Artificial Intelligence day @IRCER Limoges

Machine Learning feedbacks: Reproducibility, Meta-parameters

Jean-Luc CHARLES

Retired from ENSAM Bordeaux,
I2M, UMR 5295 CNRS, TALENCE.

Jean-Luc.Charles@mailo.com

14 mars 2025

Presentation Summary

- Historical way, definitions & concepts of AI & Deep Learning (DL)
- Reproducibility in Deep Learning
- Meta-parameters
- Sharing reproducible DL training

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My professional career

- First industrial career ~10 years (Signal Processing at Thomson-SINTRA then OO C++ development at Capgemini)
- I joined the I2M lab at ENSAM (Bordeaux) as a lecturer, working on "The Contribution of OO to Simulation in Mechanics”
- I taught Scientific & OO programing in Python at ENSAM
- I started to work on AI & Deep Learning in 2015
- Now I go on working on AI as a self-worker...

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- Historical way, definitions & concepts of AI & Deep Learning (DL)
- Reproducibility in Deep Learning
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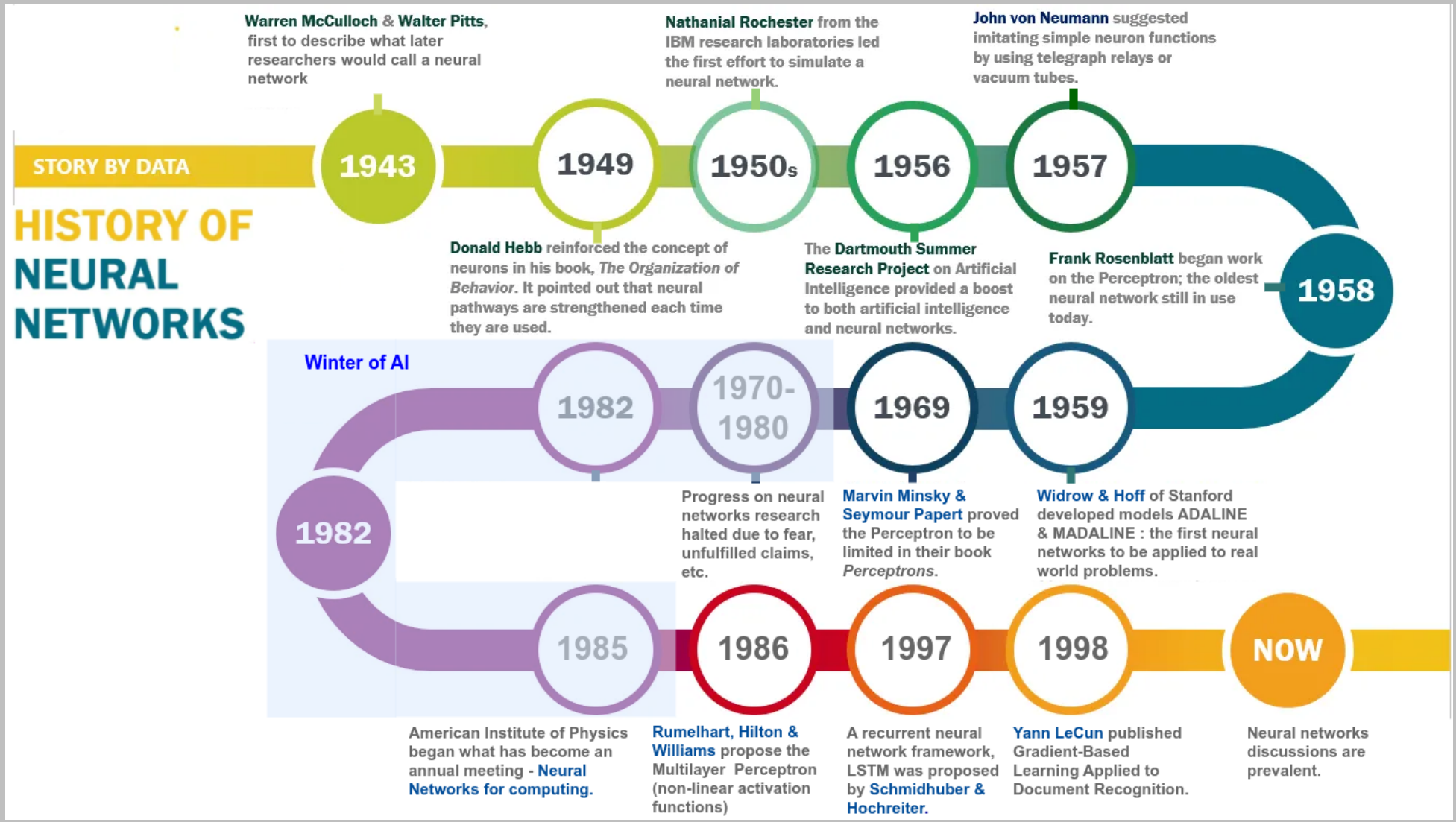
- Sharing reproducible DL training

Ressources

- GitHub repository for the PDF slides:
- GitHub repository for the example notebooks:

AI : the historical way... from 1950 to 2000s



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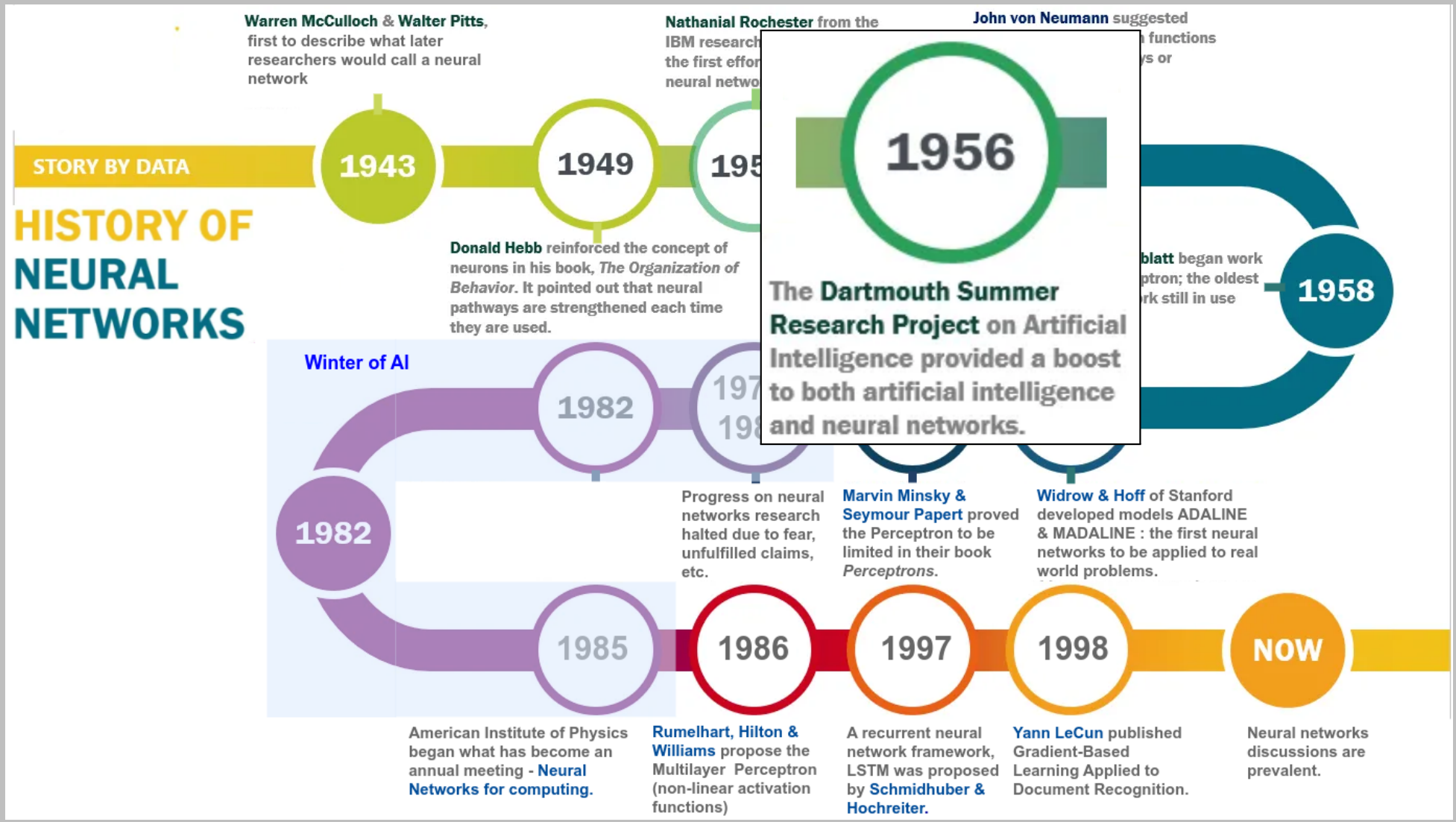

