50.039 Theory and Practice of Deep Learning

W3-S3 Introduction to Deep Learning using the PyTorch framework

Matthieu De Mari

SINGAPORE UNIVERSITY OF TECHNOLOGY AND DESIGN

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!

```python
class ShallowNeuralNet_PT(torch.nn.Module):
    def __init__(self, n_x, n_h, n_y, device):
        super().__init__()
        self.n_x, self.n_h, self.n_y = n_x, n_h, n_y
        self.W1 = torch.nn.Parameter(torch.zeros(size = (n_x, n_h), requires_grad = True, \
                                                  dtype = torch.float64, device = device))
        torch.nn.init.xavier_uniform_(self.W1.data)
        self.b1 = torch.nn.Parameter(torch.zeros(size = (1, n_h), requires_grad = True, \
                                                  dtype = torch.float64, device = device))
        torch.nn.init.xavier_uniform_(self.b1.data)
        self.W2 = torch.nn.Parameter(torch.zeros(size = (n_h, n_y), requires_grad = True, \
                                                  dtype = torch.float64, device = device))
        torch.nn.init.xavier_uniform_(self.W2.data)
        self.b2 = torch.nn.Parameter(torch.zeros(size = (1, n_y), requires_grad = True, \
                                                  dtype = torch.float64, device = device))
        torch.nn.init.xavier_uniform_(self.b2.data)
        self.loss = torch.nn.BCELoss()
        self.accuracy = BinaryAccuracy()
    def forward(self, inputs):
        return torch.sigmoid(torch.matmul(torch.sigmoid(torch.matmul(inputs, self.W1) + self.b1), self.W2) + self.b2)
    def train(self, inputs, outputs, N_max = 1000, alpha = 1, beta1 = 0.9, beta2 = 0.999, \
              batch_size = 32, lambda_val = 1e-3):
        dataset = torch.utils.data.TensorDataset(inputs, outputs)
        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)
        optimizer.zero_grad()
        self.loss_history = []
        for iteration_number in range(1, N_max + 1):
            for batch in data_loader:
                inputs_batch, outputs_batch = batch
                total_loss = self.loss(self(inputs_batch), outputs_batch.to(torch.float64))\
                    + lambda_val*sum(torch.abs(param).sum() for param in self.parameters()).item()
                self.loss_history.append(total_loss)
                total_loss.backward()
                optimizer.step()
                optimizer.zero_grad()
            if(iteration_number % (N_max//20) == 1):
                pred = self(inputs)
                acc_val = self.accuracy(pred, outputs).item()
                print("Iteration {} - Loss = {} - Accuracy = {}".format(iteration_number, total_loss, acc_val))
```

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 in research to demonstrate concepts, such as **MNIST** or **CIFAR-10**.

- For more details on the available **built-in datasets** in Pytorch, have a look at the following page: https://pytorch.org/vision/stable/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 output classes (bag, shirt, etc.) are indexed with 0-9 values, corresponding to the 10 types of fashion objects found in the dataset.

```
# Dictionary of labels and their identification
labels_map = {0: "T-Shirt",
              1: "Trouser",
              2: "Pullover",
              3: "Dress",
              4: "Coat",
              5: "Sandal",
              6: "Shirt",
              7: "Sneaker",
              8: "Bag",
              9: "Ankle Boot"}
```

```
# Define folder path as string
# Dataset will be downloaded and stored there.
folder_path = "./data"

# Download (download = True) training data (train = True)
# to folder specified in root parameter.
# The transform parameter specifies that the image samples will
# be converted to Tensors, ready to be used by models.
training_data = datasets.FashionMNIST(root = folder_path, \
                                      train = True, \
                                      download = True, \
                                      transform = ToTensor())
```

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 output classes (bag, shirt, etc.) are indexed with 0-9 values, corresponding to the 10 types of fashion objects found in the dataset.

