CSE 676-B: Deep Learning, Spring 2025

Instructor: Alina Vereshchaka

Assignment 0

PyTorch Intro, Data analysis & NN Models

Checkpoint: February 6, Thu, 11:59pm
Due date: February 13, Thu 11:59pm

Our initial assignment is focused on reviewing PyTorch, data analysis techniques, basic machine learning methods and building shallow NN. This assignment also focuses on theoretical and practical skills relating to neural networks. It consists of four parts where you derive and analyze the setup, practice dealing with various datasets and implement, train, and adjust neural network. It is expected that all coding parts of the assignment will be completed using PyTorch.

Note: You can partially reuse related implementations that you have completed for other courses with a proper citation, e.g. “Part I is based on the CSE 574 Machine Learning Assignment 1 submission by My Full Name and My Teammate Full Name”

Part I: PyTorch Intro [10 points]

1. Complete an official Pytorch tutorial “Introduction to PyTorch - YouTube Series”

   https://pytorch.org/tutorials/beginner/introyt/introyt_index.html

   Complete the following parts:

   a. Introduction to PyTorch
   b. Introduction to PyTorch Tensors
   c. The Fundamentals of Autograd
   d. Building Models with PyTorch
   e. PyTorch TensorBoard Support
   f. Training with PyTorch
      [Optional] Model Understanding with Captum & Production Inference Deployment with PyTorch

2. Use your own example values and hyperparameters, where applicable, while following the tutorial examples.

Submission Note:

- Submit Jupyter Notebook with all the saved outputs. You can combine the results into one Jupyter notebook file. There is no need to include theoretical materials. Code with your values and clear section naming is sufficient
- There is no report associated with this part.

Part II: Data analysis, ML & NN models [30 points]

Step 1: Data analysis & Pre-processing [10 points]

1. Select a real-world dataset from the source listed below. Requirements for the dataset:
   - Represent the real-world data
   - Contain at least 20k entries
   - It should be different from the one used previously for our or other courses

   The dataset should come from one of these resources:
   - Open Data Buffalo: https://data.buffalony.gov/
   - US Government's Data: https://www.data.gov/
   - Yahoo Finance: https://finance.yahoo.com/
   - Yahoo Webscope: https://webscope.sandbox.yahoo.com/
2. Read, preprocess, and print the main statistics about the dataset.
3. [If applicable] Handle missing entries. Possible solutions:
   - Drop rows with missing entries. If you have a large dataset and only a few missing features, it may be acceptable to drop the rows containing missing values.
   - Impute missing data. Replace the missing entries with the mean/median/mode of the feature. You can use the k-nearest neighbor algorithm to find the matching sample.
4. [If applicable] Handle mismatched string formats.
5. [If applicable] Handle outliers. Detect and manage outliers within the dataset. Possible solutions:
   - Remove outliers. If there are just a few outliers, you may eliminate the rows containing these outliers.
   - Impute outliers. Replace the outliers with the mean/median/mode of the feature.
6. Using any data visualization library (e.g. matplotlib, seaborn, plotly), provide at least 5 visualization graphs related to your dataset. You can utilize any columns or a combination of columns in your dataset to generate graphs. E.g. correlation matrix, features vs. the target, counts of categorical features vs. the target.
7. Identify uncorrelated or unrelated features.

   To compute the correlation matrix, load your dataset using Pandas and use the pandas.DataFrame.corr method. You can refer to the documentation here:

   https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.corr.html

   You can drop some features based on their correlation with the target.
8. Convert features with string datatype to categorical**.** Possible ways:
   - One-hot encoding, creating binary columns for each category, denoting their

presence or absence.

- Label encoding assigns unique integers to distinct feature values, useful for ordinal relationships among categories. E.g., "Small" as 0, "Medium" as 1, and "Large" as 2 can represent a "Size" feature. However, it may introduce unintended patterns.

9. [If applicable] Normalize non-categorical features.
    a. Find the min and max values for each column.
    b. Rescale dataset columns to the range from 0 to 1

    Why do we do this? Normalization is to transform features to be on a similar scale. This improves the performance and training stability of the model.

