# Transformers from Scratch with Pytorch

# Phuoc Bui, Thuong Dang

## November 2023

#### Abstract

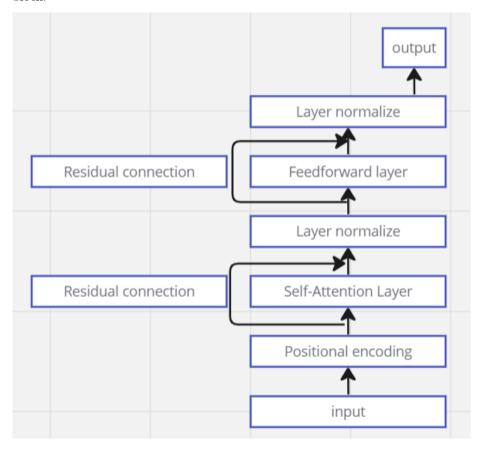
This is a documentation for our transformer model from scratch with Pytorch. In our project, we have developed a transformer model for sentiment analysis. The architecture and formulas for transformer blocks are carefully covered in this documentation.

# Contents

1	Transformer architecture	2
2	Positional encoding	3
3	Self-attention	6
4	Multihead attention	8
5	Residual connections	10
6	Layer normalization	12
7	Experiments	13

## 1 Transformer architecture

Before going to any detail, let us first look at the architecture of a transformer block.



From the picture above, we can see that our input will go through a layer for positions. It then go through the self attention layer, followed by a layer normalize. After that, our data will go through a feedforward layer and a layer normalize before producing the output via the softmax function. There will be several questions:

- 1. Why transformer models? What are they good for?
- 2. What is positional encoding?
- 3. What is self-attention?
- 4. What is a residual connection?
- 5. What is a layer normalization?

We will go through the details of those questions. But let us try to answer them quickly. For the first question, previous models such as RNN or LSTM have faced with the *bottleneck* problem, i.e. the context vector contains too much information, and also the vanishing/exploding gradients. An improvement for the bottleneck problem is the *attention mechanism*, which replaces a single context vector by weighted sum of all hidden states (see [1]-Chapter 9 for more details). The vanishing/exploding gradients can be improved by *residual connections*. Residual connections, in short, give us a shortcut through layers and they can reduce the length for the computation of the backpropagation.

Transformers models combine them both, with an important improvement: the *self-attention mechanism*. Moreover, they also solve the positional problem in previous attention models by *positional encoding*. In previous attention models, we can permute our input and the output will also be permuted in the same way. It means the models do not know the order of our input data, and this is not good, for example, for time series applications.

In the next section, let us dive into positional encoding.

## 2 Positional encoding

As we have said earlier, the attention mechanism does not know the orders of words in an input sentence. For more detail, the reader can look at our second section about the self-attention mechanism. We also note that the content of each section in our documentation is independent and the reader can start reading from Section 2. However, because we want to go with the flow of the model, we will start with positional encoding. To solve the positional problem of attention models, we need to know some important properties of positions:

- Given a sentence, a given position in this sentence uniquely determines a word. It means that for each word in a sentence, its positions must be unique, even if we have the same words in a sentence. For example, in the sentence s = "it is a very very intense situation", the word "very" appears twice, but the positions are different.
- Given two sentences  $s_1 = a_1 \cdots a_n w \cdots$ ,  $s_2 = b_1 \cdots b_n w \cdots$  where  $a_i, b_i, w$  are words, then the absolute positions of w in  $s_1, s_2$  must be the same.
- Given two sentences  $s_1, s_2$  and two words  $w_1, w_2$  in both  $s_1, s_2$ , such that  $s_1 = \cdots w_1 a_1 \cdots a_n w_2 \cdots$ ,  $s_2 = \cdots w_1 b_1 \cdots b_n w_2 \cdots$ , then the relative position of  $w_1$  and  $w_2$  in  $s_1, s_2$  must be the same. More generally, for any k and k, the k-th position and the (k + k)-th position will be different from a function depending only on k.
- Positions are easy to compute.

