

Deep Learning (IST, 2023-24)

Homework 1

André Martins, Francisco Melo, João Santinha, Duarte Alves, Margarida Campos

Deadline: Friday, December 15, 2023.

Please turn in the answers to the questions below in a PDF file, together with the code you implemented to solve them (when applicable).

IMPORTANT: Please write 1 paragraph indicating clearly what was the contribution of each member of the group in this project. A penalization of 10 points will be applied if this information is missing.

Please submit a **single zip file** in Fenix under your group's name.

Question 1 (35 points)

Medical image classification with linear classifiers and neural networks. In this exercise, you will implement a linear classifier for a simple medical image classification problem, using the OCTMNIST dataset. The dataset contains 109,309 valid optical coherence tomography (OCT) images for retinal diseases comprised of 4 diagnosis categories - **multi-class classification task**. The original training set was split with a ratio of 9:1 into training and validation set, and use its source validation set as the test set. The source images are gray-scale with sizes varying between $(384-1,536) \times (277-512)$. Images were center-cropped with a window size of length of the short edge and resize them into $1 \times 28 \times 28$. **Please do not use any machine learning library such as scikit-learn or similar for this exercise; just plain linear algebra (the numpy library is fine).** Python skeleton code is provided (hw1-q1.py).

In order to complete this exercise, you will need to download the OCTMNIST dataset. You can do this by running the following command in the homework directory:

```
python download_octmnist.py
```

1. (a) (7 points) Implement the `update_weights` method of the `Perceptron` class in `hw1-q1.py`. Then train 20 epochs of the perceptron on the training set and report its performance on the training, validation and test sets. Plot the train and validation accuracies as a function of the epoch number. You can do this with the command

```
python hw1-q1.py perceptron
```

- (b) (13 points) Repeat the same exercise using logistic regression instead (without regularization), using stochastic gradient descent as your training algorithm. Report the final test accuracies and compare, based on the plots of the train and validation accuracies, the models obtained using two different learning rates of $\eta = 0.01$ and $\eta = 0.001$. This can be solved by implementing the `update_weights` method in the `LogisticRegression` class. You can do this with the command

```
python hw1-q1.py logistic_regression -epochs 50 -learning_rate 0.01
```

2. Now, you will implement a multi-layer perceptron (a feed-forward neural network) again using as input the original feature representation (i.e. simple independent pixel values).
- (a) (5 points) Comment the following claim: “A logistic regression model using pixel values as features is not as expressive as a multi-layer perceptron using `relu` activations. However, training a logistic regression model is easier because it is a convex optimization problem.” Is this true or false? Justify.
 - (b) (10 points) **Without using any neural network toolkit**, implement a multi-layer perceptron with a single hidden layer to solve this problem, including the gradient backpropagation algorithm which is needed to train the model. Use 200 hidden units, a `relu` activation function for the hidden layers, and a multinomial logistic loss (also called cross-entropy) in the output layer (eventhough we are dealing with a binary classification this will allow you to use the same code for a multi-class problem). Don't forget to include bias terms in your hidden units. Train the model for 20 epochs with stochastic gradient descent with a learning rate of 0.001. Initialize biases with zero vectors and values in weight matrices with $w_{ij} \sim \mathcal{N}(\mu, \sigma^2)$ with $\mu = 0.1$ and $\sigma^2 = 0.1^2$ (hint: use `numpy.random.normal`). Run your code with the base command, adding the necessary arguments

```
python hw1-q1.py mlp
```

Report final test accuracy and include the plots of the train loss and train and validation accuracies as a function of the epoch number.

Question 2 (35 points)

Medical image classification with an autodiff toolkit. In the previous question, you had to write gradient backpropagation by hand. This time, you will implement the same system using a deep learning framework with automatic differentiation. Pytorch skeleton code is provided (`hw1-q2.py`) but if you feel more comfortable with a different framework, you are free to use it instead.

1. (10 points) Implement a linear model with logistic regression, using stochastic gradient descent as your training algorithm (use a batch size of 16). Train your model for 20 epochs and tune the learning rate on your validation data, using the following values: $\{0.001, 0.01, 0.1\}$. Report the best configuration (in terms of final validation accuracy) and plot two things: the training loss and the validation accuracy, both as a function of the epoch number. Report the final accuracy on the test set.

In the skeleton code, you will need to implement the method `train_batch()` and the class `LogisticRegression`'s `__init__()` and `forward()` methods.

2. (25 points) Implement a feed-forward neural network using dropout regularization. Make sure to include all the hyperparameters and training/model design choices shown in Table 1. Use the values presented in the table as default.

In the skeleton code, you will need to implement the class `FeedforwardNetwork`'s `__init__()` and `forward()` methods.

- (a) (8 points) Compare the performance of your model with batch sizes 16 and 1024 with the remaining hyperparameters at their default value. Plot the train and validation losses for both, report the best test accuracy and comment on the differences in both performance and time of execution.

You can time the execution of a program using `time`:

Number of Epochs	20
Learning Rate	0.1
Hidden Size	200
Number of Layers	2
Dropout	0.0
Batch Size	16
Activation	ReLU
L2 Regularization	0.0
Optimizer	SGD

Table 1: Default hyperparameters.

`time python hw1.py mlp`

- (b) (8 points) Train the model with learning rates: 1, 0.1, 0.01 and 0.001 with the remaining hyperparameters at their default value. Plot the train and validation losses for the best and worst configurations in terms of validation accuracy, report the best test accuracy and comment on the differences in performance.
- (c) (9 points) Using a batch size of 256 run the default model for 150 epochs. Is there overfitting? Train two similar models with the following changes: one with the L2 regularization parameter set to 0.0001 and the other with a dropout probability of 0.2. Plot the train and validation losses for the best and worst configuration in terms of validation accuracy, report the best test accuracy and comment on the differences of both techniques.

Question 3 (30 points)

1. In this exercise, you will design a multilayer perceptron to compute a Boolean function of D variables, $f : \{-1, +1\}^D \rightarrow \{-1, +1\}$, defined as:

$$f(\mathbf{x}) = \begin{cases} 1 & \text{if } \sum_{i=1}^D x_i \in [A, B], \\ -1 & \text{otherwise,} \end{cases} \quad (1)$$

where A and B are integers such that $-D \leq A \leq B \leq D$.

- (a) (5 points) Show that the function above cannot generally be computed with a single perceptron. *Hint: think of a simple counter-example.*
- (b) (15 points) Show that the function above can be computed with a multilayer perceptron with **a single hidden layer with two hidden units** and hard threshold activations $g: \mathbb{R} \rightarrow \{-1, +1\}$ with

$$g(z) = \text{sign}(z) = \begin{cases} +1 & \text{if } z \geq 0, \\ -1 & \text{otherwise,} \end{cases} \quad (2)$$

and where **all the weights and biases are integers** (positive, negative, or zero). Provide all the weights and biases of such network, and ensure that the resulting network is robust to infinitesimal perturbation of the inputs, i.e., the resulting function $h : \mathbb{R}^D \rightarrow \mathbb{R}$ should be such that $\lim_{t \rightarrow 0} h(\mathbf{x} + t\mathbf{v}) = h(\mathbf{x}) = f(\mathbf{x})$ for any $\mathbf{x} \in \{-1, +1\}^D$ and $\mathbf{v} \in \mathbb{R}^D$.

- (c) (10 points) Repeat the previous exercise if the hidden units use rectified linear unit activations instead. (You will get partial credit if you solve for $D = 2$ and $A = B = 1$ only.)