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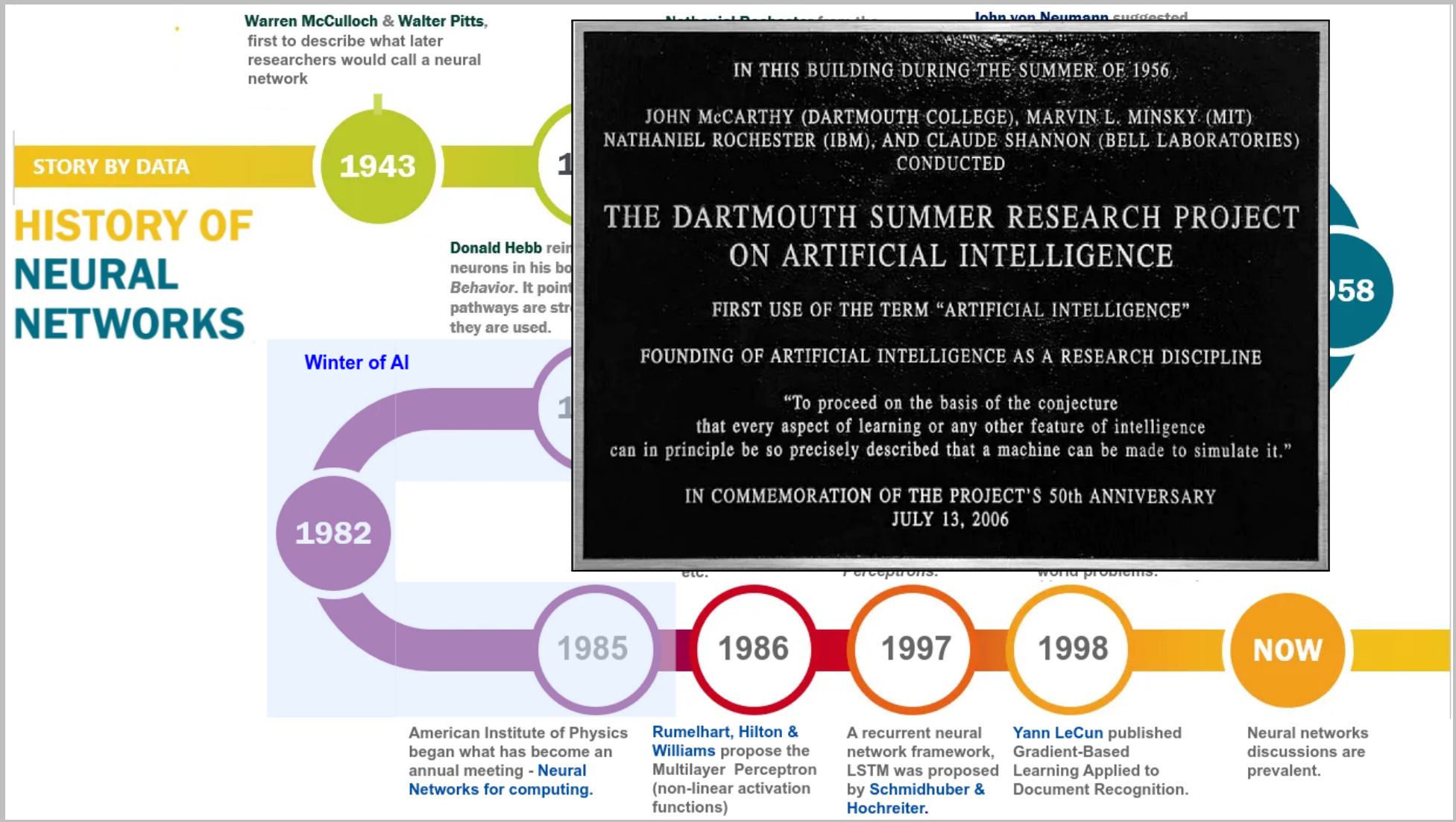

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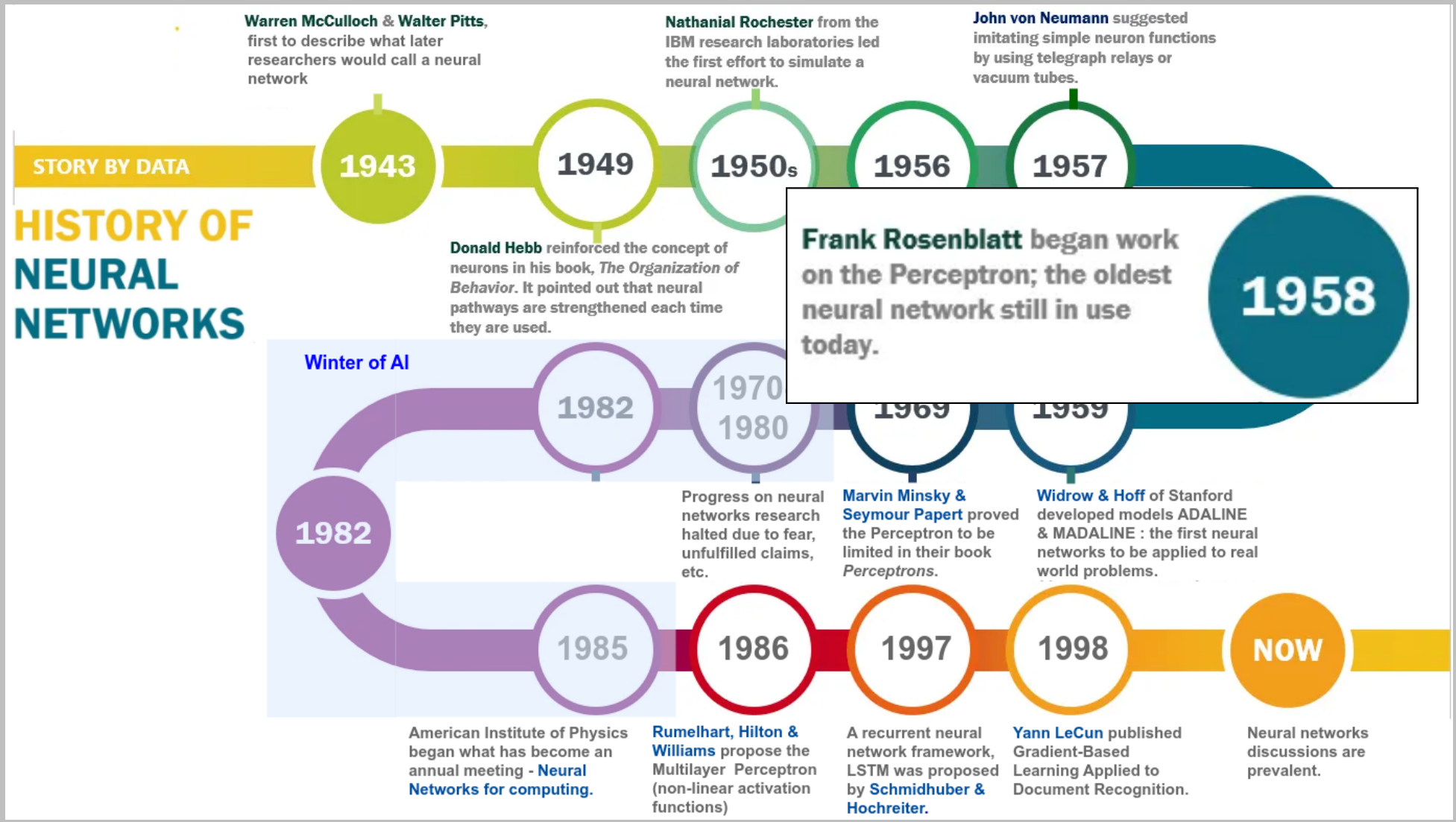

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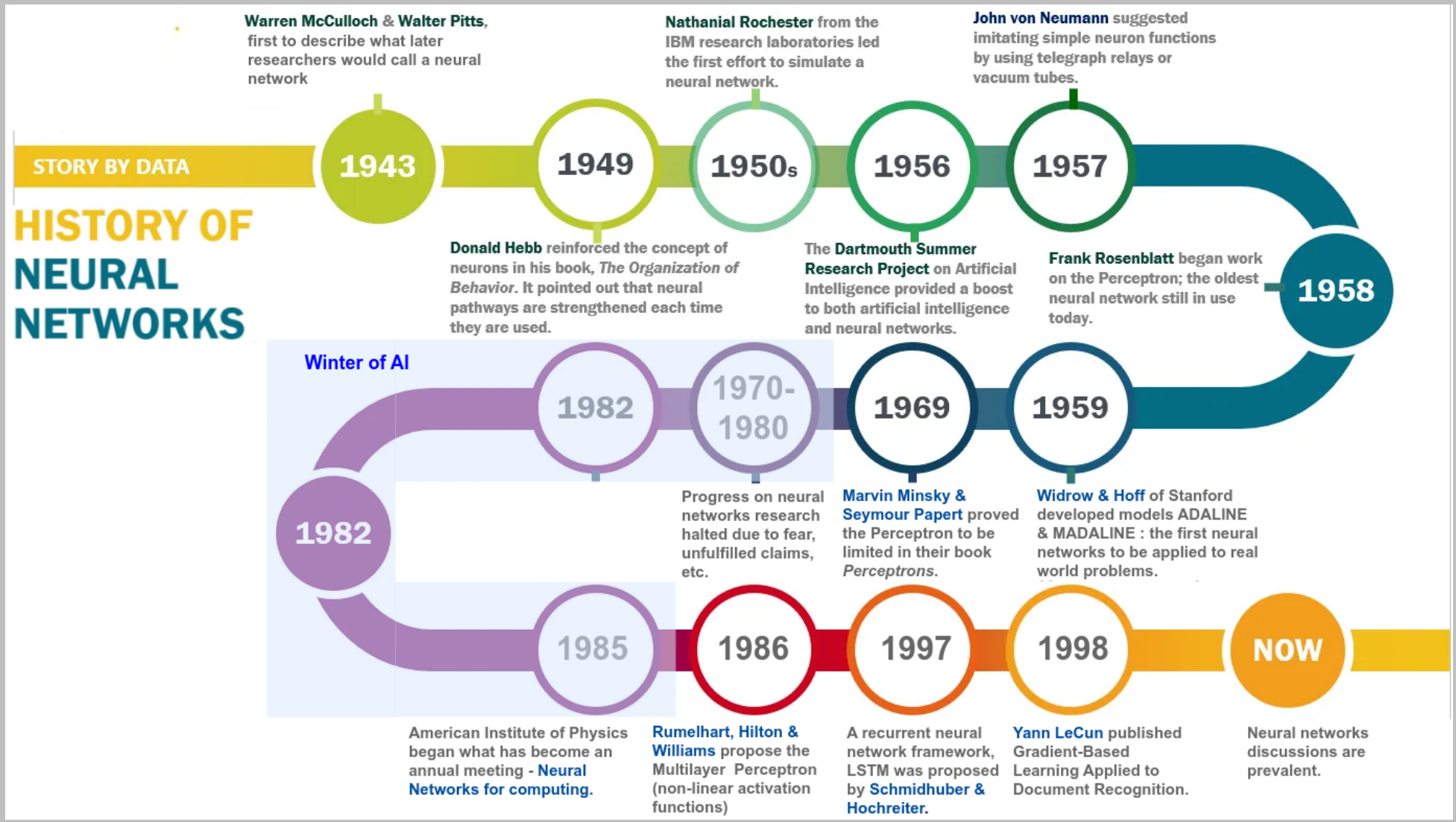

