We are starting at 14:00!

Grab a seat and get ready

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#1 Basics and Pytorch

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Agenda

14:00 - 16:00: The basics of Pytorch

16:00 - 16:30: Break

16:30 - 17:30: Neural Network

17:30 - 18:00: Challenges & Next steps

Pytorch Basics

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Pytorch

- Numpy
  - on a GPU
  - with all kinds of ANN related things
  - with a focus on tensors
  - and automatic differentiation

Alternatives to pytorch

- Tensorflow - strength in commercial applications
- JAX - strength in flexibility
- Matlab

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DL in Numpy

```python
import numpy as np

# Define sigmoid activation function and its derivative
def sigmoid(x):
    return 1 / (1 + np.exp(-x))

def sigmoid_derivative(x):
    return x * (1 - x)

# Define the NaiveNet class
class NaiveNet:
    def __init__(self, input_size, hidden_size, output_size):
        # Initialize weights and biases with random values
        self.weights_input_hidden = np.random.rand(input_size, hidden_size)
        self.bias_hidden = np.zeros((1, hidden_size))
        self.weights_hidden_output = np.random.rand(hidden_size, output_size)
        self.bias_output = np.zeros((1, output_size))

    def forward(self, inputs):
        # Forward propagation
        self.hidden_input = np.dot(inputs, self.weights_input_hidden) + self.bias_hidden
        self.hidden_output = sigmoid(self.hidden_input)
        self.final_input = np.dot(self.hidden_output, self.weights_hidden_output) + self.bias_output
        self.final_output = sigmoid(self.final_input)
        return self.final_output

    def backward(self, inputs, targets, learning_rate):
        # Backpropagation
        error = targets - self.final_output
        delta_output = error * sigmoid_derivative(self.final_output)

        error_hidden = delta_output.dot(self.weights_hidden_output.T)
        delta_hidden = error_hidden * sigmoid_derivative(self.hidden_output)

        self.weights_hidden_output += self.hidden_output.T.dot(delta_output) * learning_rate
        self.bias_output += np.sum(delta_output, axis=0, keepdims=True) * learning_rate
        self.weights_input_hidden += inputs.T.dot(delta_hidden) * learning_rate
        self.bias_hidden += np.sum(delta_hidden, axis=0, keepdims=True) * learning_rate
```

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DL in Pytorch

```
class NaiveNet(nn.Module):
  # Define the structure of your network
  def __init__(self):
    super(NaiveNet, self).__init__()

    # The network is defined as a sequence of operations
    self.layers = nn.Sequential(
        nn.Linear(2, 16),
        nn.ReLU(),
        nn.Linear(16, 2),
    )

  # Specify the computations performed on the data
  def forward(self, x):
    # Pass the data through the layers
    return self.layers(x)
```

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Everything in pytorch are tensors: how to make one

A `torch.Tensor` is a multi-dimensional (or n-dimensional) matrix containing elements of a single data type.

```
# tensor from a list
a = torch.tensor([0, 1, 2])

#tensor from a tuple of tuples
b = ((1.0, 1.1), (1.2, 1.3))
b = torch.tensor(b)

# tensor from a numpy array
c = np.ones([2, 3])
c = torch.tensor(c)
```

More tensors: common constructors

```
x = torch.ones(5, 3)
y = torch.zeros(2)
z = torch.empty(1, 1, 5)
```

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Making random tensors

```
# Uniform distribution
a = torch.rand(1, 3)

# Normal distribution
b = torch.randn(3, 4)
```

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Ranges in pytorch - just like in numpy

```
a = torch.arange(0, 10, step=1)
b = np.arange(0, 10, step=1)

c = torch.linspace(0, 5, steps=11)
d = np.linspace(0, 5, num=11)
```

Copying Tensors

As with any object in Python, assigning a tensor to a variable makes the variable a label of the tensor, and does not copy it (create a copy of it). For example:

```
a = torch.ones(2, 2)
b = a

a[0][1] = 561  # we change a...
print(b)       # ...and b is also altered
```

Out:

```
tensor([[  1., 561.],
        [  1.,   1.]])
```

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Practice

Make a couple of Tensors

(10 minutes max)

[Coding Exercise 2.1]

What can we do with tensors?

