AI539 Natural Language Processing with Deep Learning – Homework 4

Attention Mechanisms in Sequence-to-Sequence Models

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Overview and Objectives. In this homework, we'll build some intuitions for scaled dot-product attention and implement a simple attention mechanism for an RNN-based sequence-to-sequence model in a small-scale machine translation task. If you finish early, *work on your projects!*

How to Do This Assignment. The assignment has a few math questions and then walks you through completing the provided skeleton code and analyzing some of the results. Anything requiring you to do something is marked as a "Task" and has associated points listed with it. You are expected to turn in both your code and a write-up answering any task that requested written responses. Submit a zip file containing your completed skeleton code and a PDF of your write-up to Canvas.

Advice. Start early. Students will need to become familiar with `pytorch` for this and future assignments. Extra time may be needed to get used to working remotely on the GPU cluster here. You can also use GPU-enabled runtimes in Colab `colab.research.google.com`.

1 Scaled Dot-Product Attention [8 pts]

To warm up and start getting more familiar with scaled dot-product attention mechanisms, we'll do some exploratory math first.[1] Recall from the lecture the definition of a single-query scaled dot-product attention mechanism. Given a query $\mathbf{q} \in \mathbb{R}^{1\times d}$, a set of candidates represented by keys $\mathbf{k}_1, ..., \mathbf{k}_m \in \mathbb{R}^{1\times d}$ and values $\mathbf{v}_1, ..., \mathbf{v}_m \in \mathbb{R}^{1\times d_v}$, we compute the scaled dot-product attention as:

$$\alpha_i = \frac{\exp\left(\mathbf{q}\mathbf{k}_i^T/\sqrt{d}\right)}{\sum_{j=1}^{m}\exp\left(\mathbf{q}\mathbf{k}_j^T/\sqrt{d}\right)} \tag{1}$$

$$\mathbf{a} = \sum_{j=1}^{m}\alpha_j\mathbf{v}_j \tag{2}$$

where the α_i are referred to as attention values (or collectively as an attention distribution). The goal of this section is to get a feeling for what is easy for attention to compute and why we might want something like multi-headed attention to make some computations easier.

▶ `TASK 1.1 Copying [2pts]` Describe (in one or two sentences) what properties of the keys and queries would result in the output $\mathbf{a}$ being equal to one of the input values $\mathbf{v}_j$. Specifically, what must be true about the query $\mathbf{q}$ and the keys $\mathbf{k}_1, ..., \mathbf{k}_m$ such that $\mathbf{a} \approx \mathbf{v}_j$? (We assume all values are unique – $\mathbf{v}_i \neq \mathbf{v}_j,\ \forall ij$.)

In order to get the output to be equal to one of the inputs, that would require the attention to be concentrated on only one of the keys. We would want a really large dot product for one of the keys, k_j, and really small for all other keys k_i where i != j. This would set the α_k to effectively 1 and all other α values to 0 (small dot product over the sum of all dot products).

[1] These questions are adapted from CS224n at Stanford because I just liked the originals too much not to use them.

▶ TASK 1.2 Average of Two [2pts] Consider a set of key vectors $\{\mathbf{k}_1, ..., \mathbf{k}_m\}$ where all keys are orthogonal unit vectors – that is to say $\mathbf{k}_i \mathbf{k}_j^T = 0, \ \forall ij$ and $||\mathbf{k}_i|| = 1, \ \forall i$. Let $\mathbf{v}_a, \mathbf{v}_b \in \{\mathbf{v}_1, ..., \mathbf{v}_m\}$ be two value vectors. Give an expression for a query vector $\mathbf{q}$ such that the output $\mathbf{a}$ is approximately equal to the average of $\mathbf{v}_a$ and $\mathbf{v}_b$, that is to say $\mathbf{a} \approx \frac{1}{2}(\mathbf{v}_a + \mathbf{v}_b)$. You can reference the key vectors corresponding to $\mathbf{v}_a$ and $\mathbf{v}_b$ as $\mathbf{k}_a$ and $\mathbf{k_b}$ respectively. Note that due to the softmax in Eq. 1, it won't ever actually reach this value, but you can make it arbitrarily close by adding a scaling constant to your solution.

One way to accomplish this is to aim to have the attention values for a and b as 0.5 and all other values as 0.

In the previous task, we saw it was *possible* for a single-headed attention to focus equally on two values. This can easily be extended to any subset of values. In the next question we'll see why it may not be a *practical* solution.

