Deep Learning in Python

Lecture 1: PyTorch and Deep Neural Networks

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Outline

Hands-on course in Deep Learning using Python (PyTorch) with focus on computer vision.

Lecture 1	Deep Learning concepts and terminology. PyTorch commands, syntax and libraries (torch, torchvision). Building deep neural networks.
Lecture 2	Convolutional Neural Networks (CNN). Building CNN in PyTorch. Using GPUs with PyTorch.
Lecture 3	Optimisation: How to train and test neural networks robustly. Regularisation and hyper-parameter tuning.

Outline

1) Introduce concepts and aims

2) Become familiar with toolkit (PyTorch)

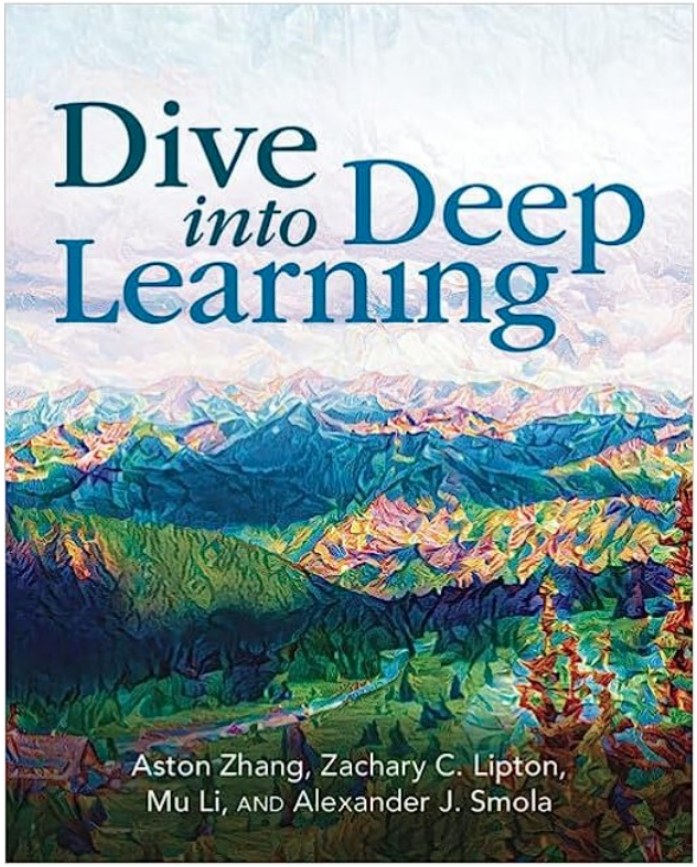
3) Combine 1 and 2 to build neural networks

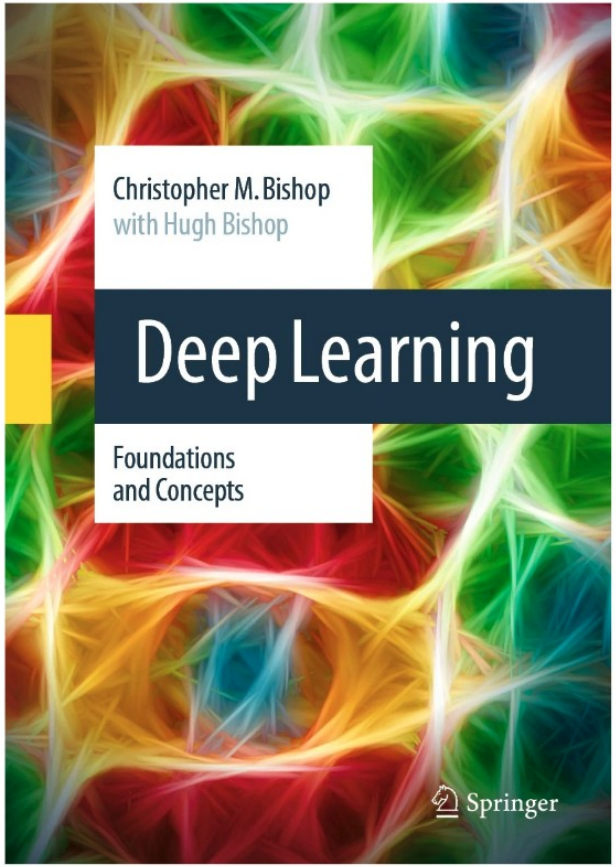
Preliminaries

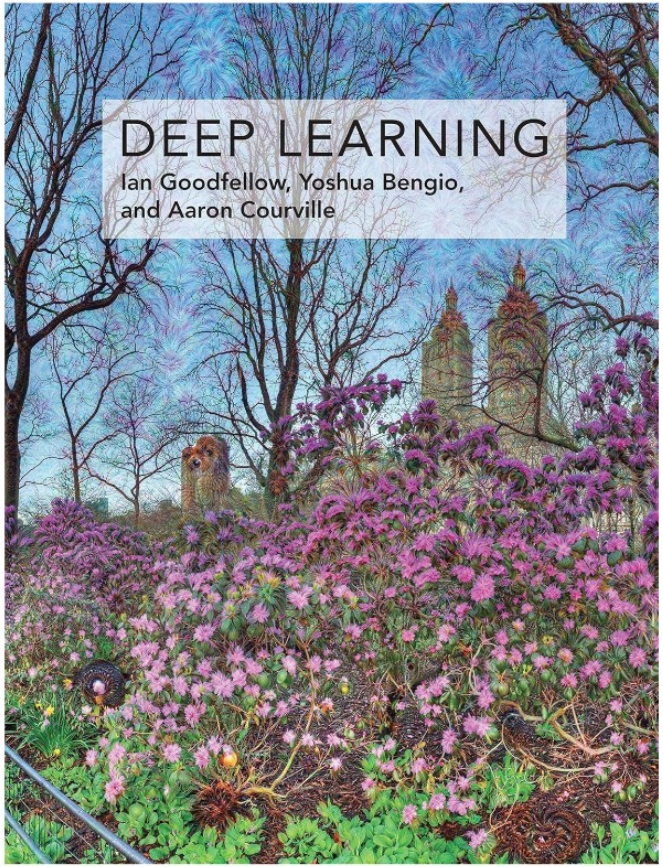
You should be familiar with

- Python3 programming (numpy, matplotlib)
- Jupyter notebooks (we run code on Google Colab)
- Basic Machine Learning and statistics terminology