Having that in mind, we can understand the positional encoding proposed in the original paper of transformers [3]. Given a word w of position k in a

sentence s, we first use a word embedding method to transform this to a vector  $v_w = (v_0, \dots, v_{d-1})$  of length d. We define the position

$$P(k,2i) = \sin\left(\frac{k}{n^{2i/d}}\right), P(k,2i+1) = \cos\left(\frac{k}{n^{2i/d}}\right)$$

for  $0 \le i \le d/2$ , and n = 10000 in the original paper. And the *positional* encoding is defined to be

positional encoding(w) = 
$$v_w + (P(k, 0), P(k, 1), \cdots)$$

Let us take a look on an example.

**Example.** Consider the sentence "i am happy", we assume that each word is embedded into a four-dimensional vector space, i.e. a word of position k is represented by a vector  $v_k = (v_{k0}, v_{k1}, v_{k2}, v_{k3})$ . Consider the word "i", which is of position 0 in the sentence. Then

$$P(0,2i) = \sin 0 = 0, P(0,2i+1) = \cos 0 = 1$$

And the positional encoding of the word "i" is

$$(v_{00}, v_{01}, v_{02}, v_{03}) + (0, 1, 0, 1)$$

Next, the word "am" is of position 1, and we have

$$P(1,0) = \sin 1, P(1,1) = \cos 1, P(1,2) = \sin \left(\frac{1}{100}\right), P(1,3) = \cos \left(\frac{1}{100}\right)$$

From this, we have the positional encoding of "am" is

$$(v_{10}, v_{11}, v_{12}, v_{13}) + \left(\sin 1, \cos 1, \sin \frac{1}{100}, \cos \frac{1}{100}\right)$$

Given a sentence s and a word w of position k in s, we will see that the positional encoding satisfies all important properties for position we listed above. First, in order to have the same vector P for two words at different positions  $k_1, k_2$ . It means, that for all i,

$$\sin\left(\frac{k_1}{n^{2i/d}}\right) = \sin\left(\frac{k_2}{n^{2i/d}}\right)$$

Because of the periodicity of the sin and cos functions, when i=d/2, we have

$$k_1 = 2\pi n + k_2,$$

which is impossible because n = 10000, and there is no sentence of length 10000.

Second, for the absolute position problem. If a word appears in two sentence in the same absolute position k, it is obvious to see that its positional encoding does not change.

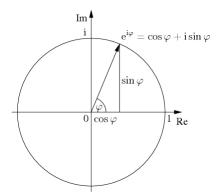
The third problem about relative positions is interesting. Assume that the relative position two words  $w_1, w_2$  in two sentences  $s_1, s_2$  are the same, let's see what we can deduce. We can first see that a pair of (even position, odd position) of the function P at position t can be represented by a complex number

$$e^{i\frac{t}{n^{2i/d}}} = \cos\left(\frac{t}{n^{2i/d}}\right) + i\sin\left(\frac{t}{n^{2i/d}}\right)$$

Here we used Euler's formula

$$e^{i\varphi} = \cos\varphi + i\sin\varphi$$

Here is how we see it in picture



Then at time k + t, we have a different complex number

$$e^{i\frac{t+k}{n^{2i/d}}} = \cos\left(\frac{t+k}{n^{2i/d}}\right) + i\sin\left(\frac{t+k}{n^{2i/d}}\right)$$

And we can see that the difference between the two numbers is exactly a rotation with angel  $\frac{k}{n^{2i/d}}$ . Therefore, if the relative positions between  $w_1$  and  $w_2$  in both sentences are k, their difference is exactly a rotation with angel  $\frac{k}{n^{2i/d}}$ .

