversation up to the last turn (as much as fits in the context) is presented to the encoder, and the decoder generates the next turn.

Beam Search. In greedy decoding discussed above, at each time step t in generation, the output $\hat{\mathbf{y}}_t$ is chosen by computing the probability for each token in the vocabulary and then choosing the highest probability token. A problem with greedy decoding is that what the argmax might turn out to have been the wrong choice once we get to token $t+1$. Instead, we model decoding as searching the space of possible generations, represented as a *search tree* whose *branches* represent actions (generating a token), and *nodes* represent states (having generated a particular prefix). We search for the the highest probability sequence, contrary to just choosing the argmax at each time.

Computing the probability of every potential sequence is time-consuming. Instead, we utilize *beam search* algorithms, where we maintain k (referred to as the *beam width*) potential tokens at each stage. Initially, we calculate a softmax across the entire vocabulary to select the top k options, known as *hypotheses*. In subsequent stages, for each of the top k hypotheses, we compute the scores for all possible extensions so far, and once again select the best k hypotheses, ensuring a consistent count of k hypotheses at each stage.

The scoring of each hypotheses is done by computing the product of the log of the probability associated with the current token choice, multiplied by the product of the log of the probabilities of the path leading to this token.

Alternatives to this version of beam search also exists, like *minimum Bayes risk* decoding, that instead of choosing the translation which is most probable, it chooses the one that is likely to have the least error.