Advanced Methods in Text Analytics

Exercise 6: Transformers - Part 2

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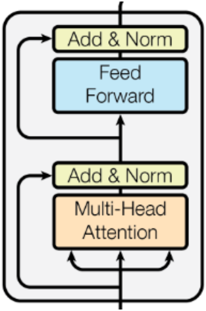
The Residual Stream

Context

- In this task, we take a closer look at both the forward and backward pass of a transformer layer (see image from original paper below).
- By *transformer layer*, we mean the combination of a multi-head self-attention followed by a feed-forward neural network, each with layer normalization applied after it, and each with a residual connection around them.



The Residual Stream

Question a)

- Let SA be a self-attention layer parameterized by $\boldsymbol{W}^Q, \boldsymbol{W}^K, \boldsymbol{W}^V$, and let $\boldsymbol{X} \in \mathbb{R}^{n \times d}$ be the d-dimensional tokens from an input sequence of length n.
- Give a formal expression for the output of SA given $\boldsymbol{X}$ as input.

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Answer a)

- We have:

$$\mathrm{SA}(\boldsymbol{X}) = \mathrm{softmax}\left(\frac{\boldsymbol{X}\boldsymbol{W}^Q(\boldsymbol{X}\boldsymbol{W}^K)^T}{\sqrt{d}}\right)\boldsymbol{X}\boldsymbol{W}^V \tag{1}$$

  where the softmax function is applied row-wise and $\boldsymbol{X}\boldsymbol{W}^Q = \boldsymbol{Q}$ is referred to as the query matrix, $\boldsymbol{X}\boldsymbol{W}^K = \boldsymbol{K}$ is the key matrix, and $\boldsymbol{X}\boldsymbol{W}^V = \boldsymbol{V}$ the value matrix.
- Recall that the factor $\frac{1}{\sqrt{d}}$ is used for numerical stability (scaled dot-product attention).

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Question b)

- Let FNN be the feed-forward neural network applied after SA in a transformer layer, and assume it projects the vectors in input $\boldsymbol{X}$ to a m-dimensional space and then back down to a d-dimensional space.
- Give a formal expression for the output of FNN given $\boldsymbol{X}$ as input.
- Assume a *ReLU* activation function is used after the first projection, and make sure to specify the size of the parameters in FNN.

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Answer b)

- We have:

$$\text{FNN}(\boldsymbol{X}) = \text{ReLU}\left((\boldsymbol{X}\boldsymbol{W}_1 + \boldsymbol{b}_1)\right)\boldsymbol{W}_2 + \boldsymbol{b}_2 \tag{2}$$

where parameters are $\boldsymbol{W}_1 \in \mathbb{R}^{d\times m}$, $\boldsymbol{b}_1 \in \mathbb{R}^{m}$, $\boldsymbol{W}_2 \in \mathbb{R}^{m\times d}$, and $\boldsymbol{b}_2 \in \mathbb{R}^{d}$.

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Question c)

- Using SA and FNN, give an expression for the output of a transformer layer TF given $\boldsymbol{X}$ as input.
- Use LN_1 and LN_2 for layer normalization after SA and FNN, respectively.

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Answer c)

- We do this in stages. First, we focus on SA, its corresponding residual connection and layer normalization LN_1. We have:

$$\boldsymbol{O}_1 = \mathrm{LN}_1(\mathrm{SA}(\boldsymbol{X}) + \boldsymbol{X}) \tag{3}$$

Then, we focus on FNN, its corresponding residual connection and layer normalization area applied. That is:

$$\boldsymbol{O}_2 = \mathrm{LN}_2(\mathrm{FNN}(\boldsymbol{O}_1) + \boldsymbol{O}_1) \tag{4}$$

All together, we have:

$$\mathrm{TF}(\boldsymbol{X}) = \mathrm{LN}_2(\mathrm{FNN}(\mathrm{LN}_1(\mathrm{SA}(\boldsymbol{X}) + \boldsymbol{X})) + \mathrm{LN}_1(\mathrm{SA}(\boldsymbol{X}) + \boldsymbol{X})). \tag{5}$$

The Residual Stream

Question d)

- What do the layer normalization operators LN_i do?
- And could we use them in a different part of the transformer layer?