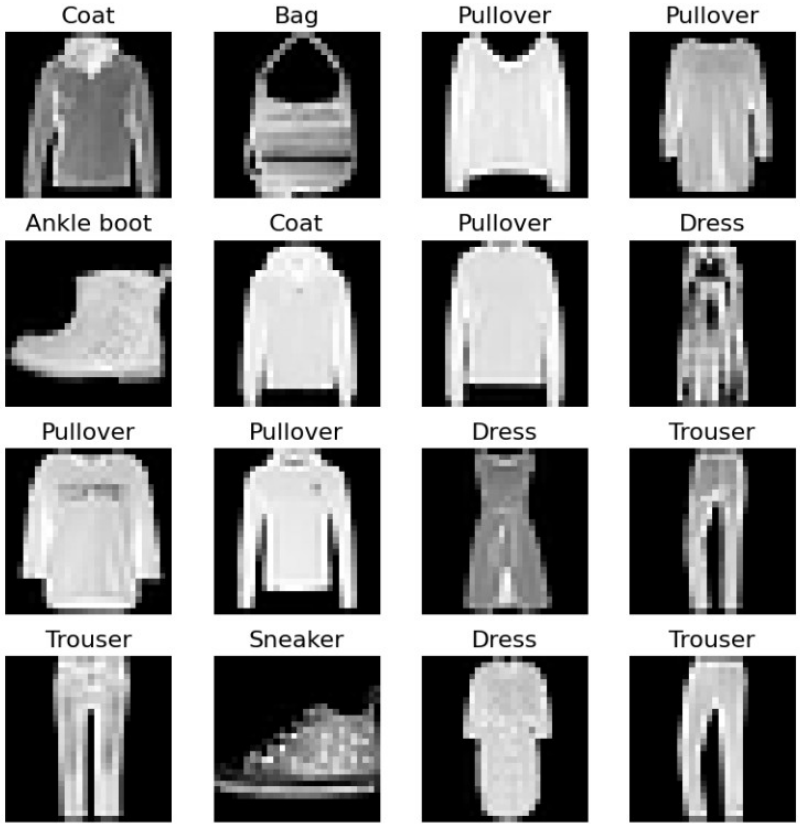
External resources





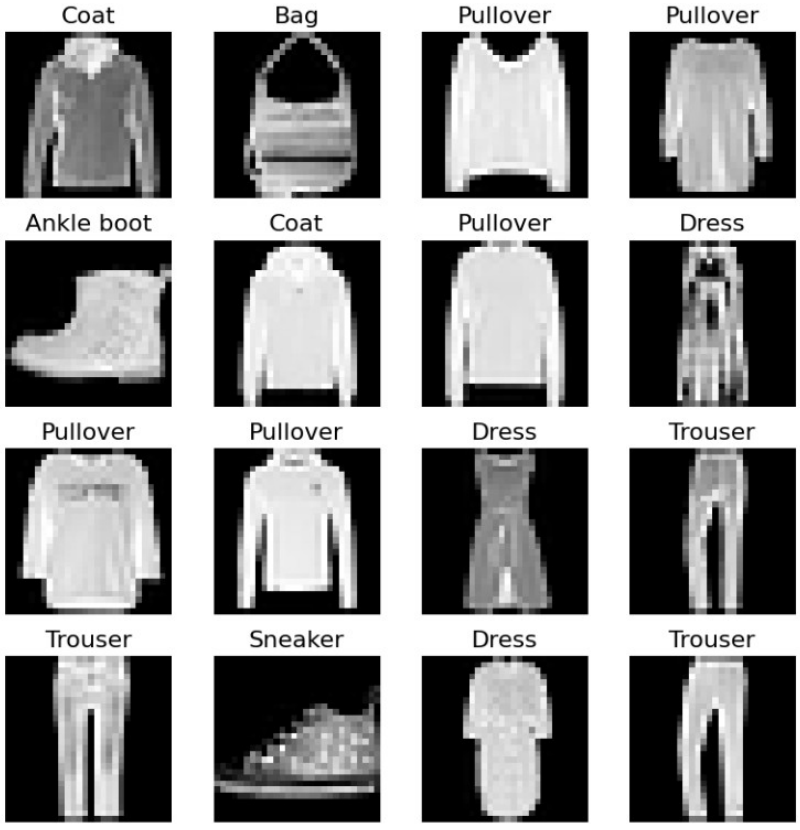


Classification, regression

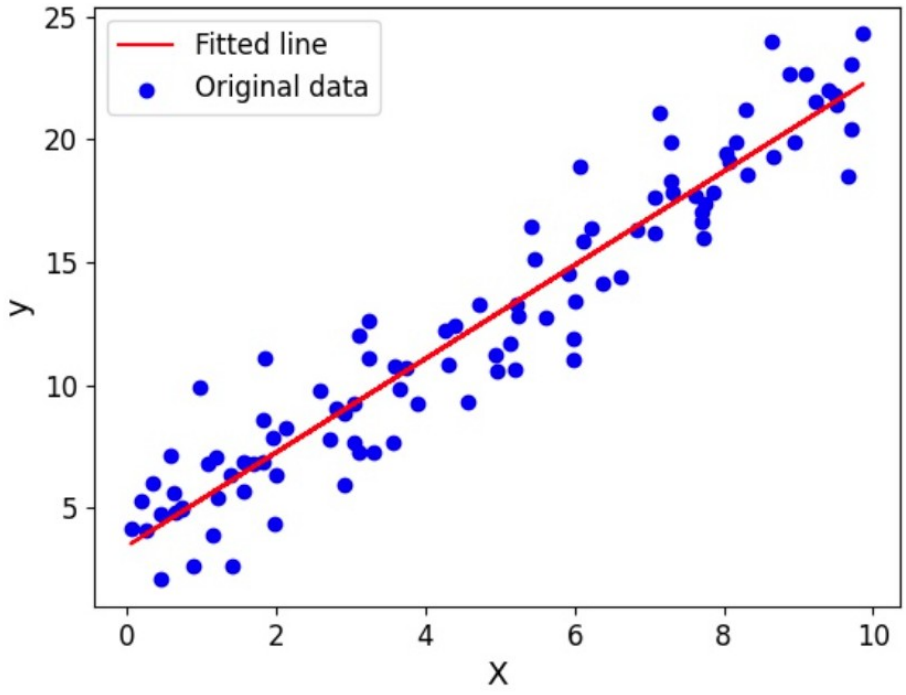


Classification: Assigning categorical labels

Classification, regression



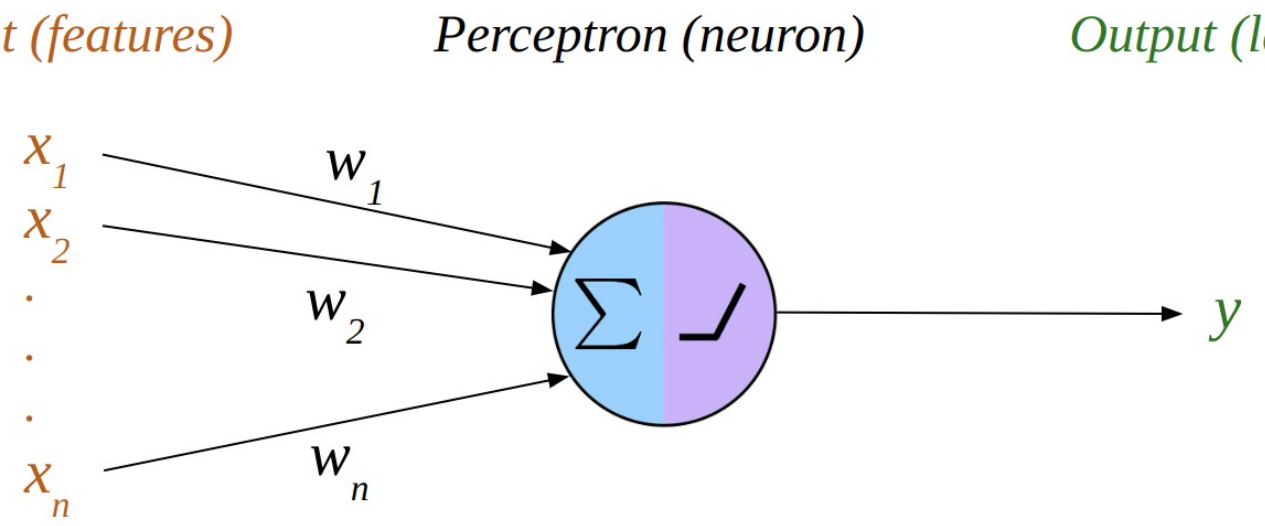
Classification: Assigning categorical labels



Regression: Predicting continuous outcomes

Deep
Neural Networks

Perceptron



Pre-activation with weights (w) and bias (b)

$$a = \sum_{i=1}^{n} w_i x_i + b$$

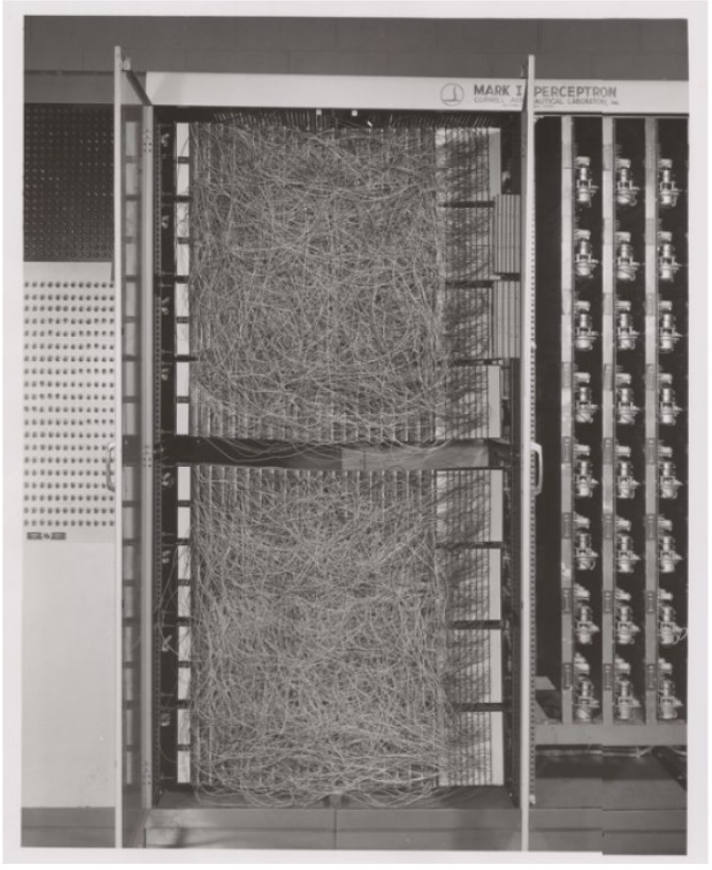
Post-activation, activation function (f)

$$y = f(a)$$

Mark I Perceptron

Why “weights” and “biases”?

In electrical engineering, you view a function as an electrical circuit with wires and biases. That’s where “**w**” and “*b*” stem from.