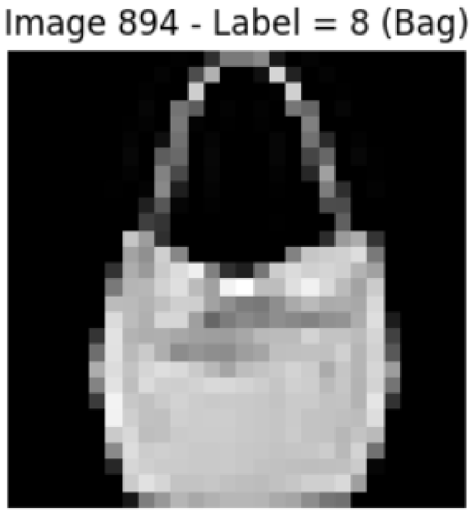
```
# Dataset contains 60000 samples, that are greyscale
# images with size 28 by 28 pixels.
print(training_data.data.shape)
```

```
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
```

```
# Display sample
sample_index = 894
img, label = training_data[sample_index]
plt.figure(figsize = (3, 3))
plt.axis("off")
plt.imshow(img.squeeze(), cmap="gray")
plt.title("Image {} - Label = {} ({})".format(sample_index, \
                                              label, \
                                              labels_map[label]))
plt.show()
```



Writing a custom Dataset object

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 company, 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

A look at our dataset Excel file

	A	B	C	D	E	F	G	H	I	J	K	
1	Lot Area	Overall Qual	Overall Cond	Year Built	Year Remod/Add	Total Bsmt SF	1st Flr SF	2nd Flr SF	Gr Liv Area	Full Bath	Half Bath	Bedro
2	31770	6	5	1960	1960	1080	1656	0	1656	1	0	
3	11622	5	6	1961	1961	882	896	0	896	1	0	
4	14267	6	6	1958	1958	1329	1329	0	1329	1	1	
5	11160	7	5	1968	1968	2110	2110	0	2110	2	1	
6	13830	5	5	1997	1998	928	928	701	1629	2	1	
7	9978	6	6	1998	1998	926	926	678	1604	2	1	
8	4920	8	5	2001	2001	1338	1338	0	1338	2	0	
9	5005	8	5	1992	1992	1280	1280	0	1280	2	0	
10	5389	8	5	1995	1996	1595	1616	0	1616	2	0	
11	7500	7	5	1999	1999	994	1028	776	1804	2	1	
12	10000	6	5	1993	1994	763	763	892	1655	2	1	
13	7980	6	7	1992	2007	1168	1187	0	1187	2	0	
14	8402	6	5	1998	1998	789	789	676	1465	2	1	
15	10176	7	5	1990	1990	1300	1341	0	1341	1	1	
16	6820	8	5	1985	1985	1488	1502	0	1502	1	1	
17	53504	8	5	2003	2003	1650	1690	1589	3279	3	1	
18	12134	8	7	1988	2005	559	1080	672	1752	2	0	
19	11394	9	2	2010	2010	1856	1856	0	1856	1	1	
20	19138	4	5	1951	1951	864	864	0	864	1	0	
21	13175	6	6	1978	1988	1542	2073	0	2073	2	0	
22	11751	6	6	1977	1977	1844	1844	0	1844	2	0	
23	10625	7	6	1974	1974	1053	1173	0	1173	2	0	

Writing a custom Dataset object

- 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, and many 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 AI models for predicting house prices, based on various house 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.

Writing a custom Dataset object

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 Flr SF**: The first floor surface, in square feet.
- **2nd Flr 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.

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 learn it, it will definitely serve you in the long run!*

https://pandas.pydata.org/docs/user_guide/10min.html)

```python
# 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  \
0     31770             6             5        1960            1960
1     11622             5             6        1961            1961
2     14267             6             6        1958            1958
3     11160             7             5        1968            1968
4     13830             5             5        1997            1998

   Total Bsmt SF  1st Flr SF  2nd Flr SF  Gr Liv Area  Full Bath  Half Bath  \
0           1080        1656           0         1656          1          0
1            882         896           0          896          1          0
2           1329        1329           0         1329          1          1
3           2110        2110           0         2110          2          1
4            928         928         701         1629          2          1

   Bedroom AbvGr  Kitchen AbvGr  TotRms AbvGrd  Garage Area  Yr Sold  \
0              3              1              7          528     2010
1              2              1              5          730     2010
2              3              1              6          312     2010
3              3              1              8          522     2010
4              3              1              6          482     2010

   SalePrice
0     215000
1     105000
2     172000
3     244000
4     189900
```

Writing a custom Dataset object

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**.

```python
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)
```

Writing a custom Dataset object

The __getitem__() and __len__() special methods will allow for **indexing** the dataset object.

