# CITS5508 Machine Learning
## Semester 1, 2024

## Assignment 1

Assessed, worth 15%. Due: 8pm, Friday 12$^{\text{th}}$ April 2024

Discussion is encouraged, but all work must be done and submitted individually. This assignment has several assessed tasks, which are total 92 marks.

## 1 Outline

In this assignment, you will develop Python code for classification tasks using logistic regression and $k$-NN classifiers. You will use Grid Search and cross-validation to find the optimal hyperparameters of the model (e.g., the regularisation hyperparameter) and discuss and interpret the different decisions and their impact on the mod [illegible]

## 2 Submission

Your submission consis [illegible] ysis/approach. Your analysis should provide [illegible] reflections about the results. Each deliverab [illegible] For instance, **D1 [3 marks]** is the first deliv [illegible]

The second file is your [illegible] alysis. It will follow the rules provided in LM [illegible]

Your report should be [illegible] `tudent_id>.pdf` (where you should repla [illegible] LMS before the due date and time. You can [illegible] vill be marked. Accordingly, your code sh [illegible] he Jupyter notebook extension.

**Important:**

- You must submit the first part of your assignment as an electronic file and use a PDF format (do not send DOCX or any other file format). Only PDF format is accepted. Any other file format will get a zero mark.
- You must deliver part one and part two to have your assignment assessed. That is, your submission should contain your analysis and your Jupyter notebook with all coding, both with appropriate formatting.
- By submitting your assignment, you acknowledge you have read all instructions provided in this document and in LMS.
- There is a section in your LMS, Assignments - Assignment 1 - Updates, where you will find updates or clarifications about the tasks when necessary. It is your responsibility to check this page regularly.

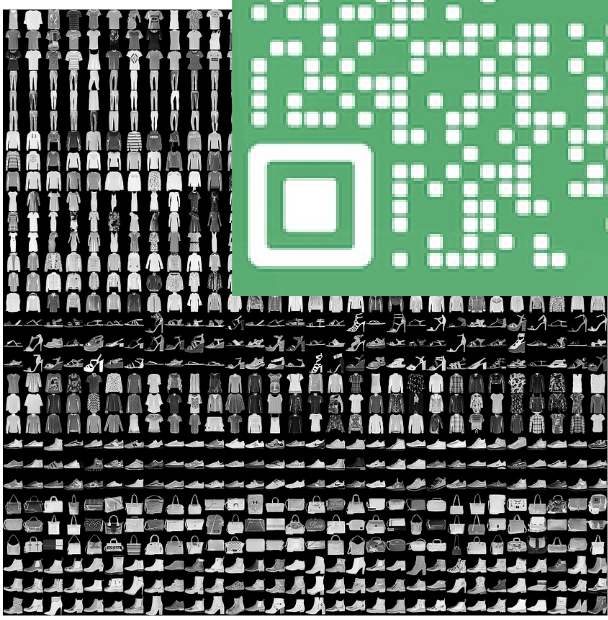
- You will be assessed on your thinking and process, not only on your results. A perfect performance without demonstrating understanding what you have done won't provide you marks.
- Your answer must be concise. Two to three sentences should be enough to answer most of the open questions. If you are writing long answers, rethink what you are doing. Probably, it is the wrong path.
- You can ask in the lab or during consultation if you need any clarification about the assignment questions.
- You should be aware that some algorithms can take a while to run. A good approach to improving their speed in Python is to use the vectorised forms discussed in class. In this case, it is strongly recommended that you start your assignment soon to accommodate the computational time.
- For the functions and tasks that require a random procedure (e.g. splitting the data into 80% training and 20% validation set), you should set the seed of the random generator to the value "5508".

## 3 Dataset

Fashion-MNIST is a [...] classify handwritten digits. It contains exa[...]ers, pullovers, etc.). Fashion-MNIST has [...]000 examples. Each example is a 28 x 28 lo[...] MNIST) associated with a label from one o[...]

References and informa[...]