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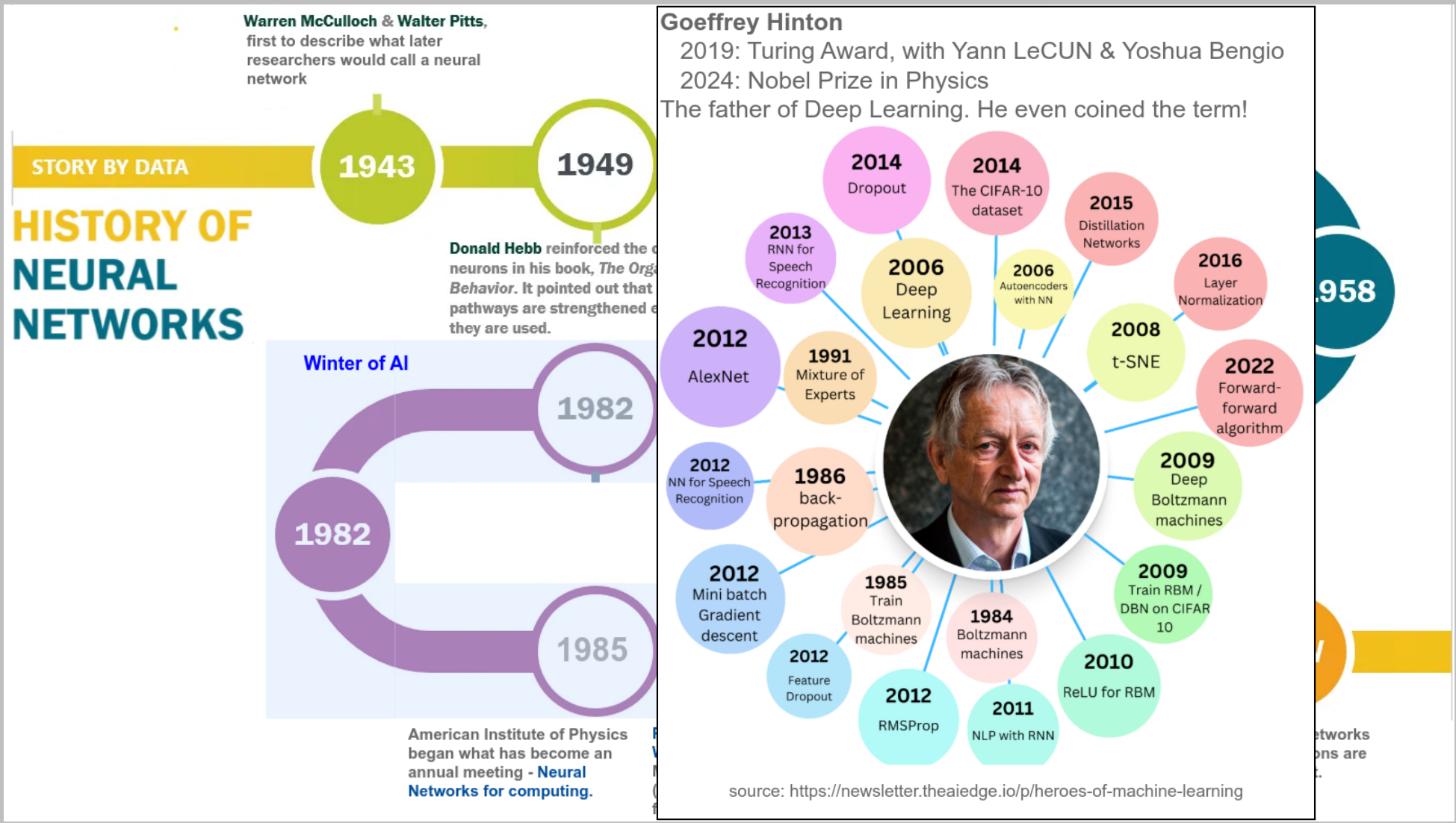

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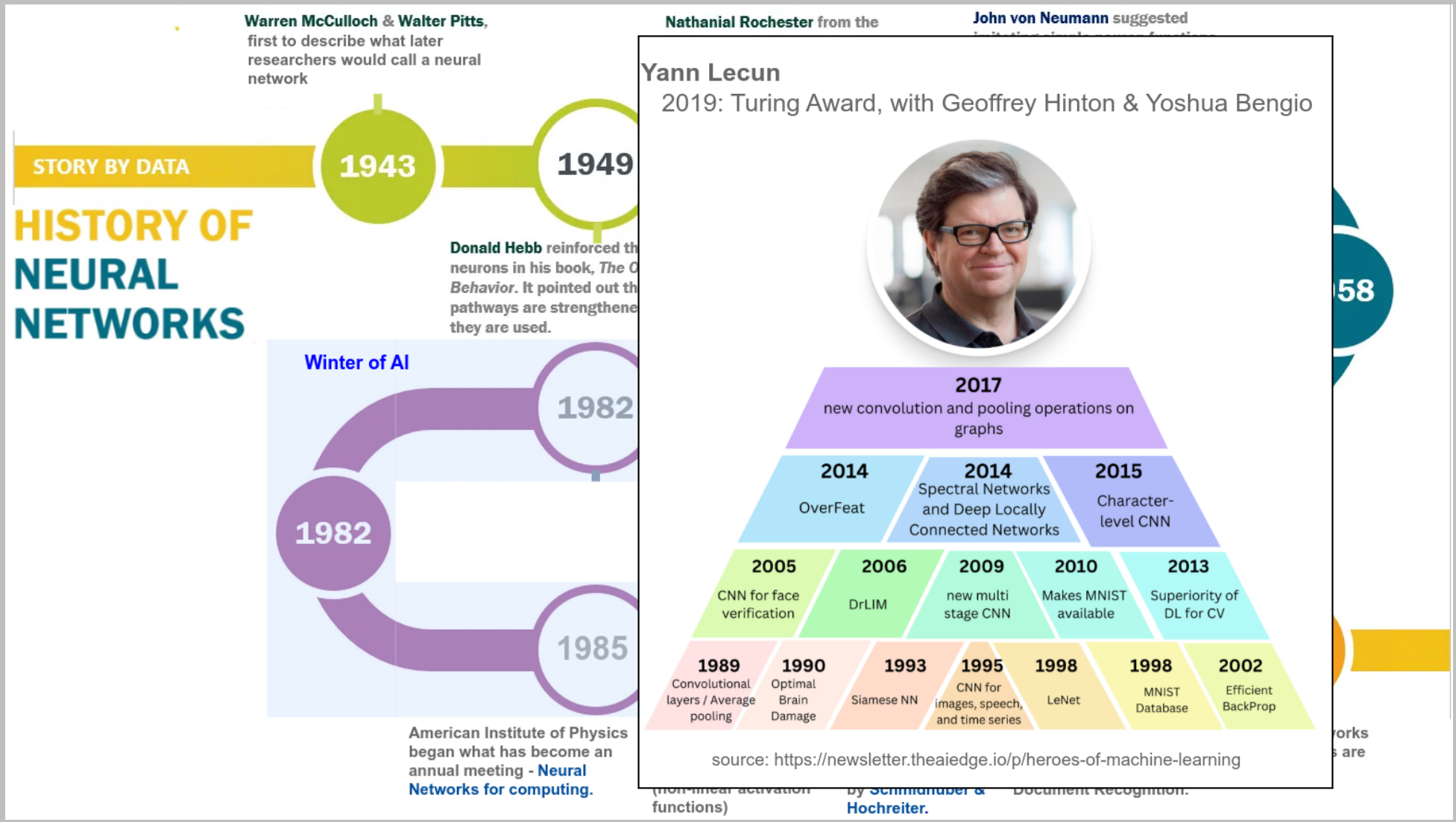