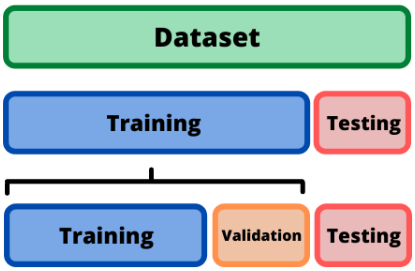
    Note: normalize() is not allowed as it is a part of *scikit-learn* **library.**

10. Choose your target Y and features $\boldsymbol{X}$

11. Split the dataset into training, testing and validation sets.

    You can use train_test_split from scikit-learn

    Hint: first you can split the dataset into 'training' and 'testing' batches. Then take the 'training' batch and split it again for 'training' and 'validation'



Why do we need to split into training, testing and validation?

- Training set: used to train the model to learn the patterns or features in the data. It is important to have a large and representative training set so that the model can learn well.
- Validation set: used to tune the model hyperparameters and to prevent overfitting. Overfitting is when the model learns the training data too well and cannot generalize to new data. Hyperparameters are parameters that are not learned from the data, but are set by the user. By tuning the hyperparameters, we can improve the model's performance on the validation set.
- Test set: used to evaluate the final model's performance on unseen data. This gives us a good idea of how well the model will perform in the real world.

The commonly used splits of 70:15:15 or 80:10:10 are good starting points, but the optimal split ratio will vary depending on the size and characteristics of the dataset.

12. Print the shape of your X_train, y_train, X_test, y_test, X_validation, y_validation

Step 2: ML Models [10 points]

1. Apply ML algorithms (min 3 different algorithms) to model the target variable. This can be either a classification or regression task. Note:
    - You can use any libraries with in-built ML functions (e.g. scikit-learn)
    - The accuracy for all models submitted should be above 65%.
2. Provide a comparison of the results of different ML models you have used:
    a. Provide the loss value and accuracy for each of the 3 methods.
    b. Include plots that compare the predictions versus the actual test data for all methods used. You can consider metrics such as accuracy, time, and loss to compare the methods.

Step 3: NN Model [10 points]

1. Apply NN model to solve this task. You may reuse the NN you defined in Part I as part of the tutorial and make any necessary modifications to the setup. The accuracy for NN model submitted should be above 75%.
2. Provide a comparison of the results of the NN model and the different ML models you used:
    a. Provide your loss value and accuracy of the NN model.
    b. Include plots that compare the predictions versus the actual test data for the NN model and all the ML models used. Consider metrics such as accuracy, time, and loss to compare the methods.

In your report for Part II:

1. Provide brief details about the nature of your dataset. What is it about? What type of data are we encountering? Provide the main statistics about the entries of the dataset (mean, std, number of missing values, etc.)
2. What kind of preprocessing techniques have you applied to this dataset?
3. Provide at least 5 visualization graphs with a brief description for each graph, e.g. discuss if there are any interesting patterns or correlations.
4. Provide brief details and mathematical representation of the ML methods you have used. What are the key features? What are the advantages/disadvantages?
5. Provide brief details of the NN model you have used.
6. Provide your loss value and accuracy for all 4 methods (3 ML models & 1 NN).

7. Show the plot comparing the predictions vs the actual test data for all methods used. Analyze the results. You can consider accuracy/time/loss as some of the metrics to compare the methods.

Checkpoint submission (Part I & Part II):

1. Report

   Submit as a PDF file: a0_report_ YOUR_UBIT.pdf
   E.g. a0_report_ avereshc.pdf

2. Code

   Submit Jupyter Notebook files with saved outputs. You can submit the files separately for Part I and II or combine them into one notebook.

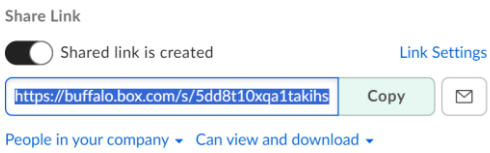
   - a0_part_1_YOUR_UBIT.ipynb
   - a0_part_2_ YOUR_UBIT.ipynb
     e.g., a0_ part_1_ avereshc.ipynb

     Or a0_part_1_2_ avereshc.ipynb

3. Saved Weights:

   - Go to UBbox > New > Folder > CSE 676-B Assignment 0 by YOUR NAME
   - Upload your saved weights to this folder. Include the model weights that generate the best results for your model for Part I and Part II, named as a0_part#_ YOUR_UBIT.pt

     e.g. a0_ part_2_ avereshc.pt
   - Copy a shared link to the UBbox folder, so it can be viewed by people in your company & it can be viewed and downloaded.