An example of how the [...]hree rows):



| | |
|---|---|
| 7 | Sneaker |
| 8 | Bag |
| 9 | Ankle boot |

In LMS, you will find four predefined datasets to support your tasks in this assignment:

- FMNIST_training_set.csv: Training set with 60,000 examples of the cloth items.

- FMNIST_training_set_labels.csv: Labels associated to each example in FMNIST_training_set.csv.
- FMNIST_test_set.csv: Testing set with 10,000 examples of cloth items.
- FMNIST_test_set_labels.csv: Labels associated to each example in FMNIST_test_set.csv.

Each input image in the files FMNIST_training_set.csv and FMNIST_test_set_classes.csv: follows the same representation as in the MNIST dataset; that is, each example is a 28 x 28 gray-scale image reshaped into a 784-dimensional vector. Each input image has a label associated with it, given by the files FMNIST_test_set_labels.csv (training set labels) and FMNIST_test_set_labels.csv (test set labels). Each pixel's feature value can assume values in the range of 0.0 (black) and 1.0 (white). Feature values in between this range represent the possible variation in grey. Therefore, each example $i$ has features $\mathbf{x_i} \in \mathbb{R}^{784}$ and target feature (label) $y_i \in \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$. The parametric space has *bias* and *weights*, which is in dimension 785.

## 4 Problem: Classifying `Sneakers` versus `Sandals`

We will start with a bi… this problem, your challenge is to build a l… sh `Sneakers` from `Sandals`, and you wil… a logistic regression classifier and interpret t…

### 4.1 Summarising t…

From the files provided … e to separate images from "sneakers" and "s… kers" and "sandals" only, from FMNIST_tra… each $y_i$ should be 0 (zero) for "sneakers" a… ould create a test set containing "sneakers" a… test set labels where each $y_i \in \{0, 1\}$.

You should not reorder, … lata, but the original characteristics and data …

Below are the first five … dals" and "sneakers" and relabelling). You w…

| label | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 53 | 102 | 144 | 169 | 149 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

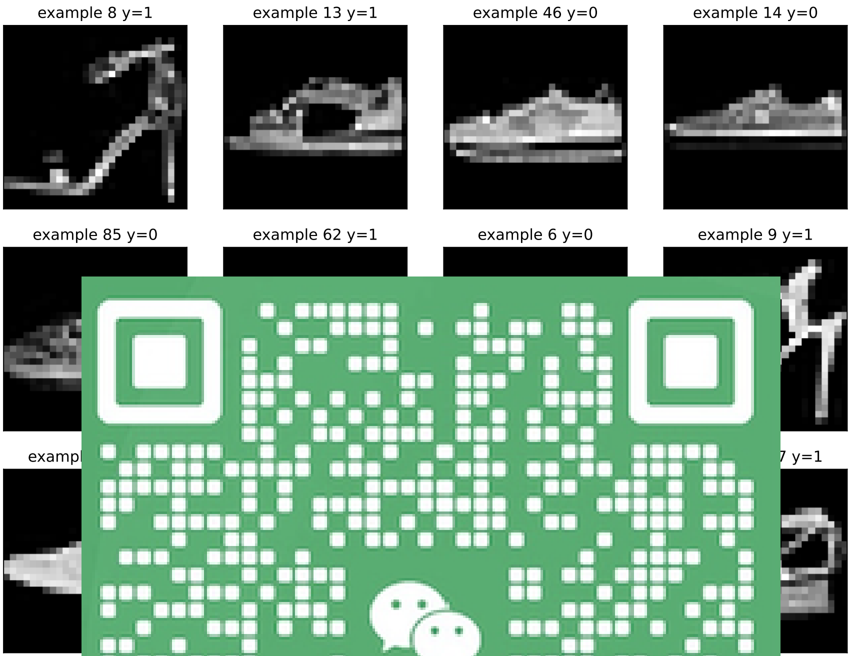
These are rows 12, 30, 36, 41, and 43 from the original training data set (remember that Python starts to count on zero). After you have built the training data, you will also need to build the test data accordingly.

