

CAS in Applied Data Science

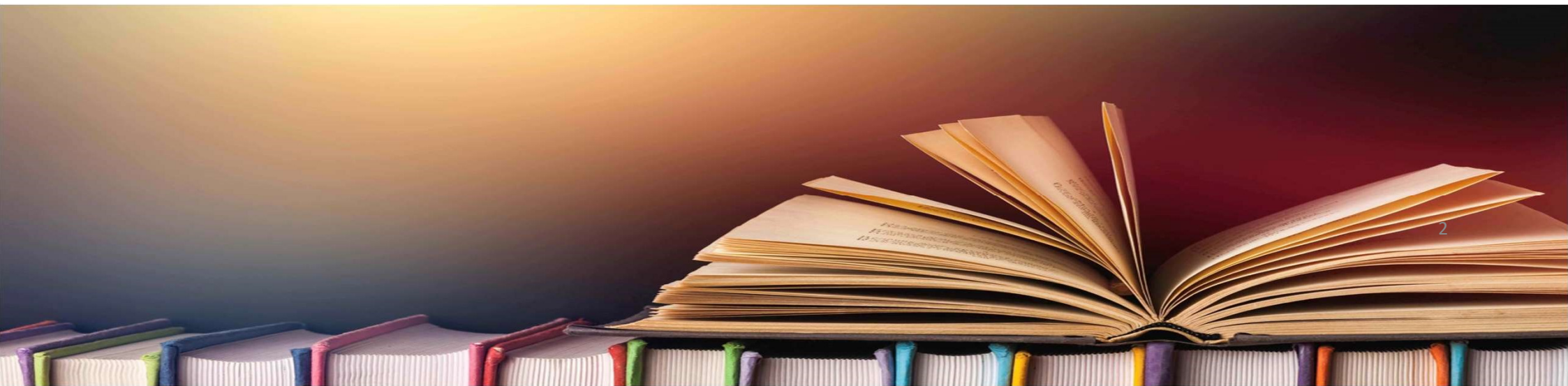
Muerren 2025



Géraldine Schaller-Conti

Bibliography

- Deep Learning book (Goodfellow, Bengio, Courville)
- Machine Learning @ Stanford (Prof Andrew Ng)
- Hands-On Machine Learning with Scikit-Learn & Tensorflow (Aurélien Géron)



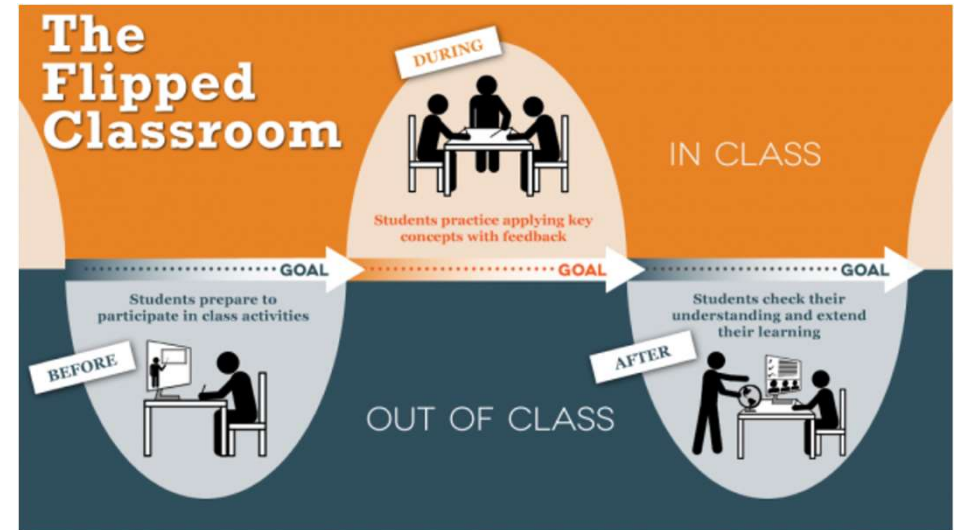
Teaching method

Inverted classroom based

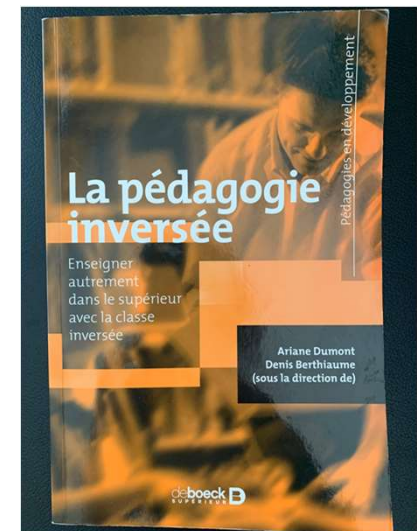
- Introduction lectures
- Real content you learn yourself with the **notebooks**. *Either to put in practice your knowledge or to learn ahead of another lecture*

Why

- Supposed to be better
- More fun
- Learning by doing



To give back sense to being present (Marcel Lebrun)



Tutorial I : Introduction to torch

[Link](#)

→ Copy to drive

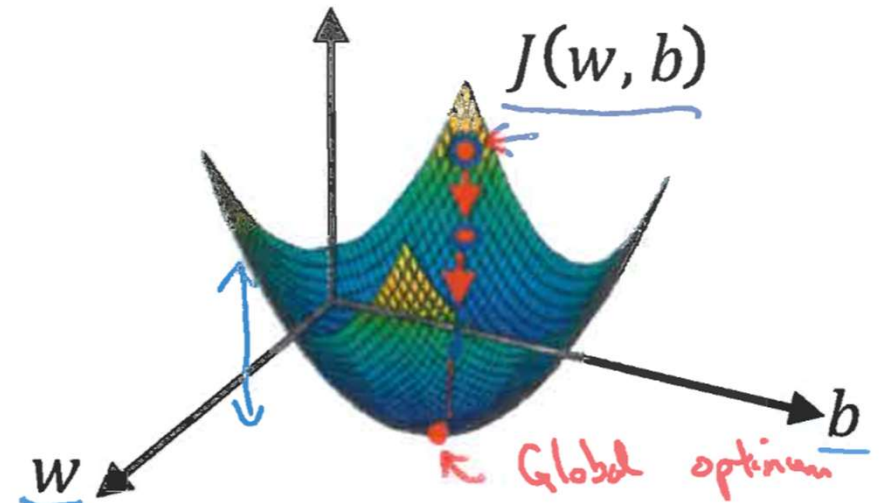
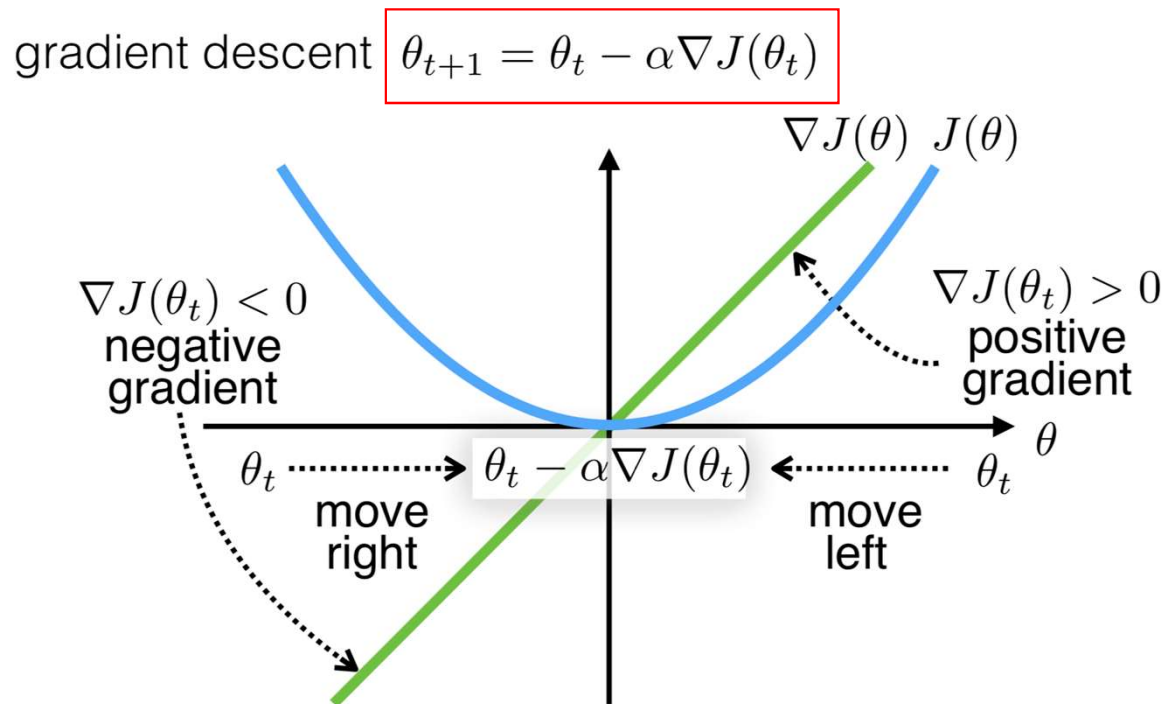
Introduction

- **Goal** : introduction to pytorch
- **Program** : inverted classroom style
 - Theory
 - Overview to get the big picture of the Notebook
 - Work alone or in groups
- **Technical** : Google Colab, Pytorch