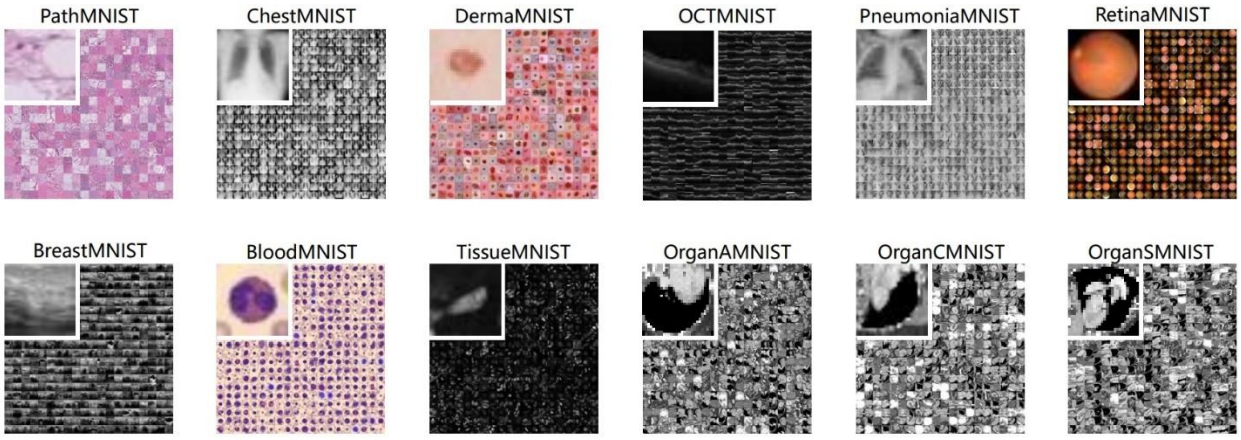
   - Add the link to the txt file, named as a0_weights_ YOUR_UBIT.txt
   - Submit this txt file as part of your submission on UBlearns

4. Dataset should NOT be submitted. Don't include as part of the submission
5. Combine all files in a single zip folder that will be submitted on UBlearns, named as assignmen0_checkpoint_YOUR_UBIT.zip

Part III: OCTMNIST Classification [40 points]

For this part, we will be working with a real-world dataset - OCTMNIST.

OCTMNIST



The OCTMNIST is based on a prior dataset of 109,309 valid optical coherence tomography (OCT) images for retinal diseases. Each example is a 28x28 image, associated with a label from 4 classes.

Getting the data:

- MedMNIST is a collection of multiple datasets, for this assignment we will be working with one dataset from the collection – OCTMNIST
- pip install medmnist

References:

- https://medmnist.com/
- https://github.com/MedMNIST/MedMNIST
- Direct download - https://zenodo.org/record/6496656

Step 1: Loading the dataset and preparing for training

1. Load OCTMNIST 2D dataset
2. Analyze the dataset, e.g., return the main statistics.
3. Provide at least 3 visualization graphs with a short description
4. Preprocess the dataset. E.g. normalizing the pixel values to a standardized range, typically between 0 and 1.
    a. [If needed] Address class imbalance in the target column. Possible solutions: oversampling; undersampling; data augmentation techniques for the minority

class; assign higher weights to the minority class and lower weights to the majority class, etc.

b. [If needed] Convert categorical variables to numerical variables using one-hot encoding. You can use OneHotEncoder from scikit-learn

5. Split the dataset into training, testing and validation sets.

   You can use train_test_split from scikit-learn

   Note: you are welcome to reuse your code for data preprocessing from Part II of this assignment with a proper citation, e.g. "Code is based on Part II of this assignment"