Everything we do with numpy otherwise.

```
# this only works if c and d already exist
torch.add(a, b, out=c)

# Pointwise Multiplication of a and b
torch.multiply(a, b, out=d)
```

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By default everything is pointwise

```
x + y, x - y, x * y, x / y, x**y  # The `**` is the exponentiation operator
```

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Sums, means etc

Just like in numpy

```
print(f"Sum of every element of x: {x.sum()}")
print(f"Sum of the columns of x: {x.sum(axis=0)}")
print(f"Sum of the rows of x: {x.sum(axis=1)}")
```

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Practice

Do a few things with Tensors

(10 minutes max)

[Coding Exercise 2.2]

Manipulating tensors: indexing

```
x = torch.arange(0, 10)
print(x)
print(x[-1])
print(x[1:3])
print(x[:-2])
```

```
tensor([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
tensor(9)
tensor([1, 2])
tensor([0, 1, 2, 3, 4, 5, 6, 7])
```

Similar logic as numpy for n-dimensional tensors

```python
# make a 5D tensor
x = torch.rand(1, 2, 3, 4, 5)

print(f" shape of x[0]:{x[0].shape}")
print(f" shape of x[0][0]:{x[0][0].shape}")
print(f" shape of x[0][0][0]:{x[0][0][0].shape}")
```

```
 shape of x[0]:torch.Size([2, 3, 4, 5])
 shape of x[0][0]:torch.Size([3, 4, 5])
 shape of x[0][0][0]:torch.Size([4, 5])
```

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Flattening/ Reshaping

```
z = torch.arange(12).reshape(6, 2)
print(f"Original z: \n {z}")

# 2D -> 1D
z = z.flatten()
print(f"Flattened z: \n {z}")
```

```
Original z:
 tensor([[ 0,  1],
        [ 2,  3],
        [ 4,  5],
        [ 6,  7],
        [ 8,  9],
        [10, 11]])
Flattened z:
 tensor([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11])
```

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Reshaping

```python
# and back to 2D
z = z.reshape(3, 4)
print(f"Reshaped (3x4) z: \n {z}")
```

```
Reshaped (3x4) z:
 tensor([[ 0,  1,  2,  3],
        [ 4,  5,  6,  7],
        [ 8,  9, 10, 11]])
```

Irrelevant dimensions

```
x = torch.randn(1, 10)
# printing the zeroth element of the tensor will not give us the first number!

print(x.shape)
print(f"x[0]: {x[0]}")
```

```
torch.Size([1, 10])
x[0]: tensor([ 0.7274, -0.1908,  1.1524,  0.0241,  0.7664,  1.0263, -1.2895,  0.2036,
         0.5379, -0.7962])
```

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Squeezing

```python
# Let's get rid of that singleton dimension and see what happens now
x = x.squeeze(0)
print(x.shape)
print(f"x[0]: {x[0]}")
```

```
torch.Size([10])
x[0]: 0.7273916602134705
```

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Dimension permutation

E.g. going from RGB in dimension 1 to in dimension 3

```
# `x` has dimensions [color,image_height,image_width]
x = torch.rand(3, 48, 64)

# We want to permute our tensor to be [ image_height , image_width , color ]
x = x.permute(1, 2, 0)
# permute(1,2,0) means:
# The 0th dim of my new tensor = the 1st dim of my old tensor
# The 1st dim of my new tensor = the 2nd
# The 2nd dim of my new tensor = the 0th
print(x.shape)
```

```
torch.Size([48, 64, 3])
```