Cf. Cornell University Library

Activation functions

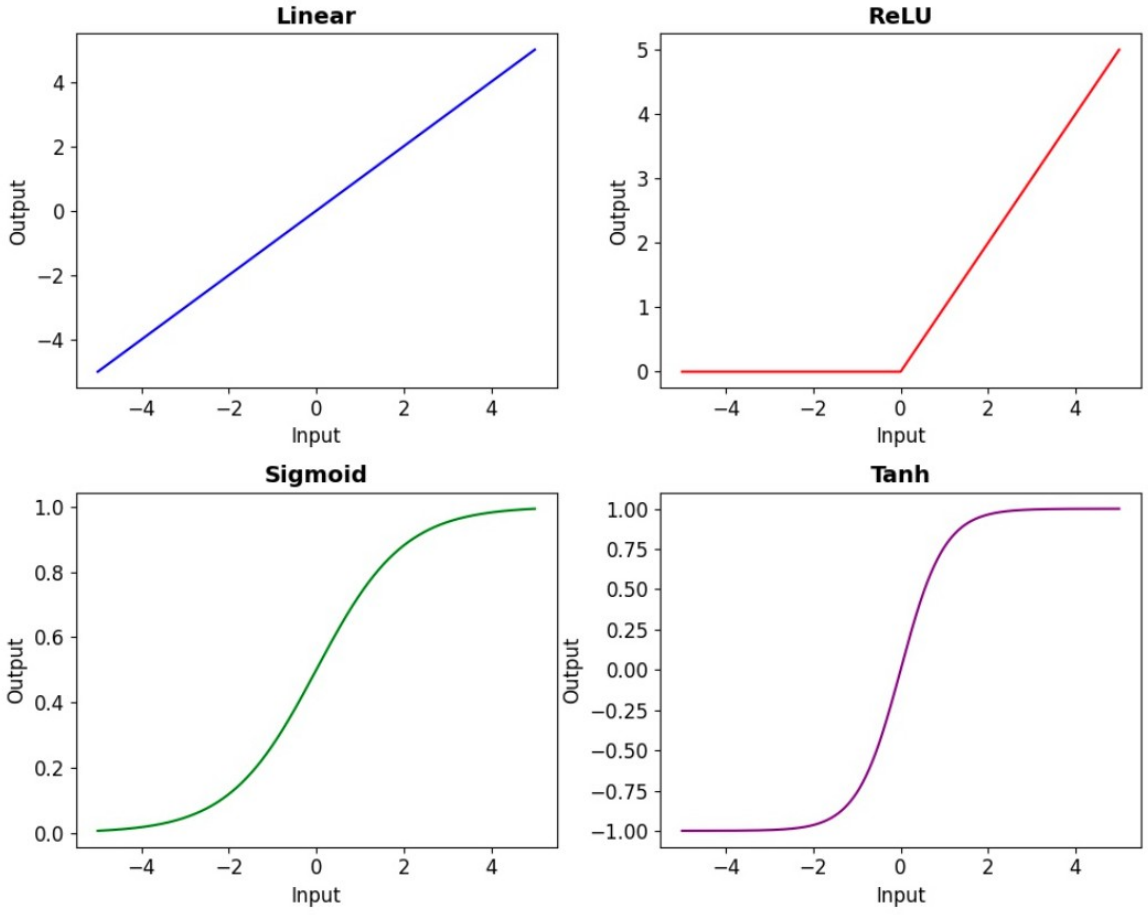
Activation functions may introduce non-linearity and determine neuron outputs.

Linear: Returns input.

ReLU (Rectified Linear Unit): Returns zero for negative inputs and the input value for positive inputs.

Sigmoid and **Tanh (Hyperbolic Tangent):** Smoothen outputs. Suffer from vanishing gradients for extreme inputs.

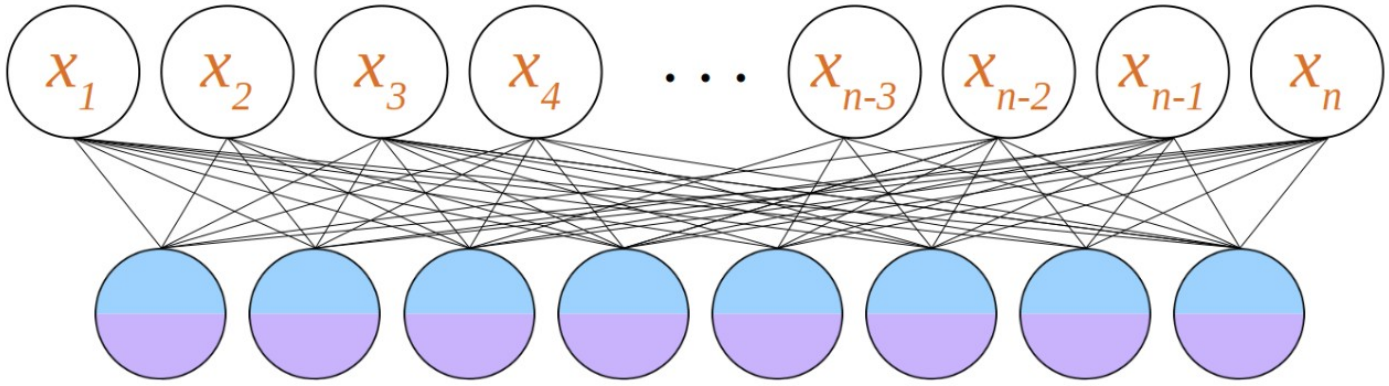
Softmax: Converts raw scores into probabilities (used for classification output).