Step 2: Defining the Neural Network

1. Decide your NN architecture. Design a model architecture that consists of at least three layers, including convolutional layers and fully connected layers. You can build an FC NN or CNN model.
   - How many input neurons are there?
   - How many output neurons are there?
   - What activation function is used for the hidden layers?
     - Suggestion: try ReLU, ELU, Sigmoid, click here for the full list
   - What activation function is used for the output layer?
   - What is the number of hidden layers?
     - Suggestion: start with a small network, e.g., 2 or 3 hidden layers
   - What is the size of each hidden layer?
     - Suggestion: try 64 or 128 nodes for each layer
   - Do you include Dropout? (details)
3. Define your NN architecture using PyTorch (basic building blocks in PyTorch).
4. Return the summary of your model. You can use Torchinfo package

Step 3: Training the Neural Network

1. Define a loss function (loss_function) that will be used to compute the error between the predicted output and the true labels of the training data. List of loss functions (PyTorch). For binary classification problems, a commonly used loss function is Binary Cross Entropy Loss (Details).
2. Choose an optimizer and a learning rate. It will update the weights of the NN during training. SGD is one of the commonly used, you can also explore other optimizers like Adam or RMSProp.
   Check a list of optimizers (PyTorch)
3. Set up the training loop:
   a. Create a loop that iterates over the training data for a specified number of epochs.
   b. Iterate over the training data in batches.

c. Forward pass: pass the input data through the neural network.

```
outputs = model(inputs)
```

d. Compute loss: calculate the loss using the defined loss function.

```
loss = loss_function(outputs, labels)
```

e. Backpropagation: zero the gradients, compute gradients, and perform backpropagation.

```
optimizer.zero_grad()    #Clear gradients
loss.backward()          #Backpropagation
```

f. Update the model's weights using the optimizer.

```
optimizer.step()         #Update weights
```

g. Validation phase: set the model to evaluation mode.

```
model.eval()             #Set to evaluation mode
```

During the validation phase, there will be no backward propagation to calculate the gradients and no optimizer step to update the steps.

```
with torch.no_grad(): # Disable gradients
      for val_inputs, val_labels in val_loader:
            val_outputs = model(val_inputs)
            val_loss = loss_function(val_outputs, val_labels)
```

4. Train the neural network. Run the training loop and train the neural network on the training data. Select the number of epochs and batch size. Monitor the training loss and the validation loss at each epoch to ensure that the model is not overfitting. Estimate the time it takes to train the model, e.g. using time.time().
5. Save the weights of the trained neural network that returns the best results. Saving and loading models in PyTorch
6. Evaluate the performance of the model on the testing data. Suggested metrics:
   - Accuracy (PyTorch functions)
   - Precision, recall and F1 score (more details). You can use sklearn.metrics.precision_recall_fscore_support
   - In case you need to convert the output of sigmoid() to 0 or 1, you can use torch.round() function

   Note: The expected accuracy on the testing dataset for this task is > 75%.
7. Visualize the results. Include the following graphs:
   a. A graph that compares training, validation and test accuracy on the same plot with clear labeling.
   b. A graph that compares training, validation and test loss on the same plot with a clear labeling.

Note: your test accuracy and loss are obtained during the prediction phase and it is a single value. To plot it on the same graph, you can repeat this value for the same number of epochs as training, to get a straight line and plot all of them in the same graph.

c. Confusion matrices on the test data (seaborn.heatmap() or PyTorch)

d. ROC curve (receiver operating characteristic curve).
   - Details about ROC
   - PyTorch ROC function

8. Further improve your model. Select a different loss function from your initial choice and use it to train your model. Compare the model's performance for each loss function and visualize the results. Include the following graphs:
   a. A graph that compares training, validation and test accuracy on the same plot with clear labeling.
   b. A graph that compares training, validation and test loss on the same plot with a clear labeling.
9. There are a few methods which can help increase the training speed, accuracy, etc. Find and try at least four different methods (e.g. earlystopping, k-fold, learning rate scheduler, batch normalization, data augmentation, gradient accumulation, more details on performance tuning)
   a. Choose a method that can improve the performance of the model. Add it to your 'base model, finalized in Step 5.
   b. Train the model with a new method. Provide a graph that compares test accuracy for a 'base' model and an improved version. You can also provide a comparison w.r.t training time and other parameters.
   c. Go to Step 8a. Try four various methods or tools that aim to improve the performance of your model.
   d. After you explore various methods, finalize your NN model that returns the best results, named as 'best model'.