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Concatenation

```python
# Create two tensors of the same shape
x = torch.arange(12, dtype=torch.float32).reshape((3, 4))
y = torch.tensor([[2.0, 1, 4, 3], [1, 2, 3, 4], [4, 3, 2, 1]])

# Concatenate along rows
cat_rows = torch.cat((x, y), dim=0)

# Concatenate along columns
cat_cols = torch.cat((x, y), dim=1)

# Printing outputs
print('Concatenated by rows: shape{} \n {}'.format(list(cat_rows.shape), cat_rows))
print('\n Concatenated by colums: shape{}  \n {}'.format(list(cat_cols.shape), cat_cols))
```

```
Concatenated by rows: shape[6, 4]
 tensor([[ 0.,  1.,  2.,  3.],
        [ 4.,  5.,  6.,  7.],
        [ 8.,  9., 10., 11.],
        [ 2.,  1.,  4.,  3.],
        [ 1.,  2.,  3.,  4.],
        [ 4.,  3.,  2.,  1.]])

 Concatenated by colums: shape[3, 8]
 tensor([[ 0.,  1.,  2.,  3.,  2.,  1.,  4.,  3.],
        [ 4.,  5.,  6.,  7.,  1.,  2.,  3.,  4.],
        [ 8.,  9., 10., 11.,  4.,  3.,  2.,  1.]])
```

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torch and numpy are friends

```
x = torch.randn(5)
print(f"x: {x}  |  x type:  {x.type()}")

y = x.numpy()
print(f"y: {y}  |  y type:  {type(y)}")

z = torch.tensor(y)
print(f"z: {z}  |  z type:  {z.type()}")
```

```
x: tensor([ 0.5728,  0.6117,  1.1747, -2.2578, -0.0359])  |  x type:  torch.FloatTensor
y: [ 0.5728153   0.61165035  1.1746601  -2.2578378  -0.0358642 ]  |  y type:  <class 'numpy.ndarray'>
z: tensor([ 0.5728,  0.6117,  1.1747, -2.2578, -0.0359])  |  z type:  torch.FloatTensor
```

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Practice

Do the tensor manipulation exercise

Trust me, these "easy" things are where the errors often happen

Coding Exercise 2.3

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Graphics cards: using GPUs

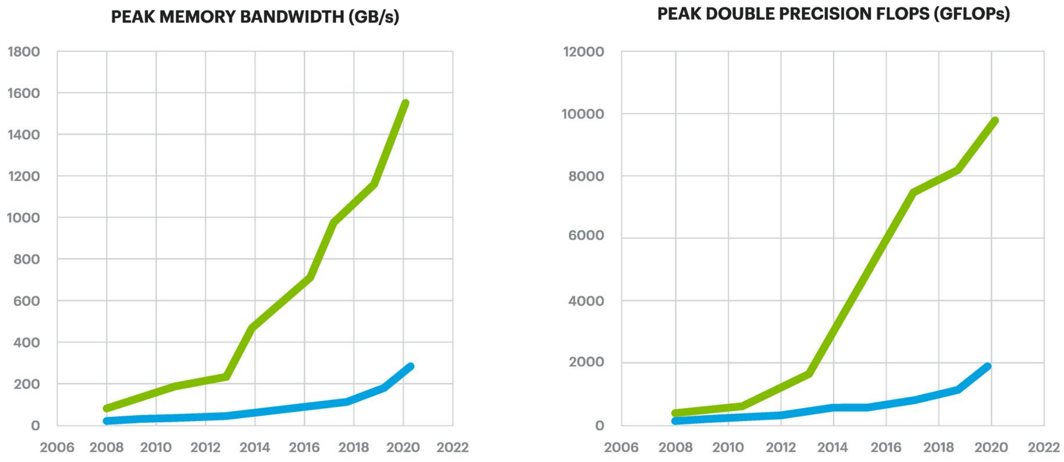

Figure 2. Comparison of evolution of memory bandwidth (left) and double precision flops (right) on GPU and CPU

