Deep Learning (IST, 2021-22)

Homework 2

André Martins, Rita Ramos, João Santinha, José Moreira, Ben Peters, Francisco Melo

Deadline: Monday, January 31, 2022.

Please turn in the answers to the questions below in a PDF file, together with the code you implemented to solve them (when applicable).
Please submit **a single zip file** in Fenix under your group's name.

Question 1

1. (10 points) Consider a convolutional neural network (CNN) that takes as input images of size 28x28x3 and has the following layers:

   - One convolutional layer with 8 kernels of shape 5x5x3 with stride of 1, and a padding of zero (i.e., no padding).
   - A max-pooling layer with kernel size 4x4 and stride of 2 (both horizontally and vertically).
   - A linear output layer with 10 outputs followed by a softmax transformation.

   How many parameters are there in total in this network?

   Solution: We need $5 \times 5 \times 3 = 75$ parameters for each kernel, since we have 8 kernels this gives $8 \times 75 + 8 = 608$ parameters (where we included one bias parameter for each kernel). With a padding of zero and stride of 1, the output after this convolution layer will be an image of size 24x24x8, as $24 = 28 - (5 - 1)$. The max-pooling layer with kernel size 4x4 and stride of 2 has no parameters, and it maps this image to one of size 11x11x8, as $11 = (24 - 4)/2 + 1$. Finally, the output layer takes as input vectors of dimension $11 \times 11 \times 8 = 968$ and maps them to a vector of dimension 10, including a bias vector of dimension 10, leading to $968 \times 10 + 10 = 9690$ parameters. Therefore, we have a total of $608 + 9690 = 10298$ parameters.

2. (10 points) Suppose that we replace the convolutional and max-pooling layers above by a feedforward, fully connected layer with hidden size 100 and output size 10 (followed by the softmax transformation). How many parameters are there in total? Compare to the previous answer and comment.

   Solution: With a single feedforward layer with hidden size 100, we need $28 \times 28 \times 3 \times 100 + 100 = 235300$ parameters in the first layer, and $100 \times 10 + 10 = 1010$ parameters in the second layer, which gives a total of 236310 parameters. Therefore, we see that the feedforward neural network has many more parameters, as it does not do the parameter sharing done by the CNN.

3. Let $\boldsymbol{X} \in \mathbb{R}^{L \times n}$ be an input matrix for a sequence of length L, where n is the embedding size. We are going to look at the *self-attention* for this sequence. Assume two self-attention heads have projection matrices $\boldsymbol{W}_Q^{(h)}, \boldsymbol{W}_K^{(h)}, \boldsymbol{W}_V^{(h)} \in \mathbb{R}^{n \times d}$ for $h \in \{1, 2\}$, with $d \leq n$.

   1. (5 points) Show that the self-attention probabilities for each head can be written as the rows of a matrix of the form

$$\boldsymbol{P}^{(h)} = \text{Softmax}(\boldsymbol{X}\boldsymbol{A}^{(h)}\boldsymbol{X}^\top) \tag{1}$$

   where $\boldsymbol{A}^{(h)} \in \mathbb{R}^{n \times n}$ has rank $\leq d$ (in the above expression, Softmax is applied row-wise). Provide an expression for the matrix $\boldsymbol{A}^{(h)}$.

   Solution: We have, with $\beta = \sqrt{d}$,

$$\begin{aligned}
\boldsymbol{P}^{(h)} &= \text{Softmax}(\beta^{-1}\boldsymbol{Q}^{(h)}(\boldsymbol{K}^{(h)})^\top) \\
&= \text{Softmax}(\beta^{-1}\boldsymbol{X}\boldsymbol{W}_Q^{(h)}(\boldsymbol{X}\boldsymbol{W}_K^{(h)})^\top) \\
&= \text{Softmax}(\beta^{-1}\boldsymbol{X}\boldsymbol{W}_Q^{(h)}(\boldsymbol{W}_K^{(h)})^\top\boldsymbol{X}^\top) \\
&= \text{Softmax}(\boldsymbol{X}\boldsymbol{A}^{(h)}\boldsymbol{X}^\top),
\end{aligned}$$

   with $\boldsymbol{A}^{(h)} = \beta^{-1}\boldsymbol{W}_Q^{(h)}(\boldsymbol{W}_K^{(h)})^\top$. Since $\boldsymbol{W}_Q^{(h)}$ and $\boldsymbol{W}_K^{(h)}$ are n-by-d matrices with $d \leq n$, $\boldsymbol{A}^{(h)}$ has rank $\leq d$.