Theory

Gradient Descent

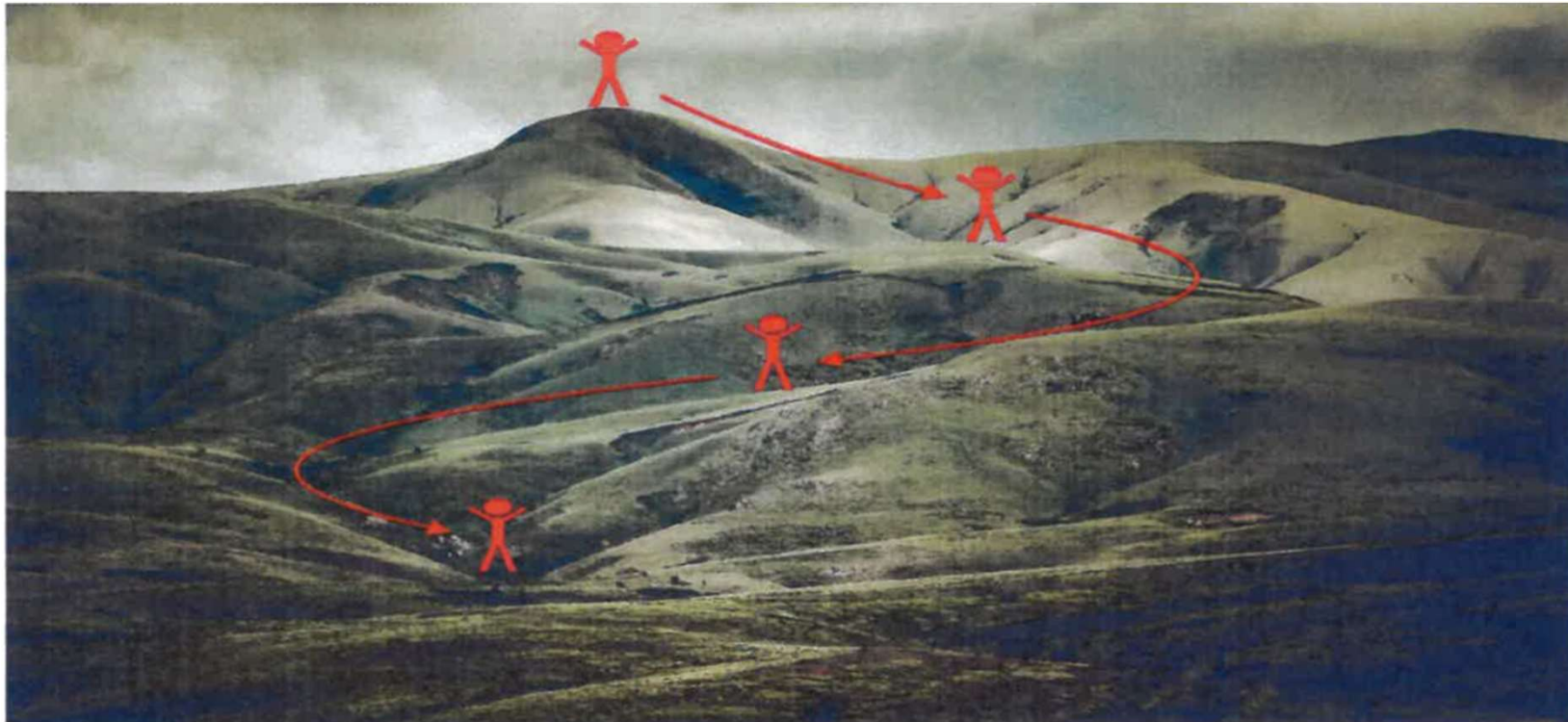
- **Iterative method** to find the parameters $\theta = (w, b)$ that minimize $J(\theta)$



$$\nabla J(w) = \frac{dJ(w, b)}{dw}$$

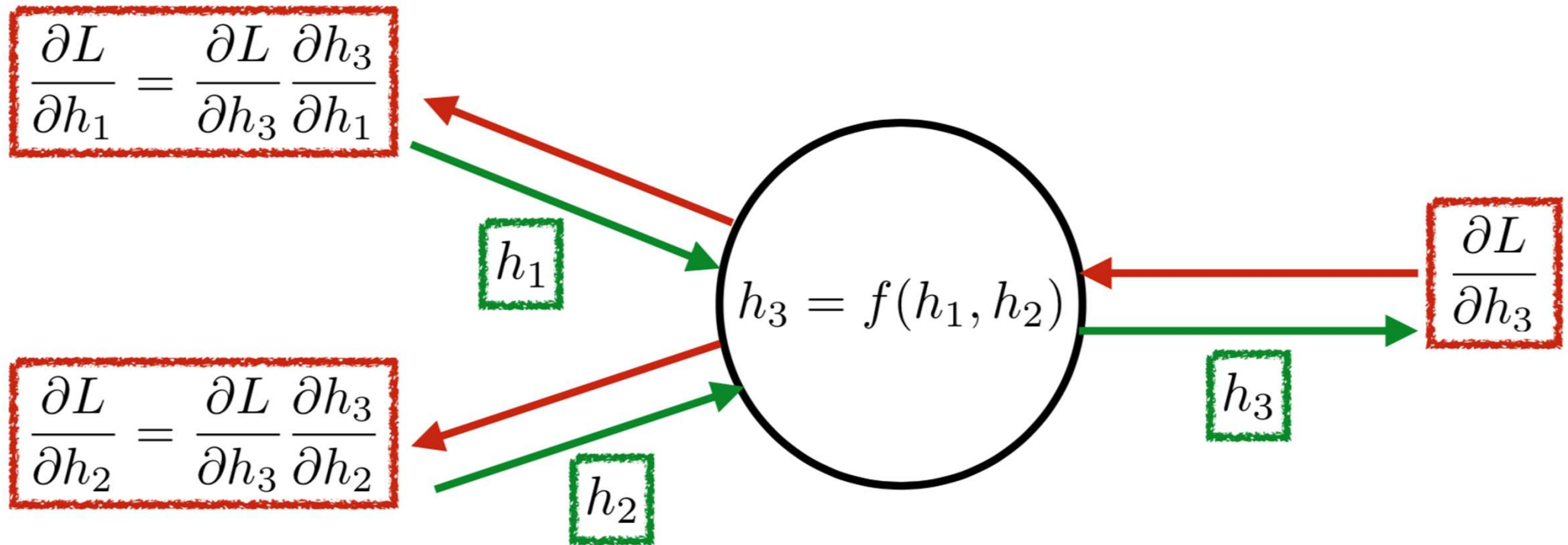
$$\nabla J(b) = \frac{dJ(w, b)}{db}$$

Gradient Descent Illustration



Backpropagation

- Efficient implementation of the **chain-rule** to compute derivatives with respect to network weights



Training

- *Iterative* process



Forward propagation

$$Z = w^T x + b$$

$$A = \sigma(Z)$$



Cost function
 $J(w, b) = J(\theta)$

epochs

Parameter update
(gradient descent)

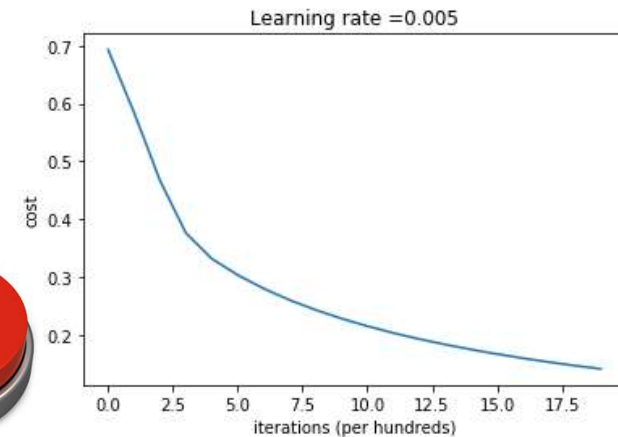
learning rate α

$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

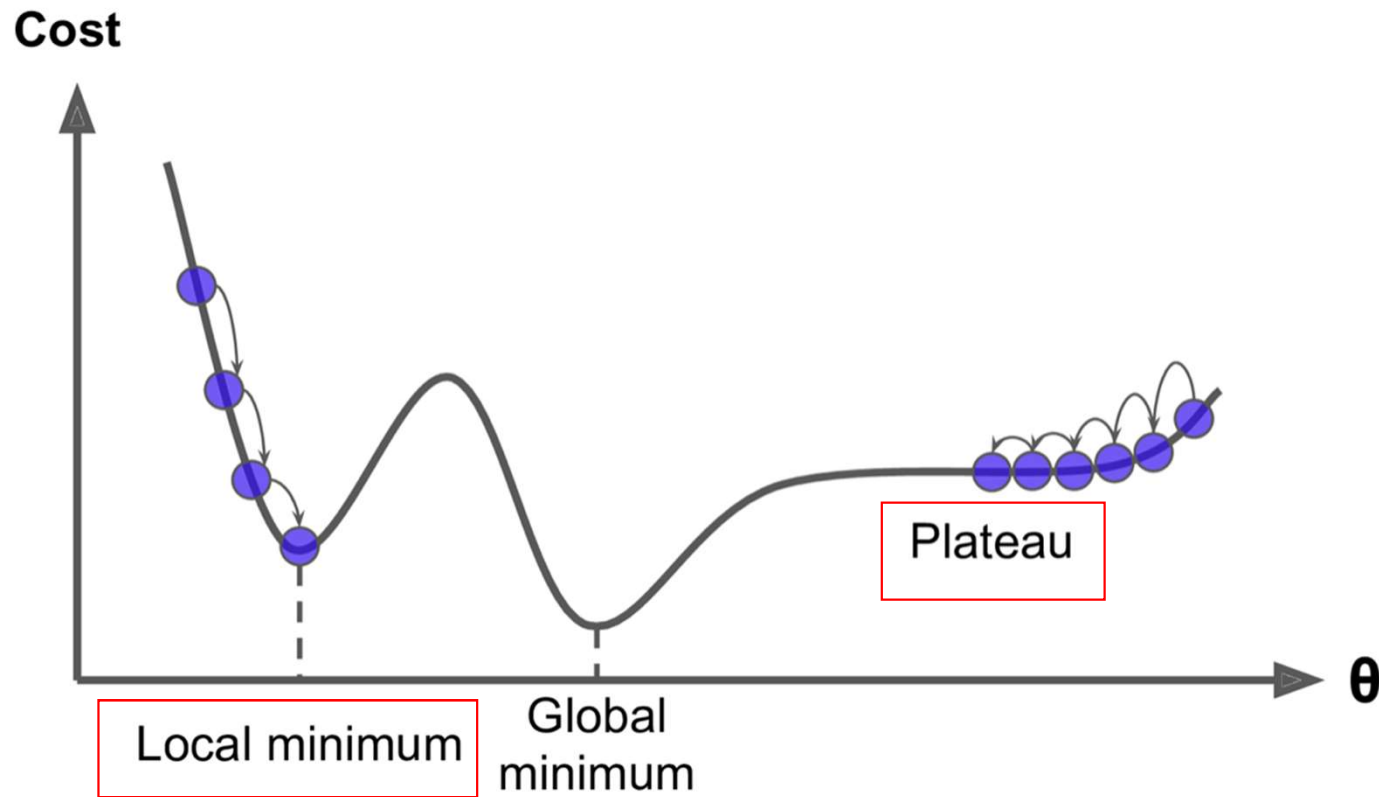


Backward propagation
(dJ/dw , dJ/db)

