# 50.039 Theory and Practice of Deep Learning

W3-S3 Introduction to Deep Learning using the PyTorch framework

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# Introduction (Week 3)

- 1. What is the **PyTorch library** and its **benefits**?
- 2. What is a **PyTorch tensor object** and its typical **attributes**?
- 3. How to implement some typical **tensor operations**?
- 4. What is **broadcasting** on tensors?
- 5. What are **tensor locations** in terms of computation?
- 6. How to transform our original NumPy shallow Neural Network class so it uses PyTorch now instead?
- 7. How to implement a **forward**, **loss** and **accuracy** metric in PyTorch?
- 8. What are some measurable **performance benefits** of using **PyTorch** over NumPy and **GPUs** over CPUs?

# Introduction (Week 3)

- 9. What is the **autograd/backprop** module in PyTorch, and how does it use a **computational graph** to **compute all derivatives**?
- 10. How to use the autograd to implement derivatives and a vanilla gradient descent?
- 11. How to implement **backprop** in PyTorch for our **shallow Neural Network** class?
- 12. How to use **PyTorch** to implement **advanced optimizers**?
- 13. How to use **PyTorch** to implement **advanced initializers**?
- 14. How to use **PyTorch** to implement **regularization**?
- 15. How to finally revise our **trainer** function to obtain a minimal, yet complete Neural Network in PyTorch?

# Introduction (Week 3)

- 16. What are the **Dataset** and **Dataloader** objects in **PyTorch**?
- 17. How to implement a custom **Dataloader** and **Dataset** object in PyTorch?
- 18. How to move from binary classification to multi-class classification?
- 19. How to adjust output probabilities using the **softmax** function?
- 20. How to change the **cross-entropy loss** so it works in **multi-class classification**?
- 21. How to implement **building blocks** in PyTorch?
- 22. How to implement and train our first **Deep Neural Network**?
- 23. What are additional good practices in PyTorch?

## To summarize (last two sessions)

We now have a full Neural Network class, in PyTorch, with:

- 2 linear layers, sigmoid activation functions,
- Xavier uniform initialization on trainable parameters,
- Forward pass method,
- Autograd backpropagation and trainer method,
- Adam optimizer,
- Dataloader allowing for stochastic mini-batches,
- Cross entropy loss and accuracies,
- L1 regularization.

And it runs/trains at the speed of light (almost...) on GPU!

```
class ShallowNeuralNet PT(torch.nn.Module):
       def __init__(self, n_x, n_h, n_y, device):
 2
           super(). init ()
 3
           self.n x, self.n_h, self.n_y = n_x, n_h, n_y
 4
           self.W1 = torch.nn.Parameter(torch.zeros(size = (n_x, n_h), requires_grad = True, \
                                                     dtype = torch.float64, device = device))
 6
 7
           torch.nn.init.xavier_uniform_(self.W1.data)
           self.b1 = torch.nn.Parameter(torch.zeros(size = (1, n h), requires grad = True, \
 8
 9
                                                     dtype = torch.float64, device = device))
           torch.nn.init.xavier uniform (self.b1.data)
10
11
           self.W2 = torch.nn.Parameter(torch.zeros(size = (n_h, n_y), requires_grad = True, \
                                                     dtype = torch.float64, device = device))
12
13
           torch.nn.init.xavier uniform (self.W2.data)
           self.b2 = torch.nn.Parameter(torch.zeros(size = (1, n_y), requires_grad = True, \
14
15
                                                     dtype = torch.float64, device = device))
           torch.nn.init.xavier_uniform_(self.b2.data)
16
17
           self.loss = torch.nn.BCELoss()
18
           self.accuracy = BinaryAccuracy()
19
       def forward(self, inputs):
           return torch.sigmoid(torch.matmul(torch.sigmoid(torch.matmul(inputs, self.W1) + self.b1), self.W2) + self.b2)
20
21
       def train(self, inputs, outputs, N_max = 1000, alpha = 1, beta1 = 0.9, beta2 = 0.999, \
22
                 batch_size = 32, lambda_val = 1e-3):
23
           dataset = torch.utils.data.TensorDataset(inputs, outputs)
24
           data loader = torch.utils.data.DataLoader(dataset, batch size = batch size, shuffle = True)
           optimizer = torch.optim.Adam(self.parameters(), lr = alpha, betas = (beta1, beta2), eps = 1e-08)
25
26
           optimizer.zero grad()
27
           self.loss history = []
           for iteration number in range(1, N max + 1):
28
29
               for batch in data_loader:
30
                    inputs_batch, outputs_batch = batch
31
                   total_loss = self.loss(self(inputs_batch), outputs_batch.to(torch.float64))\
32
                       + lambda_val*sum(torch.abs(param).sum() for param in self.parameters()).item()
33
                    self.loss_history.append(total_loss)
34
                   total loss.backward()
35
                   optimizer.step()
                   optimizer.zero_grad()
36
37
               if(iteration_number % (N_max//20) == 1):
38
                    pred = self(inputs)
                    acc_val = self.accuracy(pred, outputs).item()
39
                    print("Iteration {} - Loss = {} - Accuracy = {}".format(iteration_number, total_loss, acc_val))
40
```

#### Built-in datasets

- Pytorch has a few built-in datasets, ready to be downloaded and used on models: typically the most common ones that have been used to demonstrate concepts, such as MNIST or CIFAR-10.
- For more details on the available built-in datasets, have a look at the following page: <a href="https://pytorch.org/vision/stable">https://pytorch.org/vision/stable</a> /datasets.html.