▶ TASK 1.3 Noisy Average [2pts] Now consider a set of key vectors $\{\mathbf{k}_1, ..., \mathbf{k}_m\}$ where keys are randomly scaled such that $\mathbf{k}_i = \mu_i * \lambda_i$ where $\lambda_i \sim \mathcal{N}(1, \beta)$ is a randomly sampled scalar multiplier. Assume the unscaled vectors $\mu_1, ..., \mu_m$ are orthogonal unit vectors. If you use the same strategy to construct the query q as you did in Task 1.2, what would be the outcome here? Specifically, derive $\mathbf{q}\mathbf{k}_a^T$ and $\mathbf{q}\mathbf{k}_b^T$ in terms of μ's and λ's. Qualitatively describe what how the output a would vary over multiple resamplings of $\lambda_1, ..., \lambda_m$.

As we just saw in 1.3, for certain types of noise that either scale (shown here) or change the orientation of the keys, single-head attention may have difficulty combining multiple values consistently. Multi-head attention can help.

▶ TASK 1.4 Noisy Average with Multi-head Attention [2pts] Let's now consider a simple version of multi-head attention that averages the attended features resulting from two different queries. Here, two queries are defined ($\mathbf{q}_1$ and $\mathbf{q}_2$) leading to two different attended features ($\mathbf{a}_1$ and $\mathbf{a}_2$). The output of this computation will be $\mathbf{a} = \frac{1}{2}(\mathbf{a}_1 + \mathbf{a}_2)$. Assume we have keys like those in Task 1.3, design queries $\mathbf{q}_1$ and $\mathbf{q}_2$ such that $\mathbf{a} \approx \frac{1}{2}(\mathbf{v}_a + \mathbf{v}_b)$.

With multiple attention heads, it is easier to have one head select for a and the other select for b. The queries can be created around the features to easily discard all unwanted values.

2 Attention in German-to-English Machine Translation [12 pts]

In this part of the homework, we are going to get some experience implementing attention mechanisms on top of familiar components. In HW2 we used bidirectional encoders for Part-of-Speech tagging and in HW3 we decoded unconditional language models. Here we'll combine these into a sequence-to-sequence model that translates German sentences to English. The skeleton code already provides the data loading (using torchtext and spacy), training / evaluation infrastructure, and encoder/decoder model structure. This code relies on some extra dependencies so you'll want to execute `sh setup.sh` before starting.

To keep training time short (~5-10 minutes), we are using a small-scale translation datasets called Multi30k [1] that contains over 31,014 bitext sentences describing common visual scenes in both German and English (split across train, val, and test). It is intended to support multimodal translation (i.e. utilizing an image of the described scene to make translation easier) but we will just use it as a text problem for simplicity.

Students can look through the provided code for the implementation details; however, the computation our model is performing is summarized in the following equations. Consider a training example consisting of a source language sentence $w_1, ..., w_T$ and a target language sentence $m_1, ..., m_L$. Let $\mathbf{w}_t$ and $\mathbf{m}_t$ be one-hot word encodings.

Encoder. Out encoder is a simple bidirectional GRU model. While we write the forward and backward networks separately, PyTorch implements this as a single API.

$$\mathbf{z_t} = \mathbf{W}_e \mathbf{w}_t \quad \text{(Word Embedding)} \tag{3}$$

$$\overrightarrow{\mathbf{h}}_t^{(e)}, \overrightarrow{\mathbf{c}}_t^{(e)} = \overrightarrow{\text{LSTM}}\left(\mathbf{z}_t, \overrightarrow{\mathbf{h}}_{t-1}^{(e)}, \overrightarrow{\mathbf{c}}_{t-1}^{(e)}\right) \quad \text{(Forward LSTM)} \tag{4}$$

$$\overleftarrow{\mathbf{h}}_t^{(e)}, \overleftarrow{\mathbf{c}}_t^{(e)} = \overleftarrow{\text{LSTM}}\left(\mathbf{z}_t, \overleftarrow{\mathbf{h}}_{t+1}^{(e)}, \overleftarrow{\mathbf{c}}_{t+1}^{(e)}\right) \quad \text{(Backward LSTM)} \tag{5}$$

$$\mathbf{h}_t^{(e)} = \left[\overrightarrow{\mathbf{h}}_t^{(e)}, \overleftarrow{\mathbf{h}}_t^{(e)}\right] \forall t \quad \text{(Word Representations)} \tag{6}$$

$$\mathbf{h}_{\mathbf{sent.}}^{(\mathbf{e})} = \text{ReLU}\left(\mathbf{W}_e \left[\overrightarrow{\mathbf{h}}_T, \overleftarrow{\mathbf{h}}_0\right] + \mathbf{b}_e\right) \quad \text{(Sentence Representation)} \tag{7}$$

Decoder. Our decoder is a unidirectional GRU that performs an attention operation over the encoder word representations at each time step (Eq. 12). Notice that we initialize the decoder hidden state with the overall sentence encoding from the encoder.

$$\mathbf{h}_0^{(d)} = \mathbf{h}_{sent.}^{(e)} \quad \text{(Initialize Decoder)} \tag{8}$$

$$\mathbf{b_i} = \mathbf{W}_d \mathbf{m}_i \quad \text{(Word Embedding)} \tag{9}$$

$$\mathbf{h}_i^{(d)}, \mathbf{c}_i^{(d)} = \text{LSTM}\left(\mathbf{b}_i, \mathbf{h}_{i-1}^{(d)}, \mathbf{c}_{i-1}^{(d)}\right) \quad \text{(Forward LSTM)} \tag{10}$$

$$\mathbf{a}_i = \text{Attn}\left(\mathbf{h}_i^{(d)}, \mathbf{h}_1^{(e)}, ..., \mathbf{h}_T^{(e)}\right) \quad \text{(Attention)} \tag{11}$$

$$P(m_{i+1} \mid m_{\leq i}, w_1, ..., w_T) = \text{softmax}\left(\mathbf{W}_d \left[\mathbf{a}_i, \mathbf{h}_i^{(d)}\right] + \mathbf{b}_d\right) \quad \text{(Prob. of Next Word)} \tag{12}$$

Our explorations in this assignment will be implementing and contrasting different choices for the $\text{Attn}(q, c_1, ..., c_T)$ module above. All the other elements of the encoder-decoder architecture have already been implemented.

▶ TASK 2.1 Scaled-Dot Product Attention [8pts] Implement $\text{Attn}(\cdot)$ in equation (11) as single-query scaled dot-product attention as defined in equations (1) and (2). Here, the query will be the decoder hidden state and the keys and values will be derived from the encoder representations. Implement this attention mechanism by completing the `SingleQueryScaledDotProductAttention` class in `mt_driver.py`. The skeleton code is below:

```
class SingleQueryScaledDotProductAttention(nn.Module):
    # kq_dim is the dimension of keys and queries. Linear layers should be used
    to project inputs to these dimensions.
    def __init__(self, enc_hid_dim, dec_hid_dim, kq_dim=512):
        super().__init__()
        .
        .
        .

    #hidden is h_t^{d} from Eq. (11) and has dim => [batch_size, dec_hid_dim]
    #encoder_outputs is the word representations from Eq. (6)
    # and has dim => [src_len, batch_size, enc_hid_dim * 2]
    def forward(self, hidden, encoder_outputs):

        .
        .
        .

        assert attended_val.shape == (hidden.shape[0], encoder_outputs.shape[2])
        assert alpha.shape == (hidden.shape[0], encoder_outputs.shape[0])
        return attended_val, alpha
```

The forward function takes two inputs – `hidden` is the decoder hidden state $h_j^{(d)}$ and `encoder_outputs` corresponds to encoder word representations $h_t^{(e)}$, $\forall t$. These should be converted to keys, queries, and values:

