

# Generative AI: opdracht 3: Generating text, using LSTMs, attention and multi-headed attention

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## Introduction

**Text generation** In this report I describe my ventures into the world of Generative AI. In this report I will describe 3 LSTM-based text generating models. The models gradually build upon each other.

**LSTMs** The main layer in the models will be an LSTM. So before anything else I will describe the way LSTMs work.

**Attention** As attention will be part of two out of three models, I will pay some attention to it as well.

**Three text generation models** There is a basic model using one LSTM layer. Furthermore there is a more complex model using two LSTM layers and attention. The most complex model has two LSTM layers and multi-headed attention. I will prove the models are trainable and will show some text they produced.

**Optimizers** While experimenting with a more complex, loss started oscillating, this inclined me to investigate the way optimizers work.

**Lightning** My regular training loop didn't prove to be very flexible, so I started using torch-lightning. To use this framework, I needed to refactor my training loop, which didn't work immediately.

## Long Short-Term Memory networks

Long Short-Term Memory (LSTM) networks possess several key qualities that make them well suited for modeling sequential and temporal data. LSTM networks are a special case of the more generic RNN networks. These recurrent networks are chains of LSTM cells or RNN cells respectively.

### RNNs

An RNN cell and its context is depicted in [Figure 1](#)

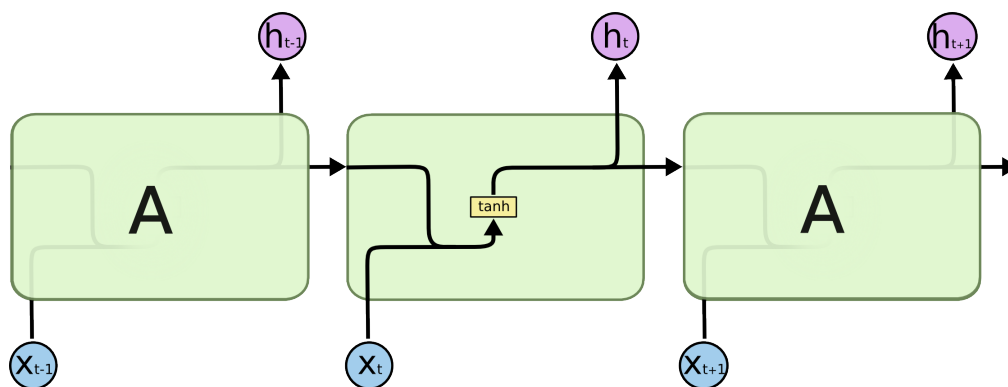


Figure 1: An RNN cell in a chain of RNN cells.

### LSTMs

The more complex LSTM cell and its context is depicted in [Figure 2](#).

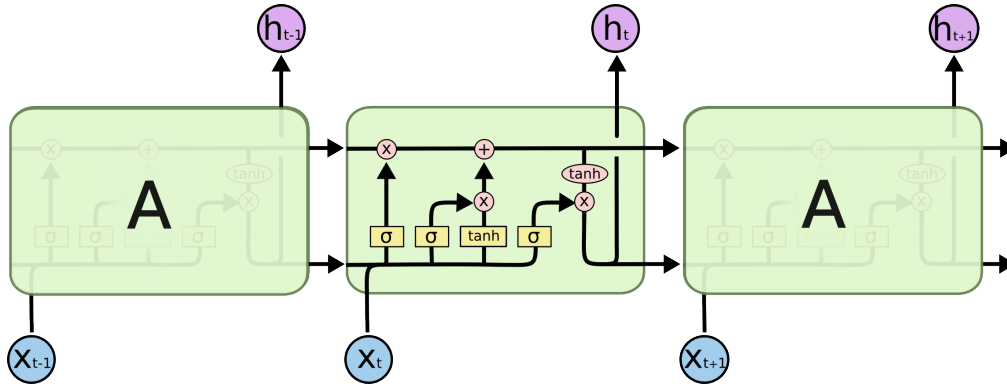


Figure 2: An LSTM cell in a chain of LSTM cells.

At each time step  $t$ , the LSTM cell receives an input vector  $x_t$ , the previous hidden state  $h_{t-1}$ , and the previous cell state  $c_{t-1}$ . It outputs an updated hidden state  $h_t$  and cell state  $c_t$ .

**Long-Term Dependency Modeling** LSTMs are specifically designed to capture long-range dependencies in sequences. The presence of a memory cell with additive updates allows gradients to flow across many time steps, mitigating the vanishing gradient problem.

**Gated Information Control** LSTMs employ gating mechanisms (forget, input, and output gates) that regulate the flow of information. These gates enable the network to selectively retain, update, or discard information based on relevance.

## Mechanism

The mechanism of an LSTM cell is explained in the following part. This part on the mechanism of LSTM cells is actually based on [this webpage](#). I did add some correct formulas. And changed the wording.

## A chain of LSTM cells

An LSTM cell differs from the RNN cell's structure. Instead of having a single gate, there are four. And this makes its structure a bit more complicated, as can be seen in [Figure 3](#).

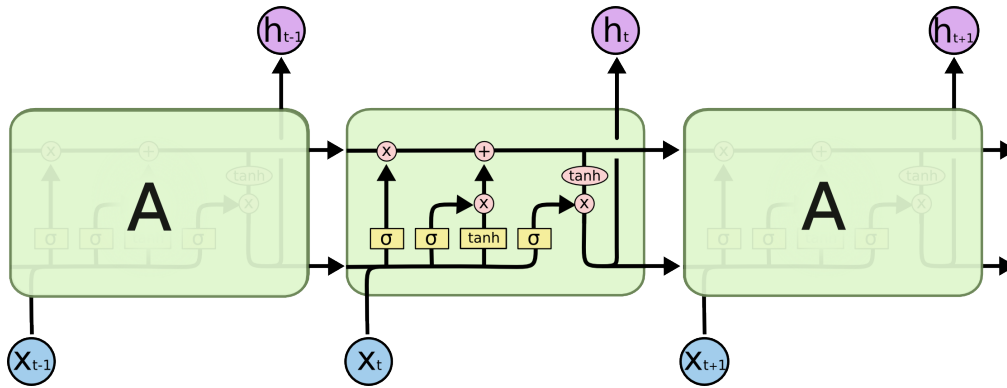


Figure 3: An LSTM cell in a chain of LSTM cells.

## Main idea

The cell state  $C_t$  serves as a long-term memory channel with controlled linear self-connections, enabling gradient preservation across long sequences. The gates learn to selectively retain, update, and expose information, allowing the LSTM to model long-range temporal dependencies effectively. The separation between memory ( $C_t$ ) and output ( $h_t$ ) is the defining feature that distinguishes LSTMs from standard recurrent neural networks.

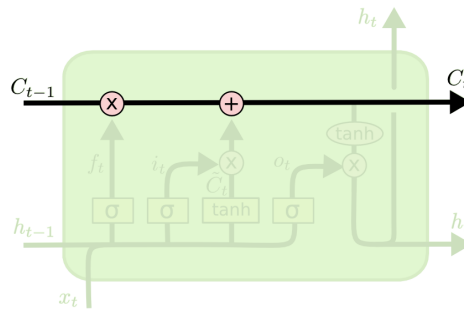


Figure 4: The cell state.

## Gates

An LSTM cell does have the ability to remove information from or add information to the cell state, carefully regulated by gates. Gates are a way to optionally let information through.

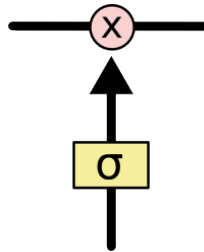


Figure 5: A gate.

**Activation layers** Something about activation layers used in the gates.

**Sigmoid** A sigmoid operation produces numbers between zero and one, describing how much of each component should be let through.

**Tanh** A tanh operation outputs numbers between -1 and 1.

## Walk Through

### What to forget?

The first step the LSTM cell needs to do is to decide what cell state information is to be forgotten. The forget vector produced by the following formula, will have the shape of  $C_{t-1}$ . The vector will contain values between 0 and 1, these values will be used to 'forget' specific information. The forget vector is calculated below:

$$f_t = \sigma(W_f x_t + U_f h_{t-1} + b_f)$$

where  $W_f$  and  $U_f$  are learned weight vectors,  $b_f$  is the bias,  $h_{t-1}$  is the hidden state from the previous time step,  $x_t$  is the current time step's input. The weight vectors aren't really visible but are part of the gate  $\sigma$ .

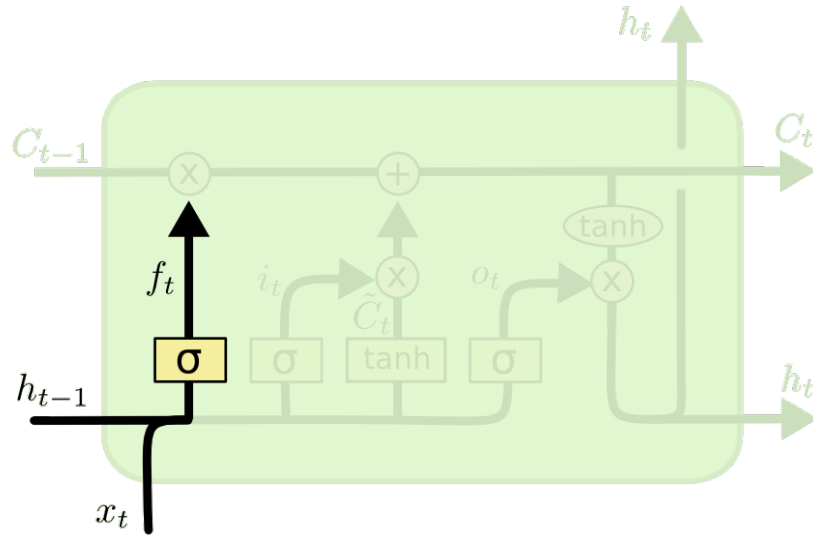


Figure 6: What to forget?

### What to update?

The next step is to decide what new information is to be stored in the cell state.

**Input gate layer** First, a sigmoid layer called the 'input gate layer' decides which values are to be updated. It is calculated using the formula below:

$$i_t = \sigma(W_i x_t + U_i h_{t-1} + b_i)$$

Where  $W_i$ ,  $U_i$  and  $b_i$  are learned,  $b_i$  is the bias. The weight vectors  $W_i$ ,  $U_i$  and  $b_i$  are part of the  $\sigma$  gate.

**New candidate layer** Next, a tanh layer creates a vector of new candidate values:

$$\tilde{C}_t = \tanh(W_c x_t + U_c h_{t-1} + b_c)$$

Where  $W_c$ ,  $U_c$  and  $b_c$  are learned,  $b_c$  is the bias. Again these values are part of the  $\tanh$  gate.