   Note: The expected accuracy on the testing dataset for improved NN is > 80%.
10. For your 'best model' defined in Step 9:
    a. Save the weights of the trained neural network
    b. Evaluate the performance of the model on the testing data
    c. Visualize the results

Note:

- You can use any inbuilt functions or define some functions from scratch.
- All libraries are allowed, except those with pre-trained models or predefined architectures. Submissions with pre-trained models or predefined architectures will not be considered.

In your report for Part III:

1. Provide a brief overview of your dataset (e.g. type of data, number of samples, and features. Include key statistics (e.g. mean, standard deviation, number of missing values for each feature).
2. Include at least 3 graphs, such as histograms, scatter plots, or correlation matrices. Briefly describe the insights gained from these visualizations.
3. Describe the NN you have defined.
4. Describe how one or more of the techniques (regularization, dropout, early stopping) you applied have impacted the model's performance.
5. Discuss the results and provide relevant graphs:
    a. Report training accuracy, training loss, validation accuracy, validation loss, testing accuracy, and testing loss.
    b. Plot the training and validation accuracy over time (epochs).
    c. Plot the training and validation loss over time (epochs).
    d. Generate a confusion matrix using the model's predictions on the test set.
    e. Report any other evaluation metrics used to analyze the model's performance on the test set.
6. Discuss all the methods you used that help to improve the accuracy or the training time (Step 9).
7. Provide a detailed description of your 'best model' that returns the best results. Discuss the performance and add visualization graphs with your analysis.

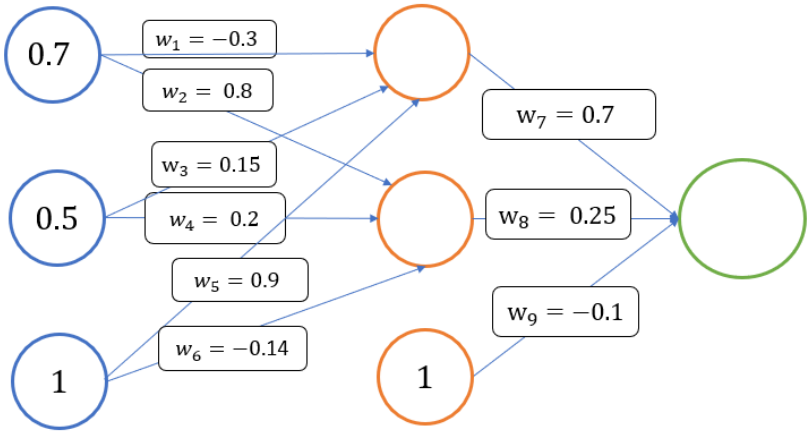
Part IV: Deep Learning Theoretical Part [20 points]

1. Forward-backward Pass [15 points]

Consider the following neural network with initialized weights.

Given the following setup:

- Hidden layer activation function: ReLU
- Output layer activation function: Linear
- Learning rate: 0.03
- Target (y): 0.5



TASK:

1. Perform a forward pass and estimate the predicted output ($\hat{y}$)
2. Estimate the MSE
3. Find the gradient using back-propagation
4. Update the weights
5. Draw a computation graph for the forward and backward pass
6. Perform a forward pass to estimate the predicted output using the updated weights.
7. Estimate the MSE and compare the results with Step 2.

2. Derivative of Tanh [5 points]

The hyperbolic tangent (tanh) activation function has the following form:

$$f(x) = \tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$$

TASK:

Prove that the derivative of Tanh has the following form:

$$f'(x) = 1 - f(x)^2$$

In your report for Part IV:

1. For this part you need to submit only the report with your solutions. You can use docx, LaTex, or hand-written and scanned format. Convert the result to .pdf
2. Include the solution for both tasks as part of your final report.

Bonus points [max 10 points]

1. Improve Buffalo using NN [5 points]

Generate a use-case scenario that uses NN can help to improve Buffalo. For example, you might develop a model that accurately predicts crime in a given region or recommend the optimal location for a new car-repair shop based on car traffic data.