The last problem about the computational aspects is also satisfied because computing sin and cos are effectively computed in python libraries, for example, numpy. Here is how positional encoding looks like in codes

#### 3 Self-attention

Self-attention is an instance of attention mechanism. In short, it tells us how much the current input depends on previous inputs. Let us dive into detail. We start with three matrices

- The query matrix  $W_q$ .
- The key matrix  $W_k$ .
- The value matrix  $W_v$ .

Let us understand those matrices this way. Given a tuple of pairs (key, value) of the form  $(k_1, v_1), \dots, (k_T, v_T)$ . Given a query q, we will compute how similar between q and each  $k_i$ . If the similar between q and  $k_t$  is high, it will most likely return  $v_t$ . It means, the weight at  $v_t$  will also be large. Here is a formula

Attention
$$(q, k, v) = \sum_{t} \text{similarity}(q, k_t) v_t$$
 (1)

The similarity function depends on our purposes, but we want it to be non-negative, convex, and  $\sum_t \text{similarity}(q, k_t) = 1$ . A natural choice is the softmax function.

Let us make it more explicitly, assume that our input X is of dimension  $T \times d$ . It means that we have T words in our sentence and each word is represented by a d dimensional vector. We can initialize  $W_q, W_k, W_v$  of size  $d \times h$ . We now compute

$$Q = XW_q, K = XW_k, V = XW_v$$

And define

$$\operatorname{Self-attention}(Q,K,V) = \operatorname{softmax} \bigg( \frac{QK^\top}{\sqrt{d}} \bigg) V$$

Let us go deeper into the definition to understand what is going on. First, we need to divide  $QK^{\top}$  by  $\sqrt{d}$  to prevent exploding by too large exponential values. If we denotes  $q_i, k_i, v_i$  columns of  $W_q, W_k, W_v$  respectively, and  $x_i$  rows of X, then

$$Q = \begin{pmatrix} x_1 q_1 & \cdots & x_1 q_h \\ \vdots & \vdots & \vdots \\ x_T q_1 & \cdots & x_T q_h \end{pmatrix}$$

$$K = \begin{pmatrix} x_1 k_1 & \cdots & x_1 k_h \\ \vdots & \vdots & \vdots \\ x_T k_1 & \cdots & x_T k_h \end{pmatrix}$$

$$V = \begin{pmatrix} x_1 v_1 & \cdots & x_1 v_h \\ \vdots & \vdots & \vdots \\ x_T v_1 & \cdots & x_T v_h \end{pmatrix}$$

The row vector  $x_iQ = (x_iq_1 \cdots x_iq_h)$  is called the *query of*  $x_i$ , and denoted  $q^i$ . Similarly we also have the *key and value*  $(k^i, v^i)$  of  $x_i$ . Then

$$QK^{\top} = \begin{pmatrix} q^1k^1 & \cdots & q^1k^T \\ \vdots & \vdots & \vdots \\ q^Tk^1 & \cdots & q^Tk^T \end{pmatrix}$$

If we apply the softmax function, we can then understand the formula as

$$\operatorname{softmax}\!\left(\frac{QK^T}{\sqrt{d}}\right) = \left(\operatorname{similarity}(q^i, k^j)\right)_{ij} = (\alpha_{ij})_{ij},$$

where  $\alpha_{ij}$  is the similarity between the query i and the key j. The i-th row in the matrix above is of the form

$$\left(q^i k^1 \cdots q^i k^T\right)$$

And the j-th column in V is of the form

$$\begin{pmatrix} x_1 v_j \\ \vdots \\ x_T v_j \end{pmatrix}$$

Multiplying them, we get

$$\left(\operatorname{softmax}\left(\frac{QK^{T}}{\sqrt{d}}\right)V\right)_{ij} = \left(\sum_{t} \alpha_{it} x_{t} v_{j}\right)_{ij}$$

Here, note that the formula does not tell us about the *positions*. If we permute  $x_j$  and  $x_l$ , the j-th row and the l-th rows of the self-attention matrix

will also be permuted as we only change  $v_j$  to  $v_l$ . And as we already discussed in Section 1, positional encoding can solve this problem.