   2. (5 points) Show that, if $\boldsymbol{W}_Q^{(2)} = \boldsymbol{W}_Q^{(1)}\boldsymbol{B}$ and $\boldsymbol{W}_K^{(2)} = \boldsymbol{W}_K^{(1)}\boldsymbol{B}^{-\top}$, where $\boldsymbol{B} \in \mathbb{R}^{d \times d}$ is any invertible matrix, then the self-attention probabilities are exactly the same for the two attention heads.

   Solution: From the previous solution, we have

$$\boldsymbol{A}^{(2)} = \beta^{-1}\boldsymbol{W}_Q^{(2)}(\boldsymbol{W}_K^{(2)})^\top = \beta^{-1}\boldsymbol{W}_Q^{(1)}\boldsymbol{B}\boldsymbol{B}^{-1}(\boldsymbol{W}_K^{(1)})^\top = \boldsymbol{A}^{(1)}.$$

Question 2

Image classification with CNNs. In this exercise, you will implement a convolutional neural network to perform classification using the Fashion-MNIST dataset. Examples of images in this dataset are shown in Figure 1.

As previously done in Homework 1, you will need to download the Fashion-MNIST dataset. You can do this by running the following command in the homework directory:

```
python download_fashion_mnist.py
```

Python skeleton code is provided (`hw2-q2.py`). You will now try out convolutional networks. For this exercise, we recommend you use a deep learning framework with automatic differentiation (suggested: Pytorch).

1. (5 points) What kind of equivariances do convolutional layers exhibit and why are they useful in CNNs for image classification?

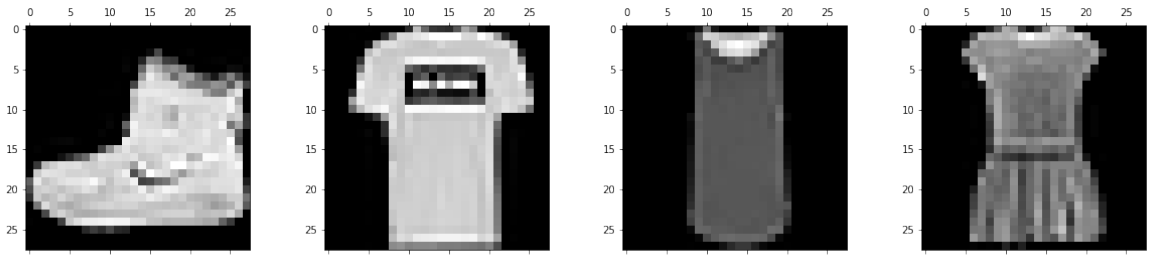


Figure 1: Examples of images from the FashionMNIST dataset.

Solution: Convolutional layers have translation **equivariance** – this is because the same filters are applied to all regions of the image; by translating the image horizontally or vertically, the response of the convolution layer is also translated by the same amount (ignoring boundary effects). When combined with pooling layers, this leads, approximately, to *invariance* to small translations. For CNNs for image classification, this leads to the CNN being (approximately) invariant to translations of the input, i.e., predicting the same label as the untranslated image. Note that convolution layers are not (in general) equivariant to rotations or scaling transformations.

(Note: While in some literature you may read that convolutional layers are *invariant* to translations, this is not rigorous. "Equivariance" to a transformation means that, when a transformation is applied to the input, the output is transformed in the same way; "invariance" to a transformation means that the output does not vary at all when the input is transformed. Convolutional layers are *equivariant* to translations; the full CNN for image classification is approximately *invariant* to translations.)

