Deep Learning 2025: Hand-in assignment 1

January 20, 2025

Individual assignment   Due: February 10, 2025

In this and individual assignment where you will implement a neural network to classify images. You will consider the so-called MNIST dataset, which is one of the most well studied datasets within machine learning and image processing. The dataset consists of 60 000 training data points and 10 000 test data points. Each data point consists of a 28×28 pixels grayscale image of a handwritten digit. The digit has been size-normalized and centered within a fixed-sized image. Each image is also labeled with the digit (0,1,...,8, or 9) it is depicting. In Figure 1, a set of 100 random data points from this dataset is displayed.

Figure 1: Some samples form the MNIST dataset used in the assignment. The input is the pixels values of an image (grayscale), and the output is the label of the digit depicted in the image (blue).

In this classification task we consider the image as our input $\mathbf{x} = [x_1, \dots x_{D_i}]^\mathsf{T}$. Each input variable x_j corresponds to a pixel in the image. In total we have $D_i = 28 \cdot 28 = 784$ input variables. The value of each x_j represents the color of that pixel. The color-value is within the interval [0,1], where $x_j = 0$ corresponds to a black pixel and $x_j = 1$ to a white pixel. Anything between 0 and 1 is a gray pixel with corresponding intensity.

The dataset is available in the file `MNIST.zip` from the course homepage. The dataset is divided into subfolders `train` and `test`, and further into subfolders `0-9` containing a number of images on the form `0000.png-xxxx.png`. (Note: Each class does not have exactly the same number of images.) All images are 28×28 pixels and stored in the png-file format. We provide a script `load_mnist.py` for importing the data, which is also available on the course homepage.

> **Tips**
>
> - **Debugging**: If something doesn't work, try to isolate the problem. Comment out code that possibly have bugs, do plenty of printouts and plots. Simplify the task until it works and then work from there. Work in small iterations.
>
> - **One-sample training**: Can the network converge if you only have one sample in the trainset and overfit to that?
>
> - **Training time**: These are very small images, the network should converge in minutes when training. If it takes longer you probably have some bug or your code is not vectorized (you're not using numpy matrix multiplication or broadcasting).

Classification of handwritten digits

In this hand-in assignment you will implement and train a feed forward neural network for solving a classification problem with multiple classes. To solve this assignment you can use combine and extend the notebooks you produced in Lab 1.

It is strongly encouraged that you write your code in a *vectorized* manner (as you did in Lab 1), meaning that you should not use `for` or `while` loops over data points or hidden units, but rater use the equivalent matrix/vector operations. In modern languages that support array processing[1] (in this case `numpy` in Python), the code will run much faster if you vectorize. This is also how modern software for deep learning works, which we will be using later in the course. Finally, vectorized code will require fewer lines of code and will be easier to read and debug. To vectorize your code, choose which dimension that represents your data points and be consistent with your choice. In machine learning and python it is common to reserve the first dimension for indexing the data points (i.e., one row equals one sample). For example, for a linear model

$$\mathbf{f}_i = \mathbf{\Omega}\mathbf{x}_i + \boldsymbol{\beta}, \qquad i = 1, \ldots, I_b,$$

the vectorized version (transposing the expression above to get each $\mathbf{f}_i$ as a row output) for a mini-batch with I_b data points would be

$$\begin{bmatrix} \mathbf{f}_1^\mathsf{T} \\ \vdots \\ \mathbf{f}_{I_b}^\mathsf{T} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^\mathsf{T} \\ \vdots \\ \mathbf{x}_{I_b}^\mathsf{T} \end{bmatrix} \mathbf{\Omega}^\mathsf{T} + \boldsymbol{\beta}^\mathsf{T} \tag{1}$$

where $\boldsymbol{\beta}^\mathsf{T}$ is added to each row (called broadcasting in Python).[2] Note that in the main optimization loop we still need a `for`-loop over the number of epochs/iterations.