- Later on, we could ask for the sample #286 using the square bracket notation, as shown on side.

```python
# Instantiate the dataset
ames_dataset = AmesHousingDataset('./ames/AmesHousing.xlsx')

# Fetch sample with index 286
sample_input, sample_output = ames_dataset[286]
# Input is a (16,) numpy array, with the following values
print(type(sample_input), sample_input.shape)
print(sample_input)
# Output is a single value, of type numpy int64
print(type(sample_output), sample_output.shape)
print(sample_output)
```

```
<class 'numpy.ndarray'> (16,)
[6858    6    4 1915 1950  806  841  806 1647    1    1    4    1    6
  216 2010]
<class 'numpy.int64'> ()
128000
```

Similarly, the two special methods are all we need to make a **for loop** that uses the dataset object as the **generator** to be looped over!

More on the for loop later!

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**.

```python
# Instantiate the dataset
ames_dataset = AmesHousingDataset('./ames/AmesHousing.xlsx')

# Create a DataLoader for the dataset
ames_dataloader = torch.utils.data.DataLoader(ames_dataset, \
                                               batch_size = 32, \
                                               shuffle = True)
```

Writing a custom Dataloader

We can then use this custom Dataloader object as the generator in a **for** loop, to generate mini-batches of samples.

- Notice how this Dataloader generates **92** (i.e. 2928/32, rounded up) **batches** of **32 samples**.
- With the exception of the **last batch** (with index 91), that only contains **16 samples** (that is 2928 % 32).

```python
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])
```

Writing a custom Dataloader

We can then use this custom Dataloader object as the generator in a **for** loop, to generate mini-batches of samples.

- **Good practice:** the custom Dataset and custom Dataloader definition should be repeated to generate **training**, **testing** and **validation sets dataloaders**.
- These Dataloaders will then be given to our **trainer** function.

```python
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])
```

Introducing the MNIST dataset

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, which allows for efficient implementations of ML/DL algorithms.

Introducing the MNIST dataset

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

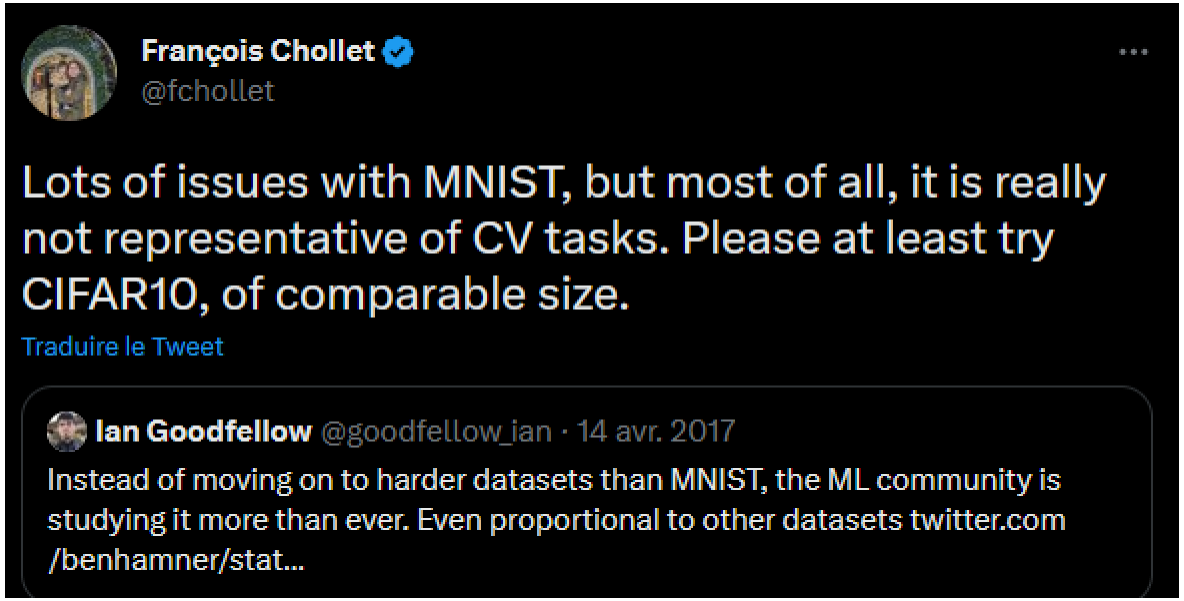
It consists of

- 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**.