2. (20 points) Implement a simple convolutional network with the following structure:

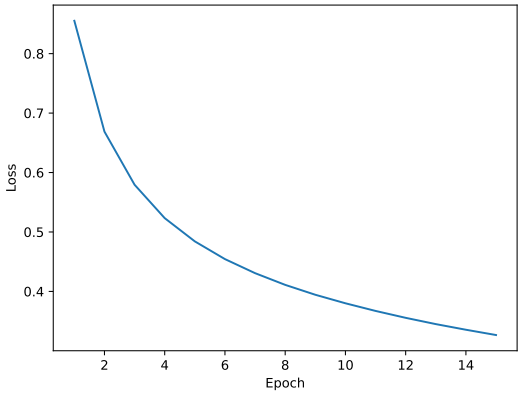
   - A first block comprising (order as provided):
     - A convolution layer with 16 output channels, a kernel of size 3x3, stride of 1, and padding chosen to preserve the original image size.
     - A rectified linear unit activation function.
     - A max pooling with kernel size 2x2 and stride of 2.
   - A second block comprising (order as provided):
     - A convolution layer with 32 output channels, a kernel of size 3x3, stride of 1, and padding of zero.
     - A rectified linear unit activation function.
     - A max pooling with kernel size 2x2 and stride of 2.
   - An affine transformation with 600 output features (to determine the number of input features use the number of channels, width and height of the output of the second block. Hint: The number of input features = $number\ of\ output\ channels \times output\ width \times output\ height$).
   - A rectified linear unit activation function.
   - A dropout layer with a dropout probability of your choice.
   - An affine transformation with 120 output features.
   - A rectified linear unit activation function.

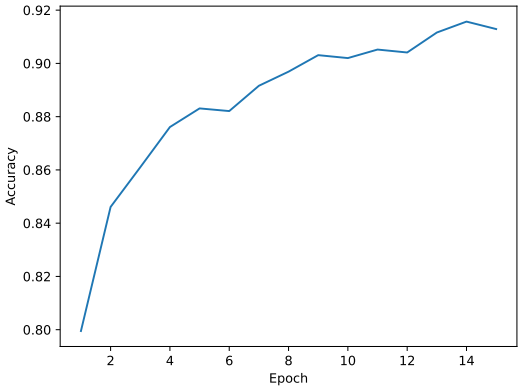
- An affine transformation with the number of classes followed by an output LogSoftmax layer.

Hint: use the functions `nn.Sequential`, `nn.Conv2d` and `nn.MaxPool2d`.

Train your model for 15 epochs using `SGD` and tune the learning rate on your validation data, using the following values: 0.001,0.01,0.1. For the best configuration, report it and plot two things: the training loss and the validation accuracy, both as a function of the epoch number.

Solution: Training 15 epochs with a learning rate of 0.01, a l2 weight decay of 0, a dropout probability of 0.3 and using the SGD optimizer we get a validation accuracy of 0.9129 and a test accuracy of 0.9053.





3. (10 points) Plot the filters in the first and second convolutional layers. In general, what kind of features are usually captured by CNNs in bottom vs top layers? (Note: for this exercise, the image resolution may be too low to notice interesting patterns in the filters.)

   NOTE: the skeleton code is designed to output the kernels of the first and second convolutions that you can use to answer the next question. Use the options `-conv_1_name` and `-conv_2_name` to save the kernels after finishing the training of the CNN. If you are using `nn.Sequential` to define each block as:

   ```
   self.convblock1 = nn.Sequential(...)
   self.convblock2 = nn.Sequential(...)
   ```

   use `-convlayer1 convblock1[0] -convlayer2 convblock2[0]`.