#### Built-in datasets

- Let us demonstrate using the FashionMNIST dataset.
- This dataset consists of 28 by 28 greyscale images.
- It is typically used to design image classification models (i.e. models that receive images as inputs), and attempt to predict what is in the image in question.
- The 10 classes (bag, shirt, etc.) are indexed with 0-9 values, corresponding to the 10 types of fashion objects found in the dataset.

Restricted

#### Built-in datasets

- Let us demonstrate this with the FashionMNIST dataset.
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- It is typically used to design image classification models (i.e. models that receive images as inputs), and attempt to predict what is in the image in question.
- The 10 classes (bag, shirt, etc.) are indexed with 0-9 values, corresponding to the 10 types of fashion objects found in the dataset.

```
# Dataset contains 60000 samples, that are greyscale
# images with size 28 by 28 pixels.
print(training_data.data.shape)
```

torch.Size([60000, 28, 28])

```
# We can then fetch a sample using the [] notations
sample_index = 894
img, label = training_data[sample_index]
print("Image: ", img.shape)
print("Label: ", label)
```

Image: torch.Size([1, 28, 28])

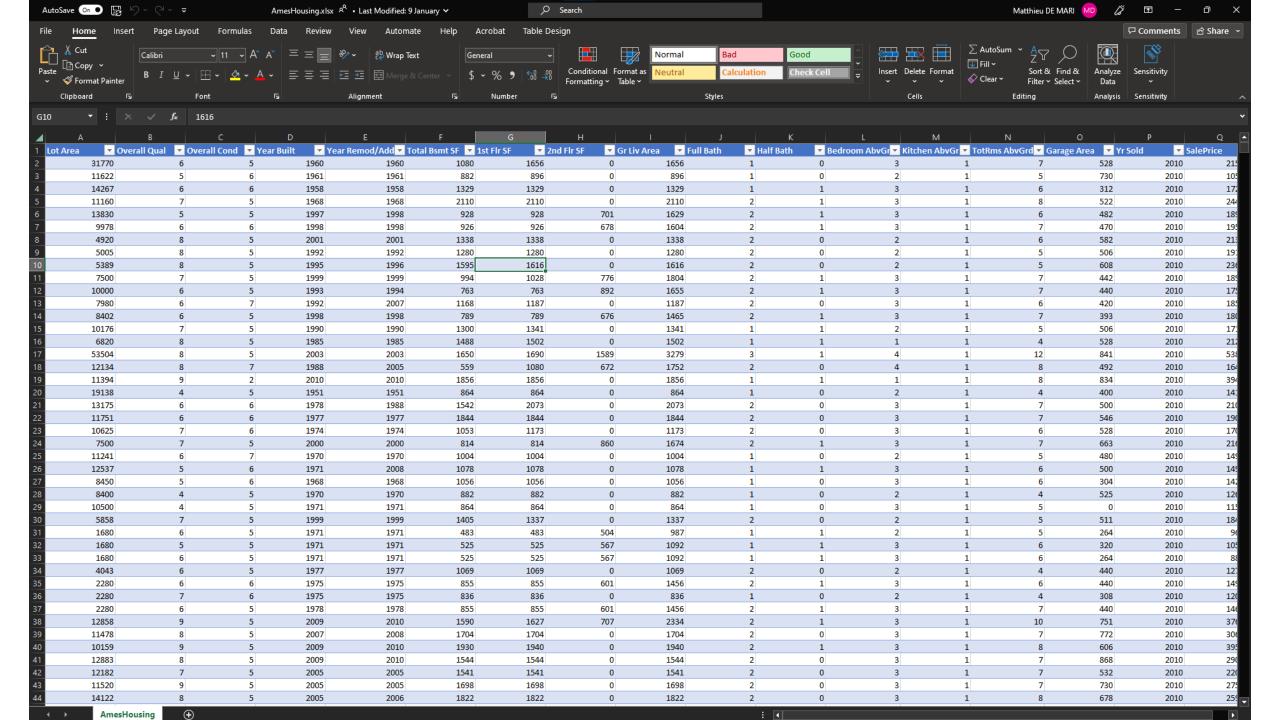
Label: 8

#### Image 894 - Label = 8 (Bag)



- Most of the time, when demonstrating concepts, we will rely on a "simple" **built-in dataset**, available in the PyTorch library.
- In practice, however, you will often play with a **custom dataset**, fitting your project needs.
- Most datasets will be provided by your future employers, or can be found on dataset search engines, such as Kaggle, Google Dataset Search, etc.
- Today, we will play with a simplified version of the **Ames Housing Dataset**, which can be found online, here:

https://www.kaggle.com/datasets/prevek18/ames-housing-dataset?resource=download



- The Ames dataset includes a variety of features for approximately 2,800 houses in Ames, Iowa.
- Features include the size of the house (in square feet), the number of bedrooms and bathrooms, the year the house was built, and more. It also includes the sale price for each house.
- The Ames Housing Dataset is a popular choice for machine learning projects, and it has been used to build models for predicting house prices based on various features.
- It consists of an Excel file (AmesHousing.xlsx) stored in the ./ames/ folder. The original dataset can be found in the AmesHousing.csv file, but we have simplified it by removing some of its features.

The features we are interested in are:

- Lot Area: The area of the lot in square feet.
- Overall Qual: A rating of the overall material and finish of the house (1-10).
- Overall Cond: A rating of the overall condition of the house (1-10).
- Year Built: The year the house was built.
- Year Remod/Add: The year the house was remodeled or had an addition added.
- **Total Bsmt SF**: The total surface of the basement, in square feet.
- **1st Fir SF**: The first floor surface, in square feet.
- **2nd Fir SF**: The second floor surface, in square feet.
- **Gr Liv Area**: The above grade (ground) living area, in square feet.