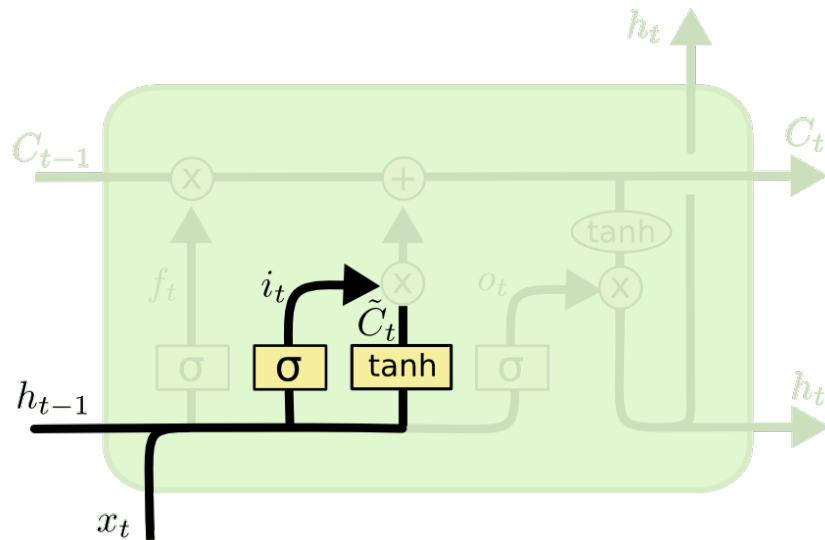


Figure 7: Creating new candidate values  $\tilde{C}_t$  and a vector that decides which values are to be updated  $i_t$

### Update

It's now time to update the old cell state,  $C_{t-1}$ , into the new cell state  $C_t$ . The previous steps already decided what to forget, what to update and with what to update. The following formula will update  $C_t$ .

$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$$

$\odot$  is a symbol for the element-wise product.

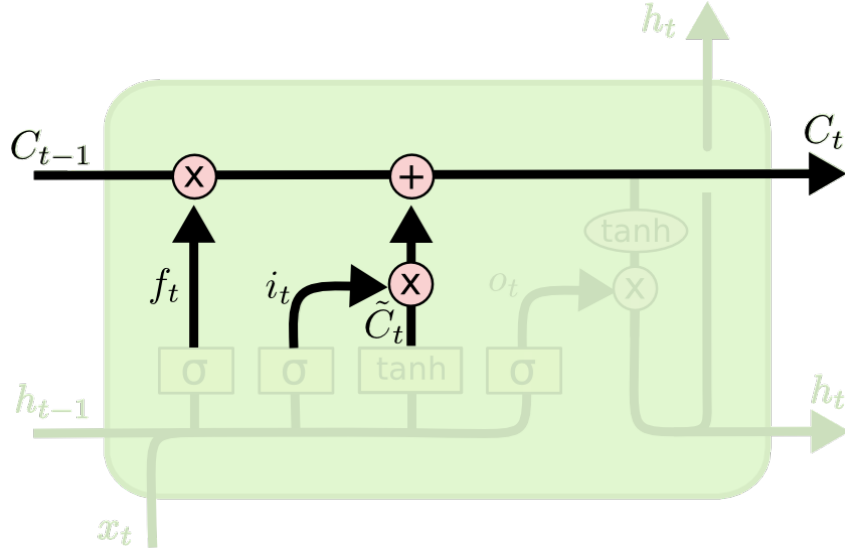


Figure 8: Updating  $C_t$

### Producing $h_t$

Finally, the LSTM cell needs to produce an output. This output is the result of 2 operations, the formulas can be found below:

$$o_t = \sigma(W_o x_t + U_o h_{t-1} + b_o)$$

$$h_t = o_t \odot \tanh(C_t)$$

where  $W_o$  and  $U_o$  are learned weight vectors,  $b_o$  is the bias,  $h_{t-1}$  is the hidden state from the previous time step,  $x_t$  is the current time step's input.

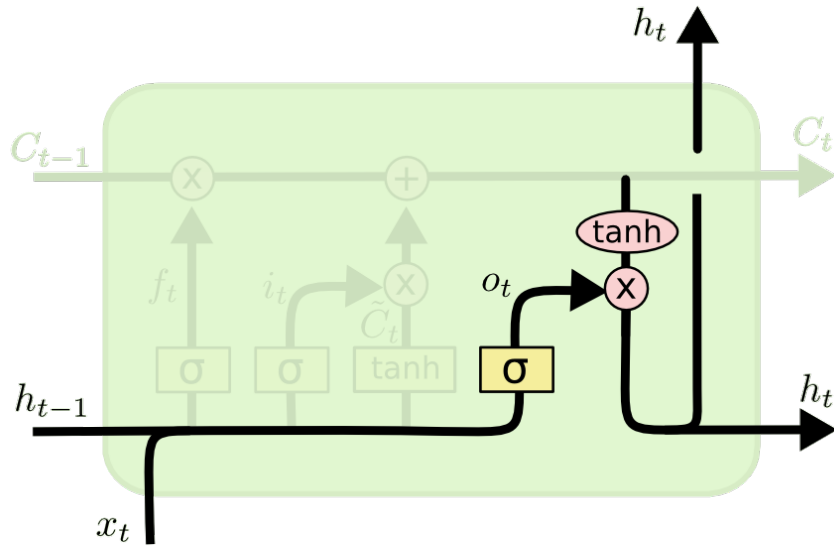


Figure 9: Producing  $h_t$

### Back-propagation

For an LSTM the vectors and values to be learned are the following.

$$\{W_f, U_f, b_f, W_i, U_i, b_i, W_c, U_c, b_c, W_o, U_o, b_o\}$$

When not in training mode, an LSTM reuses the same parameters at every time step. So at every time step the same learned parameters apply, what differs is the input at every time step  $x_t$ . As the input  $x_t$  differs,  $h_t$  and  $C_t$  differ too

of course. When training an LSTM network, loss needs to be propagated from the last time step through every cell in the recurrent network up until the first cell. Loss is propagated through  $C_t$  and  $h_t$ .

## Text generation

### A basic text generation model

The LSTM part allows the model to link a source Tensor of arbitrary length to a target Tensor of the same arbitrary length. The idea is to predict a next token for the Tensor. See Figure 10 for a visualization of this idea. The model is constructed using a multilayered LSTM to allow for some text complexity. One could think of a multilayered LSTM like multiple interconnected LSTM blocks, as to be seen in Figure 11. The outputs of a previous layer serve as input to the new LSTM layer.

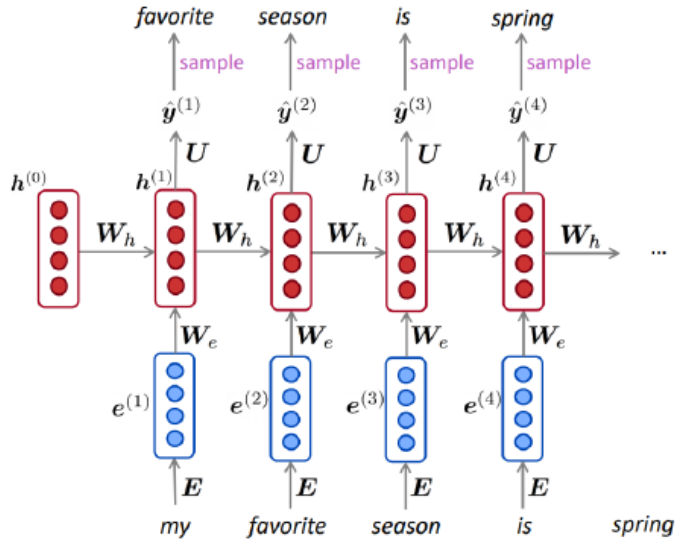


Figure 10: Visualization of text generation through an LSTM block.

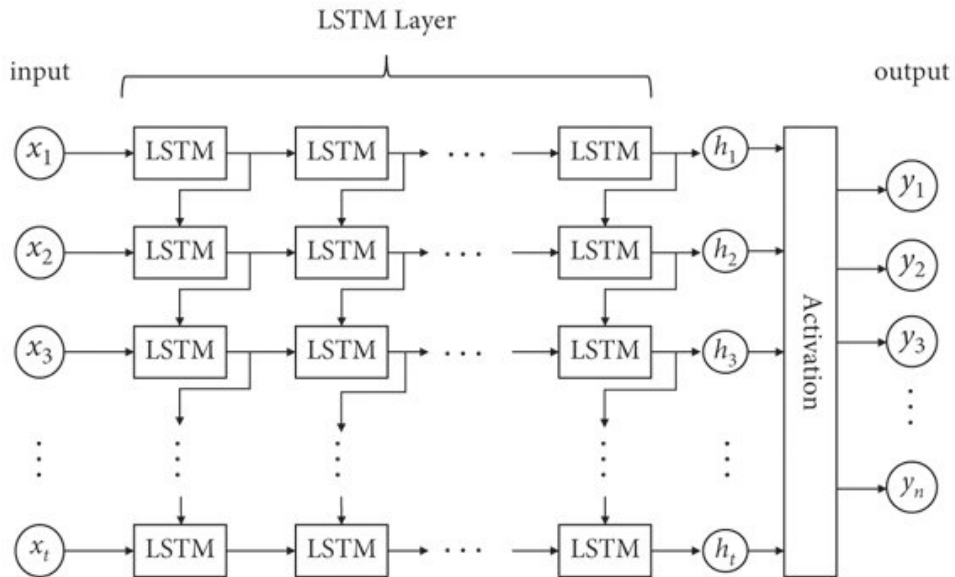


Figure 11: A multilayered LSTM block.

### How does it work

The code for a basic text generation model is to be found in Listing 1. As mentioned, the main component in this model is the LSTM part (line 12). Other parts are the embedding layer (line 11), a fully connected layer (line 17)

and a softmax layer (line 19).

**Forward method** The forward method (line 22-25) generates a complete new Tensor of Tensors, a Tensor for every embedded source token. Every Tensor produced this way, is entered into a feed forward network to produce the logits for every input token. if the length of the input is 20 tokens, output would be 20 times a logit for every token in the vocabulary.

As the model gets trained, the LSTM should get better at predicting semantically and syntactically correct words to follow a sequence of words.

**Write method** The write method (27-56) generates one token at a time. It enters a token index into an embedding block (line 37), this block converts the index into an embedding. The embedded values are fed into the LSTM block (line 38) to produce, some long- and short-term Tensors, and an output. This output is passed through a feedforward network (line 39), and the results of this operation are fed into a softmax block (line 44) to produce probabilities for every token in the corpus. Depending on the method, the token with the highest probability is selected or some randomness is allowed when it comes to selecting a next token. The write method ends when enough token indices have been generated. These indices are expanded into text on lines 53-54.