Shallow neural networks

Input layer

Output layer

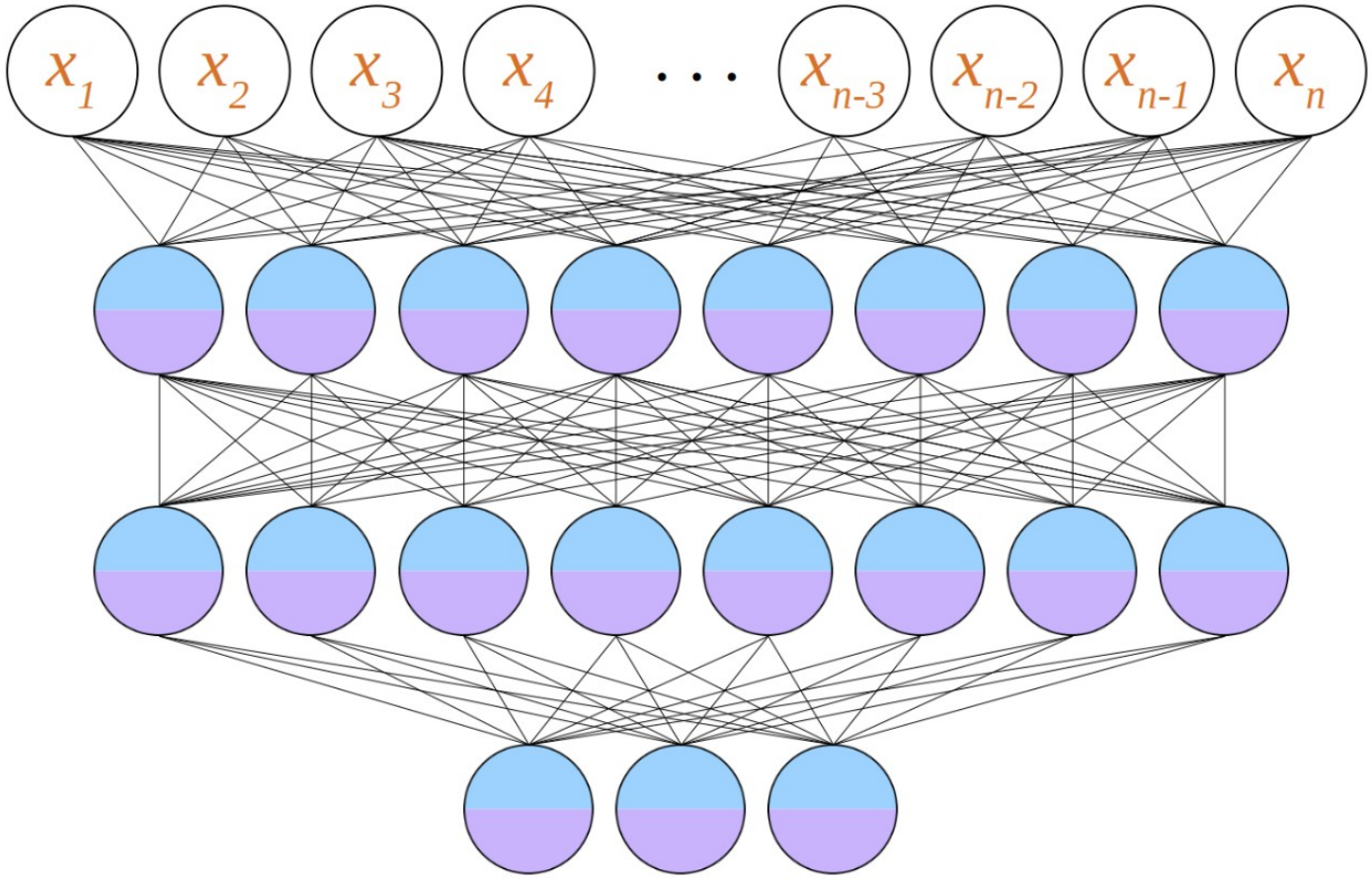


Deep neural networks

Input layer

Hidden layers

Output layer

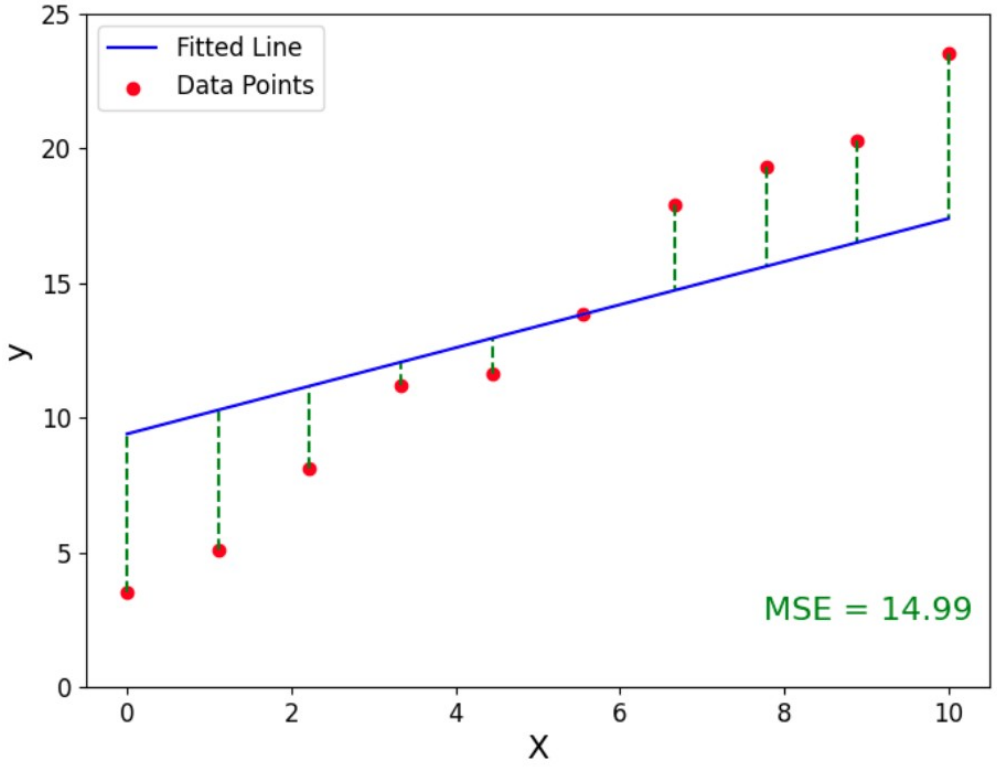


Architecture

A deep neural network transforms $\boldsymbol{x}$ stepwise, layer by layer:

$$\Phi(\boldsymbol{x}) = \phi_K(\phi_{K-1}(\dots\phi_2(\phi_1(\boldsymbol{x}))\dots))$$

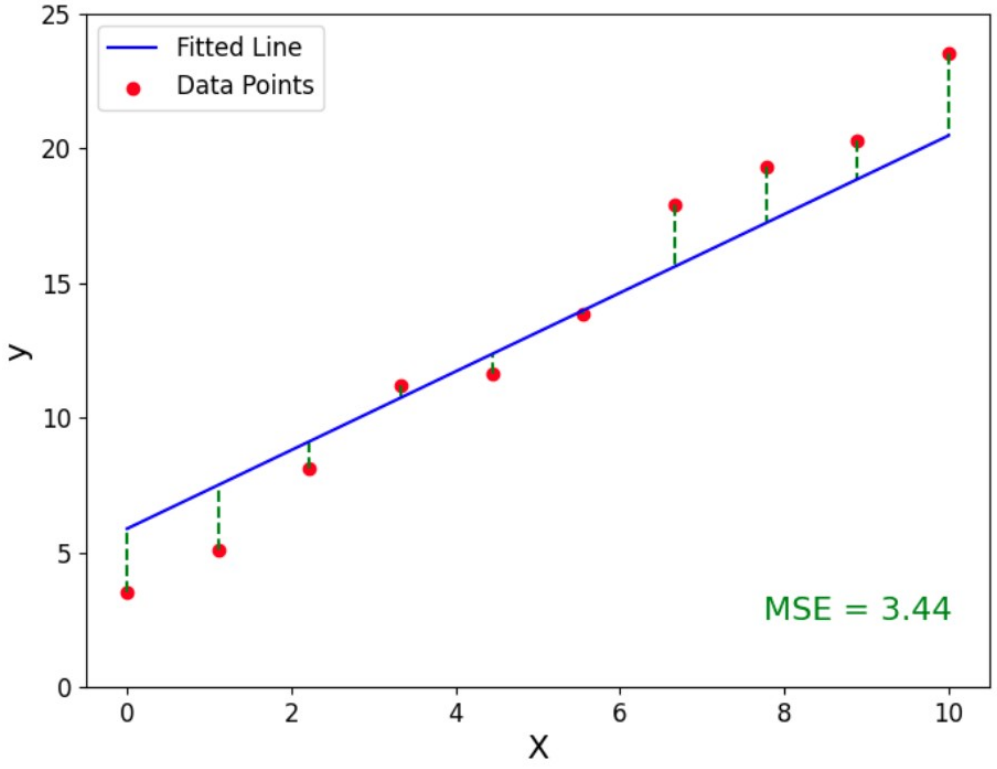
Loss functions



For regression, we use the mean squared error (MSE)

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Loss functions



For regression, we use the mean squared error (MSE)

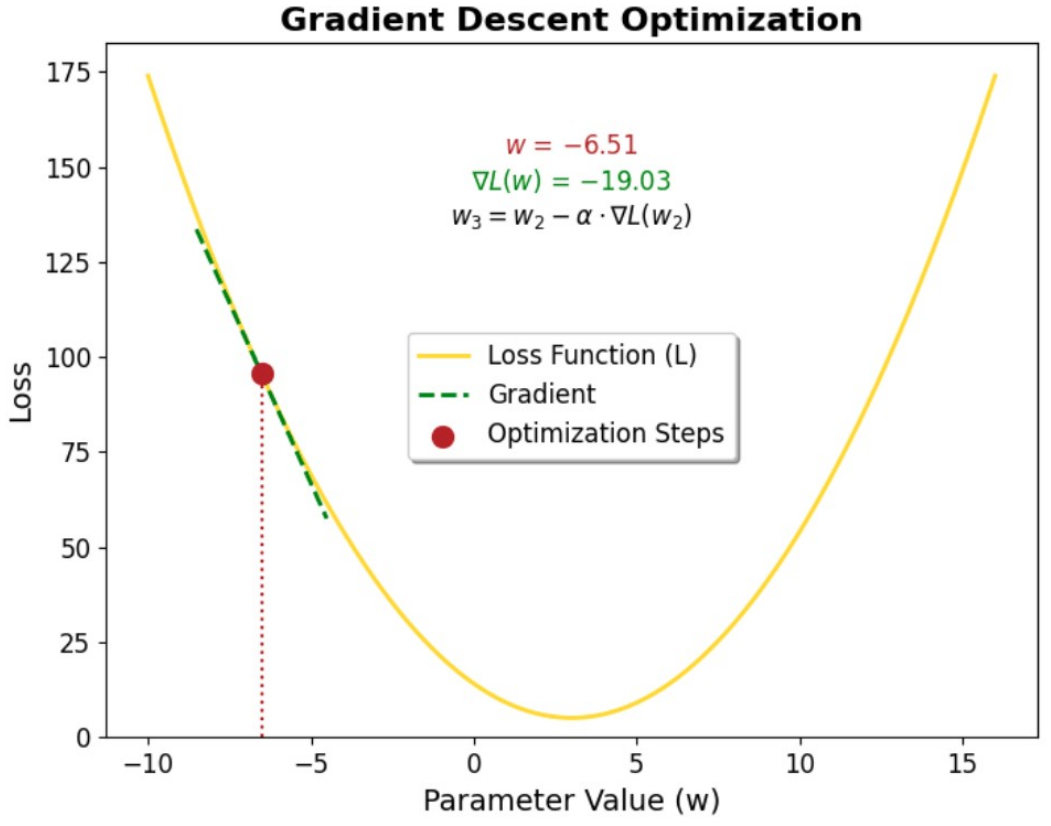
$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

For classification, we use cross entropy, quantifying the dissimilarity between the distributions over predicted labels (q) and true labels (p)

$$H(p, q) = -\sum_{i=1}^{n} p_i \log q_i$$

Optimisation

We want to **minimise the loss**, i.e., match observations as closely as possible.