- **Full Bath**: The number of full bathrooms.
- Half Bath: The number of half bathrooms.
- **Bedroom AbvGr**: The number of bedrooms.
- **Kitchen AbvGr**: The number of kitchens.
- TotRms AbvGrd: The total number of rooms (does not include bathrooms).
- **Garage** Area: The size of the garage, in square feet.
- Yr Sold: The year the property was sold.

These **16 features** will be used as **inputs**, and the **output** will consist of just **1 feature**, in the final column of the Excel file, which is:

• SalePrice: The sale price, in dollars.

#### Restricted

# Writing a custom Dataset object

Let us start by loading the **Excel** file into a pandas **DataFrame** first.

Note: Not familiar with the pandas library? Find 10 minutes to pick it up, it will definitely serve you in the long run!

https://pandas.pydata.org
/docs/user guide/10min.
html

```
# Load dataset using pandas, and showing the first five entries
 ames_dataset = pd.read_excel("./ames/AmesHousing.xlsx")
 print(ames dataset.head(5))
Lot Area Overall Qual Overall Cond Year Built Year Remod/Add \
   31770
                                             1960
                                                             1960
  11622
                                             1961
                                                             1961
  14267
                                             1958
                                                             1958
  11160
                                             1968
                                                             1968
  13830
                                             1997
                                                             1998
               1st Flr SF
                           2nd Flr SF
                                       Gr Liv Area
                                                    Full Bath Half Bath \
Total Bsmt SF
         1080
                     1656
                                               1656
                                                                        0
          882
                      896
                                                896
         1329
                     1329
                                               1329
         2110
                     2110
                                               2110
          928
                      928
                                  701
                                               1629
               Kitchen AbvGr
                              TotRms AbvGrd
                                             Garage Area
                                                           Yr Sold
                                                      528
                                                              2010
                                                      730
                                                              2010
                                                      312
                                                              2010
                                                              2010
                                                      522
                                                      482
                                                              2010
SalePrice
  215000
  105000
  172000
```

To write a custom **dataset class** in PyTorch, we need to:

- Create a class that subclasses torch.utils.data.Dataset.
- Define a an \_\_init\_\_ that takes in the required arguments, and stores them as member variables.
- Define a \_\_getitem\_\_ that takes index as input, and returns the data and label at that index as an array. This will allow to use the square bracket notation on our dataset object.
- Define a method \_\_len\_\_ that returns the number of samples in the dataset.

```
class AmesHousingDataset(torch.utils.data.Dataset):
   #The init method will simply initialize attributes, which consist
   # of the details related to the dataset.
   def init (self, file path = "./ames/AmesHousing.xlsx"):
       # Whole data as a pandas array
       self.data = pd.read excel(file path)
        self.dataset length = len(self.data) #2928
       # Extract inputs
       self.input fetaures number = 16
        self.input features = self.data.iloc[:, :16]
       # Extract outputs
       self.output_fetaures_number = 1
        self.output feature = self.data.iloc[:, 16]
   # The getitem method returns the sample with given index
    # x will consist of the 16 input features for the given sample,
   # whereas y will consist of the 1 output feature for the given sample.
   def __getitem__(self, index):
       # Fetch inputs
       x = self.input_features.iloc[index].values
       # Fetch outputs
       y = self.output feature.iloc[index]
       return x, y
   # Finally, the len special method should return the number of samples,
   # in the dataset. We could use self.dataset_length, but it is more
   # modular to use len(self.data).
   def len (self):
       return len(self.data)
```

To write a custom **dataset class** in PyTorch, we need to:

- Create a class that subclasses torch.utils.data.Dataset.
- Define a an \_\_init\_\_ that takes in the required arguments, and stores them as member variables.
- Define a \_\_getitem\_\_ that takes index as input, and returns the data and label at that index as an array. This will allow to use the square bracket notation on our dataset object.
- Define a method \_\_len\_\_ that returns the number of samples in the dataset.

```
1 # Instantiate the dataset
    ames dataset = AmesHousingDataset('./ames/AmesHousing.xlsx')
    # Fetch sample with index 286
    sample input, sample output = ames dataset[286]
 6 # Input is a (16,) numpy array, with the following values
    print(type(sample input), sample input.shape)
 8 print(sample_input)
 9 # Output is a single value, of type numpy int64
10 print(type(sample output), sample output.shape)
11 print(sample output)
<class 'numpy.ndarray'> (16,)
             4 1915 1950 806 841 806 1647
Γ6858
 216 20101
<class 'numpy.int64'> ()
128000
```

#### Writing a custom Dataloader

- Before we can feed this dataset object to Neural Networks, we need to supplement it with a Dataloader.
- The Dataloader will shuffle the samples randomly and produce mini-batches of a given size.
- This Dataloader typically allows for stochastic mini-batches, as discussed in Week 2.
- The Dataloader will also transform arrays into tensors.