## Torch code

Listing 1: A basic text generation model

```
1 class LSTMForWordGeneration(nn.Module):
2     def __init__(self, word2idx, idx2word, embedding_dim=128, hidden_size=256, n_layers=3):
3         super().__init__()
4         self.word2idx = word2idx
5         self.idx2word = idx2word
6         self.embedding_dim = embedding_dim
7         self.num_characters = len(word2idx)
8         self.hidden_size = hidden_size
9         self.n_layers = n_layers
10
11        self.embedding = nn.Embedding(self.num_characters, embedding_dim)
12        self.lstm = nn.LSTM(input_size=embedding_dim,
13                            hidden_size=hidden_size,
14                            num_layers=n_layers,
15                            batch_first=True)
16
17        self.fc = nn.Linear(hidden_size, self.num_characters)
18
19        self.softmax = nn.Softmax(dim=-1)
20
21    def forward(self, x):
22        x = self.embedding(x)
23        output, (h, c) = self.lstm(x)
24        logits = self.fc(output)
25        return logits
26
27    def write(self, text, max_words, greedy=False):
28        idx = torch.tensor([self.word2idx[w] for w in text])
29
30        for i in range(max_words):
31
32            if i == 0:
33                selected_idx = idx
34            else:
35                selected_idx = idx[-1].unsqueeze(0)
36
37            x = self.embedding(selected_idx)
38            out, (hidden, cell) = self.lstm(x, (hidden, cell))
39            out = self.fc(out)
40
41            if len(out) > 1:
42                out = out[-1, :].unsqueeze(0)
```



```

43
44 probs = self.softmax(out)
45
46 if greedy:
47     idx_next = torch.argmax(probs).squeeze(0)
48 else:
49     idx_next = torch.multinomial(probs, num_samples=1).squeeze(0)
50
51 idx = torch.cat([idx, idx_next])
52
53 gen_string = [self.idx2word[int(w)] for w in idx]
54 gen_string = " ".join(gen_string)
55
56 return gen_string

```

## Results

As I was using a corpus of length 6000000+ tokens, 28000+ unique tokens this model and write method didn't lead to interesting results. So I thought up a more advanced text generation method and implemented attention to make a better model.

## Text generation using attention

In this section an attention layer will be added to the model, but before adding this layer, let's get an idea of what attention does.

### Attention

Attention is the mathematical mechanism that allows a model to "focus" on specific words (tokens) in a sentence to understand their context and meaning. To get this more concrete. If the  $v$  matrix in the next multiplications would be a matrix of token vectors then the next explication would shed some light on this concept.

### Attention explained

Attention can be explained by some matrix multiplications. Starting with 3 matrices  $q$ (query),  $k$ (key) and  $v$ (value):

$$q = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \end{bmatrix} \quad k = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad v = \begin{bmatrix} 2 & 4 \\ 6 & 6 \\ 3 & 5 \\ 6 & 3 \\ 2 & 4 \end{bmatrix}$$

These three matrices are supposed to be learned, at least  $q$  and  $k$  are, but as  $v$  is a result of the matrix multiplication of  $q$  and  $k$ , so is  $v$ . But first things first. Multiplying the  $q$  matrix with  $k^T$  ( $k$  is transposed to fit-in this case not that essential) results in:

$$q.k^T = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

As the query is hard (not soft), and the key is hard (not soft), the resulting multiplication is just as hard. So when finally multiplying  $q.k^T$  with  $v$ , this results in:

$$q.k^T.v = \begin{bmatrix} 3 & 5 \end{bmatrix}$$

The multiplications have the effect of selecting the third row in the  $v$  matrix.

**In code** In code these kind of multiplications would be done like in [Listing 2](#).

Listing 2: Attention explained by some matrix multiplications

```

1 import torch.nn.functional as F
2 q = F.one_hot(torch.tensor([2]), 5)
3 k = F.one_hot(torch.arange(5), 5)

```

```

4 v = torch.randint(2, 8, (5,2 ))
5 q_times_k=torch.mm(q,k.T)
6 q_times_k_times_v=torch.mm(q_times_k, v)

```

### A softer query

As q is learned it could become a less clear matrix. In this case this vague or soft q matrix has its effect on the final result of the multiplications. Again, starting with 3 matrices: a softer q(uey) matrix, k(ey) and v(alue) matrices stay the same:

$$q = \begin{bmatrix} 0. & 0.3 & 0.2 & 0.4 & 0.1 \end{bmatrix} \quad k = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad v = \begin{bmatrix} 2 & 4 \\ 6 & 6 \\ 3 & 5 \\ 6 & 3 \\ 2 & 4 \end{bmatrix}$$

These three matrices are supposed to be learned, at least q and k are, but as v is a result of the matrix multiplication of q and k, so v is learned in a way. But first things first, the q matrix multiplied with  $k^T$  results in:

$$q.k^T = \begin{bmatrix} 0. & 0.3 & 0.2 & 0.4 & 0.1 \end{bmatrix}$$

As the query is soft, and the key is hard, the resulting multiplication is getting softer. So when finally multiplying  $q.k^T$  with v, this results in:

$$q.k^T.v = \begin{bmatrix} 5. & 4.4 \end{bmatrix}$$

In this case the complete operation, and especially the softer query results in a weighted mean (weighted by the q values) for every column in the v matrix.

### A softer query and softer keys

Again, starting with 3 matrices a softer q(uey) matrix and a softer k(ey) matrix, the v(alue) matrix stays the same:

$$q = \begin{bmatrix} 0. & 0.3 & 0.2 & 0.4 & 0.1 \end{bmatrix} \quad k = \begin{bmatrix} 1. & 0. & 0. & 0. & 0. \\ 0. & 0.5 & 0. & 0. & 0. \\ 0. & 0.5 & 1. & 0. & 0. \\ 0. & 0. & 0. & 1. & 0. \\ 0. & 0. & 0. & 0. & 1. \end{bmatrix} \quad v = \begin{bmatrix} 2 & 4 \\ 6 & 6 \\ 3 & 5 \\ 6 & 3 \\ 2 & 4 \end{bmatrix}$$

These three matrices are supposed to be learned, at least q and k are, but as v is a result of the matrix multiplication of q and k, so is v. But first things first. q matrix multiplied with  $k^T$  results in:

$$q.k^T = \begin{bmatrix} 0. & 0.15 & 0.35 & 0.4 & 0.1 \end{bmatrix}$$

And to get an idea of how k affects v,  $k^T$  multiplied with v results in:

$$k^T.v = \begin{bmatrix} 2. & 4. \\ 4.5 & 5.5 \\ 3. & 5. \\ 6. & 3. \\ 2. & 4. \end{bmatrix}$$

As the query is soft, and the key is soft, the resulting multiplication is also soft, even though it could even become softer. So when finally multiplying  $q.k^T$  with v, this results in:

$$q.k^T.v = \begin{bmatrix} 4.5499997 & 4.25 \end{bmatrix}$$

In this case the v matrix is influenced by both the soft query and key matrices. This manner of transforming value vectors simulates the way attention impacts vectors in a neural network.

### Attention in code

In [Listing 3](#), a difference regarding the matrix multiplications shown in [Listing 2](#) can be observed. The Attention class definition contains bmm operations, bmm is the batched version of the normal matrix multiplication.

**Torch** A MultiHeadedAttention module in torch exists, but I found it easier to use a custom class. It seemed easier to configure a custom class for my specific case. This custom class was partly found on the internet, but I needed to fit it to my needs. From what I know it is how the first Transformer had its attention calculated.

## Description

Applying this attention layer allows the model to transform initial  $h_t$  vectors. These kind of attention layers will put focus on parts of the vector that seem to lower loss production.

**Linear layers to redimension the outputs** In the code the same matrices used to describe what attention does are present as linear layers, see line 8,9,10, they are linear layers because the input and output dimensions differ, by using linear layers, the dimensions can be adapted to the output expected in the second LSTM layer. In some next development step I could try to get the right output size from the first LSTM, to not be obliged to use this kind of redimensioning.

**Redimensioning the input** On line 12,  $q$  being the output of an LSTM cell time step is being fed into a linear layer Q. The  $x$  value (an embedding vector representing a token) is being fed into two other linear layers K, V.

**Calculating raw attention and eventually normalized scores** On line 15 queries and keys returned on line 12-13 are matrix multiplied to get primary attention scores, after normalization (16), these are 'softmaxed' to get attention values.

**Applying normalization to the input token vector** On line 17, these normalized attention weights are matrix multiplied with the linearly transformed (transformed on line 14) original input token vector. By multiplying the attention weights with the original values, the original embedding is 'moved' into the direction its context seems to indicate the embedding should be moved. The attended values are returned as hidden states (line 19).

Listing 3: Attention in code

```
1 class Attention(nn.Module):
2     def __init__(self, d_in,d_out, n_layers, n_directions=2):
3         super().__init__()
4         self.d_in=d_in
5         self.d_out=d_out
6         self.n_layers =n_layers
7         self.n_directions=n_directions
8         self.Q=nn.Linear(self.n_directions*self.n_layers*d_in,d_out)
9         self.K=nn.Linear(d_in,d_out)
10        self.V=nn.Linear(d_in,d_out)
11    def forward(self,q ,x):
12        queries=self.Q(q)
13        keys = self.K(x)
14        values = self.V(x)
15        scores = torch.bmm(queries, keys.transpose(1,2))
16        scores = scores/ (self.d_out**0.5)
17        attention = F.softmax(scores,dim=2)
18        hidden_states= torch.bmm(attention,values)
19        return hidden_states
```

## A text generation model using attention

In this part I will use the attention layer in a text generation model. The two write methods will be separately covered.

**Differences compared to the simpler model** When compared to the simple model, this model has 2 LSTMs instead of 1. This to facilitate the use of attention. In this model, an attention layer is added (line 19) and a second LSTM layer is added (line 21). Other components don't really differ from the model without attention, there is an extra LogSoftmax layer (line 29) for the write\_better method. The forward method is more complex when compared to the simpler model, as I am applying the LSTM network on a per token/per time step basis.

## The forward method

The forward method will apply attention for every time step.

**Side note** The way in which I apply attention and use hidden and cell values, is sort of experimental. I commented out the experimentation as it might not be such a good idea after all.

**Manually applying attention for every time step** This because I wanted to apply the attention manually for every time step and consequently for every token embedding, this happens on line 45. The loop to go over every time step starts on line 33.

**Preparing first LSTM layer outputs for second LSTM layer input** Other steps are feeding the 'current time step token embedding vector' (line 38,40) into the first LSTM layer. Reshaping the hidden and cell LSTM outputs (line 42,43) to prepare them for input in the second LSTM layer (line 47).

**Adapting the current second LSTM's output for next time step first LSTM's input** While I was adapting values at a time step level, I wanted the second's layer's LSTM output to influence the first layers hidden and cell vectors (line 49-50) when generating outputs in a next time step. As these adapted vectors are being used in the next time step to generate new first LSTM layer's time step outputs, they need to be reshaped (line 52-53).

**Producing logits and tokens** Eventually the per time step output produced by the second LSTM layer is being concatenated with previous previous time step outputs, to form the complete output. For every output generated by the second LSTM layer, logits are generated (line 58). These logits represent probabilities for every token in the dictionary. As for every source sentence there is a target sentence, loss can be calculated by comparing the expected tokens for a source sentence, with the logit values that were returned for every token in the dictionary per time step.