For now, however, this will do.



Introducing the MNIST dataset

Nevertheless, 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 algorithms.

- 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

```python
# Define transform to convert images to tensors and normalize them
transform_data = Compose([ToTensor(),
                          Normalize((0.1307,), (0.3081,))])

# Load the data
batch_size = 64
train_dataset = MNIST(root='./mnist/', train = True, download = True, transform = transform_data)
test_dataset = MNIST(root='./mnist/', train = False, download = True, transform = transform_data)
train_loader = torch.utils.data.DataLoader(train_dataset, batch_size = batch_size, shuffle = True)
test_loader = torch.utils.data.DataLoader(test_dataset, batch_size = batch_size, shuffle = False)
```

```python
# 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])
```

Introducing the MNIST dataset

Good practice: always normalize your input data!

In general, do the following:

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

In MNIST, we will then subtract a mean of 0.1307 and divide by a standard deviation of 0.3081.

These values are the original mean and standard deviation of the dataset before normalization!

```
# Define transform to convert images to tensors and normalize them
transform_data = Compose([ToTensor(),
                          Normalize((0.1307,), (0.3081,))])
```

Writing the MNIST Dataset and Dataloader

```
# Define transform to convert images to tensors and normalize them
transform_data = Compose([ToTensor(),
                          Normalize((0.1307,), (0.3081,))])

# Load the data
batch_size = 64
train_dataset = MNIST(root='./mnist/', train = True, download = True, transform = transform_data)
test_dataset = MNIST(root='./mnist/', train = False, download = True, transform = transform_data)
train_loader = torch.utils.data.DataLoader(train_dataset, batch_size = batch_size, shuffle = True)
test_loader = torch.utils.data.DataLoader(test_dataset, batch_size = batch_size, shuffle = False)
```

```
# 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

Recall (Binary classification probabilities as output):

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

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

From binary to multi-class classification

Problem (How could we produce multi-class classification probabilities for all possible $N > 2$ classes as outputs?):

Unfortunately, when we have more than 2 classes, **we can no longer rely on a single output value $\boldsymbol{p}$**.

- Instead, it is often preferable to have the model output **10 values**:

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

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

From binary to multi-class classification

Unfortunately, this is not good enough.

- The p_i are **probabilities** and **their sum should therefore be equal to 1**, i.e.

$$\sum_{i=0}^{9} p_i = 1$$

A **fully connected layer** $(WX + b)$ cannot do that on its own, as it might produce negative values as probabilities p_i, and those 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.

It has two effects:

- It will force the values of the p_i to fall in the range of [0, 1].
- It will force their sum to be equal to 1, that is

$$\sum_{i=0}^{9} p_i = 1$$

Softmax function

Definition (the softmax function):

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

$$Y = (y_0, y_1, y_2, \dots y_K),$$

into another vector of N values

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

The new vector $\boldsymbol{P}$ **is guaranteed to contain positive values summing up to 1**, i.e.

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

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, i.e.:

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

Softmax function

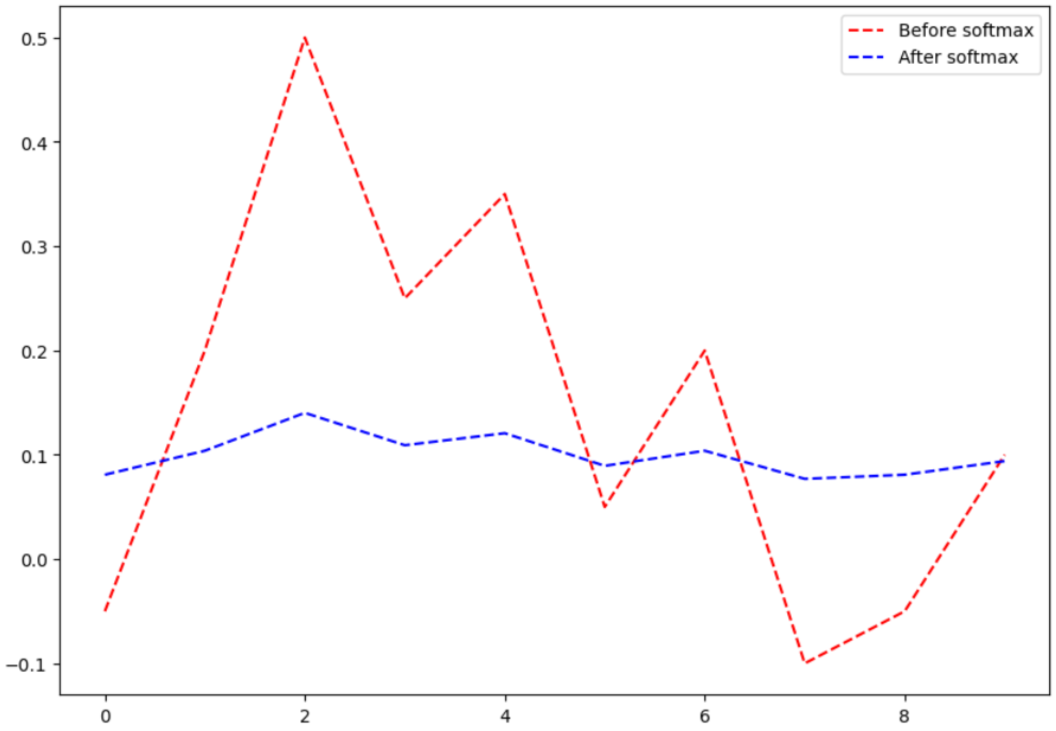
Softmax can be manually implemented as:

```python
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)
```

```python
# Ten values that do not sum up to 1
Y = np.array([-1, 4, 10, 5, 7, 1, 4, -2, -1, 2])/20
print(sum(Y))
P = softmax(Y)
print(P)
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]
0.9999999999999999
```

Softmax effect: It will rescale values so that the trend is preserved, but the new vector consists of positive values that sum up to 1.



Softmax function and prediction

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 positive values,

$$P = (p_0, p_1, p_2, \ldots p_9),$$

Which can be used as the **probabilities for sample of being of class $\boldsymbol{i}$.**

The **predicted class according to the model** is then defined as the variable $\boldsymbol{pred}$, corresponding to the index i of the highest probability value p_i, i.e.:

$$pred = \arg\max_i [p_i] \,.$$

Softmax function and prediction

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

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

No final softmax 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 ($= 28 \times 28$).

```python
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)
        x = x.view(x.size(0), -1)
        # First Wx + b operation
        out1 = self.fc1(x)
        # Using ReLU operation as activation after first layer
        act1 = torch.relu(out1)
        # Second Wx + b operation anbd return
        out2 = self.fc2(act1)
        return out2
```

Softmax function

Consider a neural network model, with **784 input size**, **128 hidden size**, and **10 output size**, eventually transferring the model to a device (CPU/CUDA).

- 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))
data, target = sample
print(data.shape)
print(target.shape)
data1 = data[0].to(device)
target1 = target[0].to(device)
print(data1.shape)
print(target1)

# Forward pass
out2 = model(data1)
act2 =  torch.nn.functional.softmax(out2, dim = 1)
print(out2)
print(act2)
print(act2.sum())
```

```
torch.Size([64, 1, 28, 28])
torch.Size([64])
torch.Size([1, 28, 28])
tensor(4, device='cuda:0')
tensor([[-0.2145, -0.0527, -0.1197, -0.0488,  0.2503, -0.1870, -0.1401,  0.1202,
          0.1220,  0.1017]], device='cuda:0', grad_fn=<AddmmBackward0>)
tensor([[0.0812, 0.0954, 0.0892, 0.0958, 0.1292, 0.0834, 0.0874, 0.1134, 0.1136,
         0.1113]], device='cuda:0', grad_fn=<SoftmaxBackward0>)
tensor(1., device='cuda:0', grad_fn=<SumBackward0>)
```

Softmax function

- Next, perform a forward pass through the model, storing the **output** in the variable **out2**.
- Apply the **softmax** operation on **out2**. PyTorch offers a functional implmentation of the softmax:

torch.nn.functional.softmax()