#### Restricted

# Writing a custom Dataloader

- We can then this custom
   Dataloader to generate minibatches using a for loop.
- Notice how this Dataloader generates 92 (= 2928/32, rounded up) batches of 32 samples.
- With the exception of the **last** batch (with index 91), that only contains **16 samples** (= 2928 % 32).

```
for batch_number, batch in enumerate(ames_dataloader):
    inputs, outputs = batch
    print("---")
    print("Batch number: ", batch_number)
    print(inputs.shape)
    print(outputs.shape)
```

```
Batch number: 0
torch.Size([32, 16])
torch.Size([32])
Batch number: 1
torch.Size([32, 16])
torch.Size([32])
Batch number: 2
torch.Size([32, 16])
torch.Size([32])
Batch number: 3
torch.Size([32, 16])
torch.Size([32])
Batch number: 4
              Batch number: 91
              torch.Size([16, 16])
              torch.Size([16])
```

#### Restricted

# Writing a custom Dataloader

- We can then this custom
   Dataloader to generate minibatches using a for loop.
- Good practice: the custom
   Dataset and custom Dataloader
   definition should be repeated to
   generate training, testing and
   validation sets dataloaders.
- This (or these) Dataloader(s) will then be fed to our **trainer** function later on.

```
for batch_number, batch in enumerate(ames_dataloader):
    inputs, outputs = batch
    print("---")
    print("Batch number: ", batch_number)
    print(inputs.shape)
    print(outputs.shape)
```

```
Batch number: 0
torch.Size([32, 16])
torch.Size([32])
Batch number: 1
torch.Size([32, 16])
torch.Size([32])
Batch number: 2
torch.Size([32, 16])
torch.Size([32])
Batch number: 3
torch.Size([32, 16])
torch.Size([32])
Batch number: 4
              Batch number: 91
              torch.Size([16, 16])
              torch.Size([16])
```

MNIST is a widely-used dataset for the benchmarking of machine learning and computer vision algorithms.

It consists of

- a **training set** of 60,000 examples,
- and a **testing set** of 10,000 examples.

All samples consist of 28x28 pixel grayscale images of handwritten digits (0 to 9).

MNIST is often used as a "Hello, World!" example, due to its simplicity and the availability of efficient implementations of various learning algorithms.



**MNIST** is a widely-used dataset for the benchmarking of machine learning and computer vision algorithms.

It consists of

- a **training set** of 60,000 examples,
- and a **testing set** of 10,000 examples.

All samples consist of 28x28 pixel grayscale images of handwritten digits (0 to 9).

Careful however: the MNIST dataset is often accused of having been overused (which is true) and of being too simple.



- It is a good dataset to use for testing and comparing the performance of different models, as well as for getting familiar with the basics of machine learning and deep learning.
- The images serve as inputs, and the task is therefore to predict which of the ten digits appears in the image.

 This is therefore a classification task, like before, except that it consists of 10 different classes (corresponding to the 0-9 digits) instead of just two like in binary classification.



### Writing the MNIST Dataset and Dataloader

```
# Try the dataloader
for batch_number, batch in enumerate(train_loader):
    inputs, outputs = batch
    print("---")
    print("Batch number: ", batch_number)
    print(inputs.shape)
    print(outputs.shape)
    break
```

---

```
Batch number: 0
torch.Size([64, 1, 28, 28])
torch.Size([64])
```

In general, it is good to do the following:

- Scale the data (pixel values) to the [0,1] range.
- Normalize the data to have zero mean and unit standard deviation.

We will then subtract a mean of 0.1307 and divide by a standard deviation of 0.3081.

These values are basically the mean and the standard deviation of the dataset divided by 255 (original max pixel value).

### Writing the MNIST Dataset and Dataloader

```
# Try the dataloader
for batch_number, batch in enumerate(train_loader):
    inputs, outputs = batch
    print("---")
    print("Batch number: ", batch_number)
    print(inputs.shape)
    print(outputs.shape)
    break
```

---

```
Batch number: 0
torch.Size([64, 1, 28, 28])
torch.Size([64])
```

## From binary to multi-class classification

In **binary classification**, we would produce **a single value** p as **output**, with p between 0 and 1.

- This value p would correspond to the probability of being of class 1.
- The probability of being of class 0 would then simply be 1 p.
- We would then use a **threshold 0.5** to decide if the sample is predicted of class 0 or 1.

- Unfortunately, when we have more than 2 classes, we can no longer rely on a single output value p.
- Instead, it is often preferable to have the model output **10 values**:

$$(p_0, p_1, p_2, \dots p_9)$$

- Where each  $p_i$  corresponds to the probability of being of class i.
- This could typically be done by asking for the final layer to produce  $n_y = 10$  values instead of just a single  $n_v = 1$  value.

# From binary to multi-class classification

- Unfortunately, this is not good enough.
- The  $p_i$  are probabilities and their sum should be equal to 1, i.e.

$$\sum_{i}^{9} p_i = 1$$

• A fully connected layer (WX + b) is not smart enough to do that on its own: it might produce values that may not sum up to 1.

 To normalize the outputs produced by the final fully connected layer, we will use the softmax operation, which is a special activation function.

#### **Definition (the softmax function):**

The **softmax function** transforms a vector of *N* values

$$Y = (y_0, y_1, y_2, ... y_K),$$

into another vector of N values

$$P = (p_0, p_1, p_2, ... p_K).$$

The new vector **P** is guaranteed to be summing up to 1, i.e.