Listing 4: A basic text generation model with attention

```
1 class LSTMForWordGenerationWithAttention(nn.Module):
2     def __init__(self, word2idx, idx2word, embedding_dim=128, hidden_size=256, bidirectional=
3         ↪ False, n_layers=3):
4         super().__init__()
5         self.word2idx = word2idx
6         self.idx2word = idx2word
7         self.embedding_dim = embedding_dim
8         self.num_words = len(word2idx)
9         self.hidden_size = hidden_size
10        self.n_layers = n_layers
11        self.num_directions = 2 if bidirectional else 1
12
13        self.embedding = nn.Embedding(self.num_words, embedding_dim)
14        self.lstm = nn.LSTM(input_size=embedding_dim,
15            hidden_size=hidden_size,
16            num_layers=n_layers,
17            batch_first=True,
18            bidirectional=bidirectional)
19
20        self.attention = Attention(self.embedding_dim, self.n_layers * self.num_directions * self.
21            ↪ embedding_dim, self.n_layers, self.num_directions)
22
23        self.lstm2 = nn.LSTM(input_size=self.n_layers * self.num_directions * self.embedding_dim,
24            hidden_size=self.n_layers * self.num_directions * self.hidden_size,
25            num_layers=1,
26            batch_first=True,
27            bidirectional=False)
28
29        self.fc = nn.Linear(self.n_layers * self.num_directions * self.hidden_size, self.num_words)
30        self.softmax = nn.Softmax(dim=-1)
31        self.log_softmax = nn.LogSoftmax(dim=-1)
32
33    def forward(self, x):
34        batch_size = x.size(0)
35        output_enc_dec = FloatTensor()
36        for i in range(x.shape[1]):
```

```

34 x_i = self.embedding(x[:, i])
35 x_i = x_i.unsqueeze(1)
36
37 if i == 0:
38     out, (hidden, cell) = self.lstm(x_i)
39 else:
40     out, (hidden, cell) = self.lstm(x_i, (hidden, cell))
41
42 hidden = hidden.reshape(1, -1, self.n_layers * self.num_directions * self.hidden_size)
43 cell = cell.reshape(1, -1, self.n_layers * self.num_directions * self.hidden_size)
44
45 attention_output = self.attention(out, x_i)
46
47 out_lstm2, (h, c) = self.lstm2(attention_output, (hidden, cell))
48
49 #hidden = torch.div(torch.add(hidden, h), 2, rounding_mode=None)
50 #cell = torch.div(torch.add(cell, c), 2, rounding_mode=None)
51
52 hidden = hidden.reshape(self.n_layers * self.num_directions, batch_size, -1)
53 cell = cell.reshape(self.n_layers * self.num_directions, batch_size, -1)
54
55 output_enc_dec = torch.cat([output_enc_dec, out_lstm2.unsqueeze(1)], dim=1)
56
57 output_enc_dec = output_enc_dec.squeeze(2)
58 logits = self.fc(output_enc_dec)
59 return logits

```

## Write

The original write method, is adapted to deal with attention. It is to be seen in [Listing 5](#).

**Apply attention to output of first lstm** On line 22 the output from the first lstm layer is transformed by the attention layer. This output is then used as input for the second lstm layer. This is the main difference from the simple text generation model.

**Detach, clone, reshape and rename hidden and cell outputs** The hidden and cell outputs from the first lstm layer are detached and cloned, renamed, reshaped and detached (line 19-20). Detached implies, released from the back-propagation cycle. In this way they can serve as inputs for the second LSTM layer (line 23), while the original hidden and cell tensors (still in the back-propagation cycle) remain available as input for the first lstm layer in the next time step.

**Second lstm produces its output for the fully connected layer** As all parameters for the second LSTM are fed into it (line 23), the output of this second LSTM is input for the fully connected layer (line 25).

**Producing a distribution over all tokens in the dictionary** After some dimensions adaptations (line 26 and possibly 29) the output becomes suitable for becoming a distribution over every token in the dictionary (line 31).

**Picking the next word by chance or the most probable** Now depending on the chosen method (line 33-36), the most probable word or a word is randomly chosen using it's possibility as a chance for it to be chosen. The index for the word is concatenated to the previously chosen index (line 38).

**Translating the indices into a sentence** When the for loop described here is finished. The only thing needed now is the translation from numbers to words using the dictionary (line 40).

Listing 5: Write with attention

```

1 def write(self, text, max_words, greedy=False):
2     idx = torch.tensor([self.word2idx[w] for w in text])
3     hidden = Tensor()
4     cell = Tensor()
5     for i in range(max_words):

```

```

6  if i == 0:
7      selected_idx = idx
8  else:
9      selected_idx = idx[-1].unsqueeze(0)
10
11  x = self.embedding(selected_idx)
12  x = x.unsqueeze(0)
13
14  if i == 0:
15      out, (hidden, cell) = self.lstm(x)
16  else:
17      out, (hidden, cell) = self.lstm(x, (hidden, cell))
18
19  hidden1 = hidden.detach().clone().reshape(1, 1, -1)
20  cell1 = cell.detach().clone().reshape(1, 1, -1)
21
22  attention_output = self.attention(out, x)
23  out_lstm2, (h, c) = self.lstm2(attention_output, (hidden1, cell1))
24
25  out = self.fc(out_lstm2)
26  out = out.squeeze(0)
27
28  if len(out) > 1:
29      out = out[-1, :].unsqueeze(0)
30
31  probs = self.softmax(out)
32
33  if greedy:
34      idx_next = torch.argmax(probs).squeeze(0)
35  else:
36      idx_next = torch.multinomial(probs, num_samples=1).squeeze(0)
37
38  idx = torch.cat([idx, idx_next])
39
40  gen_string = [self.idx2word[int(w)] for w in idx]
41  gen_string = " ".join(gen_string)
42  return gen_string

```

## Write better

In this part the write better method will be elaborated on. The write better method is an integral part of the model. As the write.better method is based on the Beam search algorithm, the Beam search algorithm is illustrated using a simple example.

**Beam search:simplified example** To get an idea of how beam search works, see [Figure 12](#), the beam search illustrated here represents a beam search with width 2. At the first time step, A and B would be retained, as these have the least negative log probabilities. At the second time step, as only A and B have been kept, only children of these nodes need to be considered. A B and B A have the least negative cumulative probability so these paths are retained. Only nodes that are descendants of A B and B A are considered next. Of those descendants A B B and B A C prove to be the most interesting hypotheses. As all other paths have a higher negative cumulative log-probability. As not all paths are being considered, beam search is no guarantee to finding the most optimal path overall, but at least it gives a chance to paths that initially look less fruitful. And in this example an initially less fruitful alternative (B) eventually proves to be just as fruitful as the initially most interesting node to investigate (A).

## Code

In the text generation model, the write.better method needs to consider thousands of tokens every time step, for every word generated. It generates a next word from previously generated/selected words. The code keeps track of the path probabilities. To describe the process of this method I will describe every step of the code and share the shape, and sometimes the content.

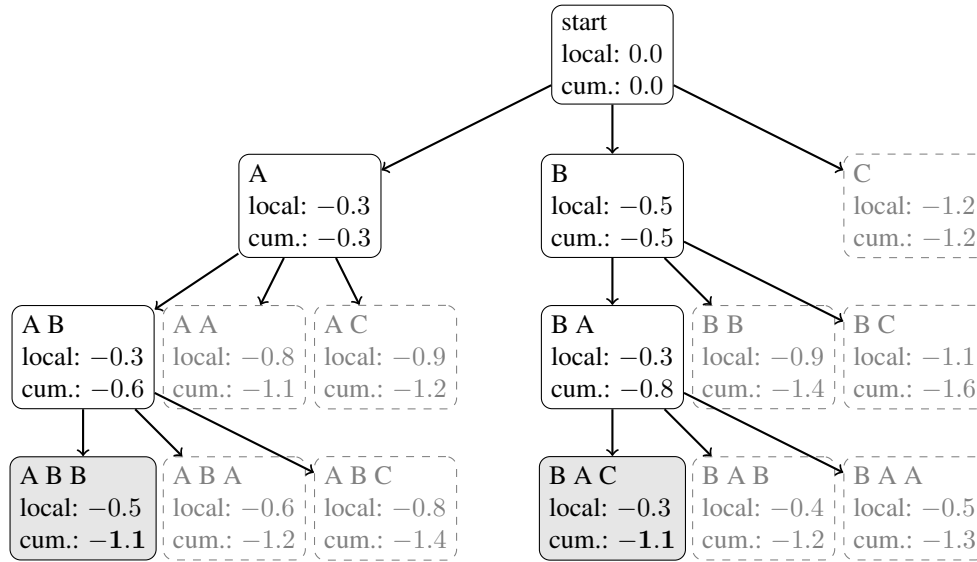


Figure 12: Beam search tree with beam width of 2. Each node displays the local log-probability and the cumulative log-probability. Pruned hypotheses are dashed, the 2 best sequences are darkened.

**Some parameters** The example beam width used here will be 3, the embedding dimension will be 128, and the first LSTM's hidden dimension will be 256, the first LSTM will be bidirectional, the number of layers in the first LSTM will be 2, the number of items in the token dictionary is 6916.

**Initializing** As beam width is 3, and our algorithm wants to return 3 fruitful paths. The algorithm needs to create a tensor 3 times the first index from which to generate the next time steps. For the first time step, as the initial input is "Spells", the initial tensor created on line 3 looks like this.

$$[[6080] [6080] [6080]]$$

6080 is the index in the dictionary for the token "Spells".

The initial tensor to hold the probabilities for each path looks like

$$[[0.] [0.] [0.]]$$

The variables set to hold the indices and the probabilities are set on line 3 and 6.

**Some background** The matrix holding the initial word indices will be fed into the LSTM like it was a sort of batched input. At this moment the indices are the same, so this seems a bit useless. But after generating a new word for each path, three different word indices will be fed into the LSTM, and those 3 indices will eventually produce 3 different distributions for the next word. The LSTM will also produce different hidden and cell outputs for every other word per time step. This is the main complicating factor when applying the beam search algorithm in this situation.

**Embedding** For the three indices an embedding is created (line 15). The embedding for this complete tensor has a shape:

$$[3 \ 1 \ 128]$$

128 representing the embedding size, 3 the number of indices/beams for which the embedding is produced.

**Feeding the embedding into the first LSTM** On line 16-19, the embedding is fed into the first LSTM. Some conditions are used here. This demands some explication, by default an LSTM will create hidden and cell vectors if none are given. The values are all zeros for these vectors. In the first time step this is a good thing, but as of the second time step the hidden and cell values will depend on the chosen beam paths. The shape of the out, hidden and cell tensors are:

$$\text{out.shape} = [3 \ 1 \ 512]$$

3 from the number of beams

512 is the hidden dimension (256) times the number of directions (2)

$$\text{hidden.shape} = [4 \quad 3 \quad 256]$$

4, as the number of layers for the LSTM is 2 and the number of directions is 2, and 2 times 2 is 4

3, as the number of beams is 3

256 as the hidden dimension for the LSTM is 256

$$\text{cell.shape} = [4 \quad 3 \quad 256]$$

4, as the number of layers for the LSTM is 2 and the number of directions is 2

3, as the number of beams is 3

256 as the hidden dimension for the LSTM is 256

**Reshaping hidden and cell vectors** On line 21 and 22 the hidden and cell vectors are detached, cloned and reshaped. After reshaping, both cell1 and hidden1 have the same shape:

$$\text{cell1.shape} = \text{hidden1.shape} = [1 \quad 3 \quad 1024]$$

3 is the number of beams

1024 is 4\*256, the same data is available as before, only dimensions have changed

The second LSTM needs the vector to be in this shape. But in the next time step, the original hidden and cell shapes are needed, that is why they are cloned and detached for reshaping.