The Residual Stream

Answer d)

- Layer normalization is used to normalize the vectors it is given as input.
- Concretely, given a vector $\boldsymbol{x} \in \mathbb{R}^d$, the layer normalization operation is given by:

$$\mathsf{LN}(\boldsymbol{x}) = \frac{\boldsymbol{x} - \mu}{\sigma}\gamma + \beta \tag{6}$$

  where γ and β are learned parameters.
- This operation can be seen as a form of data centering and is commonly used so keep training stable, sometimes at the cost of performance on some downtream tasks.
- It can be applied anywhere in a network/transformer.
- In fact, a common variant is the *pre-norm* transformer, which applies layer normalization *before* each of SA and FNN.
- Typically, this variant also includes a single final layer normalization operation applied only to the output of the last transformer layer.

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Question e)

- Let us now focus on the backward pass.
- Recall that during backpropagation, we apply the chain rule of calculus to compute the gradients of all parameterized operators used in the forward pass, usually w.r.t. some loss function L.
- In the context of some transformer layer $\mathrm{TF_i}$, these operators are $\mathrm{SA}, \mathrm{FNN}, \mathrm{LN}_1$ and LN_2.
- Give a formal expression for the gradient needed to update parameters θ_{SA} of operator SA w.r.t. some loss function L.
- Omit the use of layer normalization and residual connections for simplicity.
- Indicate which part of the expression is "received" from the FNN layer above during backpropagation.

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Answer e) (1)

- To update parameters θ_{SA} of SA w.r.t. some loss function L during training, we need:

$$\frac{\partial L}{\partial \theta_{SA}} = \frac{\partial L}{\partial \, \mathrm{SA}(\boldsymbol{H})} \frac{\partial \, \mathrm{SA}(\boldsymbol{H})}{\partial \theta_{SA}}, \tag{7}$$

  where $\boldsymbol{H}$ is the input to SA, which in turn is the output of the previous transformer layer $\mathrm{TF}_{\text{i-1}}$.
- The term $\frac{\partial L}{\partial \, \mathrm{SA}(\boldsymbol{H})}$ is the partial gradient received during backpropagation from the upper layer, the FNN operator in the context of a transformer layer.
- Let's try to visualize this in the next slide.

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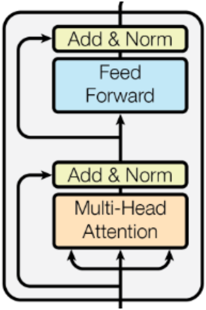
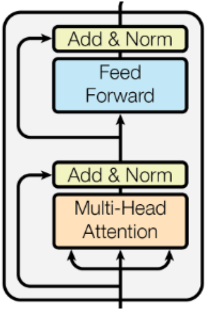
Answer e) (2)



Forward Pass



Backward Pass

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Question f)

- Following your previous answer, what is the gradient that is passed down to lower layers, e.g. the lower transformer layer TF_{i-1}?
- Give a formal expression for this gradient and briefly describe why this gradient is needed during training.

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Answer f)

- Just as we received a gradient from the upper layer during training, we pass down the following gradient to the lower transformer layer $\mathrm{TF}_{\text{i-1}}$ during backpropagation:

$$\frac{\partial L}{\partial \boldsymbol{H}} = \frac{\partial L}{\partial \, \mathrm{SA}(\boldsymbol{H})} \frac{\partial \, \mathrm{SA}(\boldsymbol{H})}{\partial \boldsymbol{H}}. \tag{8}$$

- This is the gradient of the output of $\mathrm{TF}_{\text{i-1}}$ w.r.t. L, and is needed to compute the weight updates of the operators in lower layers that contribute to the computation of the input to TF_{i}, i.e. $\boldsymbol{H}$.

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Question g)

- Now rewrite your previous answer while considering the residual connection around SA.
- Simplify the resulting expression as much as possible with the goal of answering the question: what happens during training to the gradient that we received from higher layers as it's passed through an SA operator that uses residual connection?
- **Hint:** No need to compute any gradients, but do use the fact that the gradient is a linear operator.