Requirements:

1. Define the use-case scenario. Explain how it can benefit the city or its residents or the business.
2. Select a dataset or combine multiple datasets relevant to your use-case scenario. At least one dataset should come from Open Data Buffalo: https://data.buffalony.gov/
3. Preprocess the datasets and prepare them for training.
4. Desing and train the NN. You are welcome to reuse your structure from Part III.

Note: Accepted accuracy is above 75%.

5. Evaluate the performance and analyze your results, follow guidelines from Part III.

Submission:

- Create a separate folder named as Your_UBIT_assignment0_bonus1 e.g., avereshc_ assignment0_bonus1
- You can duplicate code from your Part 3 if needed
- Include all the files needed in the folder

In your report for Bonus Task 1:

1. Provide details of the Buffalo-related case scenario and how it can benefit the city or a local business
2. Provide a brief overview of your dataset (e.g. type of data, number of samples, and features. Include key statistics (e.g. mean, standard deviation, number of missing values for each feature).
3. Include at least 3 graphs, such as histograms, scatter plots, or correlation matrices. Briefly describe the insights gained from these visualizations.
4. Describe the NN you have defined.
5. Discuss the results and provide relevant graphs
6. Summarize your findings in a business context. Explain how your NN prediction can be applied to make data-driven decisions that benefit Buffalo or its local businesses. Make a concise summary that business owners can easily understand and use.

2. Deploy the model [5 points]

Deploy a model you defined in Part III on the server using any tools/methods.

Hint: You can refer to demo tutorials on “Deploying deep learning models” in our Code Demos folder

Submission:

- Create a separate folder named as Your_UBIT _assignment0_bonus2 e.g., avereshc_ assignment0_bonus2
- You can duplicate code from your Part 3 if needed
- Include all the files needed in the folder
- You can deploy locally or directly on the server
- Make a 3-4 mins video recording showing how it works
- Share the publicly available recording link.

In your report for Bonus Task 2:

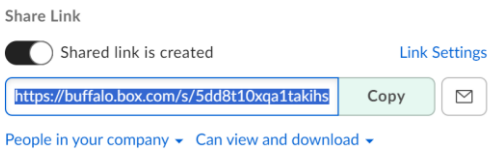
- Include a link to your recording
- Report is not required, you can include all the analysis as part of your .ipynb file

Final submission (all parts)

Please reupload your work for Part I & Part II and include your completed work for Part III & Part IV along with the final report. Follow these guidelines for submitting your assignment:

1. Report (PDF File):
    - Combine the reports for all parts (Part II, Part III, and Part IV + Bonus [optional]) into a single PDF file. Name as
      a0_report_ YOUR_UBIT.pdf
      e.g., a0_report_ avereshc.pdf
2. Code (Jupyter Notebooks with saved outputs).
    - Part I: Save as a separate Jupyter Notebook file, named as
      a0_part_1_ YOUR_UBIT.ipynb
      e.g., a0_part_1_ avereshc.ipynb
    - Part II: Save as a separate Jupyter Notebook file, named as
      a0_part_2_ YOUR_UBIT.ipynb
    - Part III: Save as a separate Jupyter Notebook file, named as
      a0_part_3_ YOUR_UBIT.ipynb
3. Saved Weights:
    - Reuse the same UBbox folder that you created during the Checkpoint, if you haven't created it yet, go to UBbox > New > Folder > CSE 676-B Assignment 0 by YOUR NAME
    - Upload your saved weights to this folder. Include the model weights that generate the best results for your model for Part III, named as a0_part#_ YOUR_UBIT.pt

      e.g. a0_ part_3_ avereshc.pt
    - Copy a shared link to the UBbox folder, so it can be viewed by people in your company & it can be viewed and downloaded.



    - Add the link to the txt file, named as a0_weights_ YOUR_UBIT.txt
    - Submit this txt file as part of your submission on UBlearns
4. Dataset should NOT be submitted. Don't include as part of the submission
5. Combine all files in a single zip folder that will be submitted on UBlearns, named as assignment0_final_YOUR_UBIT.zip

Notes:

- Large files: any individual file that is larger then 10MB (e.g. your model weights) should be uploaded to UBbox and you have to provide a link to them. A penalty of -10pts will be applied towards the assignment if there is a file submitted that is bigger than 10MB.