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Ask torch where a variable is

```
x = torch.randn(10)
print(x.device)
```

```
cpu
```

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Ask torch if we have a GPU

```
print(torch.cuda.is_available())
```

```
True
```

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Specifying devices

```python
# common device agnostic way of writing code that can run on cpu OR gpu
# that we provide for you in each of the tutorials
DEVICE = set_device()

# we can specify a device when we first create our tensor
x = torch.randn(2, 2, device=DEVICE)
print(x.dtype)
print(x.device)

# we can also use the .to() method to change the device a tensor lives on
y = torch.randn(2, 2)
print(f"y before calling to() | device: {y.device} | dtype: {y.type()}")

y = y.to(DEVICE)
print(f"y after calling to() | device: {y.device} | dtype: {y.type()}")
```

```
torch.float32
cuda:0
y before calling to() | device: cpu | dtype: torch.FloatTensor
y after calling to() | device: cuda:0 | dtype: torch.cuda.FloatTensor
```

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Device matters: no mix and match

We can not just mix and match devices - it would be undefined where the computation happens

```
x = torch.tensor([0, 1, 2], device=DEVICE)
y = torch.tensor([3, 4, 5], device="cpu")

z = x + y
```

```
---------------------------------------------------------------------------
RuntimeError                              Traceback (most recent call last)
<ipython-input-27-3ae8fe7d9873> in <cell line: 4>()
      2 y = torch.tensor([3, 4, 5], device="cpu")
      3
----> 4 z = x + y

RuntimeError: Expected all tensors to be on the same device, but found at least two devices, cuda:0 and cpu!
```

SEARCH STACK OVERFLOW

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Moving CPU<->GPU is easy

```python
x = torch.tensor([0, 1, 2], device=DEVICE)
y = torch.tensor([3, 4, 5], device="cpu")
z = torch.tensor([6, 7, 8], device=DEVICE)

# moving to cpu
x = x.to("cpu")  # alternatively, you can use x = x.cpu()
print(x + y)

# moving to gpu
y = y.to(DEVICE)  # alternatively, you can use y = y.cuda()
print(y + z)
```

```
tensor([3, 5, 7])
tensor([ 9, 11, 13], device='cuda:0')
```

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Practice

Test the GPU effect

I promise you GPUs are faster

[Coding Exercise 2.4]

Datasets

Data

+

Model

+

Training

=

DL system

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Doing data - basics

- Data science =
- 50% figure out the question you want to answer
- 35% sweat the data
- 10% ML
- 5% glorious DL

How to get data

A lot of data is easy to load for our DL experiments

```
# Download and load the images from the CIFAR10 dataset
cifar10_data = datasets.CIFAR10(
    root="data",            # path where the images will be stored
    download=True,          # all images should be downloaded
    transform=ToTensor()  # transform the images to tensors
)
```

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Practice

Display the CIFAR image

Let us look into this

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Data

- Data is not made in heaven
- Data is made to answer questions
- We need to be agile with data
- When we try to answer questions we do not want to lie to ourselves