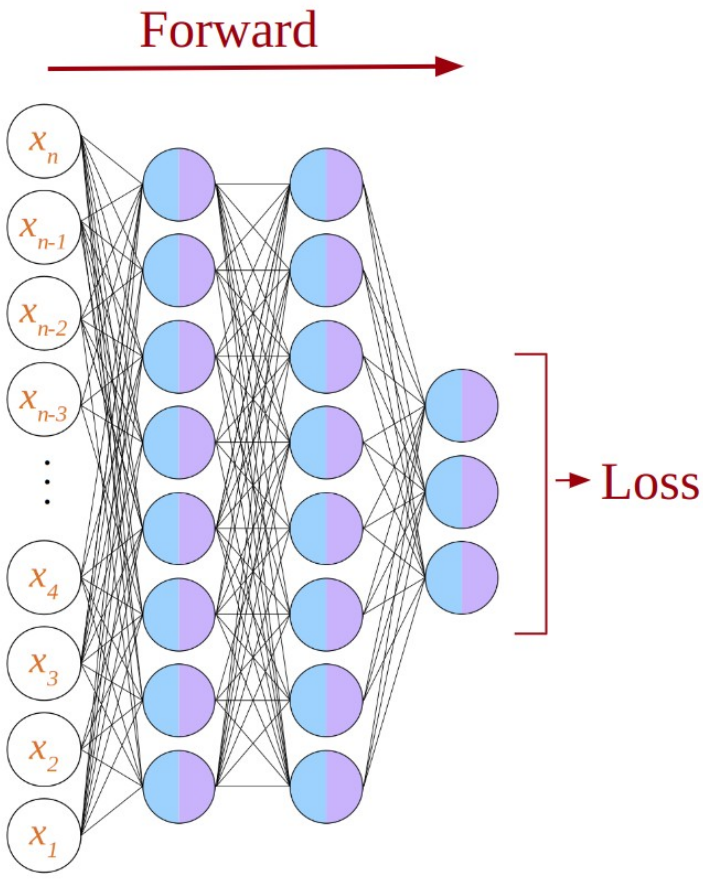


Backpropagation

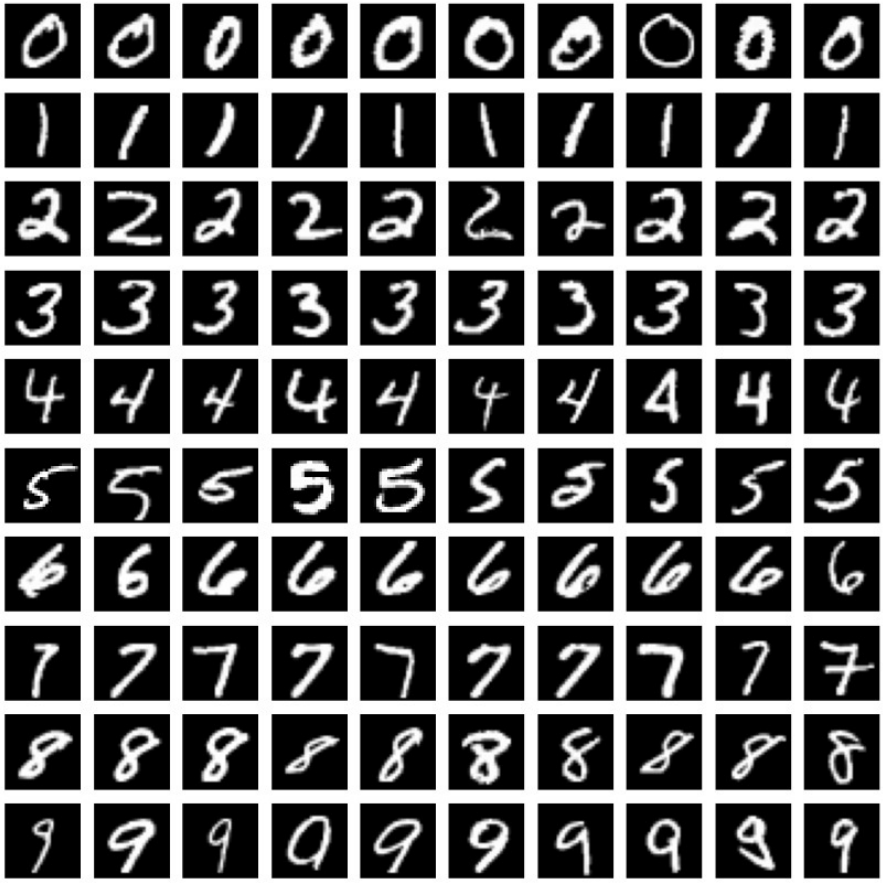
We want to compute the gradient of the loss to optimise the parameters of the neural network.

$$\frac{\partial L_i^k}{\partial w_{pq}^k}$$

The loss is a function final output of the neural network and propagate the errors in the loss “backwards” through the network.

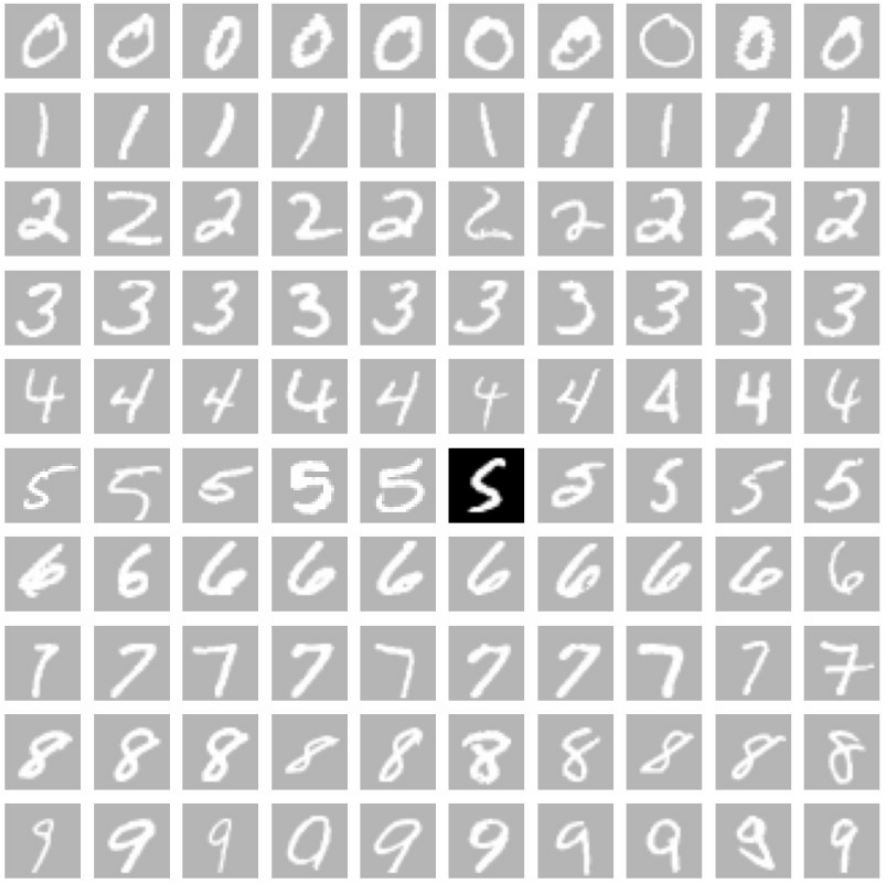


Batches and SGD



We could compute gradients based on the whole data set. But that’s computationally expensive.

Batches and SGD



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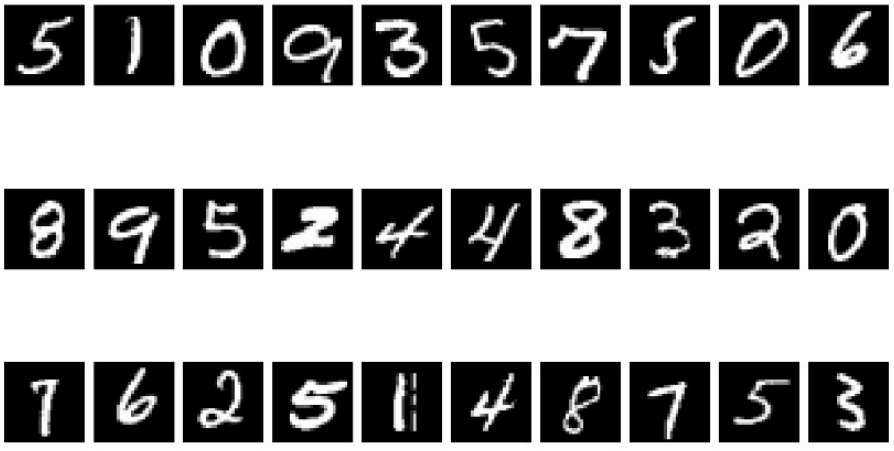
We could use a single, randomly chosen (stochastic) sample to compute the gradients. But that will be a not be representative.

Batches and SGD



~~We could compute gradients based on the whole data set. But that's computationally expensive.~~

~~We could use a single, randomly chosen (stochastic) sample to compute the gradients. But that will be a not be representative.~~

Mini-batches: We could randomly shuffle the data and compute the gradients based on and a small number (batch) of samples. That's fast and representative!

Training

1) Initialise weights ($\boldsymbol{W}$) and biases ($\boldsymbol{b}$)

2) In each epoch, loop over all mini-bashes. For each mini-batch,

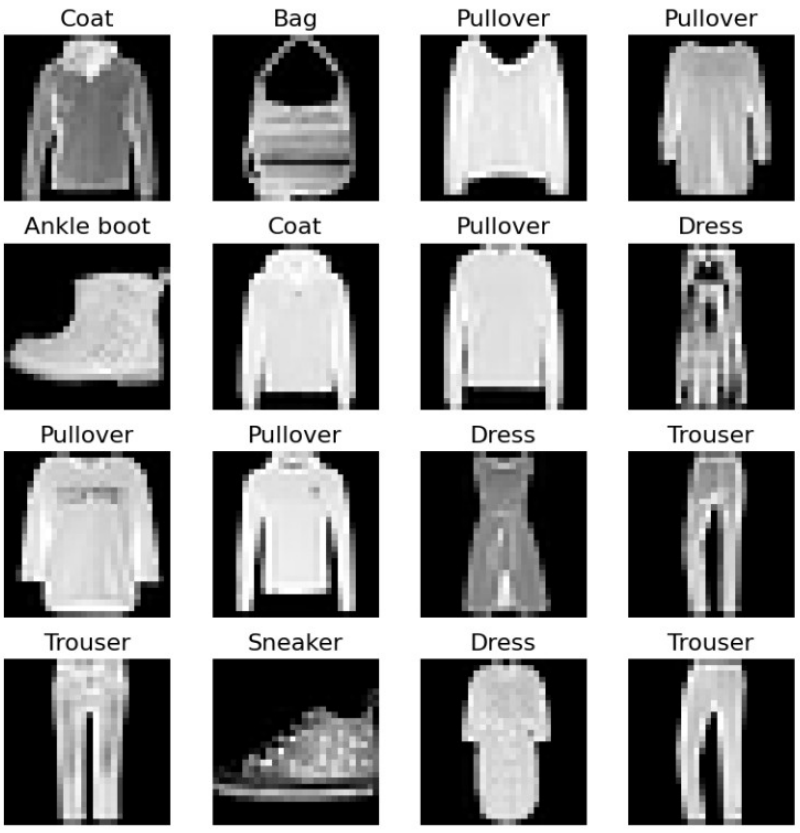
   a) Feedforward: Use current $\boldsymbol{W}$ and $\boldsymbol{b}$ to make model predictions.

   b) Compute the loss, L.

   c) Backpropagation: Compute the gradient of the loss w.r.t. $\boldsymbol{W}$ and $\boldsymbol{b}$ layer by layer.

   d) Update $\boldsymbol{W}$ and biases $\boldsymbol{b}$ for each layer.