- We can then verify that **softmax will adjust the output of the neural network correctly**.

```python
# 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)
target1 = target[0].to(device)
print(data1.shape)
print(target1)

# Forward pass
out2 = model(data1)
act2 =  torch.nn.functional.softmax(out2, dim = 1)
print(out2)
print(act2)
print(act2.sum())
```

```
torch.Size([64, 1, 28, 28])
torch.Size([64])
torch.Size([1, 28, 28])
tensor(4, device='cuda:0')
tensor([[-0.2145, -0.0527, -0.1197, -0.0488,  0.2503, -0.1870, -0.1401,  0.1202,
          0.1220,  0.1017]], device='cuda:0', grad_fn=<AddmmBackward0>)
tensor([[0.0812, 0.0954, 0.0892, 0.0958, 0.1292, 0.0834, 0.0874, 0.1134, 0.1136,
         0.1113]], device='cuda:0', grad_fn=<SoftmaxBackward0>)
tensor(1., device='cuda:0', grad_fn=<SumBackward0>)
```

Forward implementation

Our model is however implementing the same forward method as before.

In fact, we will not use the softmax operation as the final activation function in the forward method.

This is normal as **the softmax operation** will be applied **in the loss function instead**, that is the **cross_entropy() function**, which will be summoned in the **trainer**() later.

```python
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)
        x = x.view(x.size(0), -1)
        # First Wx + b operation
        out1 = self.fc1(x)
        # Using ReLU operation as activation after first layer
        act1 = torch.relu(out1)
        # Second Wx + b operation anbd return
        out2 = self.fc2(act1)
        return out2
```

From binary cross entropy...

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

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

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

How does the loss function change now that we have $N > 2$ classes?

…To multi-class cross entropy!

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

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

In the formula above, $p_i(x_k)$ denotes the **probability for sample $\boldsymbol{x_k}$ of being of class $\boldsymbol{i}$**.

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 to the output $\boldsymbol{o_i}$ of the forward method of the model**.

...To multi-class cross entropy!

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

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

Similarly, 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 $y_k = 2$, we have:

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

We say that Y_k is the **one-hot vector** for the sample k with class 2.

Setting a model in train/eval 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

```python
# Training model
num_epochs = 5
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)
        # Compute loss
        loss = torch.nn.functional.cross_entropy(outputs, labels)
        # Backward and optimize
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        # Display
        if (i+1) % 300 == 0:
            print (f'Epoch [{epoch+1}/{num_epochs}], Step [{i+1}/{len(train_loader)}], Loss: {loss.item():.4f}')
```

```
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
Epoch [4/5], Step [600/938], Loss: 0.0339
```

Eval mode and accuracy after training

After training, we will evaluate our trained model to check its accuracy on test set.

- 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).
- **97% accuracy = a rather nicely trained model!**

```python
# 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)
        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
        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**.

Definition (Deep Neural Networks):

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

To demonstrate, 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**.

It is now time…

In general, **it is good practice to have the size of layers decrease progressively by a factor of at least 2**.

- the first layer has inputs size 784 and outputs size 80,
- the second layer has inputs size 80 and outputs size 40,
- the third layer has inputs size 40 and outputs size 20,
- and the fourth layer has inputs size 20 and outputs size 10, matching the number of classes in the dataset.

Note: a layer-by-layer model summary can be seen by printing the model object!

```
print(model)
```

```
DeepNeuralNet(
  (layer1): DenseReLU(
    (fc): Linear(in_features=784, out_features=80, bias=True)
  )
  (layer2): DenseReLU(
    (fc): Linear(in_features=80, out_features=40, bias=True)
  )
  (layer3): DenseReLU(
    (fc): Linear(in_features=40, out_features=20, bias=True)
  )
  (layer4): DenseNoReLU(
    (fc): Linear(in_features=20, out_features=10, bias=True)
  )
```

Creating blocks

Good practice: create building blocks for modularity.

- 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.

Important note: not using softmax as final activation, for the same reasons as before.

```python
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))
```

```python
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** blocks,
- And one **DenseNoReLU** block.

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, using the following steps:

- The input image is flattened, transforming a 2D tensor image into a 1D tensor,
- It is then passed through the combined layers/blocks we have assembled in Sequential().

```python
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
```

```python
# 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

Good practice: This modular approach, which

- **Defines blocks of layers,**
- And eventually **assembles them in a larger Deep Neural Network network**,

is very common in deep neural networks, especially when the architectures are very heavy and include many layers.

Helps to organize the mess!