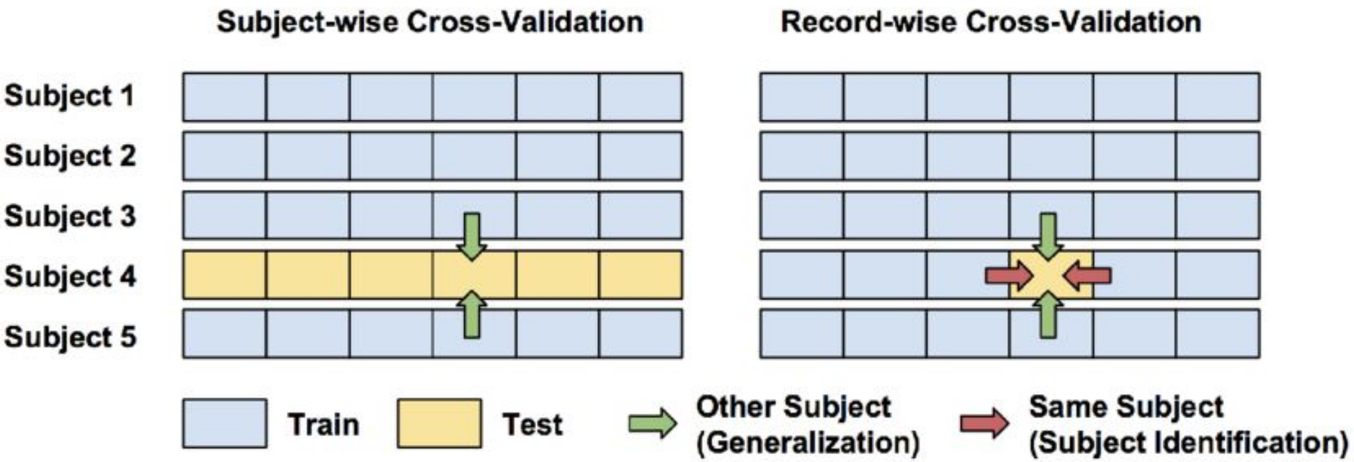
Let us not lie about data

- In DL we generally do prediction
- Caution with Causality
- The real world differs from our dataset (external validity)

Let us not lie about data: Validation

- Always have a validation/ Test set not used for training.
- Train on training set, test on test set
- For hyperparameter optimization you need to further divide the training set
- Match the cross-validation strategy to the use case

The cross-validation strategy must match the use case



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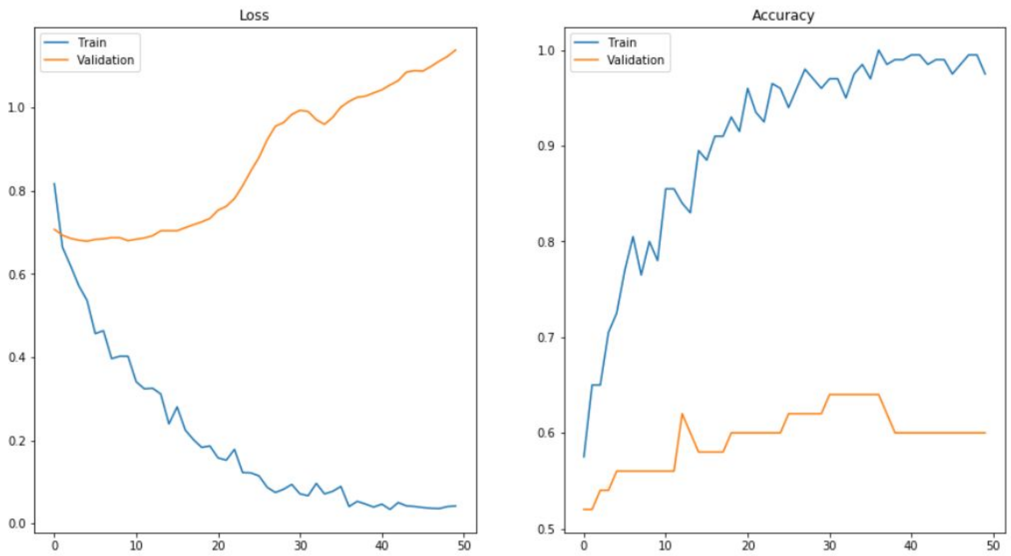
Overfitting! Validation set

- Don’t trust yourself
- Overfitting is massive for smaller datasets
- Ideally have a part of the dataset you don’t
- have access to
- Even some signs for *huge* datasets (imagenet)



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Always have both training and test data

```
# Load the training samples
training_data = datasets.CIFAR10(
    root="data",
    train=True,
    download=True,
    transform=ToTensor()
    )

# Load the test samples
test_data = datasets.CIFAR10(
    root="data",
    train=False,
    download=True,
    transform=ToTensor()
    )
```