**D1 [3 marks]**: In a table, describe:

- The number of instances in the training set;
- The number of instances in the test set;
- The total number of instances.

**D2 [2 marks]**: Provide a bar plot showing the number of instances for each class label. Do you have an imbalanced training set?

**D3 [3 marks]**: Plot the first six images/examples from each class with the corresponding *example id* and associated label on the top of the plot. Use Python function `imshow()` (you may need to adjust some values for the arguments in the function `imshow()` to better visualise the resulting image). Hint: use a 3 x 4 grid. In the example below, we attributed class '1' to the `sandals` and class '0' to the `sneakers`.




## 4.2 Fitting your log...

In this part, you will ch... ...tion algorithm to fit the training data. You w... ...Gradient Descent.

Split your training data (that you constructed on "summarising the datasets") into two sets: training and validation. Select randomly 80% for training and 20% for validation. You must set the random generator seed to "5508" before the splitting. Ensure your validation set is fixed and does not change each time you run your algorithm.

Your implementation should initialise $\eta$ (the learning rate) and $\theta$ (the parameter vector). Then, in each iteration, the main steps will look like:

```
gradients = ... # calculate the gradient vector using all instances
theta = ... # update the parameter vector
est_p = ... # compute the estimated probability for each instance
lr_cost_function = ... # calculate the logistic regression cost function
```

The probability $\hat{p}$ estimated by the logistic regression model is given by:

$$\hat{p} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \sigma(\boldsymbol{\theta}^\top \mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^\top \mathbf{x})}$$

We calculate the logistic regression cost function as follows:

$$J(\boldsymbol{\theta}) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(\hat{p}^{(i)}) + (1-y^{(i)})\log(1-\hat{p}^{(i)})\right]$$

Run your algorithm for 10000 iterations and provide the following results and plots.

**D4 [3 marks]**: Experiment with some values for $\eta$, the learning rate of the gradient descent. Provide plots to support your decision for the final value and justify your choice.

**D5 [10 marks]**: Set $\eta = 10^{-5}$. Provide two (by-side) plots:

- In the left plot, show the values of the cost function (y-axis) for each iteration (x-axis) for the training and validation sets. That is, your plot should contain two results.
- In the right plot, show the fraction of misclassifications (y-axis) for each iteration (x-axis) using the logistic regression model prediction for a threshold of 0.5. Similarly, you should provide two results (one for the training and one for the validation set).

**D6 [3 marks]**: Give a s … s?

### 4.3 Using cross-val … .

You will incorporate a … an optimal value for the regularisation hyper… raining set using the fixed validation set. Yo… lore penalty strength values in the range give… generate 30 numbers spaced evenly on a log …

```
C_range = np.log…

for C in C_grid:
# Train your mod…
# Compute the co…
# Compute the co…
```

**D7 [6 marks]**: Provide …

- In the left plot, show the values of the cost function (y-axis) for each $C$ value (x-axis) for the training and validation sets. That is, your plot should contain two results.
- In the right plot, show the fraction of misclassifications (y-axis) for each $C$ value (x-axis) using the logistic regression model prediction for a threshold of 0.5. Similarly, you should provide two results (one for the training and one for the validation set).

For the next task, you will use `sklearn.linear_model.LogisticRegressionCV`, using 10-fold cross-validation and specifying the same range for the regularisation hyperparameter as before. Similarly, you will use this function to explore penalty strengths, but now using cross-validation.

**D8 [4 marks]**: Provide two (by-side) plots:

- In the left plot, show the values of the cost function (y-axis) for each $C$ value (x-axis). Note that you will have ten values for each $C$ value (10 folds). Therefore, you should report the average value.

- In the right plot, show the fraction of misclassifications (y-axis) for each $C$ value (x-axis) using the logistic regression model prediction for a threshold of 0.5.

**D9 [3 marks]**: Give a short interpretation of your results. Which regularisation hyperparameter value would you select and why? What was the impacting of using 10-fold cross-validation instead of a fixed validation set?