```
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
num_epochs = 10
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)
        # Compute loss
        loss = torch.nn.functional.cross_entropy(outputs, labels)
        # Backward and optimize
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        # Display
        if (i+1) % 25 == 0:
            print (f'Epoch [{epoch+1}/{num_epochs}], Step [{i+1}/{len(train_loader)}], Loss: {loss.item():.4f}')
```

```
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
Epoch [2/10], Step [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 the dataset.
- In general, deep neural networks with many layers (tens or even hundreds) 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**.

Another No Free Lunch: 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. It 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)

```python
# 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)
        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
        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: 0.9649
```

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

```python
# 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)
        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
        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}')
```

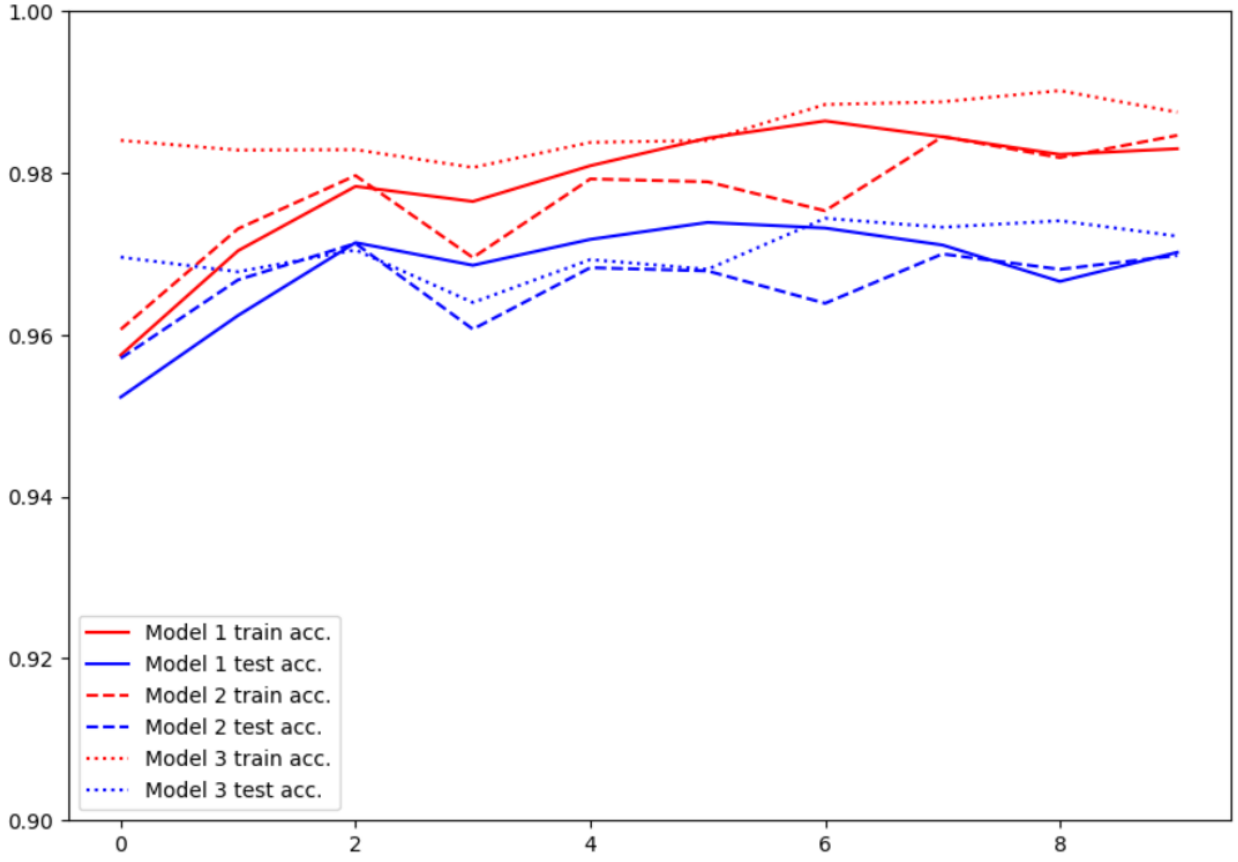
```
Evaluation after training, test accuracy: 0.9367
```

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!



Important lesson: Larger and deeper network does not necessarily mean better performance!

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

Project announcement!

Let us discuss it now.