**Applying attention to the output of the first LSTM** On line 24 attention is applied, after having applied attention shape of the weighted output is

$$\text{weighted\_output.shape} = [3 \quad 1 \quad 512]$$

This weighted output could be seen as the contextualized primary input for the second LSTM. It is the query for which a next token in the sentence should be predicted. The hidden1 and cell1 vectors are unattended to, but could/should contain additional information from a previous time step.

**Feed into the second LSTM** The cell1, hidden1 and weighted\_output are fed into the second LSTM (line 25). After this shapes of the vectors looks like this:

$$\text{lst2\_out.shape} = [3 \quad 1 \quad 1024]$$

3, is the number of beams

1024, is the number of layers (2) times the number of directions (2) times the hidden size (256)

$$\text{h.shape} = \text{c.shape} = [1 \quad 3 \quad 1024]$$

3, is the number of beams

1024, is the number of layers (2) times the number of directions (2) times the hidden size (256)

After application of line 26 all three vectors h, c and lst2\_out have the same shapes.

**Feed lst2\_out into the fully connected layer and applying softmax** The output of the second LSTM is fed into a fully connected layer (line 27). The resulting vector's shape is:

$$[1 \quad 3 \quad 6916]$$

3, for the beam width

6916, the number of tokens present in the dictionary

After feeding the fully connected return into the softmax layer (line 32), the shape remains the same. It is from this moment on, that a distribution for every word in the dictionary exists for every different path, these distributions depend on the previous inputs (hidden, cell, token index embedding) for every beam respectively.



**Add previous path probabilities to newly create distribution** To compare path probabilities, the newly created distributions for the tokens needs to be increased by the already existing path probabilities (line 33). By using the right dimensions, the path probability for each path only gets broadcast added to the right distribution. As the softmax layer we're using is a LogSoftmax layer, probabilities can be added.

## Beam search

It is from this moment on that the most fruitful paths for generating a new word in the sequence should be chosen. As it is possible an unfruitful path can be canceled, it is important to know for which paths to keep the sequence running and for which not.

**Selecting the most probable indices and their probabilities** Some background, as the distributions (adapted by the existing path probabilities) that exist for every path in our beam search can and will differ, and the 3 most fruitful paths need to be chosen, every probability for the 3 beams need to be compared, that's why the probabilities for the 3 beams need to be flattened, to compare them over distribution boundaries.

The flattened probabilities tensor has a shape of

$$[20748]$$

20748, 6916 times the number of beams 3

This comparison happens on line 35. The resulting top probabilities could look like this:

$$[0.0002 \quad 0.0002 \quad 0.0002]$$

The resulting top indices could look like this, in this case every index lies on another path:

$$[11975 \quad 14804 \quad 5194]$$

Line 37 is the code to get the global indices translated to their original distributions. The result of this line looks like this:

$$\text{indexes} = \begin{bmatrix} [0 & 0 & 5194] \\ [0 & 1 & 5059] \\ [0 & 2 & 972] \end{bmatrix}$$

After merging probabilities into this matrix (line 39) and sorting on the second column (41), the matrix looks like this.

$$\text{indexes} = \begin{bmatrix} [0 & 0 & 5194 & 0.0002] \\ [0 & 1 & 5059 & 0.0002] \\ [0 & 2 & 972 & 0.0002] \end{bmatrix}$$

11975, refers to token index 5059 in the second distribution

14804, refers to token index 972 in the third distribution

5194, refers to token index 5194 in the first distribution

The indices of the 3 most probable new path tokens can be found on the 3 column of the indexes matrix. So this column is selected on line 42. These new token indices are concatenated to the already present token indices, line 44. To keep track of the newly calculated cumulative path probabilities, path probabilities are taken from the indexes\_ext matrix and kept in a variable (line 46).

**Adapting hidden and cell vectors** As paths are chosen others are left closed, hidden and cell values should disappear as their distribution contains no relevant probability and token index, this is done on lines 47-48. Remember the shape of hidden and cell

$$\text{hidden.shape} = \text{cell.shape} = [4 \quad 3 \quad 256]$$

It is only for relevant distributions hidden and cell values are being kept. In case the distribution indices were [1, 2, 2], hidden matrix for every beam is adapted by moving the relevant parts of the matrix around. So in the next time step the hidden and cell values are relevant and are set correct for the respective paths.

**Generate text** After the loop has generated the correct number of words for all beams, the different sequences of indices are expanded into real texts, line 50-54.

Listing 6: Write better with attention

```
1 def write_better(self, text, max_words, k=1):
2     idx = torch.tensor([self.word2idx[w] for w in text])
3     k_times_idx = idx.repeat(1, k).unsqueeze(2).squeeze(0)
4     hidden = Tensor()
5     cell = Tensor()
6     k_times_probs = Tensor([0]).repeat(k).unsqueeze(1)
7
8     for i in range(max_words):
9         # print("i: ", i)
10        if i == 0:
11            selected_idx = k_times_idx
12        else:
13            selected_idx = k_times_idx[:, -1].unsqueeze(1)
14
15        x = self.embedding(selected_idx)
16        if i == 0:
17            out, (hidden, cell) = self.lstm(x)
18        else:
19            out, (hidden, cell) = self.lstm(x, (hidden, cell))
20
21        hidden1 = hidden.detach().clone().reshape(1, k, -1)
22        cell1 = cell.detach().clone().reshape(1, k, -1)
23        # apply attention
24        weighted_output = self.attention(out, x)
25        out_lstm2, (h, c) = self.lstm2(weighted_output, (hidden1, cell1))
26        out_lstm2 = out_lstm2.permute(1, 0, 2)
27        out = self.fc(out_lstm2)
28
29        if len(out) > 1:
30            out = out[-1, :].unsqueeze(0)
31
32        probs = self.log_softmax(out)
33        probs.add_(k_times_probs)
34
35        probs_top, i = torch.topk(probs.detach().flatten(), k=k, dim=-1, sorted=False)
36        i = i.detach()
37        indexes = np.array(np.unravel_index(i.numpy(), probs.shape)).T
38        # extend indexes with probs
39        indexes_ext = np.concatenate((indexes, probs_top.unsqueeze(1)), axis=1)
40        # sort extended indexes
41        sorted_indexes = indexes_ext[np.argsort(indexes[:, 1])]
42        indices = torch.tensor(sorted_indexes[:, 1]).type(dtype='torch.IntTensor')
43        idx_next = torch.from_numpy(sorted_indexes[:, 2]).type(dtype='torch.IntTensor').unsqueeze
44        ↪ (1)
45        k_times_idx = torch.cat([k_times_idx, idx_next], dim=1)
46        #update path probs
47        k_times_probs = torch.from_numpy(sorted_indexes[:, 3]).unsqueeze(1)
48        hidden = torch.index_select(hidden, 1, indices)
49        cell = torch.index_select(cell, 1, indices)
50
51        gen_strings = []
52        for i, idxs in enumerate(k_times_idx.numpy()):
53            gen_string = [self.idx2word[int(w)] for w in idxs]
54            gen_strings.append(" ".join(gen_string))
55        probs=torch.exp(k_times_probs.squeeze(1))
56        return gen_strings, probs
```

## Text generation using multiheaded attention

In the previous section attention was discussed and used in a model. In this section multi-headed attention added to the model.

## Multi-headed attention in code

Basically plain attention allows one channel of attention, and multi-headed attention allows for more channels. The code in [Listing 7](#) shows a custom multi-headed attention layer. Parameter `d_in` and `d_out` are the in and output dimensions for the module and hence the complete multi-headed attention. As the attention layer is placed between two lstms `d_in` depends on the outputs of the first lstm layer and `d_out` depends on the second lstm layer's input dimensions.

**ModuleList** The `attention_heads` are created inside a `ModuleList` (line 5). This torch construct allows for the same handling of the layers inside this list as for simple `nn.Modules`.

Listing 7: Multiheaded attention

```
1 class MultiHeadAttentionWrapper(nn.Module):
2     def __init__(self, d_in, d_out, n_layers, n_directions, num_heads):
3         super().__init__()
4         self.heads = nn.ModuleList(
5             [Attention(d_in, d_out, n_layers, n_directions) for _ in range(num_heads)]
6         )
7
8     def forward(self, q, x):
9         return torch.cat([head(q, x) for head in self.heads], dim=-1)
```

## A text generation model using multi-headed attention

The `__init__` method and the forward method don't differ that much from the simpler method with attention. That is why I will not elaborate on them. For the model's code see [Listing 8](#).

Listing 8: A basic text generation model with multiheaded attention

```
1 class LSTMForWordGenerationWithMHAttention(nn.Module):
2     def __init__(self, word2idx, idx2word, embedding_dim=128, hidden_size=256, bidirectional=
3         ↪ False, n_layers=3, n_heads=2):
4         super().__init__()
5         self.word2idx = word2idx
6         self.idx2word = idx2word
7         self.embedding_dim = embedding_dim
8         self.num_words = len(word2idx)
9         self.hidden_size = hidden_size
10        self.n_layers = n_layers
11        self.n_heads = n_heads
12        self.num_directions = 2 if bidirectional else 1
13
14        self.embedding = nn.Embedding(self.num_words, embedding_dim)
15        self.lstm = nn.LSTM(input_size=embedding_dim,
16                            hidden_size=hidden_size,
17                            num_layers=n_layers,
18                            batch_first=True,
19                            bidirectional=bidirectional)
20
21        self.attention = MultiHeadAttentionWrapper(self.embedding_dim, self.n_layers * self.
22            ↪ num_directions * self.embedding_dim, self.n_layers, self.num_directions, self.n_heads)
23
24        self.lstm2 = nn.LSTM(input_size=self.n_heads * self.n_layers * self.num_directions * self.
25            ↪ embedding_dim,
26                            hidden_size=self.n_layers * self.num_directions * self.hidden_size,
27                            num_layers=1,
28                            batch_first=True,
29                            bidirectional=False)
30
31        self.fc = nn.Linear(self.n_layers * self.num_directions * self.hidden_size, self.num_words)
32        self.softmax = nn.Softmax(dim=-1)
33        self.log_softmax = nn.LogSoftmax(dim=-1)
34
35    def forward(self, x):
36        batch_size = x.size(0)
37        output_enc_dec = FloatTensor()
38        for i in range(x.shape[1]):
```

```

35     x_i = self.embedding(x[:, i])
36     x_i = x_i.unsqueeze(1)
37
38     if i == 0:
39         out, (hidden, cell) = self.lstm(x_i)
40     else:
41         out, (hidden, cell) = self.lstm(x_i, (hidden, cell))
42
43     hidden = hidden.reshape(1, -1, self.n_layers * self.num_directions * self.hidden_size)
44     cell = cell.reshape(1, -1, self.n_layers * self.num_directions * self.hidden_size)
45
46
47     attention_output = self.attention(out, x_i)
48
49     out_lstm2, (h, c) = self.lstm2(attention_output, (hidden, cell))
50
51     hidden = torch.div(torch.add(hidden, h), 2, rounding_mode=None)
52     cell = torch.div(torch.add(cell, c), 2, rounding_mode=None)
53
54     hidden = hidden.reshape(self.n_layers * self.num_directions, batch_size, -1)
55     cell = cell.reshape(self.n_layers * self.num_directions, batch_size, -1)
56
57     output_enc_dec = torch.cat([output_enc_dec, out_lstm2.unsqueeze(1)], dim=1)
58
59     output_enc_dec = output_enc_dec.squeeze(2)
60     logits = self.fc(output_enc_dec)
61     return logits

```

## Write better and write

These methods don't differ that much from the methods in the model with attention, so I will not add the code for them.