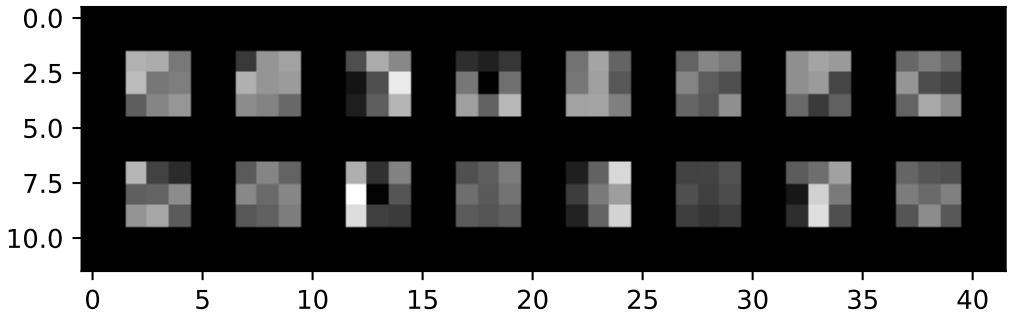
   If not using `nn.Sequential` and the layers are defined as:

   ```
   self.convlayer1 = nn.Conv2(...)
   ...
   self.convlayer2 = nn.Conv2(...)
   ```

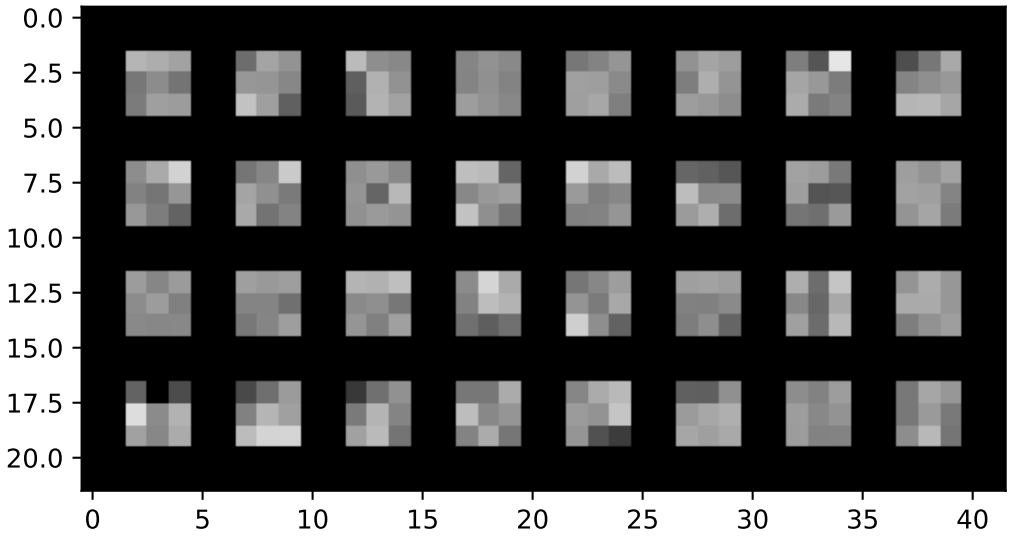
   use `-convlayer1 convlayer1 -convlayer2 convlayer2`.

   Solution: Features from the first convolutional layer capture low-level characteristics like edges, lines, corners, and other small features, while features from subsequent convolutional layers capture higher-level characteristics like parts of objects like car wheel, window of house, cat eye, etc..

   Filters of first convolutional layer:



Filters of second convolutional layer:



Question 3

Image Captioning. Image captioning is the problem of automatically describing an image with a short text description. This task is usually addressed with an encoder-decoder model. Typically, the encoder is a CNN model that processes and summarises the input image into relevant feature representations. The representations are then passed to a language decoder, commonly an LSTM model, which generates the respective caption word-by-word given the previous words and the image encoder representations.

1. You are going to implement an image captioning model for this task concerning aerial images, thus actually addressing remote sensing image captioning. The input and output should respectively be an image (i.e., remote sensing image) and the corresponding text description. The evaluation metric is BLEU-4 (which calculates precision between n-gram occurrences in the generated and reference captions.).