$$\mathbf{q} = W_q \mathbf{h}_j^{(d)} \tag{13}$$

$$\mathbf{k}_t = W_k \mathbf{h}_t^{(e)} \tag{14}$$

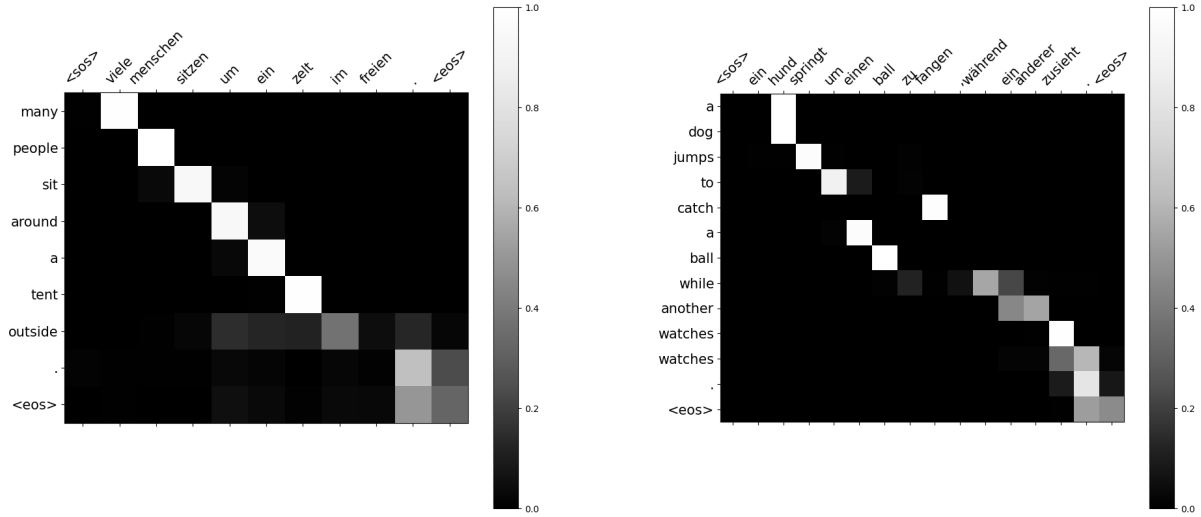
$$\mathbf{v}_t = \mathbf{h}_t^{(e)} \tag{15}$$

And the output – `attended_val` and `alpha` – correspond to the attended value vector ($\mathbf{a}$) and the vector of attention values (α) computed from as in equations (1) and (2). The expected dimensions are asserted above. Note that this is intended to be a batched operation and the equations presented are for a single instance. `torch.bmm` can be very useful here.

Train this model by executing `python mt_driver.py`. Record the perplexity and BLEU score on the test set. These are automatically generated in the script and printed after training.

The code is implemented in $\text{mt}_d irver.py, class SingleQueryScaledDotProductAttention.$
Two linear networks are used to project the decoder inputs into the keys and queries. The attention values tensor was calculated using batch matrix multiply (torch.bmm) and the alpha values were calculated according to equations 1 and 2. After 10 epochs of training, the perplexity score was 10.829 and the BLEU score was 19.22. This score is roughly what the dummy attention network scored, so something was not quite right in my setup (was aiming for a score in the 30s).

After implementing the scaled dot-product attention mechanism, running `python mt_driver.py` will execute training the model with your attention mechanism. The code saves the checkpoint with the lowest training validation [2] Afterwards, it will report BLEU on the test set as well as produce a number of examples (printed in console) with attention diagrams (saved in `examples` folder) like those shown below