  It's ok if your final combined zip folder is larger then 10MB.
- Ensure your code is well-organized and includes comments explaining key functions and attributes.
- After running the Jupyter Notebooks, all results and plots used in your report should be generated and clearly displayed.
- The zip folder should include all relevant files, clearly named as specified.
- Only files uploaded on UBlearns and a submitted link to UBbox for saved weights are considered for evaluation.

ASSIGNMENT STEPS

1. Submit checkpoint (February 6)

- Complete Part I & II of the assignment
- Include all the references at the end of the report. There is no minimum requirement for the report size, just include all of the information required.
- Add all your assignment files in a zip folder including .ipynb files, the report and txt file with a link to UBbox at a zip folder.
- Name zip folder with all the files as

  assignment0_checkpoint_YOUR_UBIT.zip

  e.g., assignment0_checkpoint_ avereshc.zip
- Submit to UBLearns > Assignments
- Dataset should NOT be submitted. Don't include as part of the submission
- Include all the references at the end of your report that have been used to complete the assignment

2. Submit final results (February 13)

- Fully complete all parts of the assignment
- Submit to UBLearns > Assignments
- Add all your assignment files in a zip folder including ipynb files for Part I, Part II, Part III & Bonus part (optional), the report and txt file with a link to UBbox

- Name zip folder with all the files as assignment0_final_YOUR_UBIT.zip

  e.g. assignment0_final_avereshc.zip
- Dataset should NOT be submitted. Don't include as part of the submission.
- Your Jupyter notebook should be saved with the results. If you are submitting python scripts, after extracting the ZIP file and executing command python main.py in the first level directory, all the generated results and plots you used in your report should appear printed out in a clear manner.
- Include all the references at the end of your report that have been used to complete the assignment.
- You can make unlimited number of submissions and only the latest will be evaluated

Notes:

- Ensure that your code follows a clear structure and contains comments for the main functions and specific attributes related to your solution. You can submit multiple files, but they all need to be labeled with a clear name.
- Recheck the submitted files, e.g. download and open them, once submitted and verify that they open correctly

Academic Integrity

The standing policy of the Department is that all students involved in any academic integrity violation (e.g., plagiarism in any way, shape, or form) will receive an F grade for the course. The catalog describes plagiarism as "Copying or receiving material from any source and submitting that material as one's own, without acknowledging and citing the particular debts to the source, or in any other manner representing the work of another as one's own.". Refer to the Office of Academic Integrity for more details.

Important Information

This assignment should be completed individually.

- No collaboration, cheating, and plagiarism is allowed in assignments, quizzes, the midterms or final project.
- All the submissions will be checked using SafeAssign as well as other tools. SafeAssign is based on the submitted works for the past semesters as well the current submissions. We can see all the sources, so you don't need to worry if there is a high similarity with your Checkpoint submission.
- The submissions should include all the references. Kindly note that referencing the source does not mean you can copy/paste it fully and submit as your original work. Updating the hyperparameters or modifying the existing code is a subject to plagiarism. Your work has

to be original. If you have any doubts, send a private post on piazza to confirm.

- All parties involved in any suspicious cases will be officially reported using the Academic Dishonesty Report form. What does that mean?
    - In most cases, the grade for the assignment/quiz/final project/midterm will be 0 and all bonus points will be subject to removal from the final evaluation for all students involved.
    - Those found violating academic integrity more than once throughout their program will receive an immediate F in the course.

  Please refer to the Academic Integrity Policy for more details.
- The report should be delivered as a separate pdf file. You can combine report for Part I, Part II, Part III & Part IV into the same pdf file. You can follow the NIPS template as a report structure. You may include comments in the Jupyter Notebook; however, you will need to duplicate the results in a separate pdf file.
- All the references can be listed at the end of the report. There is no minimum requirement for the report size, just make sure it includes all the information required.

Late Days Policy

You can use up to 5 late days throughout the course that can be applied to any assignment-related due dates. You do not have to inform the instructor, as the late submission will be tracked in UBlearns.

Important Dates

February 6, Thu, 11:59 pm - Checkpoint Submission is Due

February 13, Thu, 11:59 pm - Final Submission is Due