## Training

### The training loop

The training loop in [Listing 9](#) looks a bit complicated, but it isn't that complicated.

### Data written to the console, to disk and saving the model

There are a multiple things exported, loss, generated text, text probabilities and loss (lines 2-18, 59-69, 74-79, 81-83). Also some data is written to the console (line 47-58). Every evaluation\_interval the trained model's parameters are saved (line 71).

### Furthermore normal training elements

Furthermore basic training elements like optimizer, loss (line 26, 27). The dataset is created (line 28). Batch is fetched (line 32-33), zero\_grad() is applied to the optimizer (line 34), loss is calculated (line 38), back-propagated over parameters (line 40) and parameters are updated (line 41).

Listing 9: Train loop

```

1 def train_(model, word2idx, idx2word, tokens, config, write_better=False):
2     training_data = {
3         "model": [],
4         "iteration": [],
5         "training data length": [],
6         "loss": [],
7         "generated text": []
8     }
9     texts_generated = {
10        "iteration": [],
11        "loss": [],

```

```

12     "probabilities": [],
13     "texts": [],
14 }
15
16 name=model.__class__.__name__
17 new_dir =Path(os.path.join(TRAINED_MODELS_DIR, name))
18 new_dir.mkdir(parents=True, exist_ok=True)
19
20 iterations = config["iterations"]
21 max_len = config["max_len"]
22 evaluate_interval = config["evaluate_interval"]
23 lr = config["lr"]
24 batch_size = config["batch_size"]
25
26 optimizer = optim.AdamW(model.parameters(), lr=lr)
27 loss_fn = nn.CrossEntropyLoss()
28 np.random.seed(0)
29 dataset = code.data.data_memmap.get_databuildermemmap(max_len, tokens, word2idx, idx2word)
30 model.train()
31 for iteration in range(iterations):
32     input_texts, labels = dataset.grab_random_batch(batch_size=batch_size)
33     input_texts, labels = input_texts, labels
34     optimizer.zero_grad()
35     output = model(input_texts)
36     output = output.transpose(1,2)
37
38     loss = loss_fn(output, labels.long())
39
40     loss.backward()
41     optimizer.step()
42
43
44     if iteration % evaluate_interval == 0:
45         model.eval()
46         torch.no_grad()
47         print("-----")
48         print(f"training data length {max_len}")
49         print(f"Iteration {iteration}")
50         print(f"Loss {loss.item()}")
51         generated_text = model.write(["Spells"], max_words=50)
52         print(generated_text)
53         if write_better:
54             generated_texts, probabilities = model.write_better(["Spells"], max_words=50, k=3)
55             print("Sample Generation")
56             for text, probability in zip(generated_texts, probabilities):
57                 print(f"text: {text} probability: {probability}")
58                 print("-----")
59             training_data["model"].append(name)
60             training_data["iteration"].append(iteration)
61             training_data["training data length"].append(max_len)
62             training_data["loss"].append(loss.item())
63             training_data["generated text"].append(generated_text)
64
65         if write_better:
66             texts_generated["iteration"].append(iteration)
67             texts_generated["loss"].append(loss.item())
68             texts_generated["probabilities"].append(probabilities)
69             texts_generated["texts"].append(generated_texts)
70
71         torch.save(model.state_dict(), os.path.join(TRAINED_MODELS_DIR, name + "/model_state-v"+
72             ↪ str(iteration)+".pth"))
73         torch.enable_grad()
74         model.train()
75         td=pd.DataFrame(training_data)
76         td.set_index(["model", "iteration"])
77         td.to_csv(os.path.join(TRAINED_MODELS_DIR, name, "training_data.csv"), encoding="utf8")
78         cd=pd.DataFrame(list(config.items()), columns=["key", "value"])

```

```

79 cd.to_csv(os.path.join(TRAINED_MODELS_DIR, name, "config_data.csv"), encoding="utf8", index=
    ↪ False)
80
81 if write_better:
82     with open(os.path.join(TRAINED_MODELS_DIR, name, 'generated_texts.pkl'), 'wb') as fh:
83         pickle.dump(texts_generated, fh, protocol=pickle.HIGHEST_PROTOCOL)

```

## Loss and generated texts

In the accompanying notebook 3 models have been created, trained and compared. In the following I will compare some results produced by the models while training. As I limited the number of training examples, limited the number of tokens (by limiting the corpus to one or two books book) and limited the hidden and embedding dimensions for the models themselves. In this way I kept total training time limited to hours. Hence the text generated by these models is equally limited.

## Configurations

In the elaborations on the different models I didn't mention the parameters that make up the different models. Most values are configurable, meaning it is possible to change a model with a small embedding\_dim to become a model with a bigger embedding\_dim without having to rewrite code in the model. The hidden\_dim being the dimension used in the first lstm layer. The first and sometimes only lstm layer contains 2 layers for all models. Learning rate or lr is 0.003. The batch size is the same for each model. Both attention models have a first lstm layer that is bidirectional. A bidirectional processes sequences in two directions, in this way data from later in a sequence influences data that is available at a previous time step. The n\_heads sets the number of attention heads for the multi-headed attention model.

Simple model		Attention model		MH Att. model	
keys	value	keys	value	keys	value
iterations	10000	iterations	10000	iterations	10000
max_len	20	max_len	20	max_len	20
evaluate_interval	1000	evaluate_interval	1000	evaluate_interval	1000
embedding_dim	128	embedding_dim	128	embedding_dim	128
hidden_size	256	hidden_size	256	hidden_size	256
n_layers	2	n_layers	2	n_layers	2
lr	0.003000	lr	0.003000	lr	0.003000
batch_size	64	batch_size	64	batch_size	64
bidirectional	False	bidirectional	True	bidirectional	True
		bidirectional	True	n_heads	2

(a) Simple model

(b) Attention model

(c) MH Attention model

Figure 13: Configurations used for the training of the different models

## Loss

The different models are trainable as can be seen from [Figure 14](#).

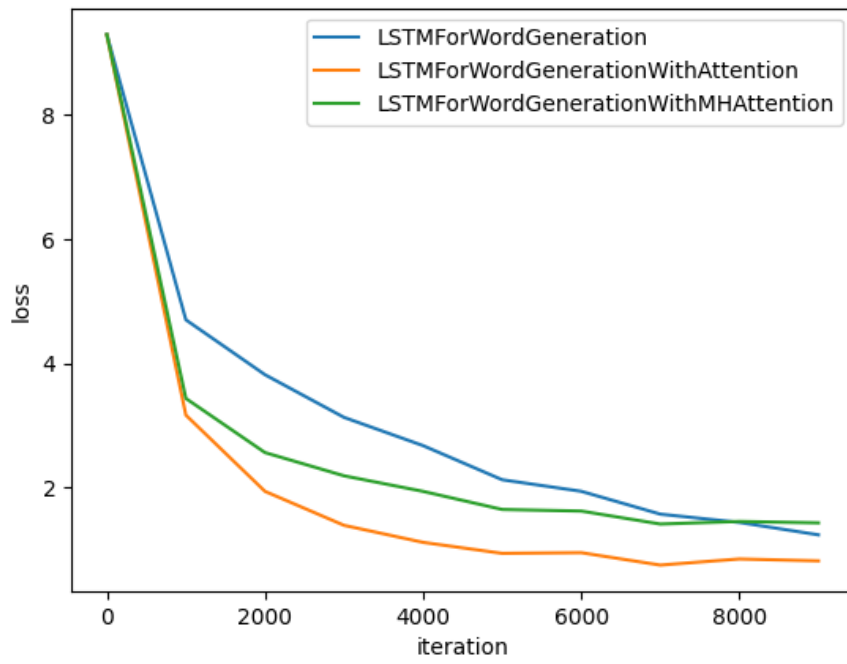


Figure 14: Visualization of training loss.

## Generated texts using Write method

After each training loop text is generated. I've always used the same input word, "Spells". For every model, configured using the values in [Figure 13](#), the quality of the text generation is poor. I must add, only the write method is considered here.

[illegible]

Figure 15: Text produced by the simple LSTM model.

[illegible]

Figure 16: Text produced by model with attention.

[illegible]

Figure 17: Text produced by model with multi-headed attention.



# Optimizers

## Adam

As I came across some difficulties while training my models, I had the idea of investigating optimizers, which I should have done earlier. It gave me a better insight into the reasons why training stops working. In machine learning, Adam (Adaptive Moment Estimation) stands out as a highly efficient optimization algorithm. It's designed to adjust the learning rates for each parameter. The text generation models I trained, in the note book were all trained using AdamW. In the accompanying notebook I apply different optimizers' calculations to simple examples to get an idea how they work. In this section I have summarized and filtered some of the information rendered by google, ai and other sources.

## Mechanics

**Moving average** Adam tweaks the gradient descent method by considering the moving average of the first and second-order moments of the gradient. This allows it to adapt the learning rates for each parameter intelligently.

**Individual learning rates** At its core, Adam is designed to adapt to the characteristics of the data. It does this by maintaining individual learning rates for each parameter in your model. These rates are adjusted as the training progresses, based on the data it encounters. Indeed, the algorithm can remember the previous actions (gradients), and the new actions are guided by the previous ones. Therefore, Adams keeps track of the gradients from previous steps, allowing it to make informed adjustments to the parameters. This memory isn't just a simple average, it's a sophisticated combination of recent and past gradient information, giving more weight to the recent.

**Cautious steps when gradients change rapidly** In areas where the gradient (the slope of the loss function) changes rapidly or unpredictably, Adam takes smaller, more cautious steps. This helps to avoid overshooting the minimum. Instead, in areas where the gradient changes slowly or predictably, it takes larger steps.

## Formula

Adam is calculated using the following formulas.

**The gradients** For each iteration  $t$ , Adam computes the gradient  $g_t$ . This gradient is the derivative of the target function (which is being minimized) concerning the current model parameters  $\theta_t$ . Therefore, it represents the direction in which the function increases most rapidly.

$$g_t = \nabla_{\theta} f_t(\theta_{t-1})$$

**Update biased first moment estimate** Updating the first-moment vector  $m$ , which stores the moving average of the gradients. This update is a combination of the previous value of  $m$  and the new gradient, weighted by parameters  $\beta_1$  and  $1-\beta_1$  respectively.  $m$  is a short-term memory of past gradients, emphasizing more recent observations. It provides a smoothed estimate of the gradient direction.