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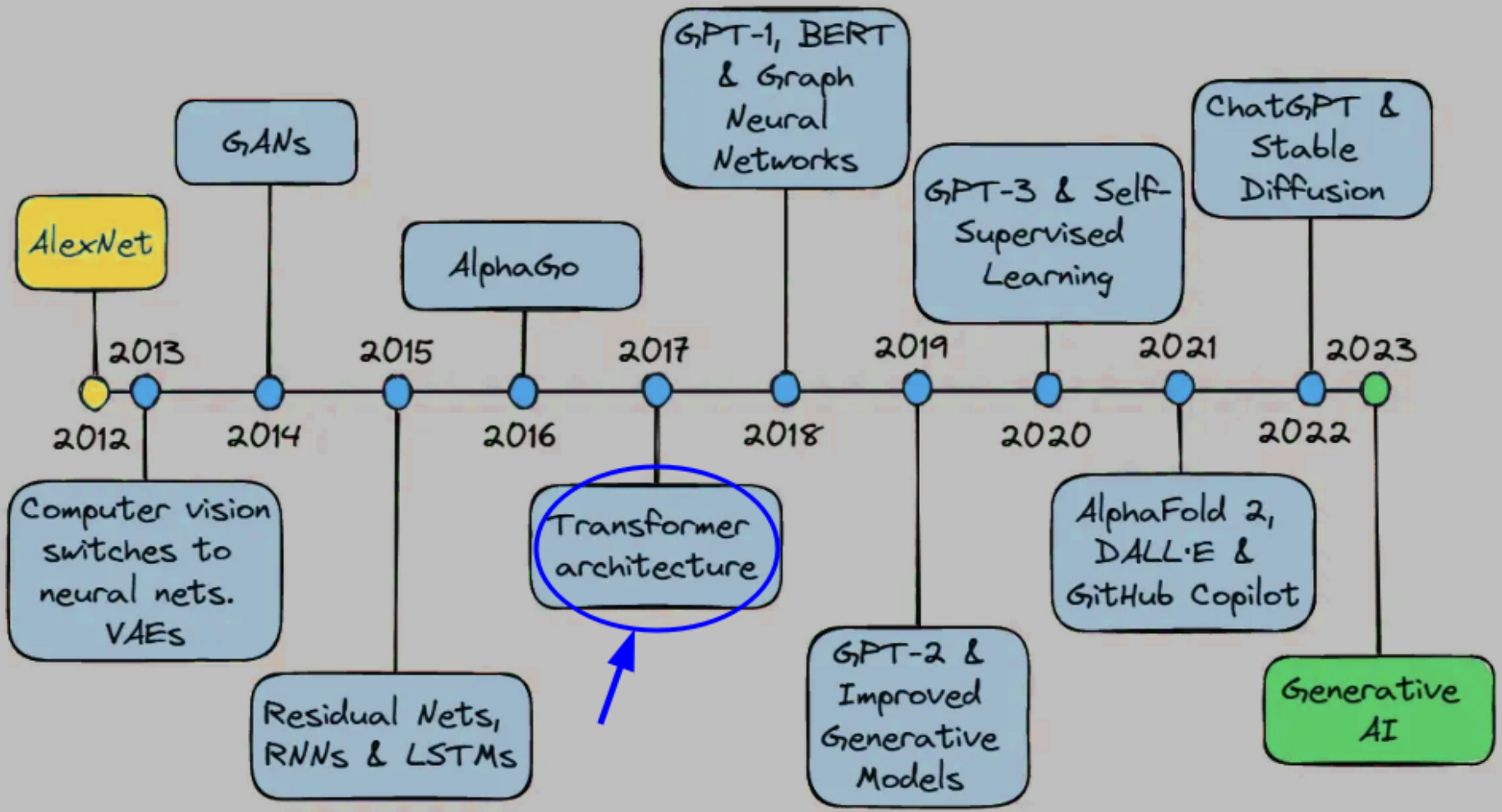
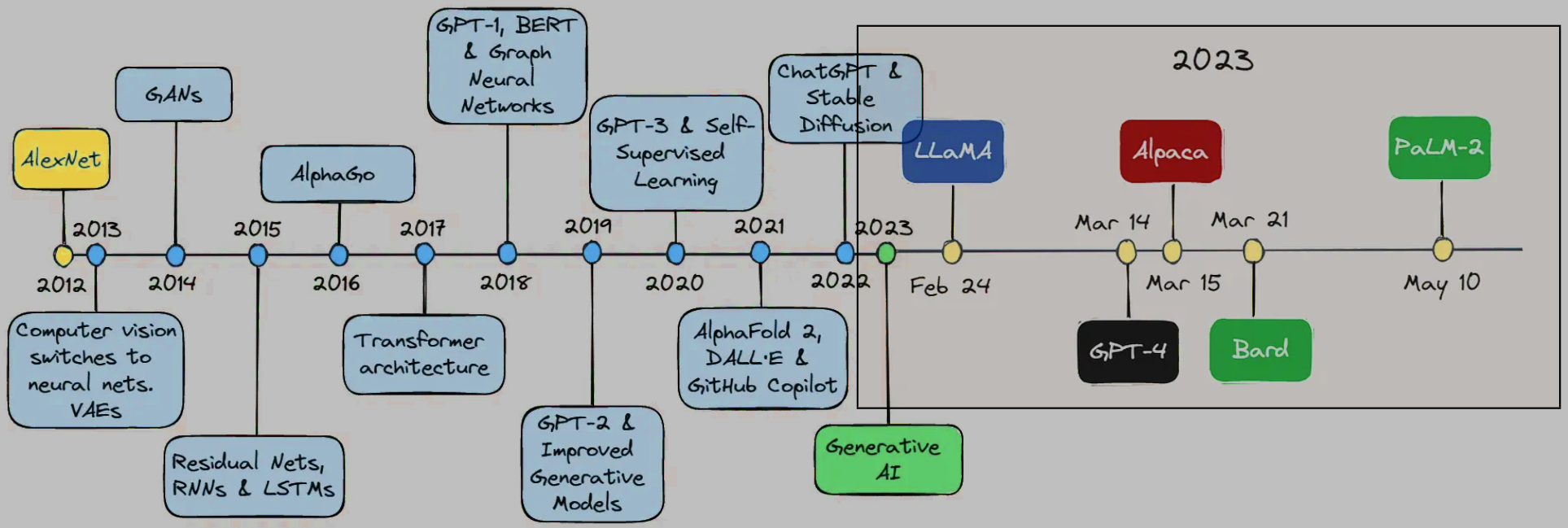
The historical way... post 2012s: the "coming-of-age" of deep learning



Source: Thomas A Dorfe: "Ten Years of AI in Review", kdnugets.com

The historical way... post 2023s, crazy acceleration



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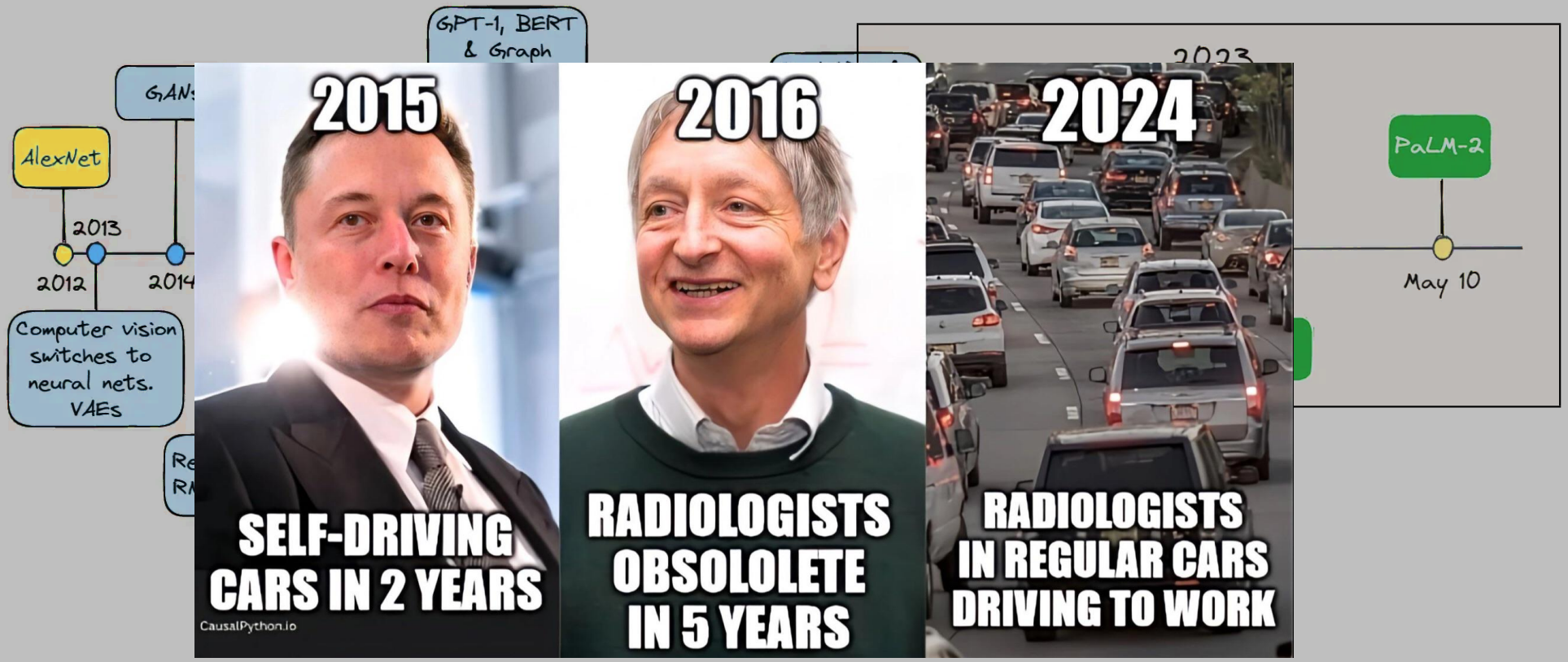

Artificial Intelligences ?

Narrow/Weak AI

Strong/General AI

Artificial Intelligences ?

Narrow/Weak AI

- AI systems designed for specific, narrow tasks:
  AlphaGo, self-driving cars, robot systems in the medical field...
- The most common form of AI that we encounter today.
- Builds systems that **behave like humans**.
- We already are there... We use it every day!
  anti-spam, facial/voice recognition, language translation...