Testing



How well does your model capture your training data?

Confront your trained network with ***unseen*** data with known labels. How does the model perform? Can it **generalise**?

You need to be careful when choosing the metrics!

Only if you pass these tests, apply to unlabelled data.

Data augmentation

Data augmentation: Techniques to artificially increase dataset size. Mitigates overfitting, improves model generalization.

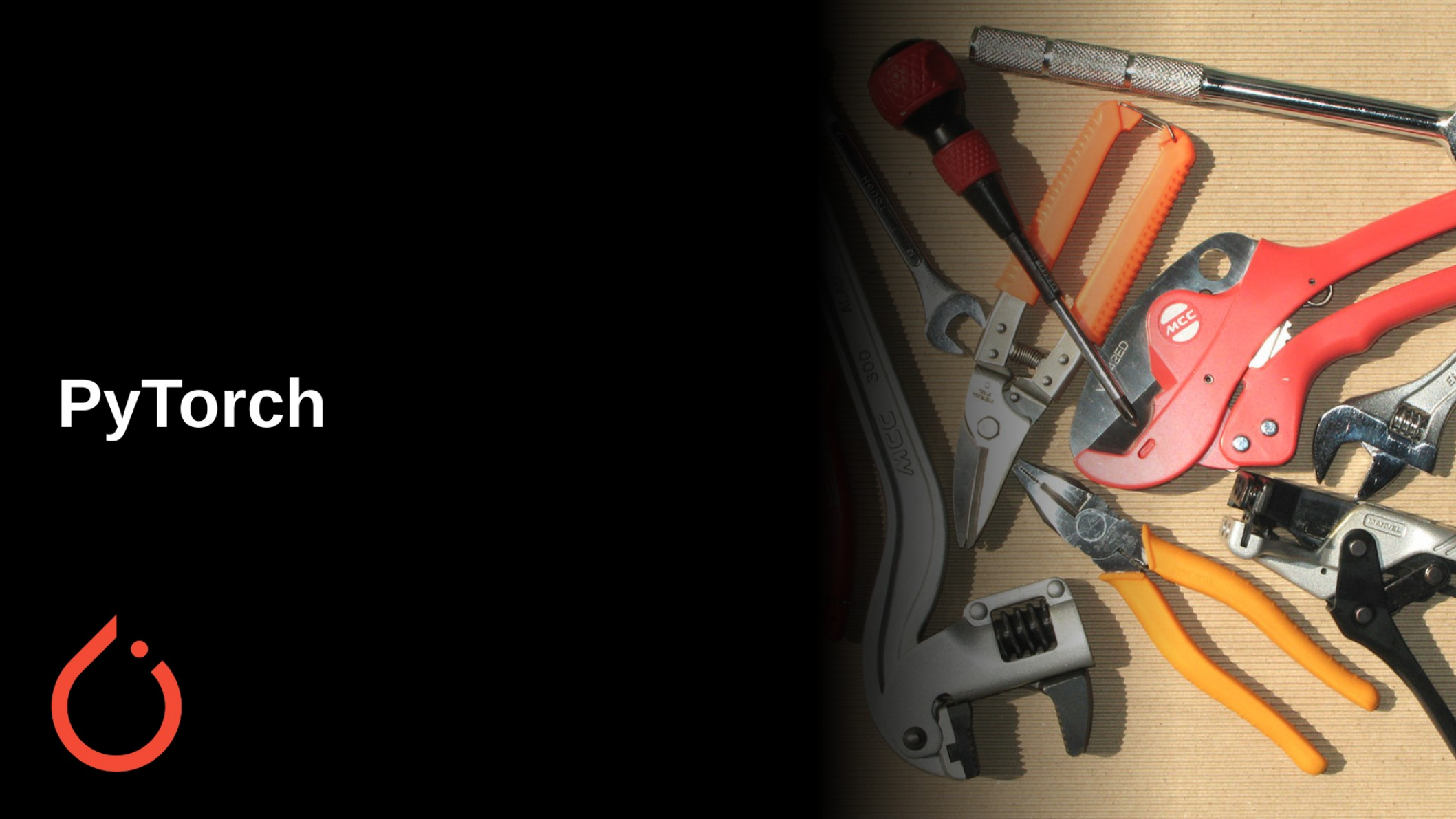
Common data augmentation techniques:

- Horizontal/Vertical Flipping
- Random Rotation
- Random Crop
- Random Resizing and Padding
- Color Jittering
- Gaussian Blur
- Random Noise Addition

Step by step guide

1) Split test and training data. Perform data augmentation.
2) Taylor the neural network architecture (layers, activation functions…)
3) Choose a meaningful loss function.
4) Choose the optimisation algorithm, batch size, learning rate …
5) Train your network
6) Test performance

PyTorch



Basics

```
import torch # PyTorch

scalar = torch.tensor(1) # Define scalar

vector = torch.tensor([1, 2]) # Define vector
```

PyTorch has its own objects (tensors) with their own methods.

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vector*vector # Example of operation

vector.argmax() # Example of method
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torch.unsqueeze(vector,dim=0) # Add dimensions

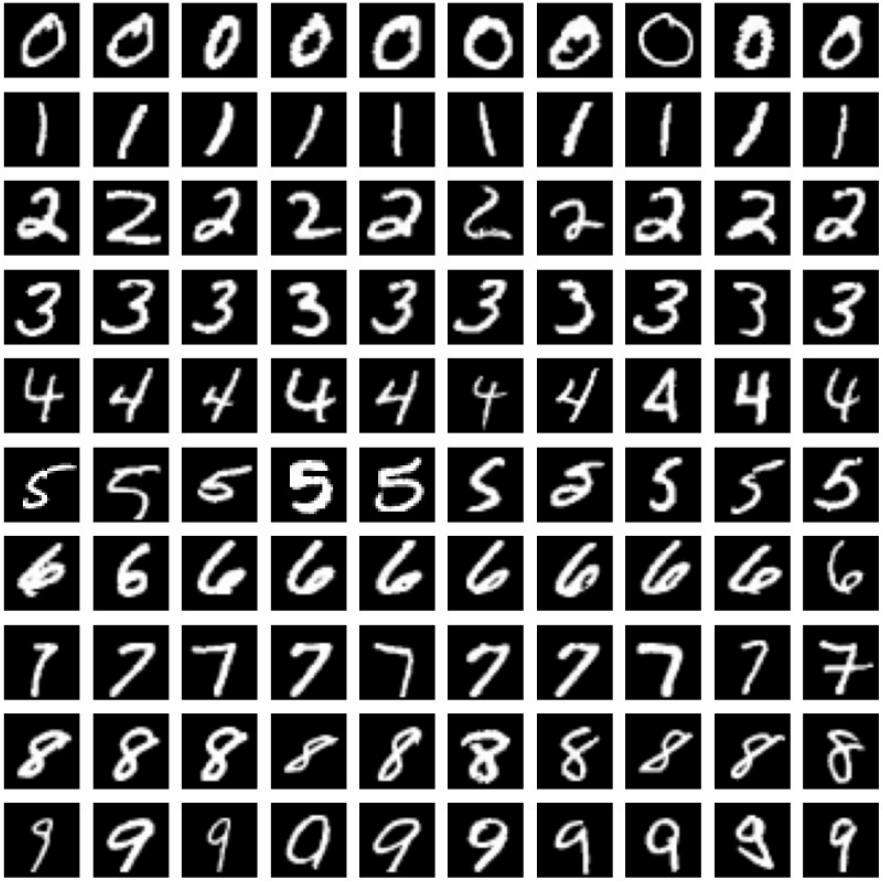
# Dealing with numpy output
array = np.arange(1,3)
torch.from_numpy(array)
```

PyTorch has its own objects (tensors) with their own methods.

Computer vision