The Residual Stream

Answer g) (1)

- Let $\boldsymbol{O}_1$ be the output of SA with a residual connection around it, i.e. $\boldsymbol{O}_1 = \text{SA}(\boldsymbol{H}) + \boldsymbol{H}$.
- Then, the gradient "received" from the upper layer is $\frac{\partial L}{\partial \boldsymbol{O}_1}$.
- Eq. 8 can then be rewritten as follows:

$$
\begin{aligned}
\frac{\partial L}{\partial \boldsymbol{H}} &= \frac{\partial L}{\partial \boldsymbol{O}_1} \frac{\partial \boldsymbol{O}_1}{\partial \boldsymbol{H}} \\
&= \frac{\partial L}{\partial \boldsymbol{O}_1} \frac{\partial (\text{SA}(\boldsymbol{H}) + \boldsymbol{H})}{\partial \boldsymbol{H}} \\
&= \frac{\partial L}{\partial \boldsymbol{O}_1} \left(\frac{\partial\, \text{SA}(\boldsymbol{H})}{\partial \boldsymbol{H}} + \frac{\partial \boldsymbol{H}}{\partial \boldsymbol{H}} \right) \\
&= \frac{\partial L}{\partial \boldsymbol{O}_1} \frac{\partial\, \text{SA}(\boldsymbol{H})}{\partial \boldsymbol{H}} + \frac{\partial L}{\partial \boldsymbol{O}_1}.
\end{aligned}
$$

- In other words, when using residual connections, the gradient $\frac{\partial L}{\partial \boldsymbol{O}_1}$ we receive from higher layers during backpropagation is passed down to lower layers by making a modification via the addition operation.

The Residual Stream

Answer g) (2)

- Note that without the residual connection, the gradient we pass down would be modified by the multiplying factor $\frac{\partial \mathsf{SA}(\boldsymbol{H})}{\partial \boldsymbol{H}}$, and the additive term would not exist.
- Since such a multiplying factor can quickly reduce the size of the gradient that is passed backward during training, the residual connection was designed by He et al. 2015 so that gradients can be more safely passed through an operator without it having a severe impact on those gradients.
- The name "residual" connection comes from the fact that, due to this change to prevent gradients from vanishing during training, the function $f(\boldsymbol{X}) = \mathsf{OP}(\boldsymbol{X})$ computed by some operator becomes $f(\boldsymbol{X}) = \mathsf{OP}(\boldsymbol{X}) + \boldsymbol{X}$.

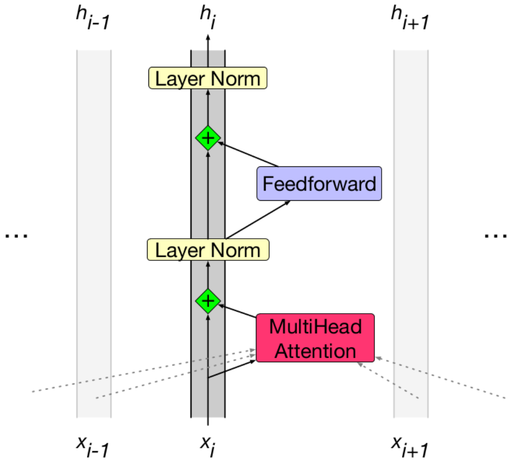
The Residual Stream

Answer g) (3)

- This means that we are learning to apply a suitable *difference* $\mathrm{OP}(\boldsymbol{X})$ that is added to given input $\boldsymbol{X}$.
- In the context of a transformer layer, $\boldsymbol{X}$ is a set of contextualized representations, so what each transformer layer learns is to add something to it *if needed*.
- If $\boldsymbol{X}$ is already suitable for the task, then a layer may make small modifications to it.
- This suggests that the main flow of information is coming from $\boldsymbol{X}$, and not from $\mathrm{OP}(\boldsymbol{X})$, or in other words, from the residual connections and not from the transformer layers.
- This perspective is known as the "residual stream" view of transformers, illustrated in the following image from Jurasfky and Martin (2024), Section 10.4.

The Residual Stream

Answer g) (4)



The Residual Stream. Main information flows through residual connections.