Strong/General AI

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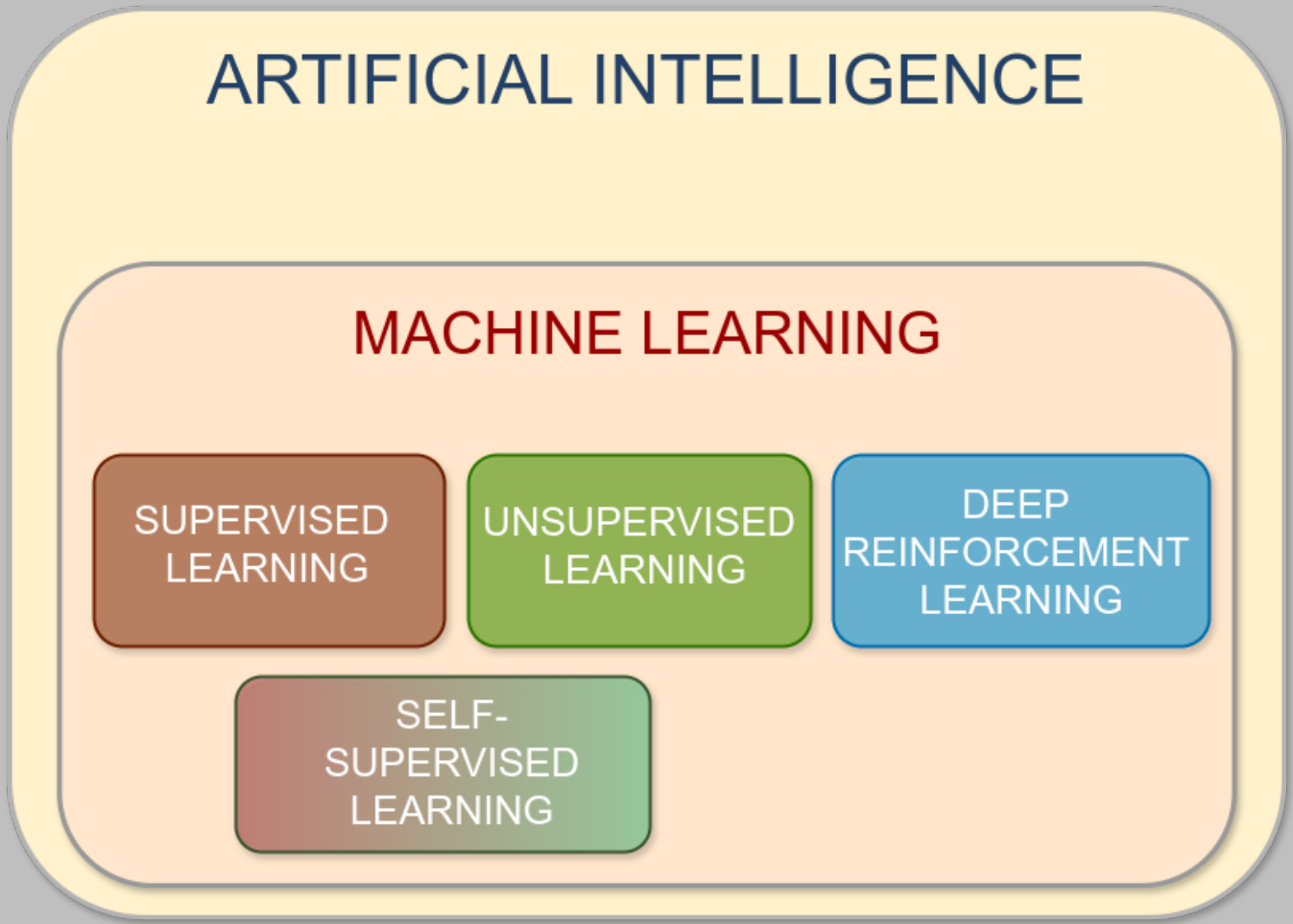
- We already are there... We use it every day!
  anti-spam, facial/voice recognition, language translation...

Strong/General AI

- Builds systems with the ability to reason in general.
- Could explain how humans think?
- Whe are not yet here... but closer and closer every day

Machine Learning: a field of AI



Branches of Machine Learning

Supervised learning

A **labeled dataset** is used to train algorithms (models):

- **Classification**
  - Images classification
  - Objects detection in images
  - Speech recognition...
- **Regression**
  - Predict a value...
- **Anomaly detection**
  - Spam detection
  - Manufacturing: finding known (learned) defects
  - Weather prediction
  - Diseases classification...

. . .

Branches of Machine Learning

Unsupervised learning

The algorithm attempts to identify patterns / structures within **unlabeled datasets**:

- **Clustering** & **Grouping**
  - Data mining, web data grouping, news grouping...
  - Market segmentation
  - Astronomical data analysis...
- **Anomaly Detection**
  - Manufacturing: finding defects (even new ones)
  - Monitoring abnormal activity: failure, hacker...
  - Fraud detection: fake account on Internet...
- **Dimensionality reduction**
  - Data compressions...

. . .

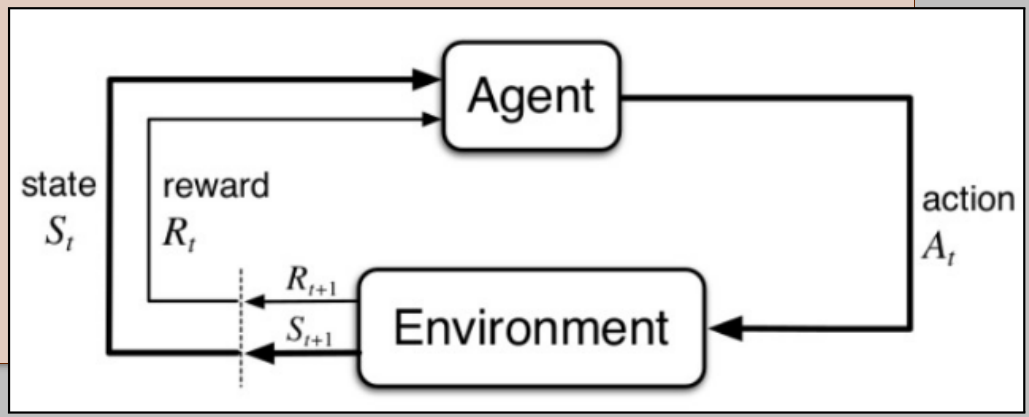
Branches of Machine Learning

Deep Reinforcement Learning DRL

An agent (the model) learns how to drive an environment within a trial and error process by maximising a cumulatd **reward**:

- **Control/command**
  - Controlling drones, mecatronic systems, electric VTVL rocket, robots
  - Factory optimization
  - Financial (stock) trading...
- **Decision making**
  - games (video games)
  - financial analysis...

. . .



Branches of Machine Learning

Self-Supervised Learning [SSL1]

- Aims to learn features/patterns from **unlabeled data without relying on human annotations**.
- Can extract data features that exhibit robust generalization.
- Technically a subset of Unsupervised Learning.
- But closely related to Supervised Learning
  $\rightsquigarrow$ optimizes performance against a self-learned ground truth.

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Branches of Machine Learning

Self-Supervised Learning

2 main stages of SSL:

- **Pre-training** (Unsupervised):
- **Fine-Tuning** (Supervised Task):

Branches of Machine Learning

Self-Supervised Learning

2 main stages of SSL:

- **Pre-training** (Unsupervised):
  The model learns useful representations from unlabeled data by solving *pretext tasks*:
  - Image-Based SSL: Predicting missing parts of an image, similarity between original and augmented images
  - Text-Based SSL: Predicting missing words in a sentence
  - Audio-Based SSL: Predicting the next segment of audio.
- **Fine-Tuning** (Supervised Task):

Branches of Machine Learning

Self-Supervised Learning

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- **Fine-Tuning** (Supervised Task):
  The model is adapted to a specific task (image classification, speech recognition) using a smaller labeled dataset.

Various approaches for ML algorithms

Supervised learning:

- Neural Networks
- Bayesian inference
- Random forest
- Decision Tree
- Support Vector Machine (SVM)
- K-Nearest Neighbor (KNN)
- Linear regression
- Logistic regression...

Unsupervised learning:

- Neural Networks
- Principal Composant Analysis (PCA)
- Singular Value Decomposition (SVD)
- K-mean & Prob. clustering...

Reinforcement learning:

- Neural Networks (Q-learning, Actor-Critic, DDPG, PPO...)
- Monte Carlo...

Self-Supervised learning:

- Neural Networks (SimCLR, Dino...)

Various approaches for ML algorithms

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Self-Supervised learning:

- Neural Networks

A large variety of possibities $\rightsquigarrow$ success of **Deep Learning** and **Neural Networks**

Fields & applications of DL

Computer Vision

- Image Classification.
- Object Detection .
- (Semantic) Segmentation.
- Pose Estimation.
- Style transfer.
- OCR (Optical Character Recognition).
- Image Generation
- ...

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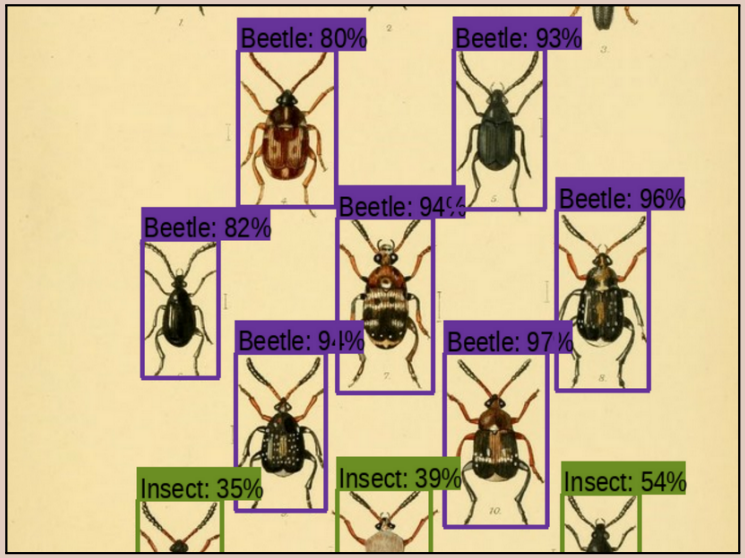

source : Tensorflow tutorials object_detection

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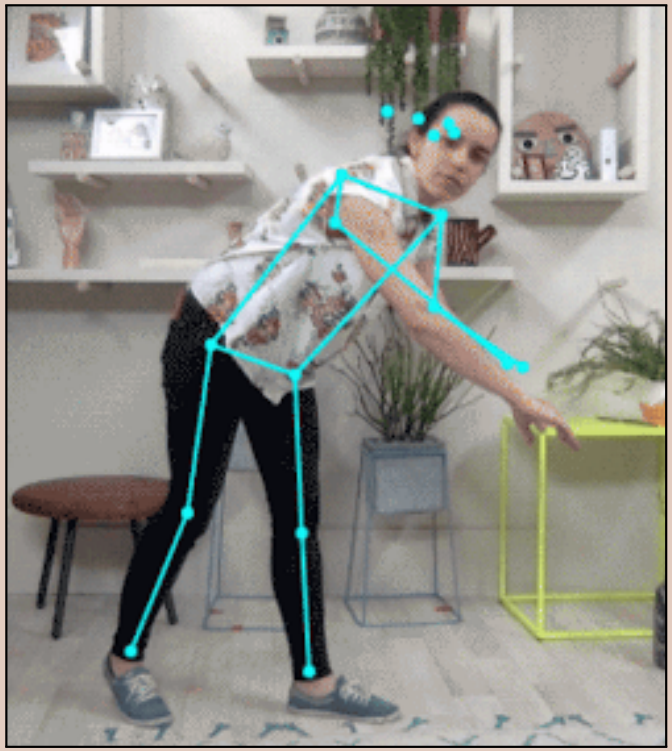

