Assignment 4: Implementing recurrent neural networks in PyTorch

Due to: December 2, 2020

Goal: Implement recurrent neural networks (RNNs) in PyTorch.

Submission: The assignment consists of two parts: implementation and an analysis. You are supposed to present results for both parts in the following manner:

1. Upload your code.
2. Prepare a report with an analysis of results obtained at home.

The code and the report must be uploaded due to the deadline to Canvas.

UPLOAD A **SINGLE FILE** (a zip file) containing your code and the report. Name your file as follows: [vunetid]_[assignment number].

changelog

25 Nov. Clarify difference between max pooling and global max pooling. Fix reference to start/end tokens.
23 Nov. First version

In this assignment, we will look at RNNs. You can choose one of two tasks:

- Task A (4 parts): Sentiment classification. A sequence-to-label task where you will learn to predict what the sentiment of a movie review is (positive of negative).
- Task B (2 parts): Autoregressive modeling. Training a model to predict the next token in a sequence given the preceding tokens.

If you're pressed for time, the first task is simpler, and more predictable to tune. The second task gives you more insight into the difficulty of training recurrent models, but it is a bit more challenging to find good hyperparameters. We recommend trying both briefly, just so you get the basic idea of each, and then polishing one of them for the final report.

The deliverable for this assignment is a single report. There are a few questions in the text of the exercise but these are meant for reflection only. Discuss them in the text of your report if it makes sense, but otherwise just make sure you can answer them for yourself.

Since a fast marking turnaround is important for this assignment, the maximum length is **two pages**, excluding references and appendix. The TAs are not required to read anything beyond the first two pages of your report.

New datasets. Before you choose your task, install the the `wget` module in your python environment with the command

```
pip install wget
```

and then download the updated dataset script:

https://gist.github.com/pbloem/bd8348d58251872d9ca10de4816945e4

Note that new functions like `load_imdb`, `load_toy` and `load_brackets` have been added.

Task A: Sentiment classification.

Part 1: Loading the data

The IMDb dataset is the sequence-learning equivalent of MNIST: a large, challenging classification dataset with plenty of examples, that is still light enough to train models for on a laptop. It contains 50 000 reviews of movies, taken from the Internet Movie Database which are either highly positive or highly negative. The task is to predict which for a given review. This is known as sentiment analysis.

> If this seems like a simple task, note that even large pretrained models like ELMo don't get far over 95% accuracy, so this is by no means a solved or a toy problem.

To simplify things we've preprocessed and tokenized the data for you. Our tokenization is a little crude: we lowercase everything, remove all non-letters and split on whitespace. It'll do for our current purposes, but in practice, you'd look to more refined tokenization strategies to extract more information from the raw text. All words have been converted to integer indices in a fixed vocabulary.

To load the data, call the load_imdb function as follows:

```
    (x_train, y_train), (x_val, y_val), (i2w, w2i), numcls =
load_imdb(final=False)
```

The return values are as follows:

- `x_train` A python list of lists of integers. Each integer represents a word. Sorted from short to long.
- `y_train` The corresponding class labels: 0 for positive, 1 for negative.
- `x_val` Test/validation data. Laid out the same as x_train.
- `y_val` Test/validation labels
- `i2w` A list of strings mapping the integers in the sequences to their original words. `i2w[141]` returns the string containing word 141.

- `w2i` A dictionary mapping the words to their indices. `w2i['film']` returns the index for the word "film".

If `final` is true, the function returns the canonical test/train split with 25 000 reviews in each. If `final` is false, a validation split is returned with 20 000 training instances and 5 000 validation instances.

To have a look at your data (always a good idea), you can convert a sequence from indices to words as follows

```
print([i2w[w] for w in x_train[141]])
```

To train, you'll need to loop over x_train and y_train and slice out batches. Each batch will need to be padded to a fixed length and then converted to a torch tensor. Implement this padding and conversion to a tensor.

Tips:

- We've included a special padding token in the vocabulary, represented by the string ".pad". Consult the `w2i` dictionary to see what the index of this token is.
- We've also included special tokens ".start" and ".end", which are only used in the autoregressive task.
- If you feed a list of lists to the function torch.tensor(), it'll return a torch tensor.
  - The inner lists must all have the same size
  - Pytorch is pretty good at guessing which datatype (int, float, byte) is expected, but it does sometimes get it wrong. To be sure, add the dataype with `batch = torch.tensor(lists, dtype=torch.long)`.
- If you're curious how the data was processed, or you want to add something, the script can be found here: `'.pad'`
-

Bonus task: Implement a loop with a *variable batch size*. That is, if the sequences are short, add many of them to the batch, and as they get longer, shrink the batch size. The simplest approach is to set a maximum number of *tokens* and to add sequences to the current batch until the maximum is reached. Then pad the batch and convert to a tensor.