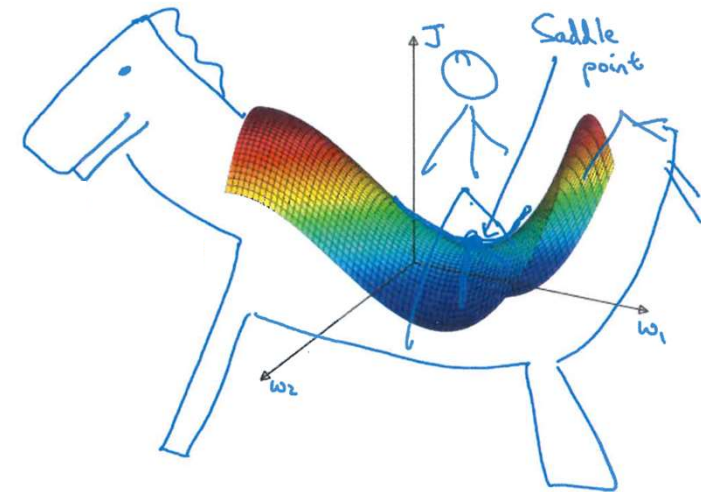
Learning curve



Optimization pitfalls



Saddle point

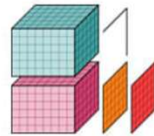


Tools

data structure & analysis

pandas

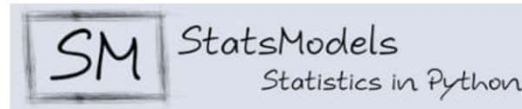
$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



xarray

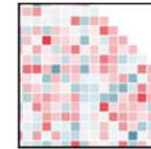


scikit-image
image processing in python



StatsModels

Statistics in Python



Seaborn

main package for scientific computing in Python



NumPy



SciPy



matplotlib



jupyter

Python-based ecosystem of open-source software for mathematics, science, and engineering.



python

IP[y]:
IPython

famous library to plot graphs in Python

provides simple and efficient tools for data mining and data analysis

interactive coding environments embedded in a webpage

h5py : common package to interact with a dataset that is stored on an H5 file

Overview of the notebook

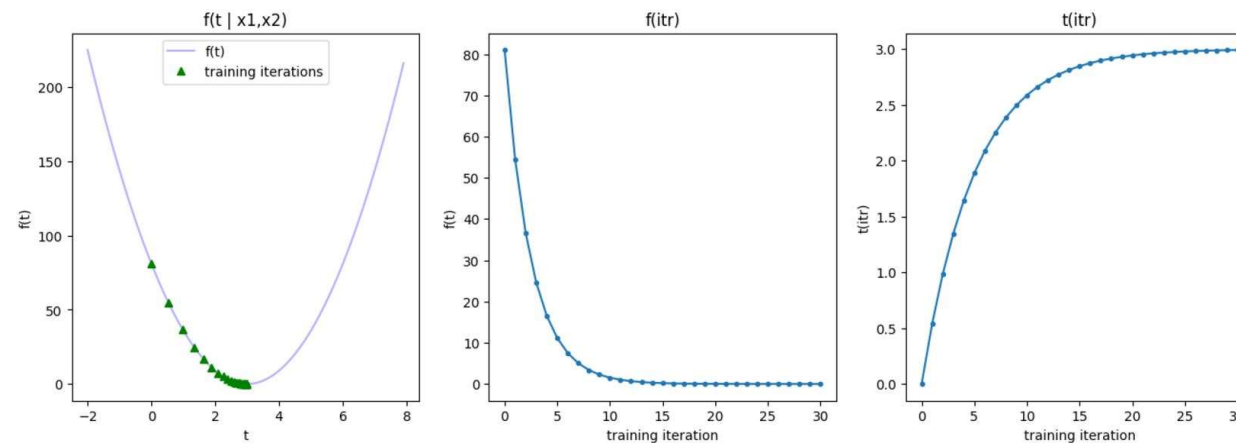
Tutorial I (1)

- 1) Load necessary **libraries** (common libraries) and data
- 2) Create **model** (**class SimpleModel**)
 - $y = x * (x+2)$
- 3) **Run** the model
 - Test it, look at the output type
- 4) **Tensor operations**
 - New model : $\sum_i (x_i + 2)$ (**class SimpleModel2**)
 - Same for several 1D arrays at one (**class SimpleMOdel3**) : add axis=1
- 5) **Exercise 1** : calculate mean of array's elements

Tutorial I (1)

6) Optimization :

- New parabolic function to optimize (`class FLayer`) – trainable parameter is t initialized to 0
- *Gradient descent* applied, SGD optimizer defined
- Plot $f(t)$ results



7) Exercise 2 : change the parabolic function, the alpha learning rate,...

Exercise 1

```
# Define the MeanModel class
class MeanModel(nn.Module):
    def __init__(self):
        super(MeanModel, self).__init__()

    def forward(self, x):
        return torch.mean(x)

# Define data
arr = torch.tensor([[1, 2, 3, 4, 5], [2, 3, 4, 5.1, 6], [25, 65, 12, 12,

# Instantiate the model
model = MeanModel()

# Run the model
result = model(arr)
```

 Copier le code



Tutorial II : Optimization and NN introduction

[Link](#)

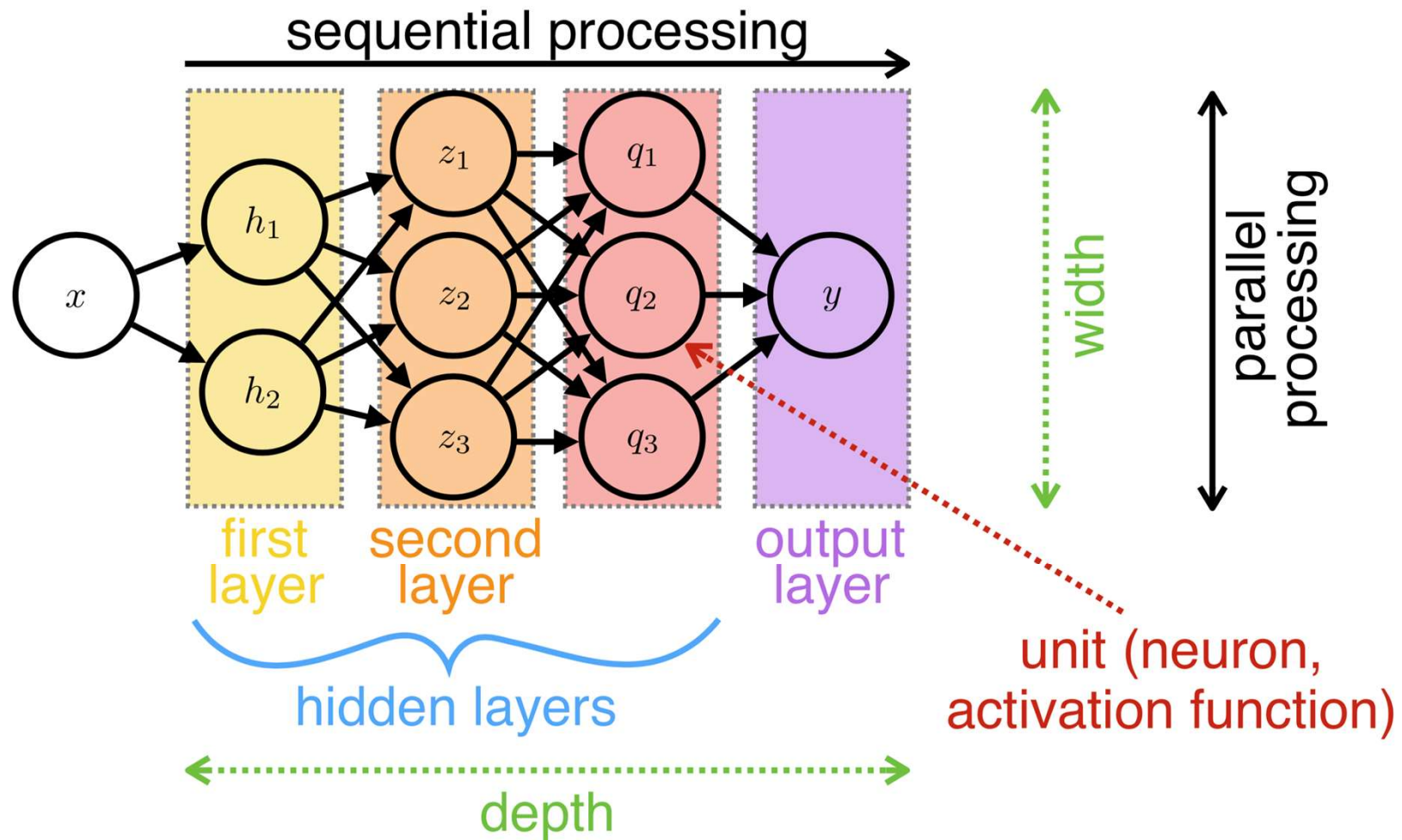
→ Copy to drive

Introduction

- **Goal** : see how to do optimization in torch and NN introduction
- **Program** : inverted classroom style
 - Theory
 - Overview to get the big picture of the Notebook
 - Work alone or in groups
- **Technical** : Google Colab, Pytorch

Theory

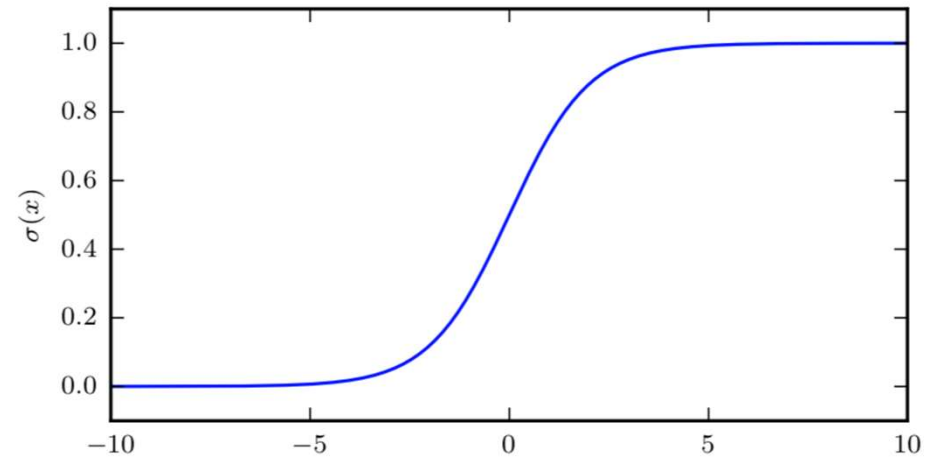
Network model



Sigmoid and softmax

Sigmoid (*two-class* classifier) :