Now you will use `sklearn.linear_model.SDGClassifier` together with `sklearn.model_selection.GridSearchCV` to find the optimal regularisation parameter according to Grid Search. `sklearn.linear_model.SDGClassifier` implements logistic regression "log loss". Remember to choose the correct strategy to evaluate the performance of the cross-validated model in the `scoring` argument of the function. (Hint: be careful how `scikit-learn` defines the Grid Search).

**D10 [5 marks]**: In a tab

- The optimal valu ... Search;
- The value of the
- The value of the
- The fraction of m
- The fraction of th

**D11 [3 marks]**: Give a ... h what you obtained in task **D8**?

Select the model you ju ... `fier` together with `sklearn.model_se` ... ue of the regularisation hyperparameter $C$ ...

**D12 [5 marks]**: With t ... dict the examples in the validation set, plot precision versus recall for different threshold values and comment on the results. How does the performance measure behave? What threshold would you choose and why?

**D13 [4 marks]**: Use a grid search (you may need to implement your own) to fine-tune the optimal threshold value using the validation set, fixing the regularisation hyperparameter $C$ as the optimal value obtained in **D10**. What value did you get? Comment comparing with your reflection in D12.

### 4.4 Analysing the performance closer

So far, we have four logistic regression models:

- LR1: The model in 4.2, which is your implementation of the logistic regression without regularisation and with a fixed validation set;

- LR2: The model in 4.3, which is your implementation of the logistic regression with regularisation and with a fixed validation set;
- LR3: The the model in 4.3 using 10-fold cross-validation and the optimal value of the regularisation hyperparameter $C$ according to Grid Search but keeping the threshold value for the logistic regression prediction model at 0.5;
- LR4: The model in 4.3 using 10-fold cross-validation and the optimal value of the regularisation hyperparameter $C$ according to Grid Search **and** threshold values according to your grid search in **D13**.

We will give a closer investigation into the classification mistakes.

**D14 [8 marks]**: Provide the model's performance on the test set. For each LR1, LR2, LR3 and LR4, provide:

- The confusion matrix;
- Precision, recall,

**D15 [3 marks]**: Briefly … capacity of the four models.

**D16 [4 marks]**: Consid… es on the test set and five images that are fals…

**D17 [2 marks]**: Briefly … istakes the model is making?

**D18 [2 marks]**: Let's … s estimated weights (parameters). Again, c… used for each image by reshaping them into … Plot the result using `imshow()`. You may … `imshow()` to better visualise the resulting i…

**D19 [3 marks]**: Inspec… what you think LR4 learned when distinguis…

## 4.5 Comparing models

Use the $k$-nearest neighbours ($k$-NN) algorithm with the Euclidean distance for the same binary classification task. Try $k$ values in the range $[1, 30]$.

**D20 [3 marks]**: Provide a plot showing the fraction of misclassifications (y-axis) for each $k$ value (x-axis) for the training and validation set. Use the same validation set you created in section 4.2. That is, your plot should contain two results.

**D21 [4 marks]**: Comment on the results. What did you observe as the value of $k$ increases? Which value of $k$ would you choose and why? How does this model compare with the one you created in section 4.2?

**D22 [2 marks]**: Provide the $k$-NN performance on the test set for the $k$ value you decided in task **D21**, providing:

- The confusion matrix;
- Precision, recall, false positive rate.

**D23 [2 marks]**: Compare these performances with the logistic regression models (LR1, LR2, LR3 and LR4) obtained on deliverable **D14**. Briefly comment on the results you see, discussing the generalisation capacity of the different models.

### 4.6 Exploring the ML pipeline

This last part of the assignment is open-ended and will assess your reflections on the machine learning pipeline. You are not restricted to the images' 784-pixel values (features). Here, the idea is to think about different strategies you can use to improve the model's performance.

We can investigate the relevant pixels for our binary classification, `sandals` and `sneakers`, and think of other information about them we could use in the classification.

**D24 [5 marks]**: Comm