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$

**Update biased second moment estimate** Similarly, the second-moment vector  $v$  is updated. This vector gives an estimate of the variance (or unpredictability) of the gradients, therefore it stores the squared gradients that are accumulated. Like the first moment, this is also a weighted combination, but of the past squared gradients and the current squared gradient.

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

**Compute bias-corrected first and second moment estimate** Since  $m$  and  $v$  are initialized to 0, they are biased toward 0, which leads to a bias towards zero, especially during the initial time steps. Adam overcomes this bias by correcting the vector by the decay rate, which is  $\beta_1$  for  $m$  (first-moment decay rate), and  $\beta_2$  for  $v$  (second-moment

decay rate). This correction is important as it ensures that the moving averages are more representative, particularly in the early stages of training.

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$
$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

As more iterations have taken place,  $1 - \beta_1^t$  and  $1 - \beta_2^t$  will approach 1.

**Update parameters** The final step is the update of the model parameters. This step is where the actual optimization takes place, moving the parameters in the direction that minimizes the loss function. The update utilizes the adaptive learning rates calculated in the previous steps.

$$\theta_t = \theta_{t-1} - \alpha \frac{\hat{m}_t}{\sqrt{\hat{v}_t} + \epsilon}$$

**Used variables** The variables used in these formula:

$\alpha$ : Learning rate.

$\beta_1$ : First moment's decay rate, typically set to 0.9.

$\beta_2$ : Second moment's decay rate, typically set to 0.999.

$\epsilon$ : A constant (eg.  $10^{-8}$ ), to prevent division by zero.

$t$ : the current time step

$t - 1$ : the previous time step

$g$ : the gradient

## Adaptive learning rates are a key feature of Adam

The key feature of Adam is its adaptive learning rates. Unlike traditional gradient descent, where a single learning rate is applied to all parameters, Adam adjusts the rate based on how frequently a parameter is updated. Like in other optimization algorithms, the learning rate is a critical factor in how significantly the model parameters are adjusted.

**Risks of high or low learning rates** A higher learning rate could lead to faster convergence but risks overshooting the minimum, while a lower learning rate ensures more stable convergence but at the risk of getting stuck in local minima or taking too long to converge.

**Updates scaled individually** The unique aspect of Adam is that the update to each parameter is scaled individually. The amount by which each parameter is adjusted is influenced by both the first moment (capturing the momentum of the gradients) and the second moment (reflecting the variability of the gradients). This adaptive adjustment leads to more efficient and effective optimization, especially in complex models with many parameters.

**Epsilon** The small constant  $\epsilon$  is added to prevent any issues with division by zero, which is especially important when the second moment estimate  $v^t$  is very small. This addition is a standard practice in numerical algorithms to ensure stability.

## Use cases for Adam

### Sparse data

Adam is particularly effective when working with data that leads to sparse gradients. This situation is common in models with large embedding layers or when dealing with text data in natural language processing tasks.

### Training large-scale models

Adam is well-suited for training models with a large number of parameters, such as deep neural networks. Its adaptive learning rate helps navigate the complex optimization landscapes of such models efficiently.

## Achieving rapid convergence

Because of its adaptive learning rate Adam achieves fast convergence.

## Limitations

### Tuning hyperparameters

While Adam is less sensitive to learning rate changes compared to other optimizers, choosing an appropriate initial learning rate is still crucial.

### Handling noisy data and outliers

While Adam is generally robust to noisy data, extreme outliers or highly noisy datasets might impact its performance. Pre-processing data to remove or diminish the impact of outliers can be beneficial.

### Computational considerations

Adam typically requires more memory than simple gradient descent algorithms because it maintains moving averages for each parameter.

## AdamW

AdamW is often superior to Adam with L2 regularization because it decouples weight decay from the gradient update process. This leads to more effective and consistent regularization, better generalization, and improved convergence. By separating the weight decay from the gradient calculation, AdamW avoids interference with the adaptive learning rates, resulting in more stable and reliable optimization across different architectures.

### Adam with L2 is outperformed by AdamW

The Adam optimizer is popular in deep learning due to its adaptive learning rate and momentum capabilities. However, regarding regularization, especially L2 regularization (also known as weight decay), a variant called AdamW often outperforms the standard Adam optimizer with L2 regularization.

## L2 regularization

$$cost = loss + \lambda * \sum_{i=1}^n w_i^2$$

Where:

Loss: The original loss function (e.g., Mean Squared Error).

$\lambda$ : The regularization parameter (a hyperparameter) that controls the strength of the penalty. A higher  $\lambda$  increases regularization, forcing weights to be smaller.

$\sum w_i^2$ : The sum of the squared weights (parameters) of the model.

$n$ : The total number of features or weights.

### L2 Calculation

Imagine a model with 3 weights:

$$w_1 = 0.5, w_2 = -0.2, w_3 = 0.1$$

and a regularization strength of

$$\lambda = 0.1$$

Square the weights:

$$0.5^2 = 0.25$$

$$(-0.2)^2 = 0.04$$

$$0.1^2 = 0.01$$

Sum the squares:

$$0.25 + 0.04 + 0.01 = 0.30$$

Multiply by  $\lambda$ :

$$0.1 \times 0.30 = 0.03$$

The L2 penalty term to be added to the loss function is 0.03.

**Preventing overfitting** L2 regularization is a method used to prevent overfitting in machine learning models.

**Penalize value of weights** It adds a penalty term to the error function that is proportional to the sum of the squares of the weights. In this way weights are kept small.

### Problem with Adam

Adds regularization (L2-penalty) direct to the gradient. As Adam adapts the learning rate per parameter based on the history of gradients (including the L2 penalty), regularization is scaled too. In this way parameters with big gradients receive less regularization than intended, reducing model generalization.

### AdamW

AdamW decouples weight decay and the gradient update. The weight decay is applied to the parameters at the end of the step, after having calculated the adaptive update. Hence regularization is constant and independent of the magnitude of the gradient. This decoupling allows the optimizer to apply weight decay uniformly across all layers without being influenced by the gradient, leading to more consistent regularization.

### Adam versus AdamW

Modern models like Transformers almost always use AdamW. The reasons for this are to be found in:

- Improved Generalization: By applying weight decay directly to the parameters rather than through the gradient, AdamW significantly reduces overfitting compared to standard Adam with  $L_2$  regularization.
- Proper weight decay (Decoupled weight decay): The core innovation is that weight decay is not influenced by the adaptive learning rate component, which means it behaves exactly as intended, ensuring effective shrinkage of weights.
- Stable training for large models: It is the preferred choice for training deep networks, transformers, and in computer vision (e.g., YOLO) because it provides better, more predictable performance.
- Easier hyperparameter tuning: Because the learning rate and weight decay are not as strongly entangled as they are in Adam, tuning the model becomes more straightforward.

Due to these advantages, AdamW has become the default optimizer in many modern deep learning applications and frameworks.

### Best practices when choosing learning rates and weight decay

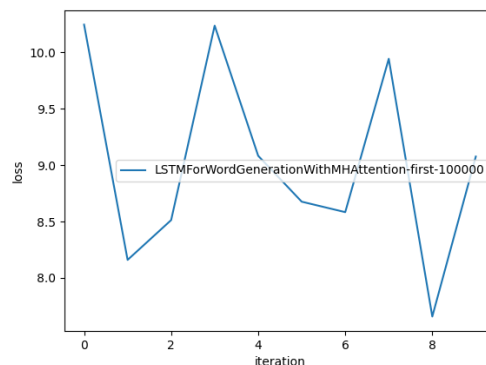
- Start with a moderate learning rate – For AdamW, a learning rate around  $1e-3$  is often a good starting point. You can adjust it based on how well the model converges, lowering it if the model struggles to converge or increasing it if training is too slow.
- Experiment with weight decay. Start with a value around  $1e-2$  to  $1e-4$ , depending on the model size and dataset. A slightly higher weight decay can help prevent overfitting for larger, complex models, while smaller models may need less regularization.
- Use learning rate scheduling. Implement learning rate schedules (like step decay or cosine annealing) to dynamically reduce the learning rate as training progresses, helping the model fine-tune its parameters as it approaches convergence.
- Monitor performance. Continuously track model performance on the validation set. If you observe overfitting, consider increasing weight decay, or if the training loss plateaus, lower the learning rate for better optimization.

## Training the module using the Lightning module

While training a more complex text generation model (for configuration see [Figure 18a](#)), using the full corpus of 7 books, I came across a situation where loss wasn't diminishing anymore [Figure 18b](#). From the plot, it looked like training still had some effect on the model.

MH Att. model	
keys	value
iterations	100000
max_len	20
evaluate_interval	10000
embedding_dim	256
hidden_size	512
n_layers	4
lr	0.003000
batch_size	4
bidirectional	True
n_heads	4

(a) Configuration used for complex model



(b) Training loss for complex model

Figure 18: Training a complex model

So I trained it anew using the same parameters, this took 10 times 2 days, 9 hours and 30 minutes. Almost a month of non-stop computer time wasted as loss kept oscillating. By changing learning rate from 0.003 to 0.002, I could train the model for 3 iterations more. After that, loss started to oscillate anew. Up until then I was using my own inflexible training loop, which didn't allow any intermediate model saving or closer monitoring of loss. But the situation forced me to do something.

## Torch-Lightning

As I didn't want to make my personal training loop more complex, I started using torch-lightning, a framework for training torch models. This framework allows one to accommodate for all kinds of additions to the training loop, effectively minimizing boilerplate code, and making logging and applying schedulers much easier. It took some time before getting it to work effectively, but it feels easier to add additions to this framework than to extend my personal monolithic training loop. In the next part I will give some idea of the way to get torch-lightning to work.

## Subclassing the torch lightning model

The first thing to do is to create a model that will become the main subject of training and validation. As a model (the multi-headed model) is already created, it can be 'embedded' into a torch lightning model, see [Listing 10](#). In the next paragraphs I will describe what needs to be done to get it to work.

**Embedding the multi-headed model** On line 4 the multi-headed attention model is embedded within a subclassed torch-lightning model. Some other things are set too (line 5-7).

**The training step** The training step (line 12-21) needs to be defined, the boilerplate code (step, backward and zerograd) doesn't need to be typed. Some basic code needs to be set, the way loss is calculated. Also the code to log some values is present, this allows for writing values to the Log.

**The validation step** In this part (line 23-30) the validation batch data is used to produce some predictions made by the model. These predictions are used to produce validation loss by comparing it to intended output.