The recommended loss function ℓ_i for a multi-output classification problem is the cross-entropy loss which, for numerical issues when $f \ll 0$, is computed *together* with the softmax function. The cost L, for an D_o-class problem, is computed by summing the loss ℓ_i over all the training points $\mathbf{x}_i$

$$\ell_i = \log\left(\sum_{k=1}^{D_o} \exp[f_{ik}]\right) - \sum_{k=1}^{D_o} \widetilde{y}_{ik} f_{ik} \qquad L = \frac{1}{I} \sum_{i=1}^{I} \ell_i \tag{2}$$

where $\widetilde{y}_i$ is the one-hot encoding of the true label y_i for data point i

$$\widetilde{y}_{ik} = \begin{cases} 1, & \text{if } y_i = k \\ 0, & \text{if } y_i \neq k \end{cases} \qquad \text{for } k = 1, \ldots, D_o$$

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[1] https://en.wikipedia.org/wiki/Array_programming

[2] You might want to consider implementing the transposed version of $\mathbf{\Omega}$ and $\boldsymbol{\beta}$ to avoid the transposes in this vectorized model.

Exercise 1. Implement a multi-layer neural network:

Implement in Python, using `numpy`, a feed forward neural network for solving the classification problem. It should involve the following functionalities, some of which have already been implemented in Lab 1:

1. **Initialize.** A function `initialize` that initializes $\boldsymbol{\Omega}_k, \boldsymbol{\beta}_k$ for each layer in the model. Note that when adding more layers it is important that the elements in the weight matrices are initialized randomly (why?). Initialize each element in $\boldsymbol{\Omega}_k$ using He initialization[3]. The offset vectors $\boldsymbol{\beta}_k$ can be initialized with zeros.

2. **Activation functions.** Two functions `sigmoid` and `ReLU` that implement each of the corresponding activation functions

$$\texttt{sigmoid}: a[x] = \frac{1}{1 + \exp[-x]}, \qquad \texttt{ReLU}: a[x] = max(0, x). \tag{3}$$

3. **Forward propagation.** A function `forward_pass` that do the forward propagation for all the layers in the model. It is recommended that the function also returns all pre-activations and activations for all layer. This will make the backward propagation more efficient.

4. **Softmax and cost.** Write a function `softmax` that computes the softmax activation function as

$$p_k = \frac{\exp[f_k]}{\sum_{l=1}^{D_o} \exp[f_l]}, \quad k = 1, \dots, D_o. \tag{4}$$

   A function `compute_cost` that computes the cost from the last layer linear output $\mathbf{f}$, as shown in Equation 2. For numerical stability when $f \gg 0$, reduce the magnitude of f by subtracting its maximum value before computing the loss (verify that adding a constant to f does not change the loss). Verify that this (stabilized) function gives the same answer (when f is not very large/small) as if computing the NLL loss based on `softmax(f)`.

5. **Backward propagation.** A function `backward_pass` that computes backward propagation for all the layers in the model.

6. **Take a step.** Write a function `update_parameters` that updates the parameters for every layer based on provided gradients. Scale the update step by the *learning rate* α, which will determine the size of the steps you take in each iteration.

7. **Predict.** A function `predict` which, using the trained model, and a data set (can be either train or test data) predicts softmax output based on corresponding inputs $\mathbf{x}_i$. Also compute the accuracy by counting the percentage of times your prediction, obtained as the maximum index in the softmax output $\mathbf{p}_i$, matches the correct class label. As a last function output, also return the cost for the data set.

8. **Mini-batch generation.** A function `random_mini_batches` that randomly partitions the training data into a number of mini-batches (`x_mini, y_mini`).

9. **Model training.** A final function `train_model` that iteratively calls the above functions that you have defined. We expect that it should have as inputs, at least:
   `x_train`: train data
   `y_train`: train labels
   `model`: defining the model architecture in some way (e.g. a vector with number of nodes in each layer)
   `iterations`: number of iterations
   `learning_rate`: learning rate α that determines the step size
   `batch_size`: number of training examples to use for each step

Note: The above function names are suggestions, you are allowed to structure your code in another way if you feel that it suits you more.

To monitor the training, you may also wish to provide test data (not used for training!):
`x_test`: test data
`y_test`: test labels
and call the `performance` function every k-th iteration. We recommended that you save and return the train and test costs and accuracies at every k-th iteration in a vector, and possibly also print or plot the results live during training.

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[3]See section 7.5 in course book

Exercise 2. Evaluate a linear model

Evaluate your code on the MNIST dataset by first considering a **linear model**, i.e. a neural network with zero layers of hidden units[4]. Use the provided code to extract the train and test data and labels in the desired format. You should be able to reach over 90% accuracy on the test data. Note that if you implemented the mini-batch generation the training will be much faster.

(a) Using `matplotlib`, produce a plot of the cost, both on training and test data, with iterations on the x-axis. Also, include a plot with the classification accuracy, also evaluated on both test and training data with iterations on the x-axis. For the training data, evaluate on the current mini-batch instead of the whole training dataset. As a help you can use the function below, it takes lists of the train and test accuracies and costs you collected along your training and plot a training curve.

```python
from matplotlib import pyplot as plt
import numpy as np
def training_curve_plot(title, train_costs, test_costs, train_accuracy, test_accuracy, batch_size, learning_rate):
        lg=18
        md=13
        sm=9
        fig, axs = plt.subplots(1, 2, figsize=(12, 4))
        fig.suptitle(title, y=1.15, fontsize=lg)
        sub = f'|  Batch size:{batch_size}  |  Learning rate:{learning_rate} |'
        fig.text(0.5, 0.99, sub, ha='center', fontsize=md)
        x = range(1, len(train_costs)+1)
        axs[0].plot(x, train_costs, label=f'Final train cost: {train_costs[-1]:.4f}')
        axs[0].plot(x, test_costs, label=f'Final test cost: {test_costs[-1]:.4f}')
        axs[0].set_title('Costs', fontsize=md)
        axs[0].set_xlabel('Iteration', fontsize=md)
        axs[0].set_ylabel('Cost', fontsize=md)
        axs[0].legend(fontsize=sm)
        axs[0].tick_params(axis='both', labelsize=sm)
        # Optionally use a logarithmic y-scale
        #axs[0].set_yscale('log')
        axs[1].plot(x, train_accuracy, label=f'Final train accuracy: {100*train_accuracy[-1]:.2f}%')
        axs[1].plot(x, test_accuracy, label=f'Final test accuracy: {100*test_accuracy[-1]:.2f}%')
        axs[1].set_title('Accuracy', fontsize=md)
        axs[1].set_xlabel('Iterations', fontsize=md)
        axs[1].set_ylabel('Accuracy (%)', fontsize=sm)
        axs[1].legend(fontsize=sm)
        axs[1].tick_params(axis='both', labelsize=sm)
```

(b) Extract each of the ten rows (or columns depending on your implementation) of your weight matrix, reshape each of them into size 28 × 28 and visualize them as 10 images. What is your interpretation of these images? Include a few of these images in the report.

Exercise 3. Evaluate your multi-layer neural network

Evaluate your **full neural network** with several layers. You should be able to get up to almost 98% accuracy on the test data after playing around a bit with the design choices. Provide a similar plot as you did in Exercise 2 a).

Exercise 4. Implement batch gradient descent with momentum

Voluntary extra task (for your own learning pleasure): Implement extensions to mini-batch gradient descent like use of *momentum* (easy) and *ADAM* (a little bit more work).

Submission instructions: Submit a pdf with answers to Exercise 1, Exercise 2, Exercise 3 and possibly Exercise 4. Also include your well commented code as appendix in your pdf **and** as a separate zip-file. Submit both files in one submission. Use the 'Assignment template' in Studium for compiling the pdf.

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[4]If your code is based on the notebooks in Lab 1, use $K = 0$ to get a linear model.

Checklist

Please check these things before handing in:

- ☐ **No miss**: Make sure you didn't miss answering any task.

- ☐ **Repeat the problem**: Start the answer to each task with the problem formulation (a short sentence where you write with your own words what you did). For example "Exercise 1: In exercise 1 we implement ... using ... since ..." instead of just "Exercise 1: Answer:..". Also provide details about learning-rate, batch-size and number of nodes in each layer when applicable.

- ☐ **Plots available** All requested plots are available and have proper figure captions, legends and axis labels. The plots are visible (not too small text) and you comment on what can be seen in the plots.

- ☐ **Reasonable accuracy**: The accuracy on the test-set of the one-layer network should be at least 90% and the multi-layer at least 95% if you implemented everything correctly. If you choose the learning rate, number of hidden nodes and layers in a good way you can get above 98% in Exercise 3. Try to experiment a bit.

- ☐ **Generative AI** You have commented if you have used any generative AI, and if so, how.[a]

- ☐ **Code** Code is both attached as appendix to the pdf and submitted as a separate zip-file.

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[a]See on Studium regarding use of generative AI.