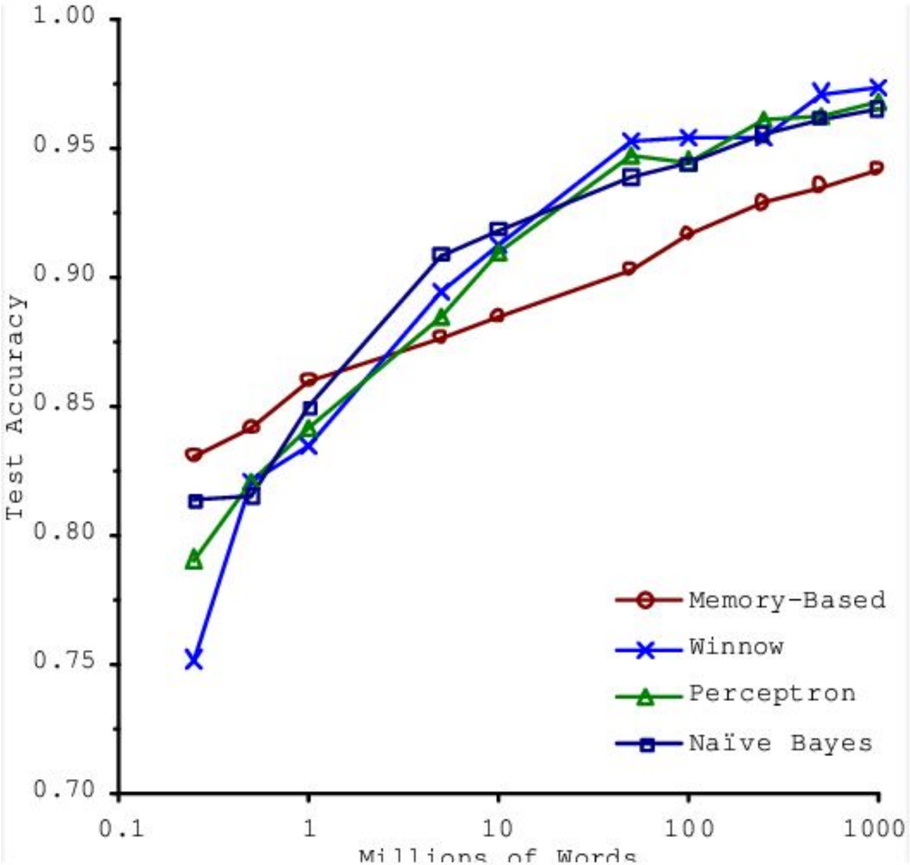
Practice

See how CIFAR train and test data are loaded

Let us load some data and divide into train and test dataset

[Coding Exercise 2.5]

More data is what it is all about



Transformations

More data = better learning

How to get more data?

Get more data

Transform the data

e.g. add color variation, etc.

Transformations are crucial across DL

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Data Loaders

- In practice we do not load all data.
- But small pieces (minibatches)
- For that we have a function that does the loading

```
# Create dataloaders with
train_dataloader = DataLoader(training_data, batch_size=64, shuffle=True)
test_dataloader = DataLoader(test_data, batch_size=64, shuffle=True)
```