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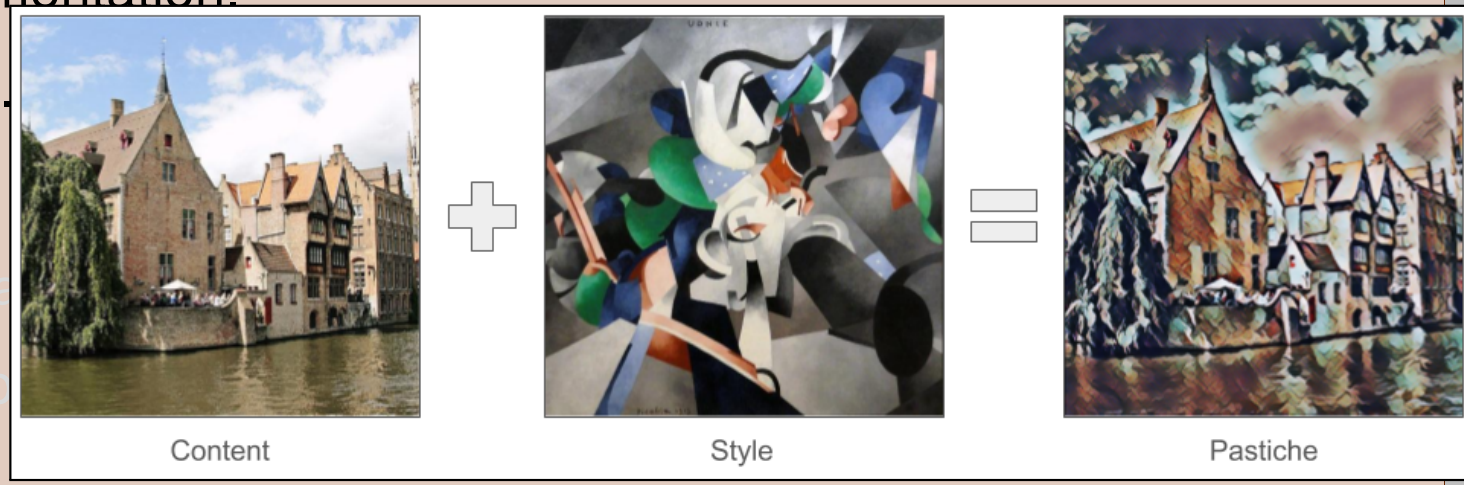

source : Tensorflow style_transfer

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source : pyimagesearch.com

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- OCR (Optical Character Recognition).
- Image Generation
- ...

source : stylegan

Fields & applications of ML

NLP(Natural Language Processing): some applications...

- Natural Language Understanding (NLU)
- Natural Language Generation (NLG)
- Speech recognition / Speech Synthesis (Text To Speech)
- Machine Translation (languages)
- Virtual agents and ChatBots
- LLM ChatBots
- ...

Societal issues: Explainabilty

Explainability is becoming a important aspect in research, referred as

- **XAI** **Explainable** Artificial Intelligence [XAI-1] [XAI-2]
- **IML** **Interpretable** Machine learning [IML-1] [IML-2] [IML-3]

Societal issues: Explainabilty

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IML **Interpretable** Machine learning [IML-1] [IML-2] [IML-3]

Explainability

- **Unexplainability** of the DL results still constitutes an obstacle to their dissemination today.
- Neural Networks are often denigrated as a **Black box** by scientists with a Cartesian approach.
- The growing complexity of NNs (LLM for example) makes the simple explanation of their outputs extremely difficult.

Societal issues: Decision-making, Certification

Decision-making

- **Decisions** in sensible fields (justice, insurance, defense...) are being ceded to ML algorithms to the detriment of human control, raising concern for loss of fairness and equity.
- Decision-making algorithms rely inevitably on assumptions (quality of training data) not always verified

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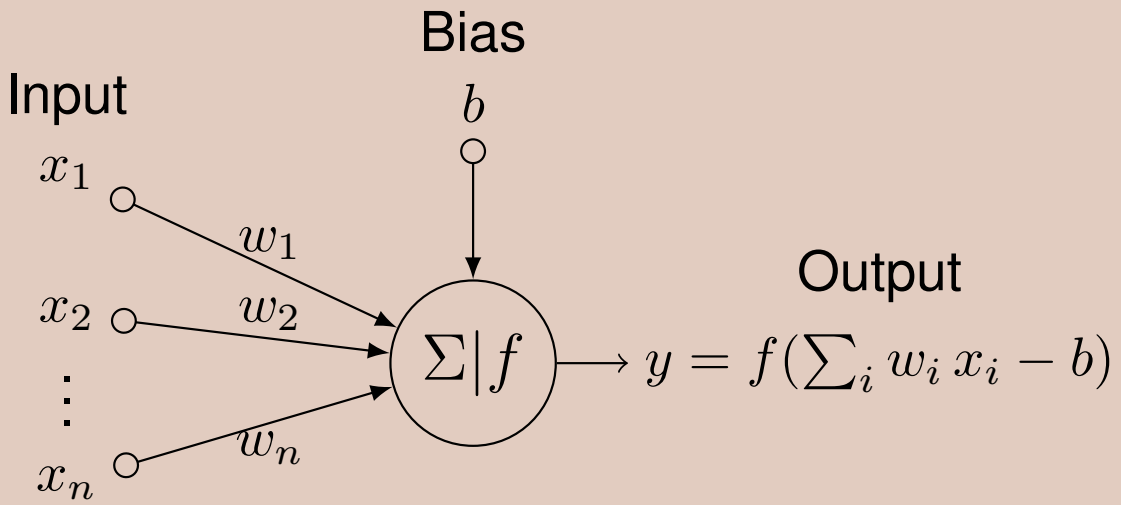
Certification

- The evaluation and the certification of AI systems remains a major issue for their integration in the industry
- Formal certification of ML algorithms still a subject of research
- Examples:
  LNE: Process certification for AI,
  Fraunhoher: Auditing and Certification of AI Systems

NN technical aspects

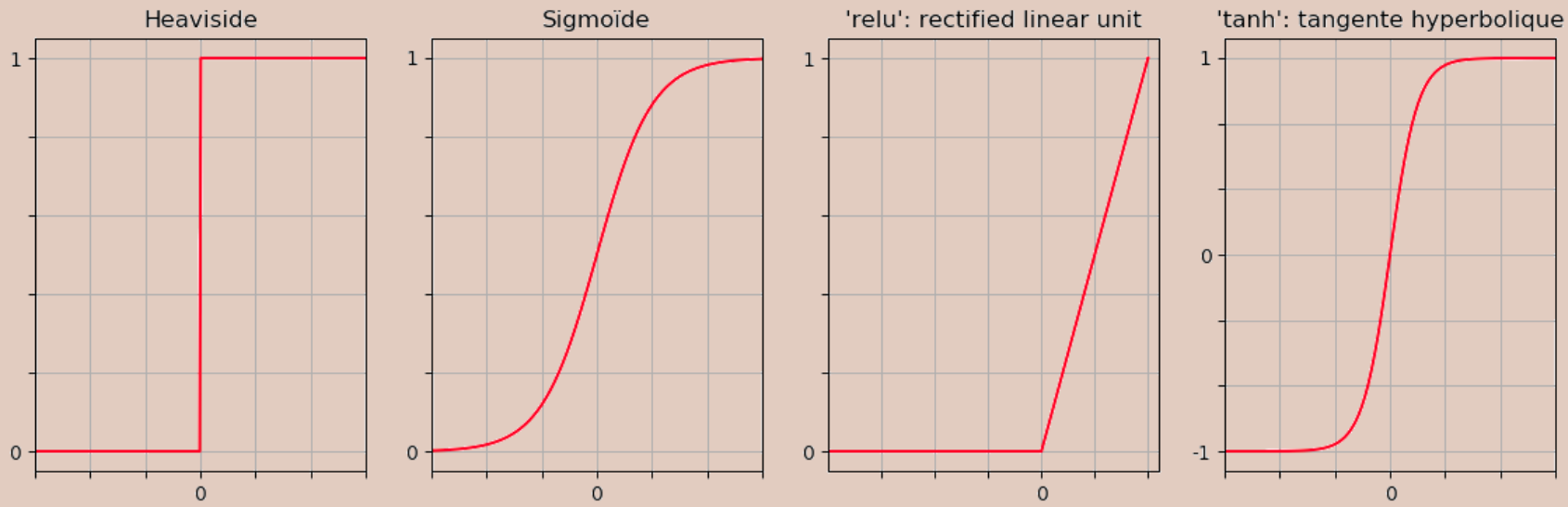
The artificial neurone



- Receives the input stimuli $(x_i)_{i=1..n}$ affected by **weights** (w_i)
- Computes the **weighted sum** of the input: $\sum_i w_i\, x_i - b$
- Outputs its activation $f(\sum_i w_i\, x_i - b)$, computed with a non-linear **activation function** f .