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



Softmax (*multi-class* classifier) :

$$\text{softmax}(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

Optimization

- Given a task we define

- Training data

$$\{x^i, y^i\}_{i=1, \dots, m}$$

- Network

$$f(x; \theta)$$

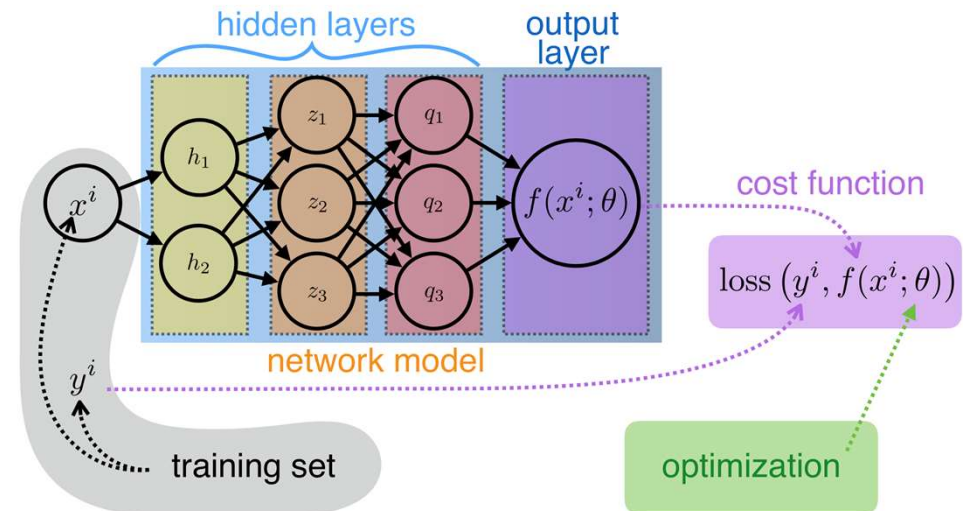
- Cost function

$$J(\theta) = \sum_{i=1}^m \text{loss}(y^i, f(x^i; \theta))$$

- Parameter initialization (weights, biases)

- random weights, biases initialized to small values (0.1)*

- Next, we *optimize the network parameters θ* (training)
- In addition, we have to set values for hyperparameters



Overview of the notebook

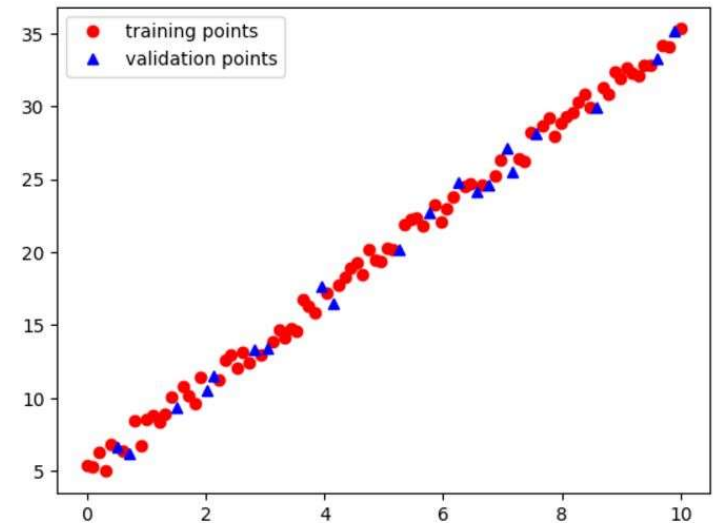
Tutorial II (1)

1) Load necessary **libraries** (common libraries)

2) **Linear regression**

- Generate data points (80 training, 20 test)
- Linear function (**class Linear**)
- Loss function (**def loss_f**)
- Train the model
- Evaluate the model

3) **Exercise 1** : play with the parameters of the linear regression and the batch size



Tutorial II (2)

4) **Explanation** of the training loop with pseudocode

5) Building blocks of a Neural network

- Model (**class Dense**)
- Forward pass

5) Build a NN

- Multilayer NN (**dense1, dense2**)
- Overall model (**class MyModel**)

Tutorial III : Fully connected NNs

[Link](#)

→ Copy to drive

Introduction

- **Goal** : handwritten digit recognition with a fully connected NN
- **Program** : inverted classroom style
 - Theory
 - Overview to get the big picture of the Notebook
 - Work alone or in groups
- **Technical** : Google Colab, Pytorch

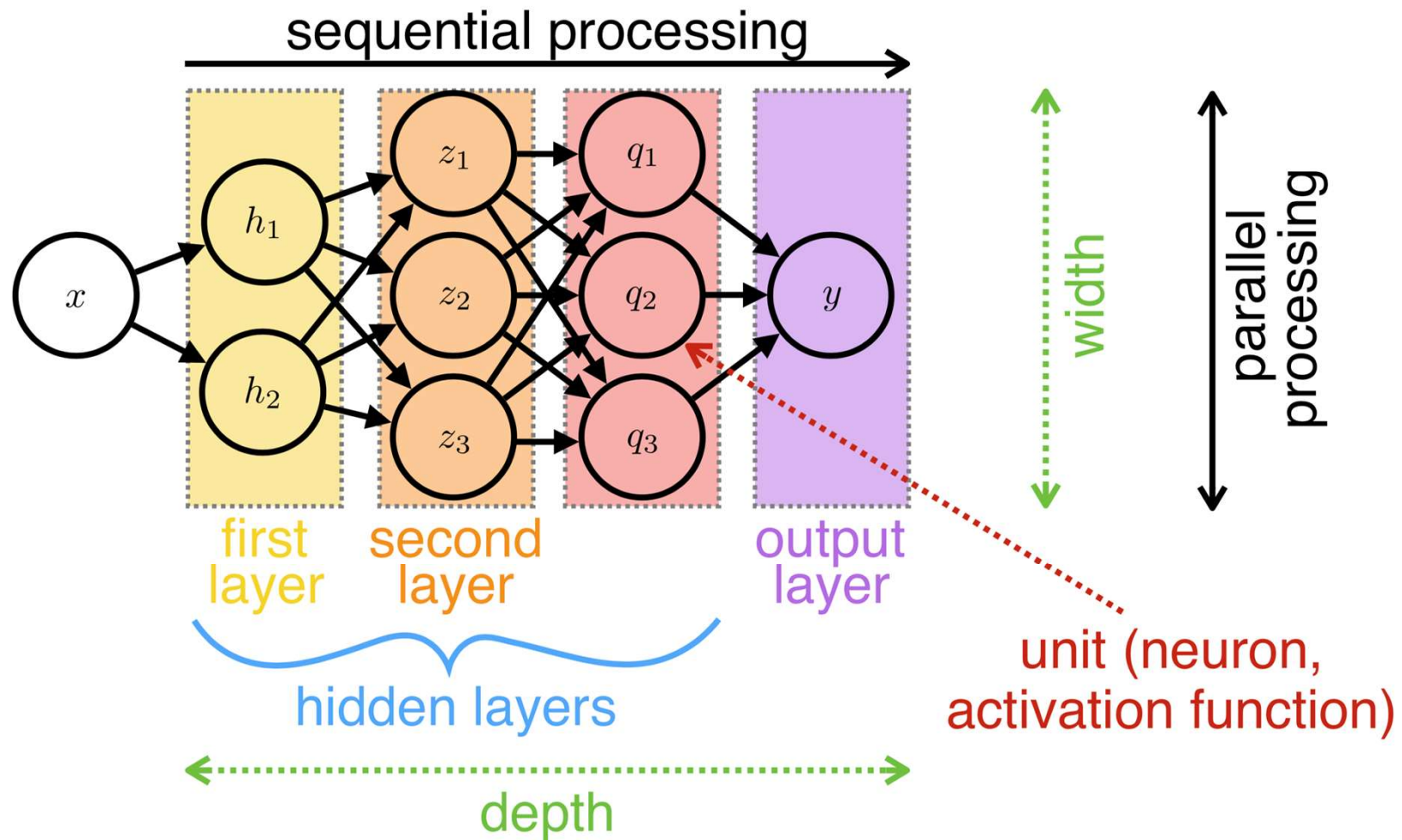
Theory

MNIST Dataset

- MNIST database with hand-written digits
- 60000 training images and 10000 testing images
- Created in 1994
- 128x128 binary images



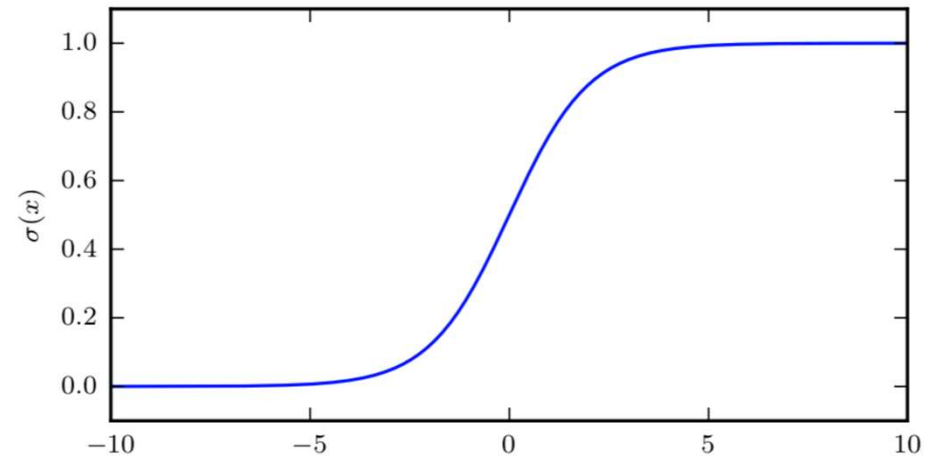
Network model



Sigmoid and softmax

Sigmoid (*two-class* classifier) :