Attention Heads are Independent

Question a)

- Let MHA be a multi-head attention layer, SA_i its i-th self-attention layer and $\boldsymbol{X} \in \mathbb{R}^{n \times d}$ the d-dimensional tokens from an input sequence of length n.
- Give a formal expression for the output of MHA as a function of its k attention heads SA_i, i.e. $1 <= i <= k$, given $\boldsymbol{X}$ as input.
- As usual, make sure to formally define all components in your expression.
- How is MHA parameterized?

Attention Heads are Independent

Answer a)

- We have:

$$\text{MHA}(\boldsymbol{X}) = (SA_1(\boldsymbol{X}) \oplus SA_2(\boldsymbol{X}) \oplus \ldots \oplus SA_k(\boldsymbol{X}))\, \boldsymbol{W}^O + \boldsymbol{X}, \tag{9}$$

  where $\oplus$ is the concatenation operator, $\boldsymbol{W}_O \in \mathbb{R}^{kd \times d}$ is a parameter matrix that projects the concatenated vector back to d-dimensional residual space, and the additive term is the residual connection around MHA.
- Note that the size of $\boldsymbol{W}^O$ is, indirectly, a design choice, as it depends on the number of attention heads (in this case k) and the size of tokens (in this case d).

Attention Heads are Independent

Question b)

- Assume MHA takes as input the output $\boldsymbol{O}^i$ of each self-attention head $\mathrm{SA}_i(\boldsymbol{X})$, i.e. $\boldsymbol{O}^i = \mathrm{SA}_i(\boldsymbol{X})$.
- Give a formal expression for the computations needed to compute a single component of the output matrix of MHA as a function of each $\boldsymbol{O}^i$.

Attention Heads are Independent

Answer b) (1)

- The operation in question here is the projection to residual space done by $\boldsymbol{W}^O$.
- As defined in the task description, let $\boldsymbol{O}^i \in \mathbb{R}^{n \times d}$ be the output of SA_i.
- After concatenating the output of each attention head, we have $\boldsymbol{O} \in \mathbb{R}^{n \times kd}$ where k is the number of attention heads.
- That is, we have the following block matrix:

$$\boldsymbol{O} = \left[\boldsymbol{O}^1 \boldsymbol{O}^2 \dots \boldsymbol{O}^k \right]. \tag{10}$$

- Now, note that when computing each element ij of $\boldsymbol{O}\boldsymbol{W}^O$, i.e. $[\boldsymbol{O}\boldsymbol{W}^O]_{ij}$, we compute the following dot product:

$$[\boldsymbol{O}\boldsymbol{W}^O]_{ij} = \sum_{h=1}^{kd} \boldsymbol{O}_{ih} \boldsymbol{W}^O_{hj}. \tag{11}$$

Attention Heads are Independent

Answer b) (2)

- We can rewrite this dot product to make use of the $\boldsymbol{O}^i$ components of $\boldsymbol{O}$ more explicitly, as follows:

$$[\boldsymbol{O}\boldsymbol{W}^O]_{ij} = \sum_{h=1}^{d} \boldsymbol{O}_{ih}\boldsymbol{W}^O_{hj} + \sum_{h=d+1}^{2d} \boldsymbol{O}_{ih}\boldsymbol{W}^O_{hj} + \ldots + \sum_{h=(k-1)d+1}^{kd} \boldsymbol{O}_{ih}\boldsymbol{W}^O_{hj} \tag{12}$$

$$= \sum_{h=1}^{d} \boldsymbol{O}^1_{ih}\boldsymbol{W}^{O_1}_{hj} + \sum_{h=1}^{d} \boldsymbol{O}^2_{ih}\boldsymbol{W}^{O_2}_{hj} + \ldots + \sum_{h=1}^{d} \boldsymbol{O}^k_{ih}\boldsymbol{W}^{O_k}_{hj}, \tag{13}$$

where we now defined $\boldsymbol{W}^{O_i} \in \mathbb{R}^{d \times d}$ as the i-th block of $\boldsymbol{W}^O$ that corresponds to $\boldsymbol{O}^i$.