NN technical aspects

Common activation functions

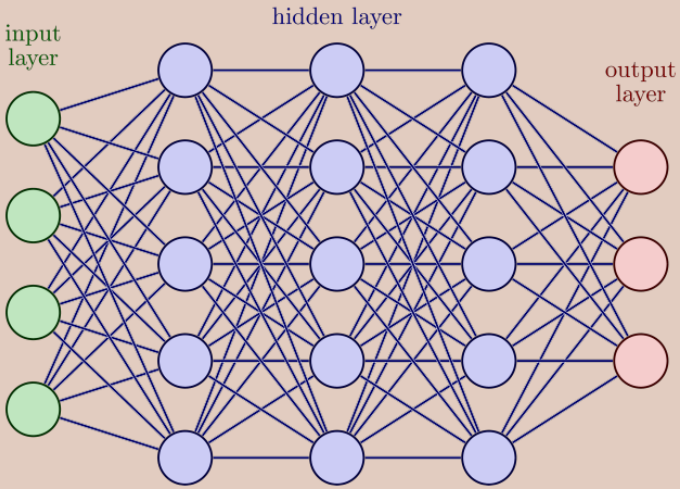


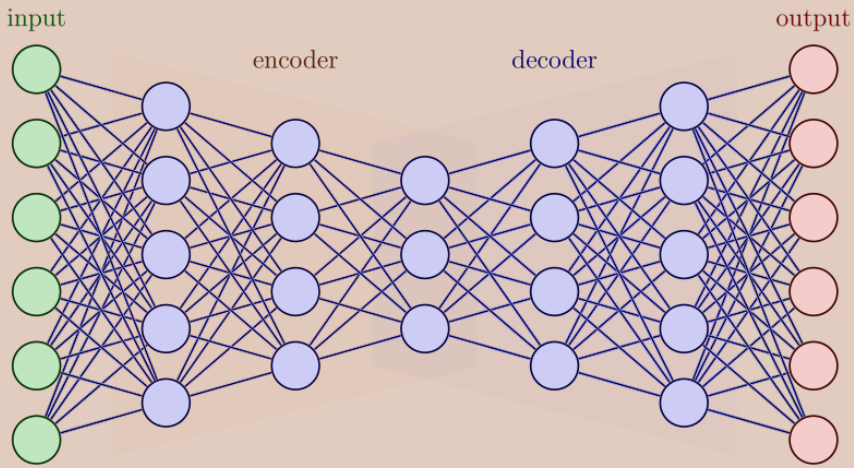
- Introduces a non-linear behavior.
- Sets the range of the neuron output: $[-1, 1]$, $[0, 1]$, $[0, \infty[$...
- The bias b sets the activation threshold of the neuron.

NN Computing aspects

Neural network

Neurons are grouped by layers to form a **Neural Network**





Neural Network Architectures

Many NN architectures for many applications (non-exhaustive list)

- ***Dense Neural Network***

  the simplest architecture made of successive layers of neurones, with *FeedForward Neural Network (FNN)* and *Back Propagation* algorithms.
- ***Convolutional** (CNN)*
- ***Recurrent** (RNN)*
- ***Auto Encoder** (AEN)*
- ***Generative Adversarial** (GAN)*
- ***Transformers***
- ***Large Language Model** (LLM)*
- ...

[Graphique synthétique animé : Saul Dobilas @ Medium]

Neural Network Architectures

Many NN architectures for many applications (non-exhaustive list)

- ***Dense Neural Network***
- ***Convolutional*** *(CNN)* - Mostly used for analyzing and classifying images.
- ***Recurrent*** *(RNN)*
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- ...

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Neural Network Architectures

Many NN architectures for many applications (non-exhaustive list)

- ***Dense Neural Network***
- ***Convolutional*** *(CNN)*
- ***Recurrent*** *(RNN)* - Used for time series, like the Long Short-Term Memory (LSTM) algorithm.
- ***Auto Encoder*** *(AEN)*
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- ...

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Neural Network Architectures

Many NN architectures for many applications (non-exhaustive list)

- ***Dense Neural Network***
- ***Convolutional*** *(CNN)*
- ***Recurrent*** *(RNN)*
- ***Auto Encoder*** *(AEN)*- Dimensionality reduction, Feature extraction, Denoising of data/images, Inputing missing data...
- ***Generative Adversarial*** *(GAN)*
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- ***Generative Adversarial*** *(GAN)*

  to generate text, images, music...
- ***Transformers***
- ***Large Language Model*** *(LLM)*
- ...

[Graphique synthétique animé : Saul Dobilas @ Medium]

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- ***Generative Adversarial*** *(GAN)*
- ***Transformers***

  (2017) Natural language processing, and also image classification
- ***Large Language Model*** *(LLM)*
- ...

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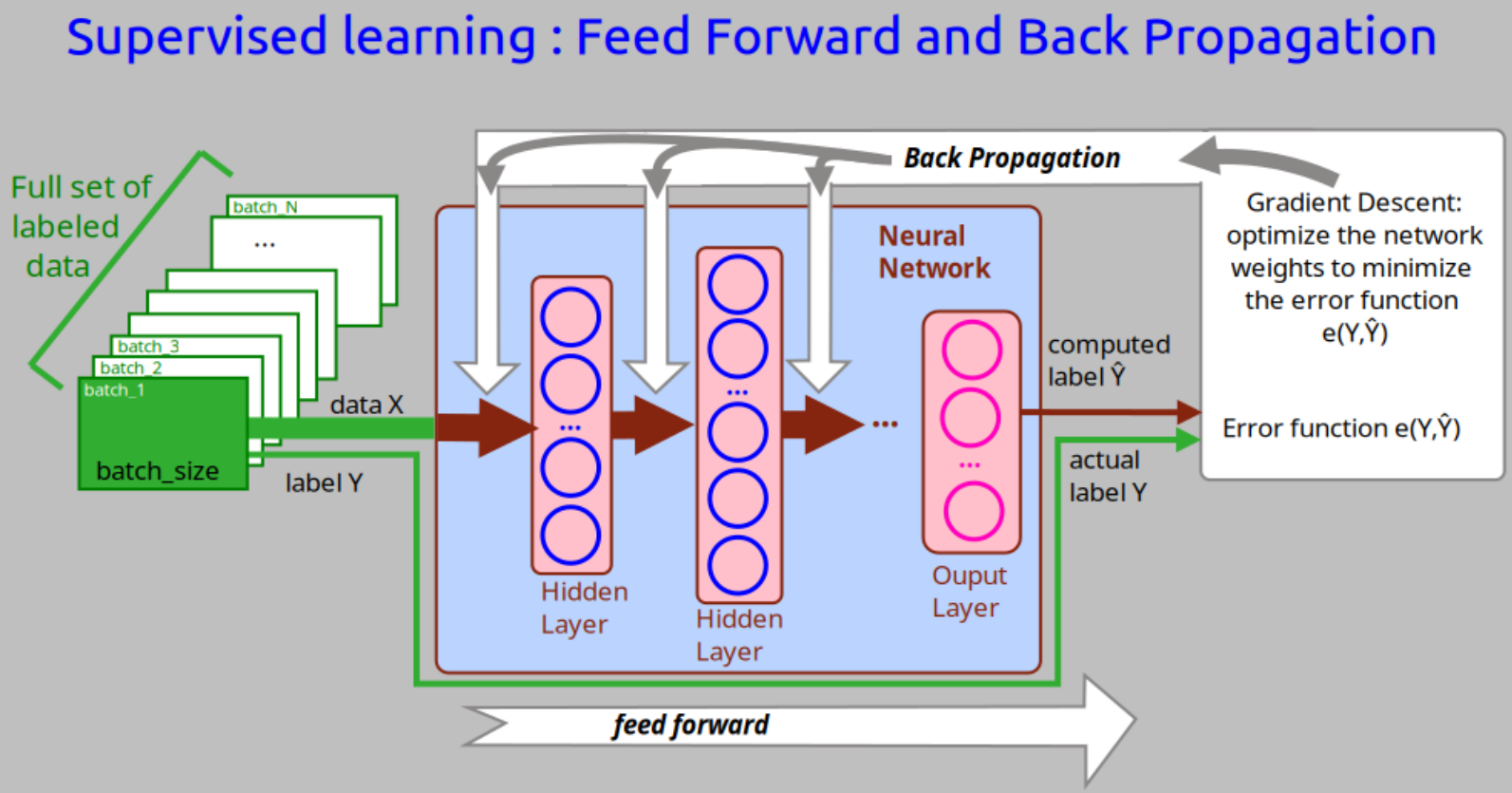
- ***Transformers***
- ***Large Language Model*** *(LLM)*
  read text, sound, write books, images, speak, make music ...
  OpenAI: ChatGPT - Anthropic: Claude, Sonnet - Google: Gemini - Mistral: mistral - Meta: LLama...
- ...

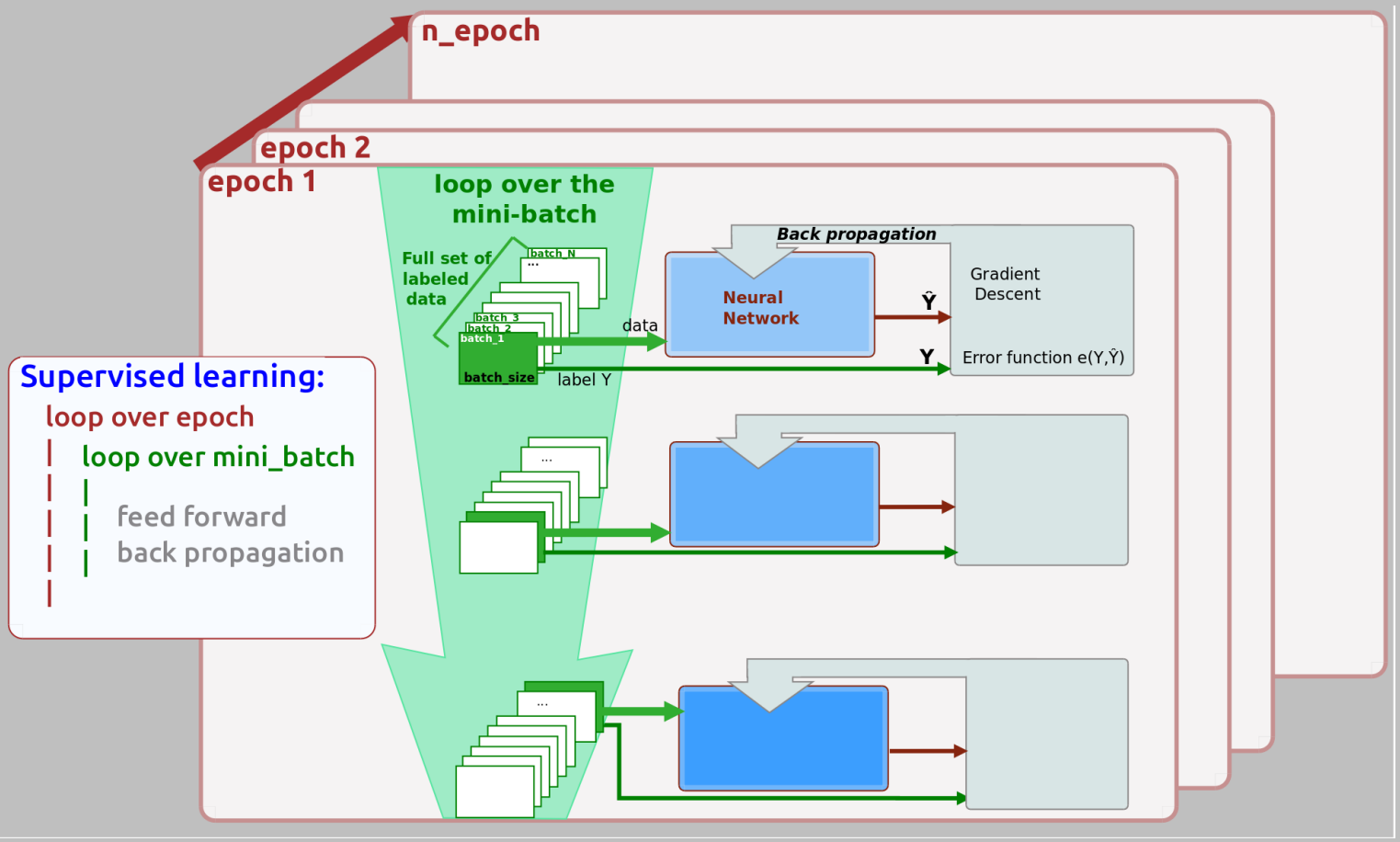
[Graphique synthétique animé : Saul Dobilas @ Medium]