Next, from the formula above, the *i*-th row of the result matrix is

$$(\alpha_{i1}x_1v_1 + \dots + \alpha_{iT}x_Tv_1 \quad \dots \quad \alpha_{i1}x_1v_h + \dots + \alpha_{iT}x_Tv_h) =$$

$$= \alpha_{i1}(x_1v_1 \dots x_1v_h) + \dots + \alpha_{iT}(x_Tv_1 \dots x_Tv_h) = \sum_t \alpha_{it}v^t$$

This is exactly the form in (1) because  $\alpha_{it}$  is the similarity between query i and key t. To summarize, the self attention formula tells us how much the current input  $x_i$  depends on other inputs.

For time series applications, we want to predict next steps based on previous steps, and not the other way around. And to deal with this, we can modify a bit by adding a masked matrix M to  $QK^T$  and then compute softmax. The masked matrix M is of size  $T \times T$  and its upper part (not including the diagonal) are all  $-\infty$  (so that after the softmax function, those values become 0) and other entries are 0. The self-attention can be now defined

$$\text{Self-attention}(\mathbf{Q},\,\mathbf{K},\,\mathbf{V}) = \text{softmax}\bigg(\frac{QK^T}{\sqrt{d}} + M\bigg)V$$

In codes, we can create the masked matrix in Pytorch as follows

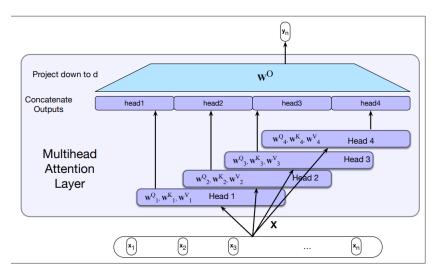
```
# Create the mask matrix with upper part is -infinity
# and other entries are 0
# First we create a matrix filled with - infinity at all entries
matrix = torch.full((self.n_heads*hidden_size, self.n_heads * hidden_size), -float('inf'))
# triu = triangular upper part, we want to fill in upper part with - infinity
matrix = torch.triu(matrix)
# Replace the diagonal by 0
matrix = matrix.fill_diagonal_(0)
self.mask = matrix
```

And here are sample codes for self-attention function

```
def self_attention(mask, Q, K, V):
   att = (Q @ K.T)/np.sqrt(Q.shape[0]) + mask
   return (torch.softmax(att, dim = 1) @ V)
```

#### 4 Multihead attention

We have finished the most two important ideas of the transformer mechanism. The multihead attention can help us program parallelly and it gives more parameters to the model. We can look at a picture taken from [1].



Let n be the number of heads, we will initialize n tupe of matrices  $(W_{qi}, W_{ki}, W_{vi})$ . Given an input X, each tupe will give us an output

$$h_i = \text{Self-attention}(Q_i, K_i, V_i)$$

And we will concatenate them

$$h = h_1 \oplus \cdots \oplus h_n$$

To project h down to the dimension we want, we will multiply it with a matrix  $W_o$ . Here is how we do it in codes. We first want to initialize query, key and value matrices for head. Note that we will initialize with Xavier initialization in Pytorch, because it is commonly used in transformer architecture. After that, we can stack heads

```
def initialize_matrix(n_rows, n_cols):
    matrix = torch.empty(n_rows, n_cols)
    init.xavier_normal_(matrix)
    matrix.requires_grad = True
    return matrix

def stack_heads(n_heads, n_rows, n_cols):
    tensors = [initialize_matrix(n_rows, n_cols) for _ in range(n_heads)]
    return tensors
```