```
from torchvision import datasets

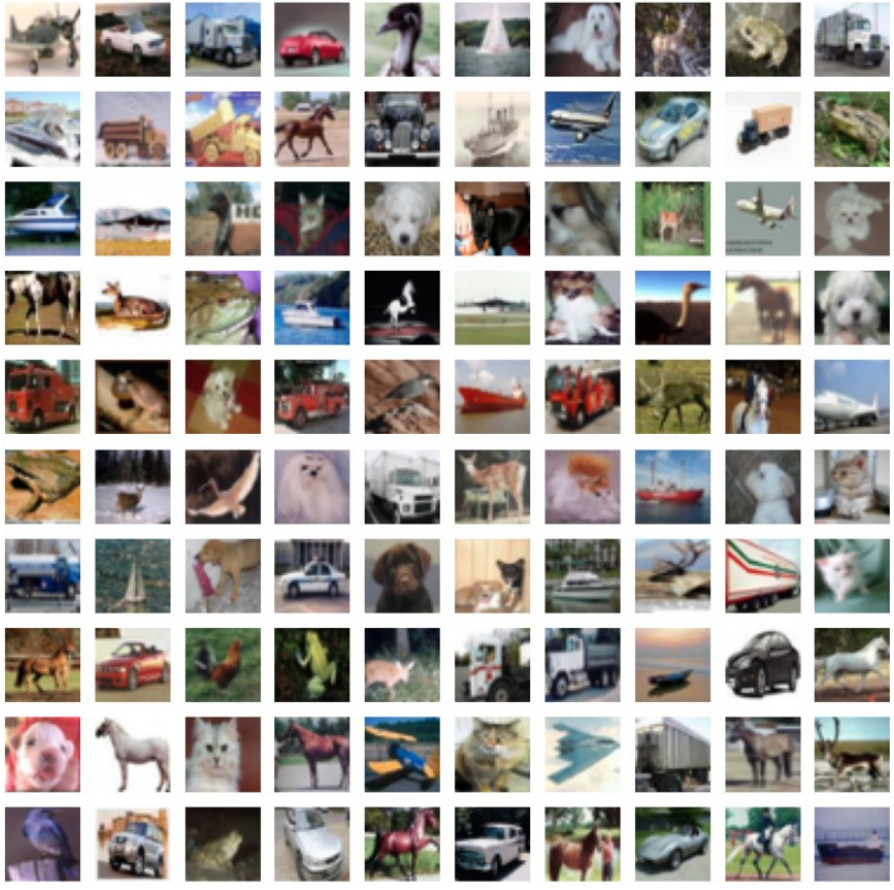
train = datasets.MNIST(root='./data', train=True, download=True)
```



Computer vision

```
from torchvision import datasets

train = datasets.CIFAR10(root='./', train=True, download=True)
```



Transforms

```
import torchvision.transforms as transforms

means = (0.5,0.5,0.5)
stds = (0.5,0.5,0.5)

# Define the data transform including normalization

transform = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize(means, stds),
])
```

Transforms preprocess data for resizing images, augmentation, and normalization.

Transforms

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```

Converts the image to a PyTorch tensor

Normalize for three channels

Transforms preprocess data for resizing images, augmentation, and normalization.

Data loaders

```
from torch.utils.data import DataLoader

Train_loader = DataLoader(dataset=train, batch_size=32,
shuffle=True)
```

PyTorch DataLoader: Batches data, shuffles, and prepares data for efficient training.

Data loaders

```
from torch.utils.data import DataLoader

Train_loader = DataLoader(dataset=train, batch_size=32,
shuffle=True)

Test_loader = DataLoader(dataset=test, batch_size=32,
shuffle=False)
```

PyTorch DataLoader: Batches data, shuffles, and prepares data for efficient training.

Step by step

1) Load your training and test data

```
from torchvision.datasets import ImageFolder
```

2) Define the required transforms and transform the data

```
trainset = ImageFolder(root='XYZ/train', transform=train_transform)
```

3) Pass the dataset to the dataloader

```
train_loader = torch.utils.data.DataLoader(dataset=train_dataset, batch_size=32, shuffle=True)
```

Building Neural Networks

A new class

```
import torch
import torch.nn as nn

# Define a neural network
class MyNet(nn.Module):
    def __init__(self):
        super().__init__()

        # Define layers and activations functions


    def forward(self, x):

        # Transform x stepwise, layer by layer:


        return x
```

We define a PyTorch neural network class inheriting from nn.Module, with initialization for layers and a forward pass method.

$$\Phi(\boldsymbol{x}) = \phi_K(\phi_{K-1}(\dots\phi_2(\phi_1(\boldsymbol{x}))\dots))$$

Linear regression

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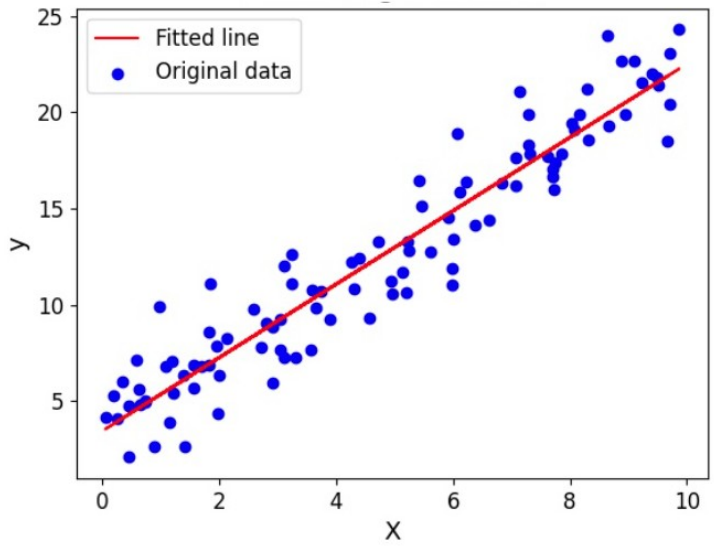
Linear regression can be viewed as a single-layer fully connected neural network, predicting a single numerical value (y), i.e. with one output neuron.



Linear regression

```
import torch
import torch.nn as nn

# Define a neural network
class MyNet(nn.Module):
    def __init__(self):
        super().__init__()

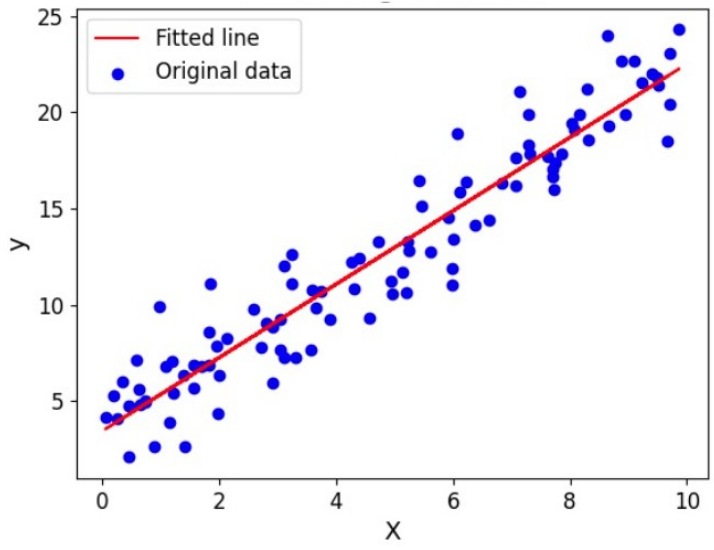
        self.linear = nn.Linear(1, 1)


    def forward(self, x):

        x = self.linear(x)


        return x
```

Linear regression can be viewed as a single-layer fully connected neural network, predicting a single numerical value (y), i.e. with one output neuron.



Initialisation

```
# Call instance of your class
model = MyNet()

# Define your loss
criterion = nn.MSELoss()

# Define your optimisation alogorithm
optimizer = optim.SGD(model.parameters(), lr=0.01)
```

Initialisation

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model = MyNet()

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```