**Configure optimizer and scheduler** On line 32-35 the optimizer is set, and a scheduler. The optimizer is an AdamW optimizer, this optimizer is accompanied by a scheduler, this scheduler reduces the learning rate when loss is on a plateau<sup>1</sup>. The optimizer and the scheduler are returned using a dictionary containing the two objects and some extra parameters. The extra parameters are:

- monitor: "val\_loss", the learning rate will be adapted monitoring validation loss
- frequency: some int value, in this case 16
- interval: "step", the value to be monitored is checked every 16 training steps

**ReduceLROnPlateau** To set the scheduler, some parameters (unset values get default values) need to be set:

- mode: the optimizer should produce models where loss is less than before, so 'min' is used to set the mode
- min\_lr: learning rate shouldn't become lower than 0.001
- patience: it is only after 3 subsequent validations moments where loss wasn't dropping anymore, the learning rate should be adapted
- threshold: the value by which the monitored value drops should be at least a value set for this threshold, in relative terms (one could set this to an absolute value too)
- factor: the value to multiply the original learning rate by

Listing 10: Embedding the multi-headed attention model into a torch-lightning model

```

1 class PLLSTMForWordGenerationWithMHAttention1(PL.LightningModule):
2     def __init__(self, word2idx, idx2word, config):
3         super().__init__()
4         self.model = LSTMForWordGenerationWithMHAttention(word2idx, idx2word, config["
           ↪ embedding_dim"], config["hidden_size"], config["bidirectional"], config["n_layers"],
           ↪ config["n_heads"])
5         self.config = config
6         self.model_name = self.model.__class__.__name__
7         self.file_columns_written=False
8
9     def get_model_name(self):
10        return self.model_name
11
12    def training_step(self, batch, batch_idx):
13        loss=None
14        self.model.train()
15        x, y = batch
16        logits = self.model(x)
17        logits = logits.transpose(1, 2)
18        loss = F.cross_entropy(logits, y.long())
19        self.log('train_loss', loss, on_step = True, prog_bar = True, logger = True)
20        self.log('num_train_items', int(x.size(0)), on_step=True, prog_bar=True, logger=True)
21        return loss
22
23    def validation_step(self, batch, batch_idx):
24        x, y = batch
25        logits = self.model(x)
26        logits = logits.transpose(1, 2)
27        loss = F.cross_entropy(logits, y.long())
28        self.log('val_loss', loss, on_step=False, prog_bar=True, logger=True)
29        self.log('num_val_items', int(x.size(0)), on_step=False, prog_bar=True, logger=True)
30        return {'val_loss': loss}
31
32    def configure_optimizers(self):
33        optimizer = AdamW(self.model.parameters(), lr=self.config["lr"])
34        scheduler = lr_scheduler.ReduceLROnPlateau(optimizer, mode="min", min_lr=0.001, patience=3,
           ↪ threshold=0.4, factor=0.98)

```

<sup>1</sup>I am kind of hoping, I will be able to train the complex multi-headed attention model, for which the loss seemed to be oscillating, using this scheduler.

```

35 return {'optimizer': optimizer, 'lr_scheduler': dict(scheduler=scheduler, monitor="
    ↪ val_loss", interval="step", frequency=16)}

```

## Creating the torch dataset and dataloader

As torch-lightning expects a torch dataset I need to create a torch Dataset. I will use the same kind of memmap as I used before to do training.

Listing 11: The dataset as a Torch Dataset

```

1 class HarryPotterDataset(Dataset):
2     def __init__(self, path_to_memmap, shape_of_memmap, seq_len):
3         self.seq_len = seq_len
4         self.number_of_tokens = shape_of_memmap[0]
5         self.path_to_memmap = path_to_memmap
6         self.shape_of_memmap = shape_of_memmap
7         self.tokens = np.memmap(self.path_to_memmap, dtype=np.int32, mode='r', shape=self.
    ↪ shape_of_memmap)
8
9     def __len__(self):
10         return self.number_of_tokens - self.seq_len
11
12     def __getitem__(self, index):
13         end = index + self.seq_len
14         text_slice = self.tokens[index:end].copy()
15         input_text = torch.from_numpy(text_slice[:-1])
16         label = torch.from_numpy(text_slice[1:])
17         return input_text, label

```

The dataset is then split into subsets using the following code:

```

train_subset, val_subset = random_split(dataset, [train_size, val_size])
train_dataloader = DataLoader(train_subset, shuffle = True, batch_size = batch_size)
val_dataloader = DataLoader(val_subset, shuffle = False, batch_size = 4)

```

## Creating a callback to generate text

To generate text at regular training step intervals a callback needs to be created. I still want to use both text generation methods (write and write\_better), so I will generate 2 text files.

Listing 12: Torch-lightning callback to generate text

```

1 class GenerateTextEveryNSteps(PL.Callback):
2     def __init__(self, every_n_step):
3         self.every_n_step = every_n_step
4         self.file_columns_written = False
5         self.file_columns_written_wb = False
6     def on_validation_end(self, trainer, pl_module) -> None:
7         if (trainer.global_step) % (self.every_n_step) == 0 and trainer.global_step != 0:
8             trainer.model.eval()
9             generated_text = pl_module.model.write(["Spells"], max_words=50)
10            generated_texts, probs = pl_module.model.write_better(["Spells"], max_words=50, k=3)
11            trainer.model.train()
12
13            with open(pathlib.Path(pl_module.logger.log_dir).joinpath("generated_text.csv"), "a",
    ↪ newline='') as f:
14                writer = csv.writer(f, delimiter='\t')
15                if not self.file_columns_written:
16                    writer.writerow(["epoch", "step", "generated_text"])
17                    self.file_columns_written=True
18                writer.writerow([str(trainer.current_epoch), str(trainer.global_step-1), generated_text
    ↪ ])
19
20            with open(pathlib.Path(pl_module.logger.log_dir).joinpath("generated_texts_write_better.
    ↪ csv"), "a", newline='') as f:
21                writer = csv.writer(f, delimiter='\t')
22                if not self.file_columns_written_wb:

```

```

23     writer.writerow(["epoch", "step", "prob", "generated_text"])
24     self.file_columns_written_wb = True
25     for generated_text, prob in zip(generated_texts, probs):
26         writer.writerow([str(trainer.current_epoch), str(trainer.global_step-1), str(np.round(
↪     prob.numpy(), 5)), generated_text])

```

## Creating an instance of the torch-lightning model

To instantiate the torch-lightning model the code in [Listing 13](#) is used.

Listing 13: Code to instantiate the torch-lightning

```

1 text = get_hp_text()
2 tokens = get_tokens()
3 word2idx, idx2word = get_2_vocabs()
4 config = get_config_mh_attention()
5 model = PLLSTMForWordGenerationWithMHAttention1(word2idx, idx2word, config)

```

## Train, monitor and checkpoint

At last, everything is more or less ready for training, validating, monitoring. Some small steps are still necessary though, see [Listing 14](#) for the steps. As I want to write logged values to a csv file I need a CSVLogger (line 3). A checkpoint callback needs to be instantiated (line 5-14). The previously coded validation callback (it will generate text at given step intervals) needs to be instantiated (line 16). A LearningRateMonitor needs to be instantiated, to see whether learning rate is being adapted. A trainer object needs to be instantiated, in which all previously created objects can be fed (line 20-31). Data needs to be available (line 33). And then finally the training can be initiated (line 36).

Listing 14: Code to train, monitor, log and checkpoint

```

1 seed_everything(42)
2
3 csv_logger = CSVLogger("lightning/logs/"+model.get_model_name(), name="csv")
4
5 checkpoint_callback = ModelCheckpoint(
6     monitor="val_loss",
7     filename="{version}/chkp_{epoch}_{step}_{val_loss:.2f}_{num_train_items}",
8     mode="min",
9     save_top_k=2,
10    dirpath="lightning/"+model.get_model_name()+"/checkpoints/",
11    every_n_train_steps=16,
12    save_last=True,
13    save_weights_only=True
14 )
15
16 val_callback = GenerateTextEveryNSteps(64)
17
18 lr_monitor = LearningRateMonitor(logging_interval='step')
19
20 trainer = Trainer(
21     logger=[csv_logger],
22     callbacks=[checkpoint_callback, val_callback, lr_monitor],
23     precision=32,
24     log_every_n_steps=1,
25     val_check_interval=0.25,
26     fast_dev_run=False,
27     max_epochs=10,
28     deterministic=True,
29     limit_val_batches=64,
30     limit_train_batches=64,
31 )
32
33 hp_train_dl, hp_val_dl = get_hp_dataloader(20, tokens, word2idx, 4)
34
35 with keep.running():
36     trainer.fit(model, hp_train_dl, val_data loaders=hp_val_dl)

```



## Some results

### Logging

The general logging for the first 16 iterations. Everything that is logged is written to the same file. The number of items used for training or validation are present too. Validation loss and training loss is present. The learning rate is present. The step number is logged. Epoch number is logged. See [Figure 19](#).

epoch	lr-AdamW	num_train_items	num_val_items	step	train_loss	val_loss
0	0.003			0	08.835014343261719	
0	0.003	4.0		1	18.825030326843262	
0	0.003	4.0		2	28.787137031555176	
0	0.003	4.0		3	38.68958568572998	
0	0.003	4.0		4	48.609517097473145	
0	0.003	4.0		5	57.9378767013549805	
0	0.003	4.0		6	67.445123672485352	
0	0.003	4.0		7	77.717151165008545	
0	0.003	4.0		8	87.181222915649414	
0	0.003	4.0		9	96.956890106201172	
0	0.003	4.0		10	107.040494441986084	
0	0.003	4.0		11	116.873996734619141	
0	0.003	4.0		12	126.387212753295898	
0	0.003	4.0		13	136.733105182647705	
0	0.003	4.0		14	147.246182918548584	
0	0.003	4.0		15	156.829124927520752	
0			16.0	15		7.064414978027344

Figure 19: Logs as produced by Lightning.

When validation loss isn't diminishing enough, according to the settings in the scheduler, learning rate is lowered. See [Figure 20](#).

1	0.003			76	765.539541721343994	
1	0.003	4.0		77	776.26999044418335	
1	0.003	4.0		78	786.5791826248168945	
1	0.003	4.0		79	795.942075252532959	
1			16.0	79		6.322289943695068
1	0.00294			80	806.200735569000244	
1	0.00294	4.0		81	815.941689968109131	
1	0.00294	4.0		82	826.3591203689575195	

Figure 20: A learning rate change on step 80.

### Generating texts

See [Figure 21](#) for the results of the `write_better` method, text is generated at the end of every epoch, every 64 steps. As results aren't that interesting, texts are limited to 25 tokens.

epoch	step	prob	generated_text
0	633e-10		Spells , Harry was Harry Harry was Harry Harry was Harry Harry was Harry Harry was Harry Harry was Harry Harry was Harry
0	630.0		Spells , Harry caught He He caught He He caught He He caught He He caught He He caught He He caught He He caught He
0	630.0		Spells , He . . was . . was . . was . . was . . was . . was . . was . . was . . was . . was . . was . . was . .
1	1270.0		Spells , and , Harry the , Harry , Harry , and , Harry the , Harry , Harry , and , Harry the , Harry
1	1270.0		Spells , Harry and said Ron , Harry and Harry and Harry and said Ron , Harry and Harry and Harry and said Ron , Harry
1	1270.0		Spells , but ! Harry Harry and Dont , the , but ! Harry Harry and Dont , the , but ! Harry Harry and Dont

Figure 21: Results for the write\_better method.