$$\sum_{k=0}^{K} p_i = 1$$

The **softmax** operation

$$p_i = s(y_i, y_{-i})$$

is defined,  $\forall i$ , as:

$$p_i = s(y_i, y_{-i}) = \frac{\exp(y_i)}{\sum_{k=0}^{K} \exp(y_k)}$$

**Note:** the  $y_{-i}$  notation comes from game theory, and consists of every element in vector Y except  $y_i$ .

$$y_{-i} = (y_1, \dots, y_{i-1}, y_{i+1}, \dots, y_K)$$

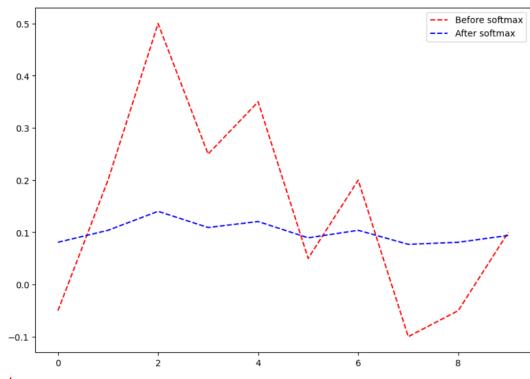
# Softmax can be manually implemented as:

```
def softmax(x):
    # Subtract the maximum value from each element of the input vector x
    # to avoid numerical instability (this is optional, but equivalent)
    x = x - np.max(x)
    # Compute the exponent of each element
    exp_x = np.exp(x)
    # Normalize the exponentiated values by their sum
    return exp_x/np.sum(exp_x)
```

```
1  # Ten values that do not sum up to 1
2  Y = np.array([-1, 4, 10, 5, 7, 1, 4, -2, -1, 2])/20
3  print(sum(Y))
4  P = softmax(Y)
5  print(P)
6  print(np.sum(P))
```

```
1.45
[0.08089815 0.10387528 0.14021696 0.10920108 0.12068586 0.08940628 0.10387528 0.0769527 0.08089815 0.09399024]
0.999999999999999
```

It will rescale values so that the trend is preserved, but the new vector sums to 1.



In the case of multi-label classification, we will use the **softmax** operation as the final activation after the last fully connected layer.

This will produce a vector of 10 values,

$$P = (p_0, p_1, p_2, ... p_9),$$

corresponding to the probability for sample of being of each class i.

The predicted class pred will be the index i of the highest  $p_i$  value, i.e.  $pred = \arg\max_i [p_i].$ 

For instance, this simple neural network consists of **two fully-connected/linear layers**.

A **single ReLU activation** is used between both layers.

#### No final activation yet.

It also consists of a **flattening** operation, which will transform our input images (2D tensors, size 28 by 28), into a "flattened" 1D tensor with size  $784 (= 28 \times 28)$ .

```
class ShallowNeuralNet(torch.nn.Module):
        def __init__(self, n_x, n_h, n_y):
            super(). init_()
            # Define two layers using the nn.Linear()
            self.fc1 = torch.nn.Linear(n x, n h)
            self.fc2 = torch.nn.Linear(n h, n y)
       def forward(self, x):
            # Flatten images (transform them from 28x28 2D
10
            # matrices to 784 1D vectors)
           x = x.view(x.size(0), -1)
11
12
            # First Wx + b operation
13
            out1 = self.fc1(x)
            # Using ReLU operation as activation after first layer
14
15
            act1 = torch.relu(out1)
            # Second Wx + b operation anbd return
16
17
            out2 = self.fc2(act1)
18
            return out2
```

- Consider a neural network model, with 784 input size, 128 hidden size, and 10 output size, eventually transferring the model to a device.
- Next, we get a single sample from the train\_loader iterator and extract sample info in the variables data and target.
- This can be simply done with the next and iter functions.

```
# Initialize model
   model = ShallowNeuralNet(n x = 784, \
                            n h = 128, \
                            n y = 10).to(device)
   # Get a single sample
   sample = next(iter(train loader))
8 data, target = sample
9 print(data.shape)
   print(target.shape)
11 data1 = data[0].to(device)
12 target1 = target[0].to(device)
13 print(data1.shape)
14 print(target1)
15
16 # Forward pass
   out2 = model(data1)
18 act2 = torch.nn.functional.softmax(out2, dim = 1)
19 print(out2)
20 print(act2)
21 print(act2.sum())
```

- Perform a forward pass through the model, storing the output in the variable out2.
- Apply the softmax operation on out2., PyTorch offers a functional implementation of the softmax:

#### torch.nn.functional.softmax()

• We can then verify that softmax will adjust the output of the neural network so that it is now summing up to 1.

```
# Initialize model.
   model = ShallowNeuralNet(n x = 784, \
                            n h = 128, \
                            n y = 10).to(device)
   # Get a single sample
   sample = next(iter(train loader))
   data, target = sample
   print(data.shape)
   print(target.shape)
   data1 = data[0].to(device)
12 target1 = target[0].to(device)
   print(data1.shape)
14 print(target1)
15
16 # Forward pass
17 out2 = model(data1)
18 act2 = torch.nn.functional.softmax(out2, dim = 1)
19 print(out2)
20 print(act2)
21 print(act2.sum())
```

#### Forward implementation

 Our model is however the same as before.

# We do not use the softmax operation in the forward.

 This is normal as the softmax operation will be used in the loss function, cross\_entropy, which will be used in the trainer() function later.

```
class ShallowNeuralNet(torch.nn.Module):
        def __init__(self, n_x, n_h, n_y):
            super(). init_()
           # Define two layers using the nn.Linear()
            self.fc1 = torch.nn.Linear(n_x, n_h)
            self.fc2 = torch.nn.Linear(n h, n y)
       def forward(self, x):
           # Flatten images (transform them from 28x28 2D
           # matrices to 784 1D vectors)
10
           x = x.view(x.size(0), -1)
11
12
           # First Wx + b operation
13
           out1 = self.fc1(x)
           # Using ReLU operation as activation after first layer
14
15
            act1 = torch.relu(out1)
           # Second Wx + b operation and return
16
17
           out2 = self.fc2(act1)
            return out2
18
```

### From binary cross entropy...

• Speaking of, in the case of the **binary classification**, we used the following loss function, namely the **log-likelihood function**.

$$L(x,y) = -\frac{1}{N} \sum_{k}^{N} y_k \ln(p(x_k)) + (1 - y_k) \ln(1 - p(x_k))$$

• But in the case of MNIST, we have more than two classes...