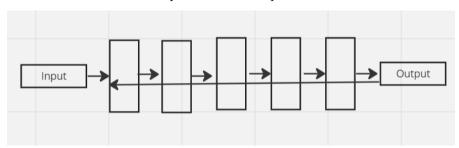
After that, we can compute the self-attention for each head and then concatenate them. Finally, we multiply the result with  $W_o$ . Here is how it is done in codes

```
# Multi-head attention
def multi_head_attention(self, inputs):
    # h is the cat matrix after we compute self attention of each head
    h = torch.empty(inputs.shape[0], 0)
    for i in range(len(self.Wq)):
        qi = inputs @ self.Wq[i]
          ki = inputs @ self.Wk[i]
        vi = inputs @ self.Wv[i]
        hi = self_attention(self.mask, qi, ki, vi)
        # We concatenate hi to h by stacking rows
        h = torch.cat((h, hi), dim = 1)
    output = h @ self.Wo
    return output
```

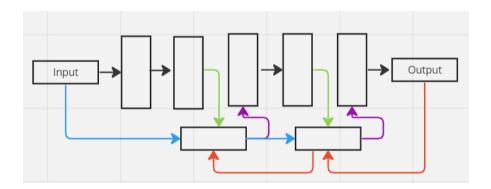
## 5 Residual connections

In deep networks, a problem we always have to deal with is vanishing/exploding gradients. The more layers our network have, the more possibility we have to deal with these problems. There are several ways to deal with this. We can clip the values whenever it is too small or too large. Another solution is to cut off the partial derivatives after long enough steps. In this section, we will discuss a solution for these problems by residual connections.

Let us look at the usual deep network in the picture below



For each layer, we will randomly initialize weights and when we have too many layers, the final input for the output contains a lot of random noises. Moreover, the backpropagation method have to go through all the way back to update parameters, and it can cause the vanishing/exploding gradients if the path is too long. An improvement for this is *residual connections*.



In a model with residual connections, after several layers, we *add/concatenate* the output and the input and make it become the input for the next layer. By this way, the random noise at the final input is reduced. Let us see why it can also reduce the vanishing/exploding gradient problem. Assume that we have a network with 3 layers. Through the first layer, we can compute

$$\operatorname{output}_1 = W_1 \operatorname{input}$$

In a residual connection network, the input of layer 2 is

$$input_2 = output_1 + input$$

Next, we have the output of the second layer is

$$output_2 = W_2 input_2$$

Again, the input for the third layer is

$$input_3 = input_2 + output_2$$

Finally, the output for the last layer is

$$output = softmax(W_3 input_3)$$

After defining the loss function L, for the backward method, to update the parameter  $W_1$ , for example, we need to compute

$$\frac{\partial L}{\partial W_1} = \frac{\partial L}{\partial \operatorname{input}_3} \frac{\partial \operatorname{input}_3}{\partial W_1} = \frac{\partial L}{\partial \operatorname{input}_3} \frac{\partial (\operatorname{input}_2 + \operatorname{output}_2)}{\partial W_1} \tag{2}$$

Note that in usual networks, the only term we have is

$$\frac{\partial L}{\partial \operatorname{input}_3} \frac{\partial \operatorname{output}_2}{\partial W_1} = \frac{\partial L}{\partial \operatorname{input}_3} \frac{\partial \operatorname{output}_2}{\partial \operatorname{input}_2} \frac{\partial \operatorname{input}_2}{\partial W_1} = \frac{\partial L}{\partial \operatorname{input}_2} \frac{\partial \operatorname{input}_2}{\partial W_1}$$

And what happens if the term  $\frac{\partial L}{\partial \text{ input}_2}$  is very small? If that happens, it is most likely that the network will not update  $W_1$ . However, in (2), we still have

the term  $\frac{\partial \text{ input}_2}{\partial W_1}$ , and we can cut off the remaining term if it is too small and obtain an approximation

$$\frac{\partial L}{\partial W_1} \approx \frac{\partial L}{\partial \text{input}_3} \frac{\partial \text{input}_2}{\partial W_1}$$

In practice, residual connections help the models converge much faster than the usual ways. The reader can take a look on [3] for more detail. Codes for residual connections will be included in the next section when we discuss about layer normalization.