```
# Synthetic data
X = 2 * torch.rand(100, 1)
y = 3 * X + 2 + 0.5 * torch.randn(100, 1)
```

Training

In each epoch (we have a single batch),

1) Feedforward: Make model predictions.

2) Compute the loss.

3) Backpropagation: Compute the gradient of the loss.

4) Update weights and biases.

Training

In each epoch (we have a single batch),

1) Feedforward: Make model predictions.

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```
num_epochs = 100

for epoch in range(num_epochs):

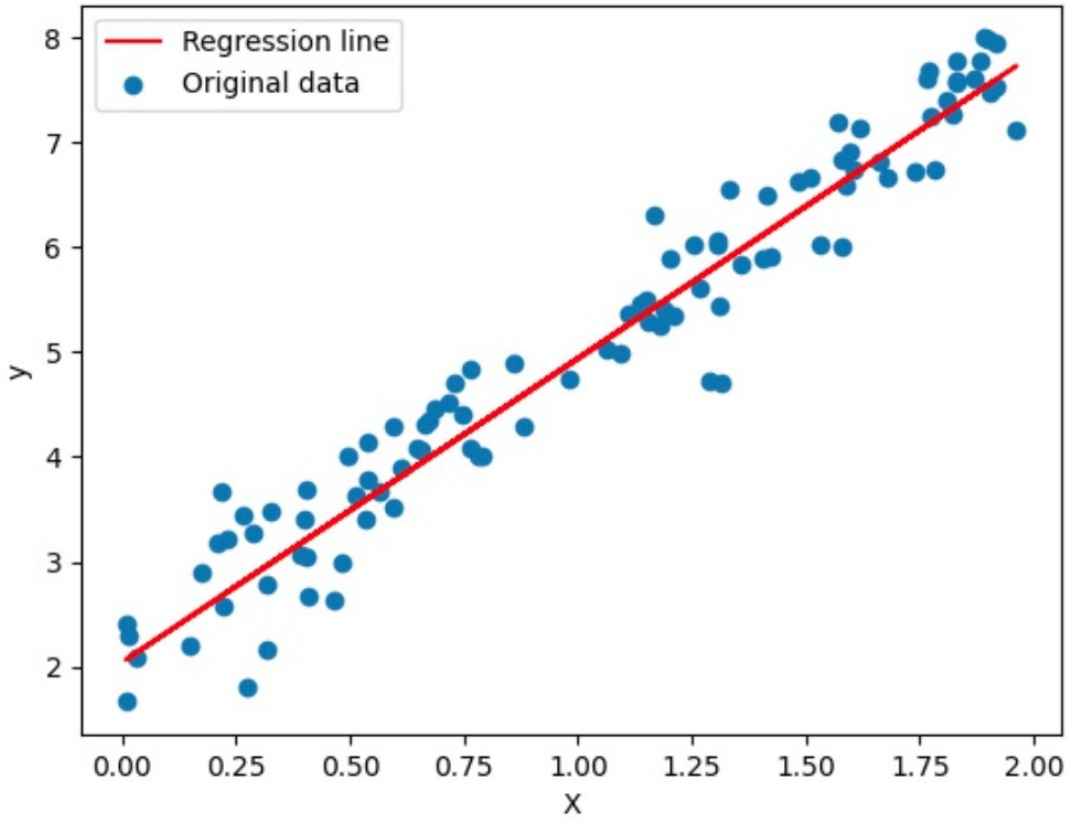
    # 1) Feedforward
    predictions = model(X)

    # 2) Compute the loss
    loss = criterion(predictions, y)

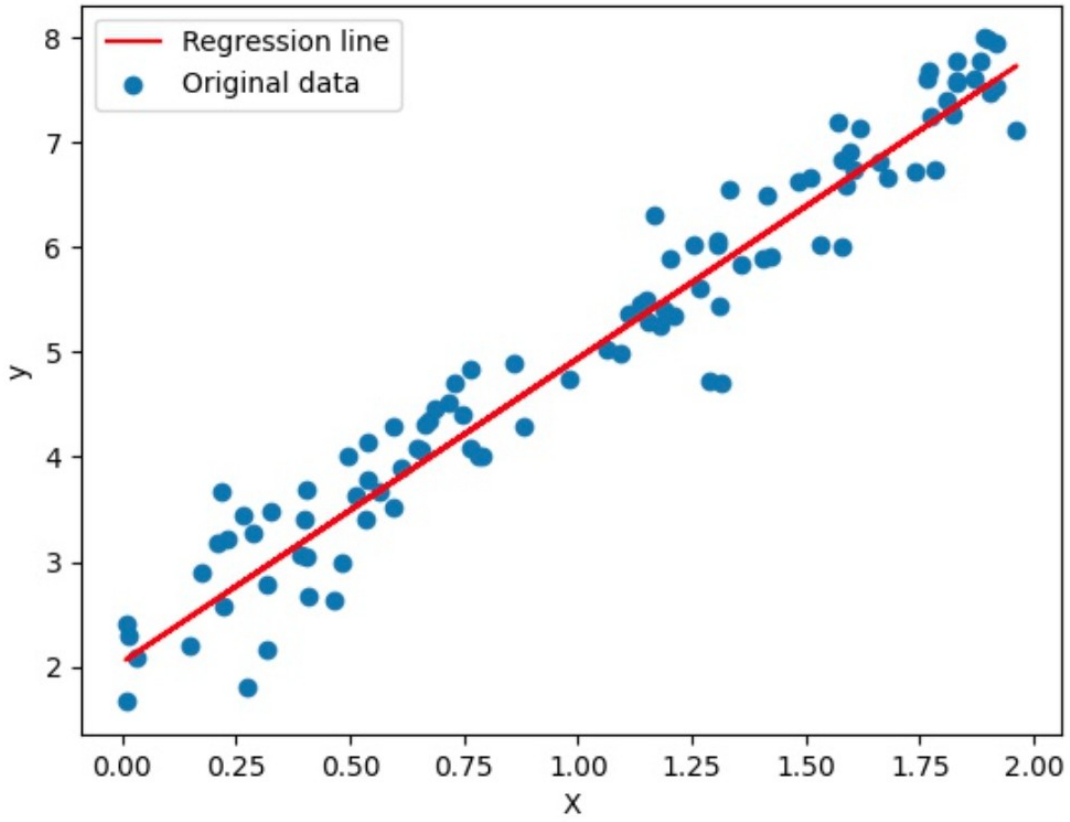
    # 3) Backpropagation of errors
    optimizer.zero_grad()
    loss.backward()

    # 4) Optimization, update W and b
    optimizer.step()
```

Final fit


Regression line
Original data
y
X
8
7
6
5
4
3
2
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00

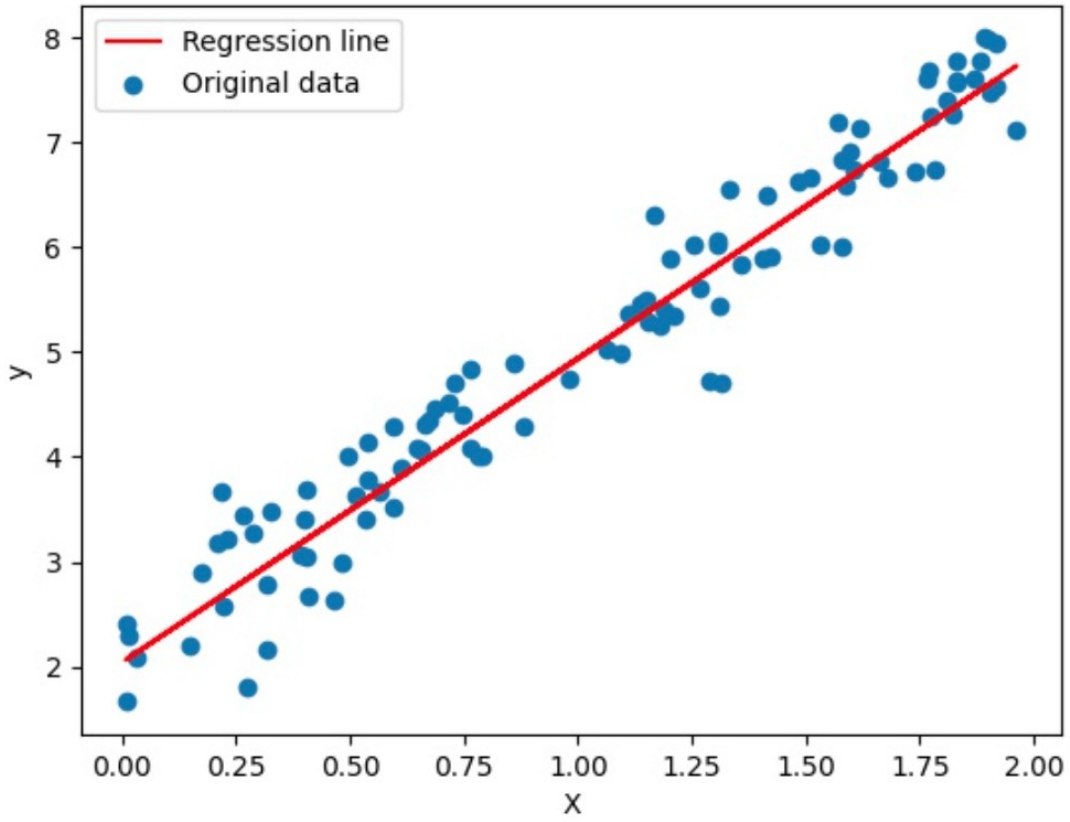
Final fit




```
print(model.linear.weight.data, model.linear.bias.data)
```

```
tensor([[2.9014]]) tensor([2.0385])
```

Final fit

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```
tensor([[2.9014]]) tensor([2.0385])
```

```
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```

Deep neural network

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```

Deep neural network

```
import torch
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# Define a neural network
class MyDeepNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.fc1 = nn.Linear(28 * 28, 128)
        self.relu = nn.ReLU()
        self.fc2 = nn.Linear(128, 10)

    def forward(self, x):
        x = x.flatten(start_dim=1)
        x = self.fc1(x)
        x = self.relu(x)
        x = self.fc2(x)
        return x
```

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        x = self.fc1(x)
        x = self.relu(x)
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        return x
```

```
# Call instance of your class
model = MyDeepNet()

# Define your loss
criterion = nn.CrossEntropyLoss()

# Define your optimisation alogorithm
optimizer = optim.Adam(model.parameters(), lr=0.01)
```

Training

```
# Set the model to training mode
model.train()

for epoch in range(num_epochs):
        for images, labels in train_loader:
                # 1) Feedforward
                outputs = model(images)

                # 2) Compute the loss
                loss = criterion(outputs, labels)

                # 3) Backpropagation of errors
                optimizer.zero_grad() # clear gradients
                loss.backward()

                # 4) Optimization, update W and b
                optimizer.step() # update weights and biases
```

The **bare bone training loop looks the same**: There are 4 steps. We now also loop over mini-batches.

Testing

```
# Set the model to evaluation mode
model.eval()
correct = 0
total = 0

with torch.no_grad():
        for images, labels in test_loader:
                outputs = model(images)
                # Determine likeliest label
                _, predicted = torch.max(outputs.data, 1)
                total += labels.size(0)
                # Is it right or wrong?
                correct += (predicted == labels).sum().item()

accuracy = correct / total
```

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There are often better choices than accuracy …

Summary

Based on this lecture, you should better be able to

1) Explain basic concepts in Deep Learning, including activation and loss functions, gradient descent, backpropagation, batching, data augmentation, and neural network architecture.

2) Outline the basic steps in training and testing neural networks.

3) Understand and point to essential commands in PyTorch (including torchvision).

4) Translate the concepts of Deep Learning into PyTorch.