How does the loss function change now that we have 10 classes?

### ...To multi-class cross entropy!

• The adjustment is actually quite simple, and the multi-class crossentropy loss function simply rewrites as shown below:

$$L(x,y) = -\frac{1}{N} \sum_{k=1}^{N} \sum_{i=0}^{9} y_k^i \ln(p_i(x_k)).$$

In the formula above,  $p_i(x_k)$  denotes the **probability for sample**  $x_k$  **of being of class** i. In other words, it is the i-th value of the output vector produced by the model for sample  $x_k$  after softmax has been applied.

The value  $y_k^i$  is the ground truth value for the probability of being of class i for sample  $x_k$ . For instance, if the sample  $x_k$  is of class 2:

$$Y_k = (y_k^0, y_k^1, y_k^2, y_k^3, \dots y_k^9) = (0, 0, 1, 0, \dots, 0).$$

#### Setting a model in train mode

**New good practice:** some operations (layers, activations, etc.) in forward will have **two different behaviors** depending on whether

- the model is currently training,
- or if we are using its trained version for evaluation.

(Note: at the moment, we have not seen such operations.)

But let us keep this in mind, and accept that is good practice to set the model to either train() or eval() mode.

```
# Initialize the model and optimizer
model = ShallowNeuralNet(n_x = 784, n_h = 64, n_y = 10).to(device)
optimizer = torch.optim.Adam(model.parameters(), lr = 1e-3)
# Set model in train mode!
model.train()
```

#### Training our model with Adam GD, as before

```
1 # Training model
 2 num epochs = 5
 3 for epoch in range(num epochs):
        # Go trough all samples in train dataset
        for i, (images, labels) in enumerate(train_loader):
            # Get from dataloader and send to device
            images = images.to(device)
            labels = labels.to(device)
            # Forward pass
            outputs = model(images)
10
            # Compute loss
11
            loss = torch.nn.functional.cross entropy(outputs, labels)
12
            # Backward and optimize
13
            optimizer.zero grad()
14
            loss.backward()
15
            optimizer.step()
16
17
            # Display
18
            if (i+1) % 300 == 0:
                print (f'Epoch [{epoch+1}/{num epochs}], Step [{i+1}/{len(train loader)}], Loss: {loss.item():.4f}')
19
Epoch [1/5], Step [300/938], Loss: 0.2895
Epoch [1/5], Step [600/938], Loss: 0.1588
Epoch [1/5], Step [900/938], Loss: 0.1753
Epoch [2/5], Step [300/938], Loss: 0.0461
Epoch [2/5], Step [600/938], Loss: 0.1251
Epoch [2/5], Step [900/938], Loss: 0.1592
Epoch [3/5], Step [300/938], Loss: 0.1241
Epoch [3/5], Step [600/938], Loss: 0.0511
Epoch [3/5], Step [900/938], Loss: 0.0553
Epoch [4/5], Step [300/938], Loss: 0.0514
Fnoch [1/5] Sten [600/938] Loss: 0 0339
```

#### Eval mode and accuracy after training

After training, we will evaluate our trained model.

- Set the model in eval() mode (good practice for later).
- Predict on test dataloader.
- Calculate accuracy manually (we could have probably also used a torch function to do that).
- Good trained model!

```
# Evaluate model accuracy on test after training
   # Set model in eval mode!
   model.eval()
   # Evaluate
   with torch.no grad():
       correct = 0
       total = 0
       for images, labels in test loader:
            # Get images and labels from test loader
            images = images.to(device)
10
            labels = labels.to(device)
11
           # Forward pass and predict class using max
            outputs = model(images)
            _, predicted = torch.max(outputs.data, 1)
14
            # Check if predicted class matches label
15
           # and count numbler of correct predictions
16
17
           total += labels.size(0)
           correct += (predicted == labels).sum().item()
   # Compute final accuracy and display
   accuracy = correct/total
   print(f'Evaluation after training, Accuracy: {accuracy:.4f}')
```

Evaluation after training, Accuracy: 0.9712

#### It is now time...

It is now time for us to define and train our first **Deep Neural Network**.

By definition, a deep neural network consists of more than two layers.

Here we will create a deep neural network with four layers:

- three linear layers with ReLU activation,
- followed by one linear layer, finished with a softmax activation.

In general, it is good practice to have the size decrease progressively by a factor of at least 2 from one layer to another.

For instance, we decided here, to have

- the first layer receive inputs of size 784 and produce outputs of size 80,
- the second layer receive inputs of size 80 and produce outputs of size 80,
- the third layer receive inputs of size 40 and produce outputs of size 40,
- and the fourth layer receive inputs of size 20 and produce outputs of size 10.

#### Creating blocks

## Good practice (another one): create building blocks for modularity in your neural networks.

- The DenseReLU class is a custom PyTorch module that consists of a linear layer followed by a ReLU activation function.
- The DenseNoRELU class is similar, but it applies no activation function after the linear layer.