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



Softmax (*multi-class* classifier) :

$$\text{softmax}(z)_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

Optimization

- Given a task we define

- Training data

$$\{x^i, y^i\}_{i=1, \dots, m}$$

- Network

$$f(x; \theta)$$

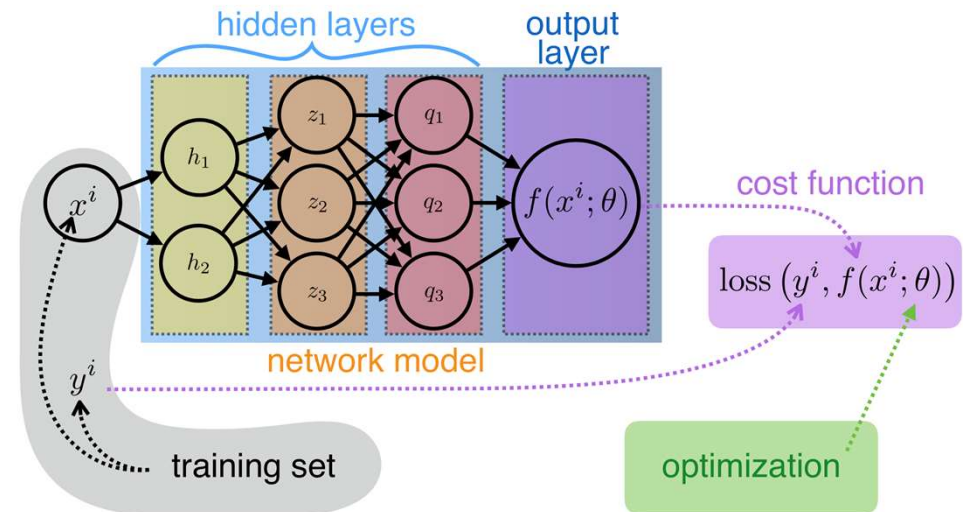
- Cost function

$$J(\theta) = \sum_{i=1}^m \text{loss}(y^i, f(x^i; \theta))$$

- Parameter initialization (weights, biases)

- random weights, biases initialized to small values (0.1)*

- Next, we *optimize the network parameters θ* (training)
- In addition, we have to set values for hyperparameters



Overview of the notebook

Tutorial III (1)

- 1) Load necessary **libraries** (common libraries) and data
- 2) **Training loop** (similar to Tutorial II)
 - Explanation
- 3) **Building blocks of a NN** (similar to Tutorial II)
- 4) **Structure of a NN**
 - Definition of a model and the forward pass (**class MyModel**)

Tutorial III (2)

5) Load the **data** (MNIST dataset)

- Training data, test data, normalization
- Plot examples

6) **Build** a NN

- Model, loss function, optimizer
- Training function
- Testing function
- Train the model (loss curves)
- Get the accuracy of the model

Tutorial III (2)

7) **Exercise 1** : build a NN with two layers

Exercises

```

import torch
import torch.nn as nn
import torch.optim as optim
from torch.utils.data import DataLoader, TensorDataset

# Définition du réseau
class SimpleNN(nn.Module):
    def __init__(self):
        super(SimpleNN, self).__init__()
        self.fc1 = nn.Linear(784, 1500) # Input size = 784 (ex: MNIST), output = 1500
        self.relu = nn.ReLU()
        self.fc2 = nn.Linear(1500, 10) # Output size = 10 (classes)
        self.softmax = nn.Softmax(dim=1)

    def forward(self, x):
        x = self.fc1(x)
        x = self.relu(x)
        x = self.fc2(x)
        x = self.softmax(x)
        return x

# Données fictives pour l'exemple
# 784 features (ex: pixels de MNIST), 1000 échantillons
X = torch.rand(1000, 784)
y = torch.randint(0, 10, (1000,)) # Classes entre 0 et 9

# Dataset et DataLoader
dataset = TensorDataset(X, y)
dataloader = DataLoader(dataset, batch_size=64, shuffle=True)

# Initialisation du modèle, de la fonction de perte et de l'optimiseur
model = SimpleNN()
criterion = nn.CrossEntropyLoss() # Perte adaptée pour classification
optimizer = optim.Adam(model.parameters(), lr=0.001) # Taux d'apprentissage initial

```

Exercise 1

```

# Entraînement du modèle
def train_model(dataloader, model, criterion, optimizer, epochs=10, lr_scheduler=None):
    for epoch in range(epochs):
        total_loss = 0
        for inputs, labels in dataloader:
            optimizer.zero_grad() # Réinitialiser les gradients
            outputs = model(inputs) # Passage avant
            loss = criterion(outputs, labels) # Calcul de la perte
            loss.backward() # Calcul des gradients
            optimizer.step() # Mise à jour des paramètres
            total_loss += loss.item()

        # Ajustement dynamique du taux d'apprentissage
        if lr_scheduler:
            lr_scheduler.step()

        print(f"Epoch {epoch+1}/{epochs}, Loss: {total_loss:.4f}, LR: {optimizer.param_groups[0]['lr']:.4f}")

# Ajustement du Learning rate avec ReduceLROnPlateau
scheduler = optim.lr_scheduler.ReduceLROnPlateau(optimizer, mode='min', factor=0.5, patience=10)

# Entraîner le modèle
train_model(dataloader, model, criterion, optimizer, epochs=10, lr_scheduler=scheduler)

```

Tutorial IV : Convolutions

[Link](#)

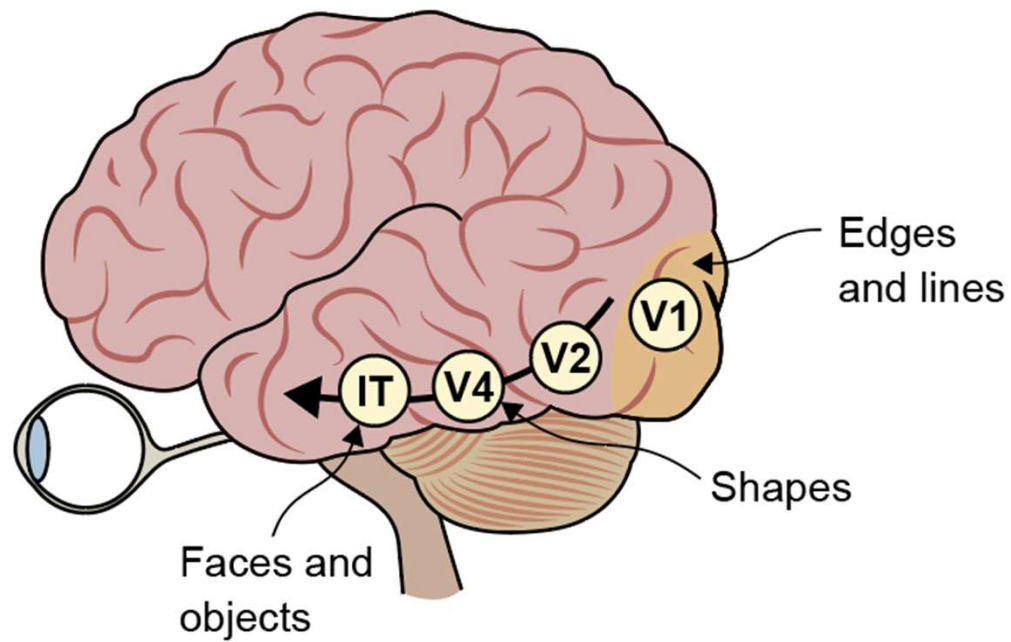
→ Copy

Introduction

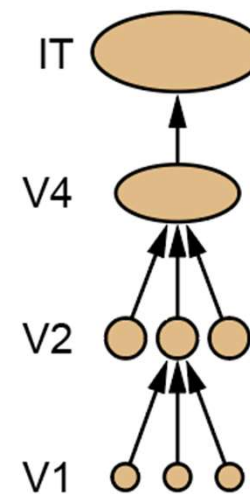
- **Goal** : basics to perform image recognition (Inception)
- **Program** : inverted classroom style
 - Theory
 - Overview to get the big picture of the Notebook
 - Work alone or in groups
- **Technical** : Google Colab, Pytorch