- That is, we can also see $\boldsymbol{W}^O$ as the following block matrix:

$$\boldsymbol{W}^O = \left[\boldsymbol{W}^{O_1}\boldsymbol{W}^{O_2} \ldots \boldsymbol{W}^{O_k}\right]^\top . \tag{14}$$

Attention Heads are Independent

Question c)

- Using the intuition built in the previous subtask, show that the output of the multi-head attention layer MHA can be expressed as the following linear combination:

$$\mathrm{MHA}(\boldsymbol{X}) = \sum_{i=1}^{k} \boldsymbol{O}^i \boldsymbol{M}^i + \boldsymbol{X}, \tag{15}$$

  and make sure to define exactly what each $\boldsymbol{M}^i$ is.
- What does this rewriting of the multi-head attention layer imply about the operations computed by each attention head?

Attention Heads are Independent

Answer c) (1)

- From the solution to the previous subtasks, it follows that we can represent the general operation of MHA as:

$$\mathrm{MHA}(\boldsymbol{X}) = \left[\boldsymbol{O}^1 \boldsymbol{O}^2 \ldots \boldsymbol{O}^k\right] \begin{bmatrix} \boldsymbol{W}^{O_1} \\ \boldsymbol{W}^{O_2} \\ \ldots \\ \boldsymbol{W}^{O_k} \end{bmatrix} + \boldsymbol{X}. \tag{16}$$

- And being as this is a matrix multiplication of block matrices, we can write this as the following linear combination:

$$\mathrm{MHA}(\boldsymbol{X}) = \sum_{i=1}^{k} \boldsymbol{O}^i \boldsymbol{W}^{O_i} + \boldsymbol{X}, \tag{17}$$

where $\boldsymbol{M}^i = \boldsymbol{W}^{O_i}$ as desired.

Attention Heads are Independent

Answer c) (2)

- This equivalence shows that the output of the multi-head attention layer MHA can be expressed as a linear combination of the outputs of each attention head $\mathrm{SA}_i(\boldsymbol{X})$, where the weights of that linear combination are learned by the layer.
- Thus, each (weighted) attention head contributes to the learned representations by *independently adding* to the representations in the residual space.
- Indeed, the field of interpretability has identified that certain attention heads learn specific roles that completely differ from other attention heads.
- For more details, see here.

Language Models With Transformers

Context

- In this exercise, we have a quick look at how to implement a language model with transformers using PyTorch.
- As before with our FNN-based and RNN-based language models, we will need to define a class for the model, a training loop and an evaluation loop.
- In addition, we also need to implement positional encodings.
- We use the ones used by the original transformer architecture.

Language Models With Transformers

Question a)

- Read the code for the class *PositionalEncoding* to make sure it's correct w.r.t. how these positional embeddings are defined.
- Then check documentation for PyTorch's Module.
- What does the method *register_buffer* do?

Language Models With Transformers

Answer a)

- Storing models during or after training is important to later be able to use them, e.g. for inference, fine-tuning or to continue training.
- PyTorch models have a state dictionary (state_dict) that is usually stored on disk in so-called *checkpoint* files.
- It's important that these files contain all the necessary information so that we may later be able to use the model.
- *register_buffer* is used to define "parameters" of a model that need to be stored in its state_dict, but that aren't actually parameters in the learning sense.
- That is, they are not changed during training.
- Since we are implementing a non-parameterized positional encoding, we register these embeddings as buffers, because we later need them for using the model.

Language Models With Transformers

Question b)

- Read the code for the TransformerModel class. What kind of architecture does it use? Encoder-decoder? Encoder-only?

Language Models With Transformers

Answer b) (1)

- The answer is not straightforward.
- If we look at the class from PyTorch that we use, it's the TransformerEncoder class.
- But, as we'll see later, we apply a mask to our attention scores, which have an impact on the type of model we are using, so we'll come back to this in the next few questions.
- In addition, the model does not have cross-attention (attention between decoder and the outputs of the encoder), so it is definitely not an encoder-decoder model either.
- The code does have a component called a decoder, but what is that exactly?

Language Models With Transformers

Answer b) (2)

- It's a linear layer that projects down to a vector space the size of our vocabulary, so while common, this naming convention can be confusing, as this decoding step refers to decoding in the tokenization sense.
- This projection, in combination with a softmax, will be used to produce probabilities over our vocabulary in order to predict the next token (if we construct the training examples correctly).
- But why isn't the softmax function there then? Well, as in our previous coding exercise, we will use CrossEntropyLoss, which includes the softmax function, so we need our model to output logits.