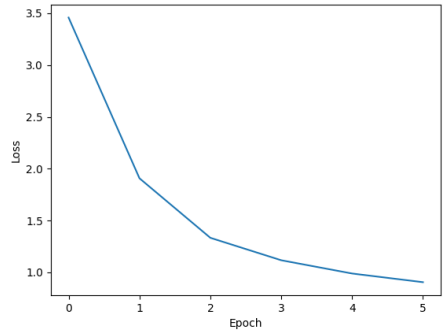
   (a) (10 points) Unzip the provided `images.zip` file and put the images at the `data/raw_dataset/images` folder. Run the file `script_features.py` (`python3 src/script_features.py`) that extract the images features using a pretrained `ResNet-18` convolutional neural network encoder model. Then, implement a vanilla image captioning model using an encoder-decoder architecture with an auto-regressive LSTM as the decoder. Specifi-

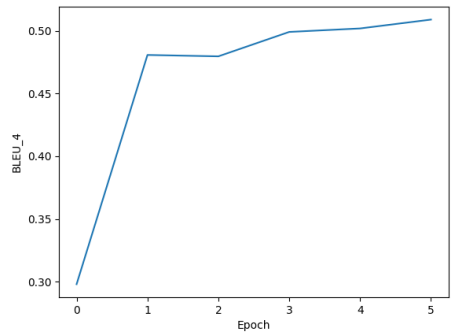
cally, in the skeleton code, you will need to implement the method `forward()` of the `decoder.py` (inside the folder `models`) and then run (`python3 src/train.py`).

Plot the training loss and the validation BLEU-4. Also, report the final BLEU-4 score in the test set.

Hint: At each time-step, the LSTM decoder `self.decode_step` receives as input the embedding of the current word (`self.embedding`), then the LSTM hidden state is processed through a dropout operation (`self.dropout`), followed by an affine transformation (`self.fc`) to produce the scores of the words of the vocabulary.

Solution:





Final BLEU-4: 0.5126

(b) (20 points) Add an attention mechanism to the decoder (additive attention), which weights the contribution of the different image regions, according to relevance for the current prediction.

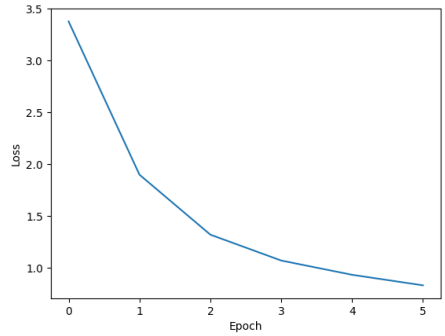
Specifically, in the skeleton code, you will need to implement the `forward()` methods of the `decoder_with_attention.py`, i.e., the forward methods of the `DecoderWithAttention` class and the `Attention class`.

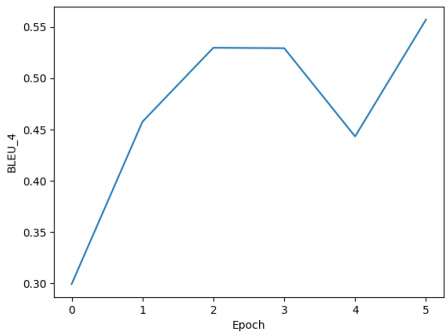
Plot the training loss and the validation BLEU-4. Also, report the final BLEU-4 score in the test set.

Hint: Now, the input of the LSTM decoder (`self.decode_step`) is the embedding of the current word (`self.embedding`) concatenated with the attention vector.

You can run the code with the command `python src/train.py -use_attention`

Solution:





Final BLEU-4: 0.522

(c) (5 points) For the previous model (encoder-decoder with neural attention), report the generated captions for the images "219.tif", "540.tif", "357.tif". For each of those images, place the image next to the corresponding caption. Hint: Use the file inside the `results` folder: `caps_generated_enc_dec_w_attention.json`.

Solution: