Machine Learning 1, Summer Term 2025
Homework 2
PCA. Neural Networks.

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Tutor:	Thomas Knoll, thomas.knoll@student.tugraz.at
Points to achieve:	30 Points
Deadline:	14.05.2025 23:59 (strict, no late submissions allowed)
Hand-in procedure:	Submit **a report (PDF)** and the following **5 Python files** to TeachCenter: `neural_net.py`, `main.py`, `mlp_classifier_own.py`, `nn_classification_sklearn.py`, `nn_classification_from_scratch.py` Do not zip them. Do not upload any folders.
Plagiarism:	If detected, 0 points on the entire assignment sheet for all parties involved. If this happens twice, we will grade the group with "Ungültig aufgrund von Täuschung"
Course info:	TeachCenter, https://tc.tugraz.at/main/course/view.php?id=1648

Contents

General remarks

Your submission will be graded based on:

- Correctness (Is your code doing what it should be doing? Is your derivation correct?)
- The depth of your interpretations (Usually, only a couple of lines are needed.)
- The quality of your plots (Is everything clearly readable/interpretable? Are axes labeled? ...)
- Your submission must run with Python 3.11.5 and the package versions listed in `requirements.txt`. These are exactly the same as in Assignment 1, i.e., if you have already setup your environment, you can simply reuse it.

Since we run automated tests, it is crucial that you keep the following in mind:

- **Do not add any additional `import` statements** anywhere in the code.
- **Do not modify the function signatures** of the skeleton functions
  - i.e., do not edit the function names and inputs

1 Neural Networks [13 points]

In this task, we will use an implementation of Multilayer Perceptron (MLP) from `scikit-learn`. The documentation for this is available at the scikit-learn website. The relevant multi-layer perceptron class is `MLPClassifier`, as we will solve a classification task.

1.1 PCA and Classification [9 points]

PCA can be used as a data preprocessing technique, to reduce the dimensionality of data. In this task, we will use an *MRI Scan Dataset*. It consists of images of brains scans that should be classified into 4 different classes, as shown in Figure 5. The images are of size $(64, 64)$ pixels, i.e., the input dimension to the neural network that we want to train to classify the images would be quite large ($64 \cdot 64 = 4096$), and hence we want to reduce their dimension by means of PCA. By doing this, the benefit will be that the model will be smaller and thus, it will take less time to train the model.

Tasks:

1. **PCA for dimensionality reduction.** Use `PCA` from `sklearn.decomposition` to reduce the dimensionality of the training data `X_train`. Create an instance of `PCA` class, and set `random_state` to 42. Choose `n_components=128`, i.e., 128 principal components. In the report, state how much percent of the original data's variance is preserved by this projection.

2. **Varying the number of hidden neurons/layers.** We will use the data with the reduced dimension (from the previous step) to train a neural network to perform classification. We will vary the number of neurons and layers in the neural network:

   $$\texttt{hidden\_layer\_sizes} \in \mathcal{H} := \{(2,),(8,),(64,),(256,),(1024,),(128,256,128)\}$$

   For this task, we will use `MLPClassifier` from `sklearn.neural_network`. Create an instance of `MLPClassifier`. Set `max_iter` to 100, `solver` to `adam`, `random_state` to 1, `hidden_layer_sizes` to be $\in \mathcal{H}$ (a value in the set above), and the other parameters should have their default values.

   For each `hidden_layer_sizes` $\in \mathcal{H}$, report the accuracy on the train and validation set, and the final training loss.

3. In general: How do we know if a model does not have enough capacity (the case of underfitting)? How do we know if a model starts to overfit?

   In your particular case: Does overfitting/underfitting happen with some of your architectures/models? (If so, say with what number of neurons that happens). Which of the trained models would you prefer? Explain why.

4. **Overfitting.** To prevent overfitting, we could use a few approaches, for example, introducing regularization and/or early stopping. Copy the code from the previous task. Try out (a) $\alpha = 0.1$ (b) `early_stopping = True`, (c) $\alpha = 0.1$ and `early_stopping = True`. Choose (a), (b), or (c) - depending on what you think works best. State your choice in your report.

   Then, using a setup as in (a), (b), or (c), report the train and validation accuracy, and the loss for each `hidden_layer_sizes` $\in \mathcal{H}$. Does this improve the results from the previous step? Which model would you choose now?

5. From all models you have trained so far, pick the one you consider best. For this model, plot the loss curve (training loss over iterations). Hint: Check the attributes of the classifier.

1.2 Model selection and Evaluation Metrics [4 points]

To find a good configuration of hyperparameters, we can use, for example, `GridSearchCV`, by trying out all the different combinations of the parameters by an automated procedure.

Tasks:

1. We want to check all possible combinations of the parameters:
   - $\alpha \in \{0.0, 0.1, 1.0\}$
   - `batch_size` $\in \{32, 512\}$
   - `hidden_layer_sizes` $\in \{(128,), (256,)\}$

   Create a dictionary of these parameters that `GridSearchCV` from `sklearn.model_selection` requires. How many different architectures will be checked? (State the number of architectures that will be checked and how you calculated it.)

2. Set `max_iter=100, solver='adam', random_state=42` as default parameters of `MLPClassifier`. Create a `GridSearchCV` object with the dictionary you have created. Run cross validation with $k = 5$ folds by setting `cv=5`. If you want a more verbose output during the search procedure, set e.g. `verbose=4`.

3. What was the best parameter set that was found in this grid search? What was the best score obtained (i.e., the mean cross-validation score)? Hint: Check the attributes of the `GridSearchCV` object.

4. Implement `show_confusion_matrix_and_classification_report`. Among all models trained so far (also the ones you have constructed without the help of `GridSearchCV`), pick the model you consider best. Then, pass this final model to the implemented function (together with the PCA-projected test set). Report the final test accuracy in your report. Also include the plot of the confusion matrix and the classification report.

5. Explain in words what *recall* measures and what *precision* measures. Which class in the test dataset was misclassified most often?

6. (Theoretical question, general) What is the difference between hyperparameters and parameters of a model (in general)? Explain then the difference using the example of neural networks (i.e., name a few hyperparameters and parameters of neural networks).

2 Neural Networks From Scratch [13 points]

In this task, we will implement a neural network from scratch, i.e., without using `MLPClassifier` from `scikit-learn`. We will again solve the same classification task as above.

In order to train the network, we will use a minimal implementation of an *automatic differentiation* framework. This will allow us the compute gradients of the loss w.r.t. the weights and biases of the neural network, which in turn allows us to perform (stochastic) gradient descent.

The central component of this framework is the `Scalar` class in the `autodiff` module. An object of this class can store a single scalar value $x \in \mathbb{R}$ and, as soon as we compute derivatives of the loss $\mathcal{L}$, this object will also contain the partial derivative $\frac{\partial \mathcal{L}}{\partial x}$ at the point x (which is again just a scalar value). The `Scalar` class keeps track of a computational graph by overloading methods like `__add__` or `__mul__` (which are called when you add or multiply two Python objects, respectively). Thus, we need to implement all computations we wish to differentiate using `Scalar` objects (i.e., the neural network forward pass, including all activation functions, and the loss function).

For example, if we wish to add two Scalar objects `s1 = Scalar(1.0)` and `s2 = Scalar(2.0)`, we just compute `s = s1 + s2`, where `s` is again a `Scalar` object which holds the result of the computation, as well as the computational graph that produced this result.

Tasks:

1. In `autodiff/neural_net.py`, implement the `__call__` method of the `Neuron` class. This method should compute the output of a single neuron, given a list of inputs. Note that the inputs are given as a list of `Scalar` objects and you should again return a `Scalar` object.

2. In `autodiff/neural_net.py`, implement the `__init__` and `__call__` method of the `FeedForwardLayer` class.

3. In `autodiff/neural_net.py`, implement the `__init__` and `__call__` method of the `MultiLayerPerceptron` class.

4. In `mlp_classifier_own.py`, you can find an implementation of a multi-class[1] classifier that uses your implementation of the MultiLayerPerceptron class under the hood. Carefully read and understand the code in this file. Note that when the MLP in `self.model` performs a forward pass, we get the *logits* at the output layer, i.e., the values that still need to be fed into the output activation function. Implement the `softmax` method and the `multiclass_cross_entropy_loss` method.

5. In `nn_classification_from_scratch.py`, implement the `train_nn_own` function. In there, create an `MLPClassifierOwn` object: We want to train for 5 epochs, set the L2 regularization coefficient $\alpha = 0$, construct a network with a single hidden layer with 16 neurons and set `random_state=42`. As input to this small network we will use the PCA-projected *Brain Scan* dataset – however, this time, we will only use 16 principle components for the PCA projection (`n_components=16`). We take these measures to keep the network size small, as our implementation is highly inefficient (no parallelization/vectorization). Also, we standardize the PCA projected training data (this is already done for you). After training, use the `score` method of the classifier to compute the accuracy on the train, validation and test set. Report the final train, validation and test accuracy in your report.

6. Right now, we can only train our network without L2 regularization ($\alpha = 0$). Implement the `l2_regularization_term` method in `mlp_classifier_own.py`. The output of this method is added to the loss during training. Specifically, let $\Omega(\boldsymbol{\theta})$ denote the output of this method. Then we have

$$\Omega(\boldsymbol{\theta}) = \frac{\alpha}{2|\mathcal{B}|}\|\boldsymbol{\theta}\|_2^2$$

   where $\boldsymbol{\theta}$ is the vector of network parameters and $|\mathcal{B}|$ is the batch size.

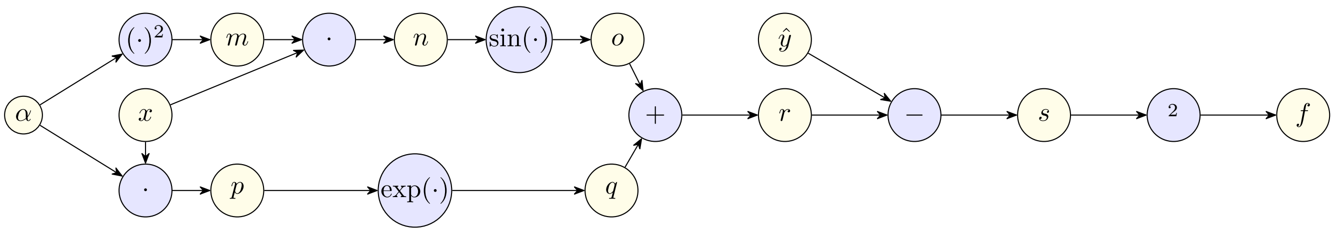
   Train the same network as before, but now set $\alpha > 0$. Pick two different values for α and see if you can observe any difference to the case where $\alpha = 0$. State which value of α you have tried. Do you think that L2 regularization is useful in this case?

[1] We will extend this to also work with binary classification in Task 3, so you can ignore any code that is run when `self.num_classes == 2` for now.

7. Answer the following questions in your report:

   (a) Compute the partial derivative of f with respect to α (i.e., $\frac{\partial f}{\partial \alpha}$) using backpropagation (i.e., the chain rule of calculus, starting from the right of the computational graph). Write down all steps in your report. Your solution should include *all* partial derviatives $\frac{\partial f}{\partial z}$ for all variable nodes z in the graph. Hint: Start from the very right and compute $\frac{\partial f}{\partial f}$. Then, compute $\frac{\partial f}{\partial s}$, after which you can use this result to compute $\frac{\partial f}{\partial r}$ and $\frac{\partial f}{\partial \hat{y}}$ using the chain rule. Repeat this until you arrive at an expression for $\frac{\partial f}{\partial \alpha}$.

$$f(\alpha) = \left(\hat{y} - \left(\sin(x\alpha^2) + \exp(x\alpha)\right)\right)^2$$



   (b) Why do we require the activation function in the hidden layers of a neural network to be nonlinear? What would happen if all activation functions in the hidden layers were linear?

   (c) What problem may arise when we increase the number of layers in a neural network?

   (d) What effect does L2 regularization have on the parameters of the trained network?

3 Binary Classification [4 points]

In this bonus task, we wish to extend `MLPClassifierOwn` to not only support multi-class classification, but also *binary classification* (i.e., `num_classes == 2`).

Tasks:

1. In `mlp_classifier_own.py`, implement the methods `sigmoid` and `binary_cross_entropy_loss`.

2. The code skeleton will create a binary classification dataset by slicing out the subset of the *Brain Scan* dataset where the label is 0 or 1 (neglecting all other classes). In `nn_classification_from_scratch.py`, use the `train_nn_own` function from the previous task to train the model on this subset of data. After training, use the `score` method of the classifier to compute the accuracy on the train and test set. Report the final train, validation and test accuracy in your report.

3. (Theory Question) Your friend comes to you and says: "I have changed the labels in the *Brain Scan* dataset in the following way: I leave every image with class 0 untouched, but I change the label of every image with a class id $\in \{1, 2, 3\}$ to class 1. Using this new dataset with binary labels, I have trained a binary classifier, which achieves a test accuracy of $\approx 75\%$. That's great, don't you think?" Is accuracy a misleading metric in this case? Explain why/why not. If you think that it is misleading, explain which performance metric is more useful in this case.

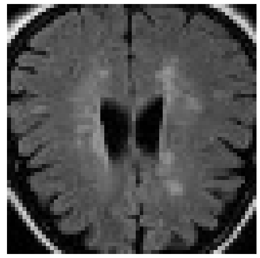


Figure 1: No tumor

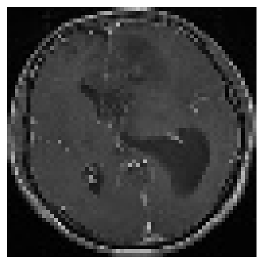


Figure 2: Glioma

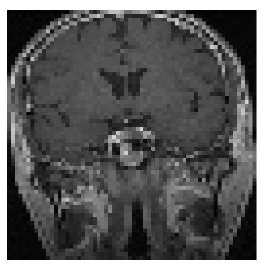


Figure 3: Pituitary

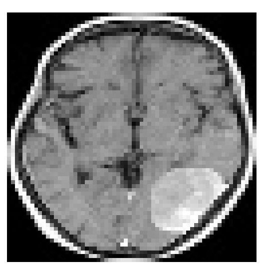


Figure 4: Meningioma

Figure 5: Example image for each class of the *Brain Scan* dataset.