**Important note:** no softmax, for the same reason as before.

```
class DenseReLU(torch.nn.Module):
    def __init__(self, n_x, n_y):
        super().__init__()
        # Define Linear layer using the nn.Linear()
        self.fc = torch.nn.Linear(n_x, n_y)

def forward(self, x):
    # Wx + b operation
    # Using ReLU operation as activation after
    return torch.relu(self.fc(x))
```

```
class DenseNoReLU(torch.nn.Module):
    def __init__(self, n_x, n_y):
        super().__init__()
        # Define Linear layer using the nn.Linear()
        self.fc = torch.nn.Linear(n_x, n_y)

def forward(self, x):
    # Wx + b operation
    # No activation function
    return self.fc(x)
```

#### Creating blocks

The DeepNeuralNet class will here represent the overall deep neural network.

It starts by initializing four layers:

- Three DenseReLU layers,
- And one DenseNoReLU.

It then combines them into a single PyTorch sequential model using torch.nn.Sequential().

```
class DeepNeuralNet(torch.nn.Module):
   def __init__(self, n_x, n_h, n_y):
        super(). init ()
       # Define three Dense + ReLU layers,
       # followed by one Dense + Softmax layer
       self.layer1 = DenseReLU(n x, n h[0])
        self.layer2 = DenseReLU(n h[0], n h[1])
       self.layer3 = DenseReLU(n h[1], n h[2])
        self.layer4 = DenseNoReLU(n h[2], n y)
       # Combine all four layers
        self.combined layers = torch.nn.Sequential(self.layer1,
                                                   self.layer2,
                                                   self.layer3,
                                                   self.layer4)
   def forward(self, x):
       # Flatten images (transform them from 28x28
        # 2D matrices to 784 1D vectors)
       x = x.view(x.size(0), -1)
       # Pass through all four layers
       out = self.combined layers(x)
       return out
```

```
# Initialize the model and optimizer
model = DeepNeuralNet(n_x = 784, n_h = [80, 40, 20], n_y = 10).to(device)
optimizer = torch.optim.Adam(model.parameters(), lr = 1e-3)
```

#### Creating blocks

The forward pass of the network is then simply defined:

- The input image is first flattened from a 2D image to a 1D vector,
- It is then passed through the combined layers we have assembled in Sequential().

This modular approach, defining blocks of layers and eventually assembling them in a larger network, is very common in deep neural networks, especially when the architectures are very heavy and include many layers.

```
class DeepNeuralNet(torch.nn.Module):
   def __init__(self, n_x, n_h, n_y):
       super(). init ()
       # Define three Dense + ReLU layers,
       # followed by one Dense + Softmax layer
       self.layer1 = DenseReLU(n x, n h[0])
        self.layer2 = DenseReLU(n h[0], n h[1])
       self.layer3 = DenseReLU(n h[1], n h[2])
        self.layer4 = DenseNoReLU(n h[2], n y)
       # Combine all four layers
       self.combined layers = torch.nn.Sequential(self.layer1,
                                                   self.layer2,
                                                   self.layer3,
                                                   self.layer4)
   def forward(self, x):
       # Flatten images (transform them from 28x28
        # 2D matrices to 784 1D vectors)
       x = x.view(x.size(0), -1)
       # Pass through all four layers
       out = self.combined layers(x)
       return out
```

```
# Initialize the model and optimizer
model = DeepNeuralNet(n_x = 784, n_h = [80, 40, 20], n_y = 10).to(device)
optimizer = torch.optim.Adam(model.parameters(), lr = 1e-3)
```

#### Training our model as before

```
# Training model
 2 num epochs = 10
 3 for epoch in range(num epochs):
        # Go trough all samples in train dataset
        for i, (images, labels) in enumerate(train_loader):
            # Get from dataloader and send to device
            images = images.to(device)
            labels = labels.to(device)
            # Forward pass
            outputs = model(images)
10
            # Compute loss
            loss = torch.nn.functional.cross entropy(outputs, labels)
13
            # Backward and optimize
14
            optimizer.zero grad()
            loss.backward()
15
            optimizer.step()
16
17
            # Display
            if (i+1) % 25 == 0:
18
                print (f'Epoch [{epoch+1}/{num epochs}], Step [{i+1}/{len(train loader)}], Loss: {loss.item():.4f}')
19
Epoch [1/10], Step [25/235], Loss: 2.2469
Epoch [1/10], Step [50/235], Loss: 2.1274
Epoch [1/10], Step [75/235], Loss: 1.9379
Epoch [1/10], Step [100/235], Loss: 1.8415
Epoch [1/10], Step [125/235], Loss: 1.6548
Epoch [1/10], Step [150/235], Loss: 1.4660
Epoch [1/10], Step [175/235], Loss: 1.2895
Epoch [1/10], Step [200/235], Loss: 1.1478
Epoch [1/10], Step [225/235], Loss: 0.9910
Fnoch [2/10] Sten [25/235] Loss: 0 8251
```

#### On Deep Neural Networks complexity

We can therefore raise a fairly important question:

### What is the appropriate number of layers to use and how many neurons should we use on each layer?

- We established in Week 2 Notebook 8, that there is no fixed rule for how many layers should be used in a deep neural network.
- Instead, the number of layers, as well as the number of neurons in each layer, should be chosen based on the complexity of the task and the amount of available data.
- In general, deep neural networks with many layers (hundreds or even thousands) can learn very complex patterns in data, but they will require a large amount of data and computational resources to train.

#### On Deep Neural Networks complexity

- More importantly, if the network is too deep, it may also be prone to overfitting, which can hinder its generalization performance on unseen data.
- On the other hand, shallow networks with fewer layers may be easier to train and require less data, but they may not be able to learn as complex patterns.

 NFL: Finding the optimal number of layers and the optimal architecture of a deep neural network is often a trade-off between model complexity, computational resources, and performance, and requires some experimentation and model selection.