## 6 Layer normalization

Layer normalization is a technique in statistics to scale the data to a specific range or distribution. In deep network, there are several normalization techniques

1. **Min-max normalization.** For a row vector  $v = (v_1, \dots, v_n)$  the min-max normalization of v is defined to be

$$\frac{(v_1 - \min, \cdots, v_n - \min)}{\max - \min},$$

where min, max are the minimum and maximum value of  $(v_1, \dots, v_n)$ , respectively.

2. z-score normalization. For a row vector  $v = (v_1, \dots, v_n)$ , let define mean and std be the mean and standard deviation of v, then the z-score of v is defined to be

$$\frac{(v_1 - \text{mean}, \cdots, v_n - \text{mean})}{\text{std}}$$

3. **Softmax normalization.** This is our familiar softmax function in deep networks.

We have to carefully chose a suitable normalization for specific problems. Note that, in the min-max and z-score normalization, we need a division, and it *can be zero*. In transformer models, the z-score normalization is commonly used. However, if we are working with classification problems with two labels, it might not be a good idea, here is why.

Assume that we have a 2-dimensional vector v=(a,b). We claim that the z-score of v is always a constant. Without loss of generality, we can assume a>b (if a=b then the vector is already normalized). Then mean =(a-b)/2, and std  $=(a-b)/\sqrt{2}$ . This follows that the z-score of v is  $(1/\sqrt{2},-1/\sqrt{2})$ , which is a constant.

And we certainly do not want constants as outputs of a layer in our deep networks. Hence, for our problem about sentiment analysis with two labels, we decided to use softmax normalization. In codes, the inputs of layer norms are the concatenated values between last outputs and last inputs, and then we apply softmax to the result. Here is the normalized layer after self-attention layer

```
# Layer norm after self-attention layer
def layer_norm_self_attention(self, previous_layer_outputs, previous_layer_inputs):
    cat_matrix = torch.cat((previous_layer_outputs, previous_layer_inputs), dim = 1)
    next_inputs = torch.softmax(cat_matrix @ self.gamma_self + self.beta_self, dim = 1)
    return next_inputs
```

And here is the normalized layer after feedforward layer

```
# Layer norm after feed_forward
def layer_norm_feed_forward(self, previous_layer_outputs, previous_layer_inputs):
    cat_matrix = torch.cat((previous_layer_outputs, previous_layer_inputs), dim = 0)
    next_inputs = torch.softmax(cat_matrix @ self.gamma_feed + self.beta_feed, dim = 1)
    return next_inputs
```

## 7 Experiments

We have finished explaining the theory behind transformer, and here is our experiment. The project is to build a transformer model for the sentiment analysis task. The source of our data can be found at [4]. It consists of simple sentences with label True for positive feeling and False for negative feeling.

For vector embedding method, we use the one hot encoding. The reader can use different methods such as Word2vec or GloVe, but it is not our main purposes, and we want to keep it simple.

The input for the forward method of the transformer class is a matrix of a whole sentence and each row represents a word embedding vector. Here is our forward method

```
def forward(self, inputs):
    # Inputs is a whole sentence at a time
    # And this sentence is represented by a matrix
    # The matrix consists of row vectors, each row is a word embedding
    np_inputs = np.array(inputs)
    torch_inputs = torch.tensor(np_inputs)
    torch_inputs = torch_inputs.to(torch.float32)
    pos_inputs = self.positional_encoding(torch_inputs)
    output_self_attention = self.multi_head_attention(pos_inputs)
    output_layer_norm_self = self.layer_norm_self_attention(output_self_attention, pos_inputs)
    output_feed_forward = self.feed_forward(output_layer_norm_self)
    output_layer_norm_feed = self.layer_norm_feed forward(output_feed_forward, output_layer_norm_self)
    output_linear = self.linear(output_layer_norm_feed)
    y_pred = torch.softmax(output_linear, dim = 1)
    return y_pred
```

And for the backward method, here is a common way to use it in Pytorch. We use torch.backward() to update parameters with requires\_grad = True. Note that we need to define loss = torch.nn.BCE() and optimizer = torch.optim.SGD([parameters], learning\_rate) outside of loops and they are initialized only once. At each step, we compute the loss L = loss(y\_pred, y\_true)

and update parameters by the optimizer.step() method. Also, do *not* forget optimizer.zero\_grad() after each step, as it will add up otherwise.