Part 2: Non-recurrent model

We'll start with the simplest sequence-to-sequence model discussed in the lectures: an Linear layer applied to each token in the sequence separately. **Build a model with the following structure:**

	input/output	layer
1	tensor of `dtype=torch.long` with size (batch, time)	**`nn.Embedding(...)`** Convert the integer indices to embedding vectors

2	tensor of `dtype=torch.float` with size (batch, time, emb)	**`nn.Linear(emb, hidden)`** Map each token by a shared MLP
3	tensor of dtype=torch.float with size (batch, time, hidden)	`ReLU`
4	"	Global max pool along the time dimension Note the difference between a max pool as used in a CNN and a *global* maxpool. There is no special layer for this in pytorch, you can just implement it manually.
5	tensor of `dtype=torch.float` with size (batch, hidden)	**`nn.Linear(emb, numcls)`** Project down to the number of classes
	tensor of `dtype=torch.float` with size (batch, num_clases)	

Notes:

- Make sure to read the documentation for the layers used carefully
- Use embedding size and hidden size 300.
- The embedding layer needs to know how many tokens there are (since that is how many embedding vectors it needs to create). How can you find this from the return values of the load_imdb function?
- Note that the second layer is a Linear layer, applied only to the last dimension of three input dimensions. That is, the first two dimensions should *both* be treated as batch dimensions.
    - One way to achieve this is to use reshapes (lecture 2.4) to fold the two into one dimension and then unfold them again afterwards. However, if you read the documentation of `nn.Linear` carefully, you'll find that for this particular layer, there's an easier way.
- The model is not memory-intensive, so you can easily go to large batch sizes to speed up training. Note however, that the amount of padding does also increase with the batch size. Can you explain why?
- It's most common not to make softmax part of the model, but to apply it as part of the loss function, since this can be done in a more numerically stable way. The function `torch.nn.functional.cross_entropy` can be used to calculate the loss here. Make sure to read the documentation carefully so that you know what it expects.
    - Note that when computing accuracy, we only need the class with the highest score, so we can just compute the argmax over the linear outputs.

Train for at least one epoch and compute the validation accuracy. It should be above 60% for most reasonable hyperparameters.

Part 3: Writing your own Elman RNN

For a sequence-to-sequence layer that propagates information over time, we'll start with a simple Elman network (the first type of simple RNN shown in the lectures).

Pytorch has these available, but it's instructive to build our own first, to see what happens under the hood. Since this can be complicated, we'll give you some skeleton code to work from:

```
class Elman(nn.Module):

   def __init__(self, insize=300, outsize=300, hsize=300):
       super().__init__()

       self.lin1 = ...
       self.lin2 = ...

   def forward(self, x, hidden=None):

       b, t, e = x.size()

       if hidden is None:
           hidden = torch.zeros(b, e, dtype=torch.float)

       outs = []
       for i in range(t):
           inp = torch.cat([x[:, i, :], hidden], dim=1)

            ...

           outs.append(out[:, None, :])

       return torch.cat(outs, dim=1), hidden
```

Fill in the missing parts of this code. And build a second model, like the one in the previous part, but replacing the second layer with an `Elman(300, 300, 300)` layer.

Notes:

- As you will see when you run the network, looping over slices of your input tensor is horribly slow (remember that every slice becomes a node in the computation graph). This is optimized a lot in the pytorch library implementations of RNNs, but fundamentally all RNNs require some level of sequential processing.

- As we saw in the slides, the first and last hidden layers can be useful for various tricks. This is why pytorch returns both the output sequence and the last hidden layer.
    - Remember this when you fit the Elman module into your larger network: it outputs a pair, and only the first element of that pair should be passed to the next layer.

Bonus task: Implement an LSTM in the same way. It may look daunting at first, but if you follow the formulae, it shouldn't take too long (although it will probably run very slow).

Part 4: Using Torch's RNNs

To speed things up, let's try again with pytorch's own RNN implementations. Take the previous model and replace layer 2 with layers of the type `torch.nn.RNN` (the torch implementation of the Elman network) and `torch.nn.LSTM`.