Language Models With Transformers

Question c)

- What is the role of the function *_generate_square_subsequent_mask*? Read the documentation for the Transformer Class to find out more.

Language Models With Transformers

Answer c)

- This function is used to construct an attention mask. Masking is the process by which we “block” some entries in a tensor.
- In this context, the forward pass of the TransformerEncoder takes a mask as input along side the input sequence.
- This mask is added to the matrix of attention *scores* in the self-attention layer.
- If scores are -*Inf*, their attention weight (via softmax) is zero.
- Entry *ij* in this matrix can be seen as how much attention input token *i* pays to *j*.
- Thus, the mask is a matrix with zeros in the lower triangular, and the rest -*Inf*.

Language Models With Transformers

Question d)

- What kind of language model is it? Causal or masked? Why?
  Hint: What does the function triu do?

Language Models With Transformers

Answer d)

- Given the attention mask we use, as explained in the answer above, this is a causal language model.
- Note that the use of this *causal mask*, in combination with the lack of cross-attention, means we have a decoder-only model, despite using a TransformerEncoder class.
- It is common to implement such a CLM using TransformerEncoder.

Language Models With Transformers

Question e)

- Complete the *forward* function of your transformer.

Language Models With Transformers

Answer e)

- See Jupyter notebook.

Language Models With Transformers

Question f)

- We can train this transformer in the same way that we trained our RNN in our last coding exercise: with *teacher forcing*.
- So, we will use the same methods for preprocessing the data, creating the batches and training the model.
- Note that the training method was modified slightly to accomodate this model's forward function (no need to pass the hidden state as with RNNs).
- Use the given code to train the transformer on the *Shakespeare* data.
- What perplexity do we get on validation data? Is it higher or lower than when using an RNN as before?
- Is the task comparable w.r.t. that case? Discuss.

Language Models With Transformers

Answer f) (1)

- We get validation perplexity (PPL) of about 500, which is somewhat higher than with the RNN, which was about 400.
- Recall that PPL can be interpreted as proportional to the vocabulary size, which is about 30K.
- In addition, and as discussed in previous tutorials, it can be interpreted as the average *branching factor*, i.e. the average number of possible next words after a given one.
- The PPL values from the RNN and this transformer are inded comparable, as both models are evaluated on the same task using the same validation data (it's virtually the same code base).

Language Models With Transformers

Answer f) (2)

- As for basic resources, they are also comparable. The embedding size is the same as the one used by the RNN, and both use dropout with default values as the only form of regularization.
- It's therefore likely can this slighly lower performance is due to the stronger inductive bias in the transformer model, i.e. it's overfitting.
- It would be nice to try to use a transformer with lower number of attention heads, or lower number of layers.
- And indeed, such tests are important to do on validation data before deciding which model will be used on test data or real-world data.
- We look at this further in the next question.

Language Models With Transformers

Question f)

- Can you modify the model so it performs better? Consider using different embedding sizes, different number of layers, etc.

Language Models With Transformers

Answer f) (1)

- See Jupyter notebook for details.
- When training longer, for 20 epochs, we see the transformer achieving a PPL of about 400, i.e. it achieves the same performance achieved by the RNN in a single epoch.
- But when training the RNN for 20 epochs, it gets a PPL of about 350, so while smaller, there is still a performance gap in favor of the RNN.
- W.r.t. changing model depth, we get slightly lower performance with a single layer, and a marginal improvement with 3 layers.
- But when using 6 layers performance drops, suggesting overfitting.

Language Models With Transformers

Answer f) (2)

- Finally, we could use a learning rate scheduler to get an increase in performance, as the learning rate is often a crucial hyperparameter in deep learning models, so stuff like a learning rate warmup are common practice when training LLMs.
- In general, the transformer does not quite achieve the performance of the RNN in our tests, but it's possible that with other modifications we can get our transformer to performn better, e.g. using smaller hidden sizes, a different number of attention heads, etc.
- And what about model stability? I.e. how large is the variance of PPL when training the same model multiple times?
- Running the models in these tests multiple times suggests they are not quite stable, i.e. it's possible that the transformer and the RNN perform similarly when comparing the mean and variance of PPL over, say, 10 different runs of each model.