Theory

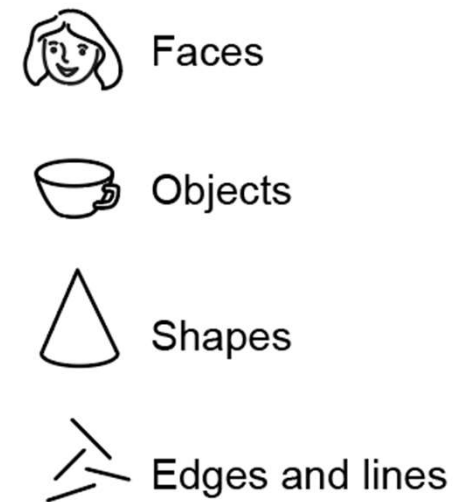
Human vision



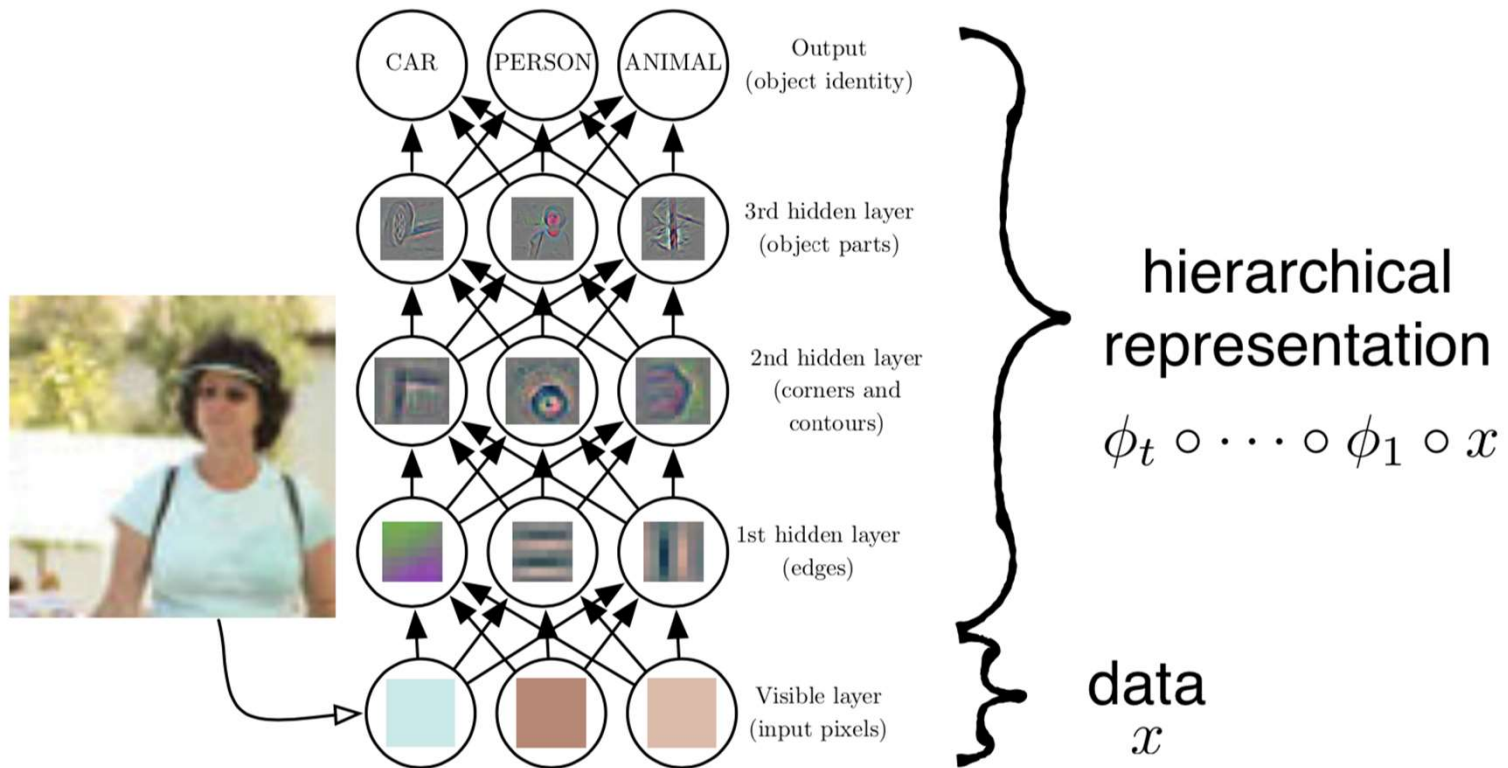
Receptive fields size



Features



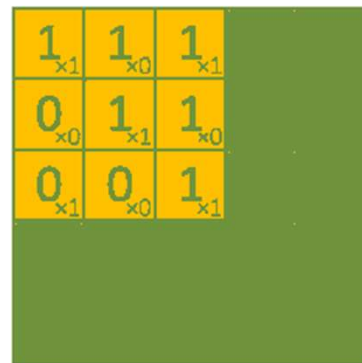
Computer vision



Kernel (filter)

- Used to **detect features** (vertical/horizontal filter,...)
- Different kernels to create different feature maps → learn to see various patterns and details in images

1	0	1
0	1	0
1	0	1



Image

4		

Convolved
Feature

how well the pattern in the kernel matches
the content in that part of the image

= Feature map

Kernel example

1	0	-1
1	0	-1
1	0	-1

Vertical

1	1	1
0	0	0
-1	-1	-1

Horizontal



Vertical edges

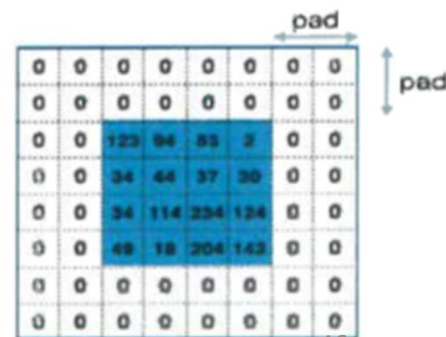
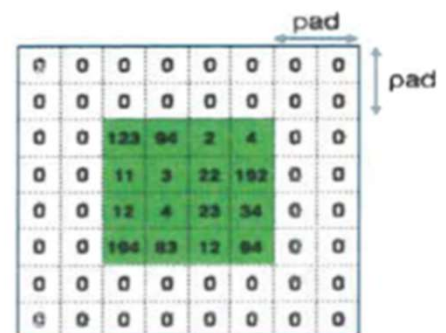
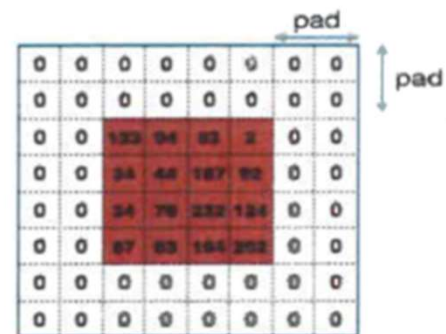
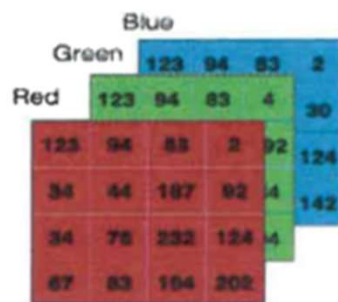


Horizontal edges

Padding, Stride, Dilation



=



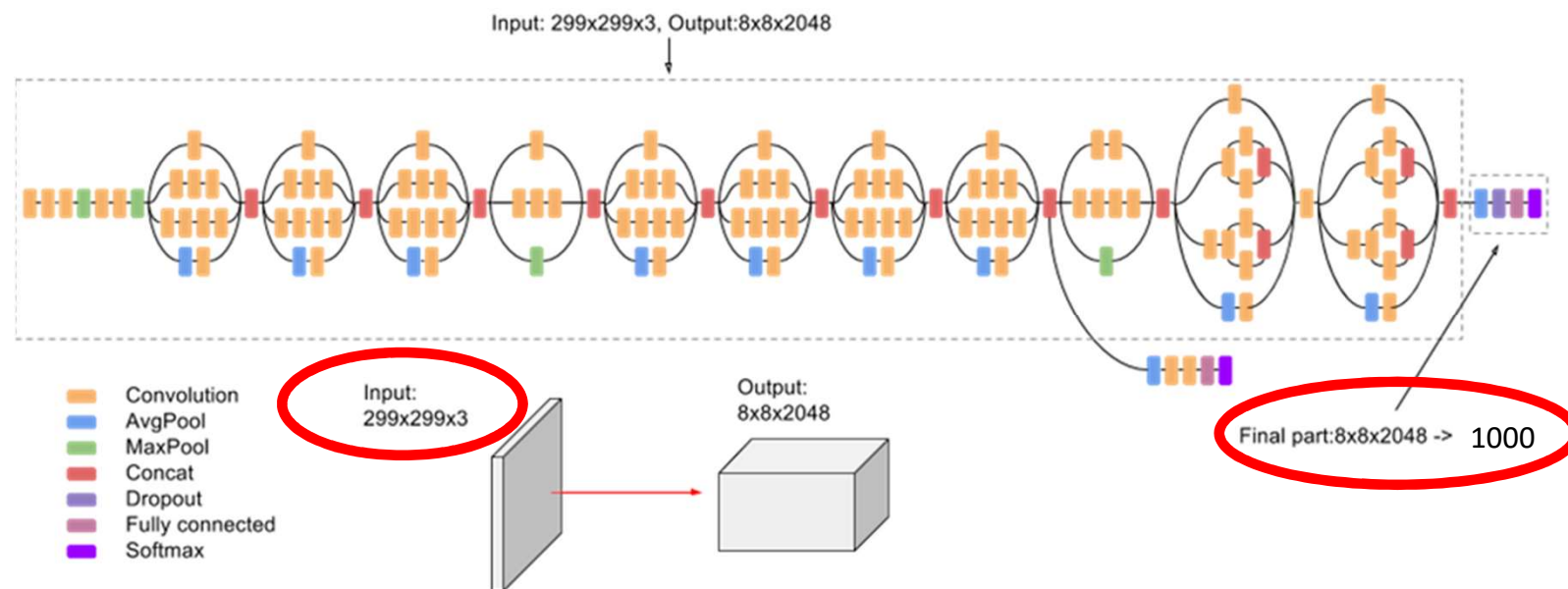
1	2	3
4	5	6
7	8	9



1		2		3				
		4		5		6		
				7		8		9

Inception V3 model

- Deep learning model based on Convolutional Neural Networks
- Used for image classification
- Released in year 2015
- It has 42 layers

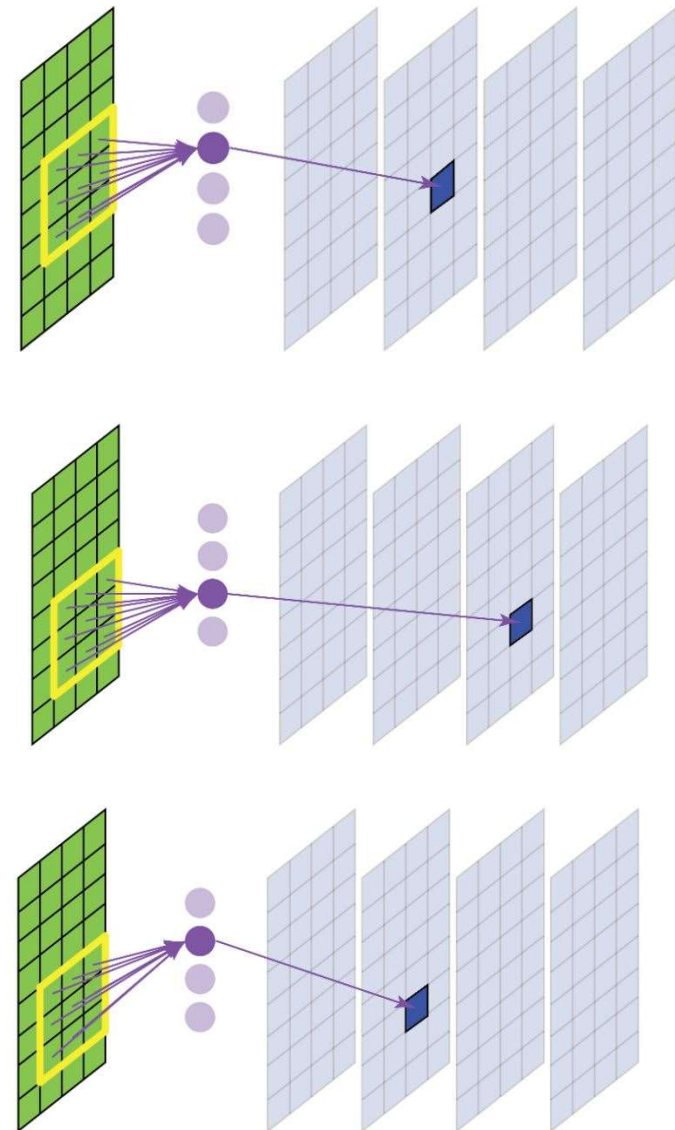
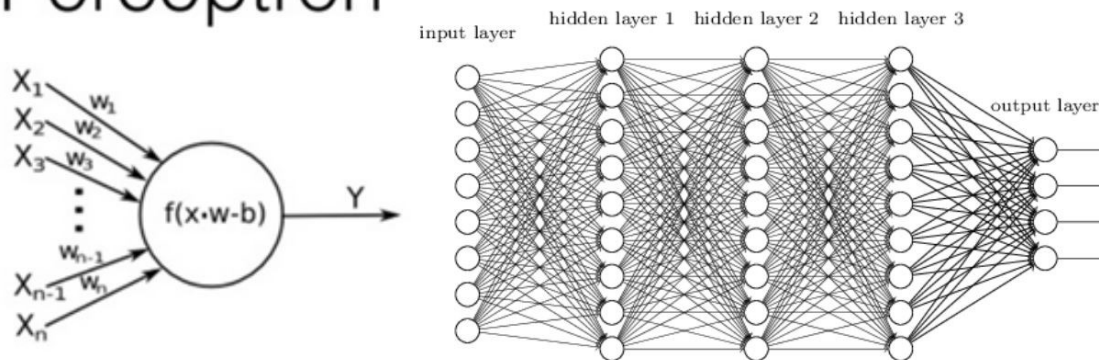