#### In fact, our DNN is overfitting at the moment!

#### Shallow Neural Net: 96.5% test acc (not too bad)

```
1 # Evaluate model accuracy on test after training
   # Set model in eval mode!
   model.eval()
   # Evaluate
   with torch.no_grad():
       correct = 0
       total = 0
       for images, labels in test loader:
9
           # Get images and labels from test loader
           images = images.to(device)
10
           labels = labels.to(device)
           # Forward pass and predict class using max
           outputs = model(images)
           _, predicted = torch.max(outputs.data, 1)
14
           # Check if predicted class matches label
16
           # and count numbler of correct predictions
           total += labels.size(0)
17
           correct += (predicted == labels).sum().item()
   # Compute final accuracy and display
   accuracy = correct/total
   print(f'Evaluation after training, Accuracy: {accuracy:.4f}')
```

#### Deep Neural Net: 93.7% test acc (lower, even though we had a lower loss!)

```
# Evaluate model accuracy on test after training
2 # Set model in eval mode!
   model.eval()
   # Evaluate
   with torch.no grad():
       correct = 0
       total = 0
       for images, labels in test loader:
           # Get images and labels from test loader
           images = images.to(device)
10
           labels = labels.to(device)
           # Forward pass and predict class using max
           outputs = model(images)
           _, predicted = torch.max(outputs.data, 1)
           # Check if predicted class matches label
           # and count numbler of correct predictions
17
           total += labels.size(0)
           correct += (predicted == labels).sum().item()
   # Compute final accuracy and display
   accuracy = correct/total
   print(f'Evaluation after training, test accuracy: {accuracy:.4f}')
```

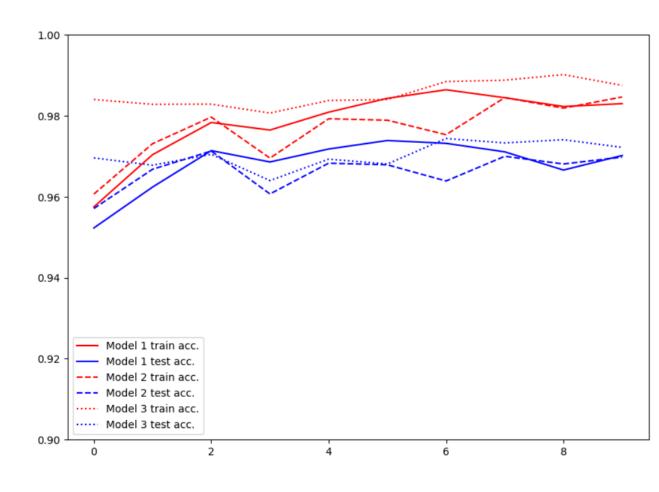
Evaluation after training, test accuracy: 0.9367

#### Experimenting on layers numbers and sizes

In fact, in Notebook 7, we trained three DNN models:

- Model 1: 6 layers (probably too many layers)
- $n_h = [320, 160, 80, 40, 20],$
- Model 2: 3 layers (layers probably too large)  $n_h = [400, 200],$
- Model 3: 3 layers (just fine?)  $n_h = [40, 20].$

While simpler, model 3 has highest test accuracy!



#### Introduction (Week 3)

- 1. What is the **PyTorch library** and its **benefits**?
- 2. What is a **PyTorch tensor object** and its typical **attributes**?
- 3. How to implement some typical **tensor operations**?
- 4. What is **broadcasting** on tensors?
- 5. What are **tensor locations** in terms of computation?
- 6. How to transform our original NumPy shallow Neural Network class so it uses PyTorch now instead?
- 7. How to implement a **forward**, **loss** and **accuracy** metric in PyTorch?
- 8. What are some measurable **performance benefits** of using **PyTorch** over NumPy and **GPUs** over CPUs?

#### Introduction (Week 3)

- 9. What is the **autograd/backprop** module in PyTorch, and how does it use a **computational graph** to **compute all derivatives**?
- 10. How to use the autograd to implement derivatives and a vanilla gradient descent?
- 11. How to implement **backprop** in PyTorch for our **shallow Neural Network** class?
- 12. How to use **PyTorch** to implement **advanced optimizers**?
- 13. How to use **PyTorch** to implement **advanced initializers**?
- 14. How to use **PyTorch** to implement **regularization**?
- 15. How to finally revise our **trainer** function to obtain a minimal, yet complete Neural Network in PyTorch?

#### Introduction (Week 3)

- 16. What are the **Dataset** and **Dataloader** objects in **PyTorch**?
- 17. How to implement a custom **Dataloader** and **Dataset** object in PyTorch?
- 18. How to move from binary classification to multi-class classification?
- 19. How to adjust output probabilities using the **softmax** function?
- 20. How to change the **cross-entropy loss** so it works in **multi-class classification**?
- 21. How to implement **building blocks** in PyTorch?
- 22. How to implement and train our first **Deep Neural Network**?
- 23. What are additional good practices in PyTorch?

#### Conclusion (Week 3)

- PyTorch library and its benefits
- Tensor objects, attributes and operations on tensors
- Converting our NumPy shallow neural network into PyTorch
- Parameter objects
- Forward method implementation
- Performance benefits of GPU acceleration
- Using autograd and compuitational graphs

- Advanced optimizers in PyTorch
- Initializers in PyTorch
- Regularization in PyTorch
- Dataset and Dataloader objects
- Multi-class classification
- Softmax function and multi-class cross entropy loss
- Building blocks in PyTorch
- Our first Deep Neural Network!
- Network size vs. overfitting tradeoff

# Homework 1 and project announcement!

Let us discuss it now.