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Practice

Load CIFAR images as grayscale

Practice transformation

Break

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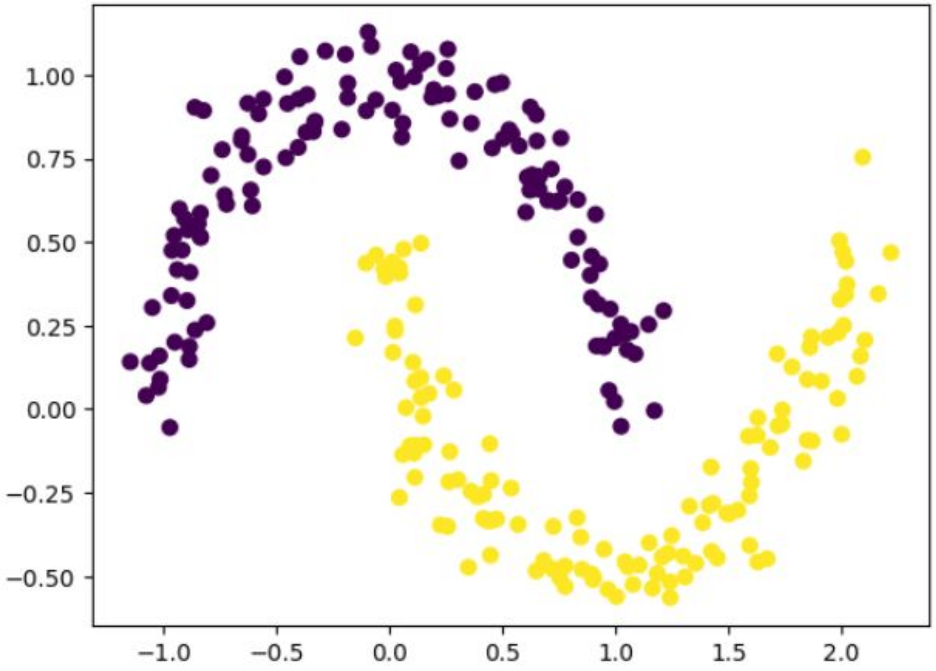
Neural Networks

Now, let us design a neural network

- (step 0) Get Data
- (step 1) All the variables and structures we need. We need to initialize them
- (step 2) And then we need to use these variables to define the compute in our network
- (step 3) And then we need gradients
- (step 4) And then we need to optimize
- (step 5) And then we need to test

Let us get the data from a csv file

Why? Because many real world datasets are in that format



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Practice

Load from csv and put on GPU into torch

Can you think of other datasets you could load this way?

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Let us see the anatomy of the network

First, we need to initialize the relevant variables

`__init__`

And then we need to specify how information travels through network

`forward`

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We will often need to make predictions

While many people just use `forward` we will separate it and use

```
predict
```

and then we need to

```
train
```

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With __init__ we make network structure

```
# Define the structure of your network
def __init__(self):
  super(NaiveNet, self).__init__()

  # The network is defined as a sequence of operations
  self.layers = nn.Sequential(
      nn.Linear(2, 16),
      nn.ReLU(),
      nn.Linear(16, 2),
  )
```

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The other components

```python
# Specify the computations performed on the data
def forward(self, x):
  # Pass the data through the layers
  return self.layers(x)

# Choose the most likely label predicted by the network
def predict(self, x):
  # Pass the data through the networks
  output = self.forward(x)

  # Choose the label with the highest score
  return torch.argmax(output, 1)

# Train the neural network (will be implemented later)
def train(self, X, y):
  pass
```

Practice

Run your first neural network

Check if it actually works and provides the outputs we expect

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Ok hold on. What has just happened

We have a neural network

It is initialized

It produces outputs

But these outputs are not better than chance yet!

Training = lots of small steps into good direction

```
# The Cross Entropy Loss is suitable for classification problems
loss_function = nn.CrossEntropyLoss()

# Create an optimizer (Stochastic Gradient Descent) that will be used to train the network
learning_rate = 1e-2
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate)

# Number of epochs
epochs = 15000
```

The anatomy of the training loop

```
for i in range(epochs):
  # Pass the data through the network and compute the loss
  y_logits = model.forward(X)
  loss = loss_function(y_logits, y)

  # Clear the previous gradients and compute the new ones
  optimizer.zero_grad()
  loss.backward()

  # Adapt the weights of the network
  optimizer.step()
```

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Practice

We give you code. What happens?

Train your network

Challenges & Next steps!

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Kahoot!

Any questions?

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THANKS

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coming soon
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