Overview of the notebook

Tutorial IV (1)

- 1) Load necessary **libraries** (common libraries and personal modules)
- 2) Images
- 3) **Convolutions**

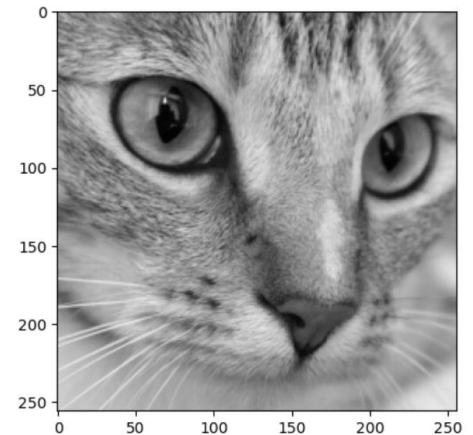
Perceptron



Tutorial IV (2)

- Pre-processing of the image

- Gray-scale, cropping, float conversion, normalization
- Add dimensions (batch, channel, height, width) (in `get_convolved`)
- Convert Numpy to pytorch (in `get_convolved`)



- Define the convolution

- Forward model (`class Model`)
- Apply 4 convolutions one after each other (inside `class Model`, call `conv_2d` function)

- Define the filter

- Identity filter
- Convert to np.array (in `get_convolved`)
- Add dimensions
- Convert Numpy to pytorch

```
flt_mtx = [  
    [ 0, 0, 0, 0, 0,],  
    [ 0, 0, 0, 0, 0,],  
    [ 0, 0, 1, 0, 0,],  
    [ 0, 0, 0, 0, 0,],  
    [ 0, 0, 0, 0, 0,],  
] # identity transformation
```

Tutorial IV (3)

- Use it ! (`ims_convolved = get_convolved(img_raw, flt_mtx)`)
 - You get back 5 figures

- Exercise :

1. experiment with different filters and understand what they do, e.g.:

- identity transformation
- identity transformation with positive non-unit values
- identity transformation with negative unit value
- identity transformation off center
- blurring with box filter
- edge detection with + and - bands
- try whatever you like

2. experiment with convolution parameters:

- padding = 1, 2, 3
- stride = 2
- dilation = 2

0	0	0	0	0
0	0	0	0	0
0	0	30	0	0
0	0	0	0	0
0	0	0	0	0

0	0	0	0	0
0	0	0	0	0
0	0	-1	0	0
0	0	0	0	0
0	0	0	0	0

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	1	0	0
0	0	0	0	0

1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1

0	-1	1	0	0
0	-1	1	0	0
0	-1	1	0	0
0	-1	1	0	0
0	-1	1	0	0

Tutorial IV (4)

filter type	effect
gaussian	blurring
first derivative of gaussian	detection of edges
second derivative of gaussian	detection of peaks

- Most common filters

- Define 1D functions
- Create 2D filters by repeating the 1D filters along axis 0 (`np.tile`)
- Multiply by `transpose()` to get the horizontal dimension (filter size does not change)
- Use them ! (`ims_convolved = get_convolved(img_raw,flt_mtx)`)

4) Homework (leave it for now)

Tutorial IV (5)

5) Load a pretrained model (inception V3) from torchhub

6) Test the model

- Preprocessing of the image (cropping, shuffle sizes, totensor, normalize adds batch size) → [1,3,299,299]
- Deactivate the gradient (eval mode)
- Get the logits (1000 values), then the probabilities (applying softmax)
- Print out the 5 most probable classes
- Do the same with 100 classes

Tutorial V : Transfer Learning

[Link](#)

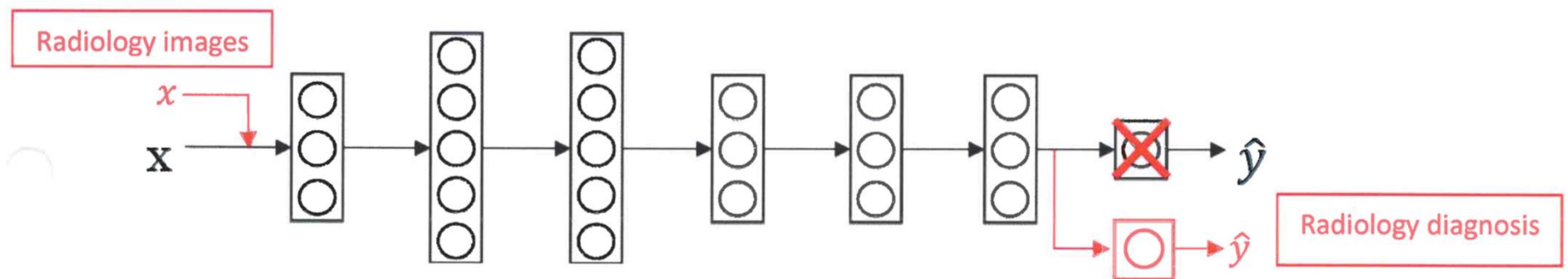
Introduction

- **Goal** : use the Inception model to classify images of different nature (it/de), learn how to save a model
- **Program** : inverted classroom style
 - Theory
 - Overview to get the big picture of the notebook
 - Work alone or in groups
- **Technical** : Google Colab, Pytorch

Theory

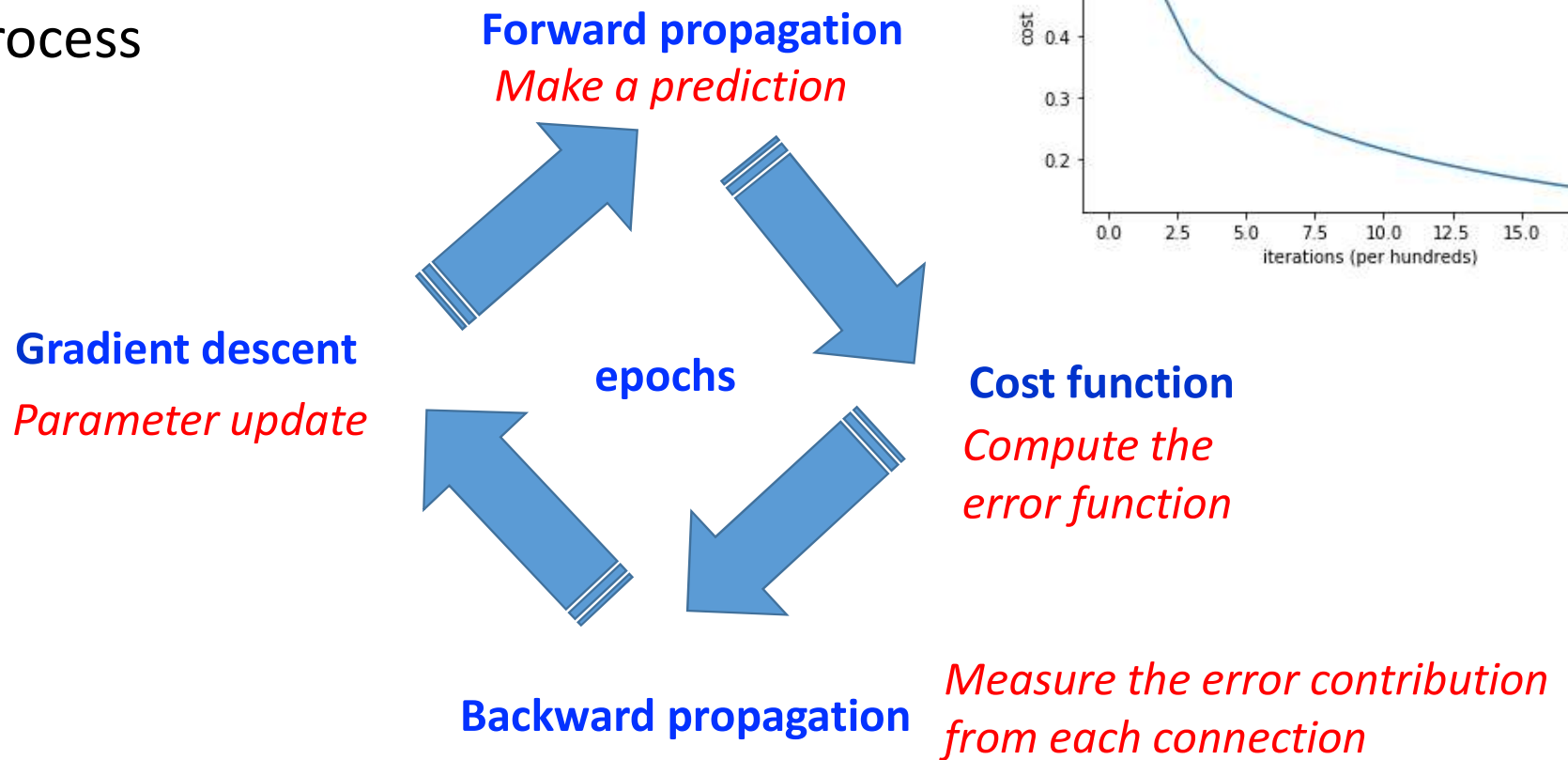
Transfer Learning

- Try to find an existing neural network that accomplishes a **similar task** to the one you are trying to tackle
- reuse the lower layers of this network
 - Output layer should usually be replaced
- **Speeds up** training and requires much fewer training data