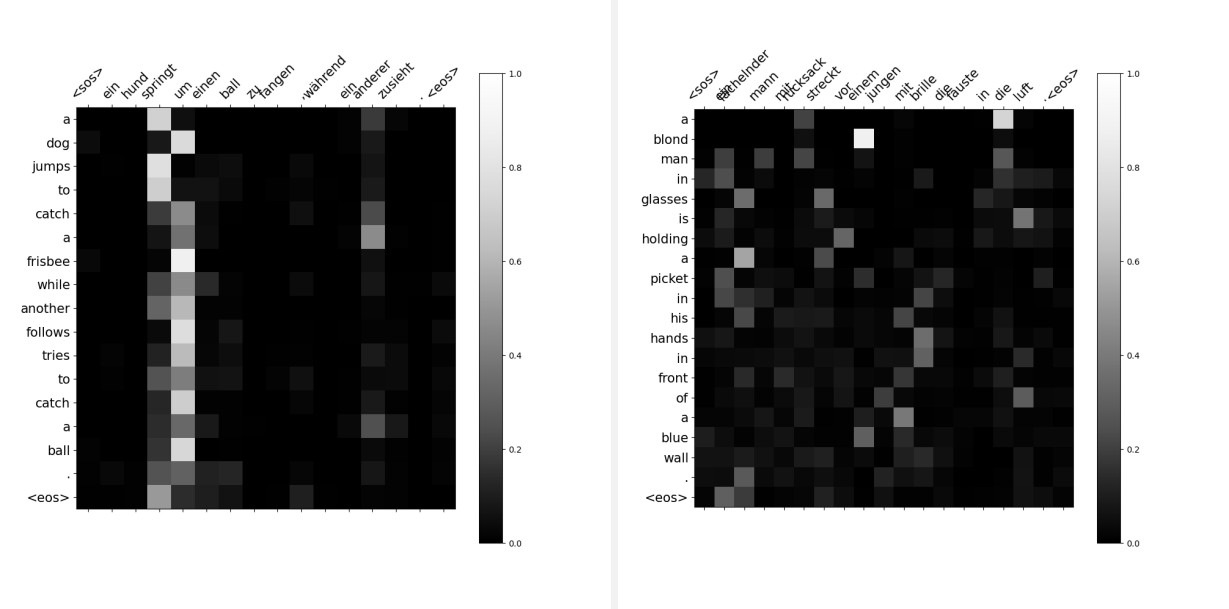


where the brighter blocks indicate high attention values over source word encodings (columns) used when generating translated words (rows). Remember that these encodings also carry information about the rest of the sentence as they come from the bidirectional encoder.

▶ TASK 2.2 Attention Diagrams [1pts] Search through the attention diagrams produced by your model. Include a few examples in your report and characterize common patterns you observe.Note that German is (mostly) a Subject-Object-Verb language so you may find attention patterns that indicate inversion of word order when translating to Subject-Verb-Object English as in the 2nd example above.

[2] The code can be run with `--eval` to load an existing checkpoint and run inference.

Two of my attention maps are shown below. The left diagram attempts to translate the German sentence "Ein hund springt um einen ball zu fangen während ein anderer zusieht." My model returned "a dog jumps to catch a frisbee while another follows, tries to catch a ball" whereas Google Translate decodes this as "a dog jumps to catch a ball while another watches". The general theme of the sentence is preserved but there is a hallucination in my model about a frisbee, but given the correlation between dogs and frisbees this could be plausible (but still an extrinsic hallucination). The attention pattern on the left diagram seems to focus almost exclusively on two phrases in the source text which seems amiss. Given the similar if not re-ordered nature of German and English, the attention should be more spread out across the input. The right diagram shows a more dispersed, but still not well-organized attention diagram. Again, if the model was performing as expected, I'd expect the attention of each column to have a single high value (single white colored box). Alas, it seems that jungen in the source has the source text has the most attention, which is odd because that translates to boy in English and that is not found in the decoded text. Given the scattered attention plots, it is not possible to find indications of German-English word inversion patterns.



The code also implements two baseline options for the attention mechanism. A `Dummy` attention that just outputs zero tensors – this effectively attends to *no* words. The `MeanPool` attention which just averages the source word encodings – this effectively attends *equally* to all words. The code will use these if run with the `--attn none` and `--attn mean` arguments respectively.

▶ TASK 2.3 Comparison [3pts] Train and evaluate models with the `Dummy` and `MeanPool` 'attention' mechanisms. Report mean and variance over three runs for these baselines and your implementation of scaled dot-product attention. Discuss the observed trends.

Three methodologies for attention were compared: Dummy (no attention), MeanPool (average of source encodings), and ScaledDotProduct (equations 1 and 2). For each configuration, three trials were run and the results are shown in the table below. The performance was measured using the BLEU metric and the MeanPool scored the highest (22.820). Ideally, the ScaledDotProduct configuration should have been able to outperform the other methods but something was wrong in my implementation. My scaled dot product's performance was on-par with the dummy / baseline model, so no ideal. Of the three models, the mean pool had the highest variance but it still consistently outperformed the other models.

	Dummy	**MeanPool**	**ScaledDotProd**
	19.23	21.57	19.22
	18.97	23.27	19.43
	18.93	23.62	18.28
Mean	19.043	22.820	18.977
Variance	0.027	1.203	0.375

▶ TASK 2.EC Beam Search and BLEU [2pts] This is an extra credit question and is optional.

In the previous homework, we implemented many decoding algorithms; however, in this work we just use greedy top-1 in the `translate_sentence` function. Adapt your implementation of beam search from HW3 to work on this model by augmenting `translate_sentence` (which is used when computing BLEU). Report BLEU scores on the test set for the scaled dot-product attention model with B=5, 10, 20, and 50.

References

[1] D. Elliott, S. Frank, K. Sima'an, and L. Specia, "Multi30k: Multilingual english-german image descriptions," in *Proceedings of the 5th Workshop on Vision and Language*, pp. 70–74, 2016.