However, because we did not use torch.nn.Module, and our stacked heads  $W_q, W_k, W_v$  are not torch tensors, we need to be extra careful. This is because in this situation, torch.optim does not accept non-tensor parameters. Indeed, they are torch lists, and each element in those lists is a tensor with require\_grad = True and we need to treat them manually. First, we can define an optimizer with other parameters

For elements in stacked heads, we can define a function to treat them separately.

```
def manually_update(tensor_list, lr):
    with torch.no_grad():
        for tensor in tensor_list:
            tensor -= lr * tensor.grad
    for tensor in tensor_list:
        tensor.grad.zero_()
```

And finally, we update them through loops

```
L = self.loss(probs, y_true_torch)
self.optimizer.zero_grad()
L.backward()
self.optimizer.step()
# Update Wq, Wk, Wv manually
manually_update(self.Wq, lr)
manually_update(self.Wk, lr)
manually_update(self.Wv, lr)
```

Here are our fit and process function, the inputs of those are

• The list X consists of matrices of all sentences. Each element of X is a matrix of a sentence.

 $\bullet$  The list y consists of true labels from the data.

```
def process(self, X, y, run backward = False, lr = None):
    accuracy = 0
    for x, y_true in zip(X,y):
        # x is a matrix of a sentence
        probs = self.forward(x)
        # True label
        true index = int(y true)
        # Accuracy
        accuracy += int(torch.argmax(probs) == true_index)
        if run backward:
            y true torch = torch.zeros((1,2))
            y true torch[0][true index] = 1
            L = self.loss(probs, y true torch)
            self.optimizer.zero grad()
            L.backward()
            self.optimizer.step()
            # Update Wq, Wk, Wv manually
            manually_update(self.Wq, lr)
            manually update(self.Wk, lr)
            manually update(self.Wv, lr)
     # Accuracy
    return float(accuracy/len(X))
```

And here are the results of our model

```
PS C:\Users\Thuong Dang\Desktop\Data Science\Projects\transformer_from_scratch_with_pytorch> python experiments.py
Step: 0
accuracy for training data: 0.43103448275862066
Step: 20
accuracy for training data: 0.5517241379310345
Step: 40
accuracy for training data: 0.5517241379310345
Step: 60
accuracy for training data: 0.5862068965517241
Step: 180
accuracy for training data: 0.5862068965517241
Step: 180
accuracy for training data: 0.8275862068965517
Step: 120
accuracy for training data: 0.83793103448275862
Step: 140
accuracy for training data: 0.93193103448275862
Step: 140
accuracy for training data: 0.93193103448275862
Step: 150
accuracy for training data: 0.9310344827586207
Step: 180
accuracy for training data: 0.9310344827586207
Accuracy for training data: 0.931
```

We hope you enjoy this documentation and our project. We very much welcome any comment or suggestion for our work. Below, you will find the list of references we have used throughout our project.

#### REFERENCES

- [1] Dan Jurafsky and James H. Martin, Speech and Language Processing, 3rd edition, available at https://web.stanford.edu/~jurafsky/slp3/.
- [2] Rupesh Kumar Srivastava, Klaus Greff, Jurgen Schmidhuber, *Highway networks*, available at https://arxiv.org/pdf/1505.00387.pdf.
- [3] Ashish Vaswani et al., Attention is all you need, available at https://arxiv.org/pdf/1706.03762.pdf.
- [4] Victor Zhou's dataset for sentiment analysis, available at https://github.com/vzhou842/rnn-from-scratch/blob/master/data.py