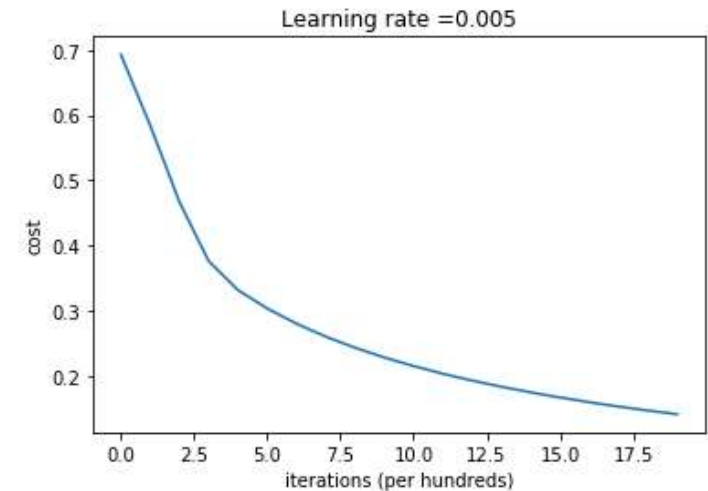


Training Loop

- *Iterative* process

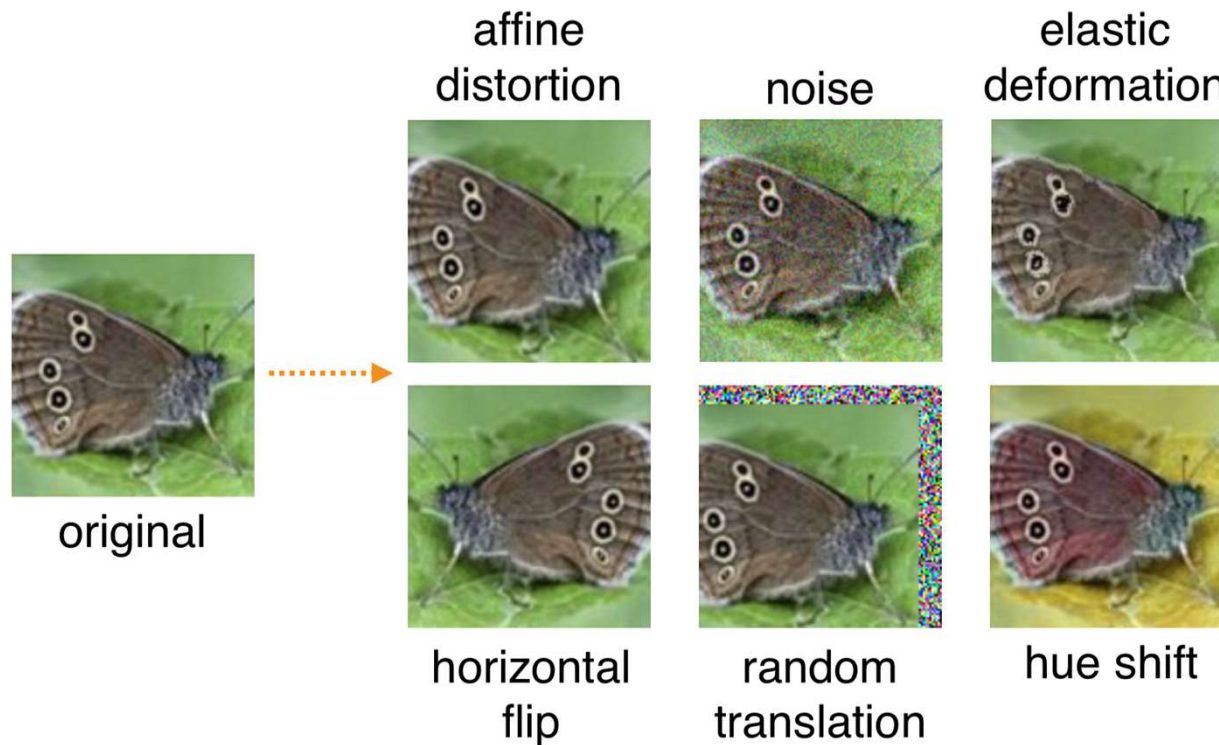


Learning curve



Dataset Augmentation

- Apply **realistic transformations** to data to create new synthetic samples, with same label



Overview of the notebook

Tutorial V (1)

1) Load necessary **libraries** (common libraries and personal modules)

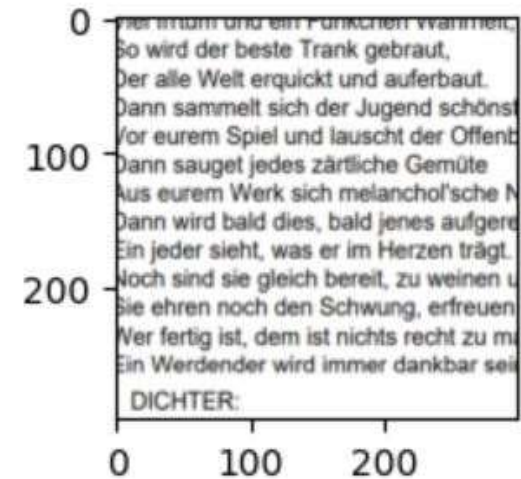
2) Transfer Learning

- Load the **inception model** (**base_model**)
- Build **new model** using the **base_model** (**model**)
 - Define a head function (in_features, n_classes=2) : use of sigmoid
- **Optimization** : define the loss function (**criterion**) and the optimizer
- **Helper functions** to get the prediction (**get_predictions**) and to compute the batch accuracy (**calculate_accuracy_batch**)

Tutorial V (2)

3) Dataset

- **Images** :
 - Get them from **ML3** folder
 - Preprocessing using **transforms.Compose (resize, tensor, normalize)**
 - Shape **[3,299,299]**
 - Transform to numpy array for display (**im_numpy**)
- **Labels**
- **Split** dataset into train/test samples
 - **Torch.utils.data.random_split**
 - **Train_test_split** with **stratify** enabled from scikit-learn
- Create **data loaders** for training/val (beware shuffle param)
- Example : batch of 10 images, plot them, print logits and output classes (**res**)



Tutorial V (3)

4) Training

- **Train_model** function
 - Contains the loop on **epochs**
 - Calls the **train** and **validate** functions (beware the params)
 - Save **history** (loss, accuracy) and model for a given epoch
- **Train function** : reset gradients, compute logits and loss, compute gradients (backward prop), update parameters, calculate accuracy of the batch (helper functions), returns train loss and train accuracy
- **Validate function**: structure BUT (no optimizer, no backward, no update of the params), returns test loss and test accuracy
- **Plot_history** function
- Run it ! **history = train_model(...)** using 70 epochs

Tutorial V (4)

5) Load trained variables from checkpoint

- Choose epochs values
- Load corresponding models
- Call validate function to get the validation loss and validation accuracy (see how it evolves)

6) Save final model for inference

7) Inference :

- Load the model, eval() mode
- Get an image, preprocess (convert to tensor, add batch dimension)
- Get the logits and associated class

Tutorial V (4)

8) Improve the results : data augmentation

- Load images from **ML3** folder
- Preprocess (**resize**, **Randomcrop**, **tensor**, **normalize**)
- Convert to Numpy for plotting purposes (**im_numpy**)
- The rest of the code is similar to previous code

9) Exercise

Tutorial VI : RNNs

[Link](#)

Introduction

- **Goal** : use Recurrent Neural Networks to predict and generate text sequence
- **Program** : inverted classroom style
 - Theory
 - Overview to get the big picture of the notebook
 - Work alone or in groups
- **Technical** : Google Colab, Pytorch

Theory

Overview of the notebook

Tutorial VI (1)

1) Load necessary **libraries** (common libraries and personal modules)

2) Text data

- Read the data (**rnn.txt**), print the first 100 words

3) Build the **dataset**

- 2 dictionaries : word → id (**dictionary**) and id → word (**reverse_dictionary**)
 - Build_dictionaries function
- Vocabulary size = 493 (0=most common word)
- Helper functions to get sequences of int or words (**text_to_ints**, **ints_to_text**)
- Print example : first 100 words (or int), length of input data=2118 (words_as_int)

Tutorial VI (2)

3) Data streaming

- Create dataset using **WordDataSet** class to create blocks of text
 - Block length = $n_input + 1 = 3 + 1 = 4$
- Create **DataLoader** with **batch size=50**, **preprocess** data (separate input and target sequences, **stack** data and convert Numpy → **tensors**, put them to **GPU**)
 - Length of dataset = Number of blocks in sequence = $\text{Total length} / \text{Block length} = 2118 / 4 = 529$
- Example : print the 50 samples that are in the 1st batch

Tutorial VI (3)

4) Construct model

- Create **class RNN**
 - Embedding layer (vocab_size, embedding_dim=128)
 - Loop to add the 3 **LSTM** layers
 - **FC** layer with vocab_size
- Define sequence of 3 words (**n_input**), define dimension of 3 LSTM, call the RNN class
- Investigate the model using **Tensorboard**
 - Create an input of size=5 (**x**), transform to tensor, add batch
 - **SummaryWriter** to save the model and be able to open it with tensorboard
 - Print the output size of **y** : [5,1,493]
- Test the **NOT trained model** and see that it is bad
 - Get the first batch (break), apply the model, get the predictions, compare to true

Tutorial VI (4)

5) Train the model

- Params : `n_input = 3`, `batch_size=50` , one LSTM layer (128), `n_epochs=200`
- Create the `data loader` (preprocess data)
- `Optimization` part : `criterion`, `optimizer` (RMSprop)
- `Training loop` on epochs, then on batches
 - Initialize gradients
 - Get the output (`seq_len`, `batch_size`, `vocab_size`), reshape it to (`seq_len*batch_size`, `vocab_size`)
 - Reshape labels (`seq_len`, `batch_size`) to (`seq_len*batch_size`)
 - Compute the loss between output and true labels
 - Backward prop, param update
 - Compute loss and accuracy
- `Plot` loss and accuracy

Tutorial VI (5)

6) Generate text with RNN

- Function to generate text (`gen_long`)
 - Input parameters : model, input sequence, number of words to generate (128)
 - `No_grad()` because we are in an evaluation mode
 - Loop on number of words, convert to tensor, predict, ...)