Tune the hyperparameters for these three models (MLP, Elman, LSTM). Machine Learning gospel tells us that with enough tuning, the LSTM will perform best, followed by the Elman network, followed by the MLP. Is this what you find as well? State your hypothesis based on your chosen hyperparameters and the validation performance. Then run all three models on the test set and report your findings.

Bonus task: Try a CNN model as well. Do you notice that the model is faster to train? If you stack multiple CNNs, at which point does the training speed become similar?

Bonus task: The Pytorch RNNs can be made bilinear with a simple constructor argument. Investigate the performance boost you get from a bilinear LSTM.

Notes:

- The default dimension order in pytorch sequence models is slightly confusing (time, batch, embedding). You can transpose the dimensions, or just pass `batch_first=True` to the constructor of your RNN.

Task B: Autoregressive modeling

Part 1: NDFA and Bracket matching

Data We will start with two simple synthetic datasets.

Load the `ndfa` dataset with

```
x_train, (i2w, w2i) = load_ndfa(n=150_000, char=True)
```

Load the `brackets` dataset with

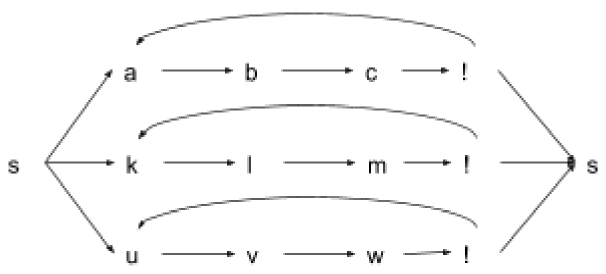
```
x_train, (i2w, w2i) = load_brackets(n=150_000, char=True)
```

This will return the following objects:

- `x_train` A list of lists of integers indices, encoding characters. Sorted from short sequences to long sequences.
- `i2w` A list mapping the indices to their characters
- `w2i` A dictionary mapping the characters to their indices.

To decode a sequence, use:

```
print(''.join([i2w[i] for i in  x_train[10_000]]) )
```



The `ndfa` dataset contains sequences sampled from the non-deterministic finite automaton. On the right.

The brackets dataset contains sequences like `()()(())`, `(((())))` and `(()())`: sequences of parentheses that are correctly matched (a so-called *Dyck language*). We will attempt to train an autoregressive LSTM to learn these grammars. We suggest starting with the NDFA data, and then moving on to the brackets.

In both cases, we will consider the learning successful if in a sample of 10 sequences, the majority is correct. This is not very strict, but it will suffice for our purposes. To check if a long string is correct for the bracket data, just check that it contains the same number of opening and closing brackets.

To load the data, we will split it into batches and *pad* the batches. However, before padding, we'd also like to prepend a `'.start'` token to each sequence and append an `'.end'` token (you can look up their indices in the `w2i` dictionary). These tokens will help the model understand where a sequence should start and end.

Batching You can split the data into batches of the same size, but then the early batches will use far less memory than the later batches. To maximise memory utilization, we recommend setting a maximum number of tokens per batch rather than a maximum number of sequences, and adding sequences to the batch until you're finished.

LSTMs can suffer from *catastrophic forgetting*. This means that if we train on short sequences for too long after seeing a long sequence, the model forgets what it has learned about the long sequences. A simple solution is to cut up your dataset into batches of similar-length sequences (and possibly variable size) before training, and to shuffle the list of batches before the start of each epoch. That way, the model will never go too long without seeing a long sequence.

Since we're training autoregressively, the target is just the batch, shifted one token to the left. Create a target tensor by removing the first column of the input tensor and appending a column of zeros.

Model Set up a model with the following structure:

	input/output	layer
1	tensor of `dtype=torch.long` with size (batch, time)	**`nn.Embedding(...)`** Convert the integer indices to embedding vectors
2	tensor of `dtype=torch.float` with size (batch, time, emb)	**`nn.LSTM(input_size=emb, hidden_size=h, numlayers=..., batch_first=True)`** Single layer LSTM
3	tensor of `dtype=torch.float` with size (batch, time, hidden)	**`nn.Linear(emb, vocab)`** Project down to the number of characters
	tensor of `dtype=torch.float` with size (batch, time, num_chars)	

The number of layers should be 1, 2 or 3. Make sure to set batch_first to True if your input tensor has shape (batch, time, emb). Omitting this argument results in silent failure that looks

The NDFA task can be learned in three epochs with a single-layer network with e=32, h=16.

For our loss function, we want to use a cross entropy loss at every point in time. This is possible with the pytorch cross entropy loss function, but if your output tensor has size (batch, time, vocab) and your target (integer) tensor has size (batch, time), you'll need to do some shuffling of dimensions. Read the documentation carefully to figure out the details.

Sampling Since this task is challenging, we will forego a proper evaluation on a test/train split. Instead, we'll *sample* some data from our model.

Start with a *seed* sequence of a number of integer encoded tokens. For instance:

```
seq = [w2i['.start'], w2i['('], w2i['('], w2i[')']]
```

Feed this sequence to the model (transform it to a tensor and add a singleton batch dimension), and observe what probabilities it predicts for the next character. That is, the probabilities from the logit vector `output[0, -1, :]`. Sample a character from this distribution and append it to the seed sequence. Repeat this process until your observe and end token, or until the sequence reaches a particular maximum length.

Generate and print 10 samples from the seed after every epoch.

For sampling from the output distribution, you can use the following function:

```python
import torch.distributions as dist

def sample(lnprobs, temperature=1.0):
    """
    Sample an element from a categorical distribution

    :param lnprobs: Outcome logits
    :param temperature: Sampling temperature. 1.0 follows the given
        distribution, 0.0 returns the maximum probability element.
    :return: The index of the sampled element.
    """
    if temperature == 0.0:
        return lnprobs.argmax()

    p = F.softmax(lnprobs / temperature, dim=0)
    cd = dist.Categorical(p)

    return cd.sample()
```

The temperature hyperparameter allows you to balance between sampling from the given probabilities (temp 1.0) and giving more weight to the high probability tokens. For the bracket task a low temperature is good, since we want to see if the model has learned to generate only correct sentences.

Notes:

- This can be a challenging training task, even on toy data. Make sure to plot your loss curves and gradient norm curves. Gradient clipping is very likely to help (this is true in general for RNNs).
    - We strongly recommend tensorboard for plotting loss curves in this exercise.

- Once you have a smoothly decaying loss curve over the first 10 or so epochs, you'll have to let the model run for around 50 or so epochs to see real progress.
- Make sure to compute the loss *per token*, so that the batch size and instance length don't affect the smoothness of the loss curve. Pass `reduction='sum'` to the loss function, and divide by the number of tokens manually.
- It's common to implement *masking*, so that the loss is only computed over the non-padded elements of the batch. You can do this by passing a weight tensor to the cross-entropy function. This is not crucial for the task, since it's relatively simple for the network to learn that an `.end` token is always followed by a string of .pad tokens. Consult the documentation of the cross-entropy loss to see how to do this.

Part 2: Natural language

Load the second toy grammar with `load_toy(n=50_000, char=True)`. This grammar generates grammatical English sentences. See how far you get with training an LSTM on these sequences. Setting char=False, gives you word-level sequences, which is an easier task.

Use the same model as in the previous part, but increase the hidden size, the embedding dimension and possibly the number of layers. Tune the hyperparameters and train until you get the model at least to produce mostly words that occur in the training data.

For the report, provide the details of your hyperparameter tuning on both tasks and provide and interpret samples from the model for all three tasks. Note that this is a very informal evaluation. In your discussion section, discuss what a proper evaluation on this task would look like (you may want to look into the notion of *perplexity*).

Bonus task If you want to try this on actual natural language, you can load the imdb dataset (see task A) with `char=True`. Be advised that you'll probably need a multi-layer LSTM, training on a GPU for a long time until you see good performance.

Notes:

- At word-level, the task should be easier, but the softmax over the 8K large vocabulary in the last layer will make this a very slow model.
- Sorting by length breaks one of the fundamental assumptions of stochastic gradient descent. A nicer solution is to shuffle the list of instances, and cute it into sequences of wildly varying length, and then to *pack* the batches instead of padding them. See the pytorch documentation for how to do this.
- One simple trick to speed up training is to use *curriculum learning*. Train the model first on only the simple, short instances (which can be done much faster) for a number of epochs, before moving on to the longer, more difficult sequences. Since the model first needs to learn basic patterns like token frequencies and first-order probabilities, it doesn't need to see the longer sequences yet.

- Another trick is to stack several LSTMs and to sum the output of each to make the output of the model (a bit like a residual connection). The num_layers keyword doesn't do this, so you'll have to create and stack the LSTMs manually.