NN Computing aspects



- The dataset is split into (mini) **batches** of size `batch_size`
- After each *feed forward* the *Back Propagation* algorithm modifies the nerons weights to minimize the error e.

NN Computing aspects



- Training with the whole dataset is repeated `n_epoch` times,
- The network state after epoch `n` becomes the initial state for epoch `n+1`.

Reproducibility

The reproducibility crisis in AI & ML is not new...

- *1500 scientists lift the lid on reproducibility*
  Nature, volume 533, pages 452–454 (2016)
- *Artificial intelligence faces reproducibility crisis*
  Science, 16 Feb 2018, Vol 359, Issue 6377, pp. 725-726
- *Reproducibility Workshops* at major AI conferences:
  - NeurIPS NeurIPS Reproducibility Challenge 2018, 2019, 2020...
  - ICML *International Conference on Machine Learning*: 2017, 2018, 2019...
  - AAAI *Association for the Advancement of Artificial Intelligence*: reproducibility checklist

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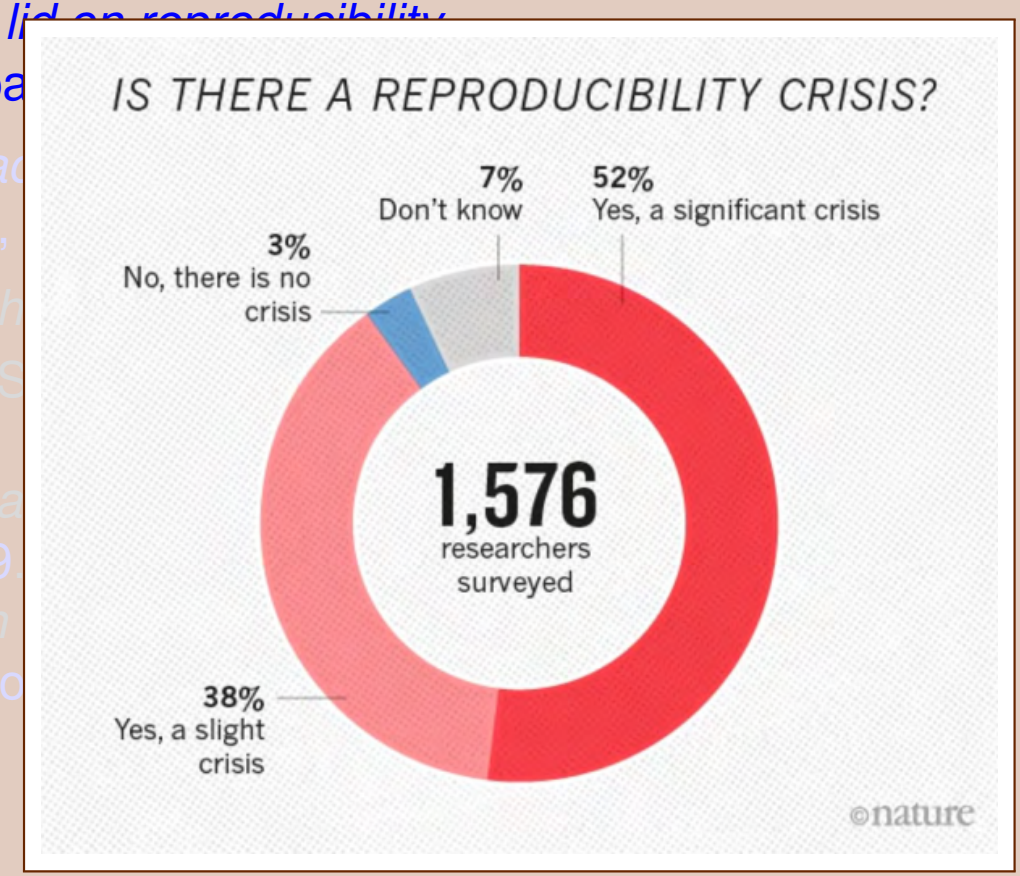

Reproducibility

The reproducibility crisis in AI & ML is not new...

- *1500 scientists lift the lid on reproducibility*
  Nature, volume 533, pages 452–454 (2016)
  70% of researchers failed to reproduce another researcher's experiments
  50% failed to reproduce one
- *Artificial intelligence fac*
  Science, 16 Feb 2018,
- *Reproducibility Worksh*
  - NeurIPS NeurIPS
    2019, 2020...
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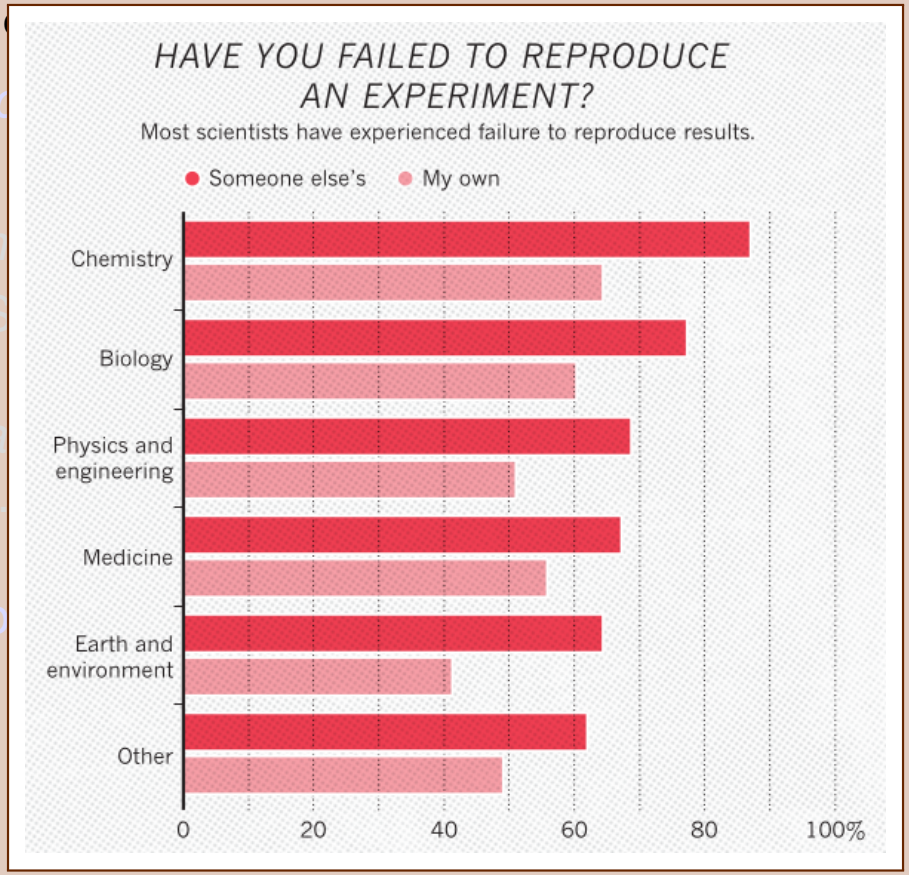

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- Many papers relate the reproducibility question in AI & ML:
  [Repro0] [Repro1] [Repro2] [Repro3] [Repro4] [Repro5] [Repro6] [Repro7]..
- Currently still a problem for trusting ML outputs.

Reproducibility - The DL context

Reproducibility - The DL context

Reproducibility for Deep Learning

refers to the ability to achieve the **same or similar results**:

- Using the same **training dataset**
- Using the same **algorithms**
  model architecture, parameters and hyperparameters, and other code
- Within the same computing **environment**
  software (Python modules) used to run the algorithm, data-preprocessing... and all pieces of code.

Reproducibility - The DL context

Reproducibility: an important issue for confidence in DL

- Necessary to trust DL outputs
- Required for the validation of published results & claims
- Helps to promote open and accessible research
- Makes published matter an educational tool for students

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Reproducibility - The DL context

2 main reasons why DL training is not reproducible

- NN training involves random draws at many stages:

- Non-determinism in hardware operations
  (floating-point ops are sensitive to computation order...)
  - Most of these cases occur on GPUs
    auto-tuning: libraries CUDA and cuDNN auto-select the optimal primitive operations at runtime $\rightsquigarrow$ different ops may occur on subsequent run
  - Forcing deterministic ops possible but $\rightsquigarrow$ slower computation ☹

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- NN training involves random draws at many stages:
  - Data augmentation [DL2]
  - Shuffling training data
  - Batch ordrering at each epoch
  - Initialisation of the NN weights
  - Exploration noise during training (DRL)
  - Specific algorithm treatments: *dropout* [DL1]
  - Optimisation algorithms: *stochastic gradient* (adam)...
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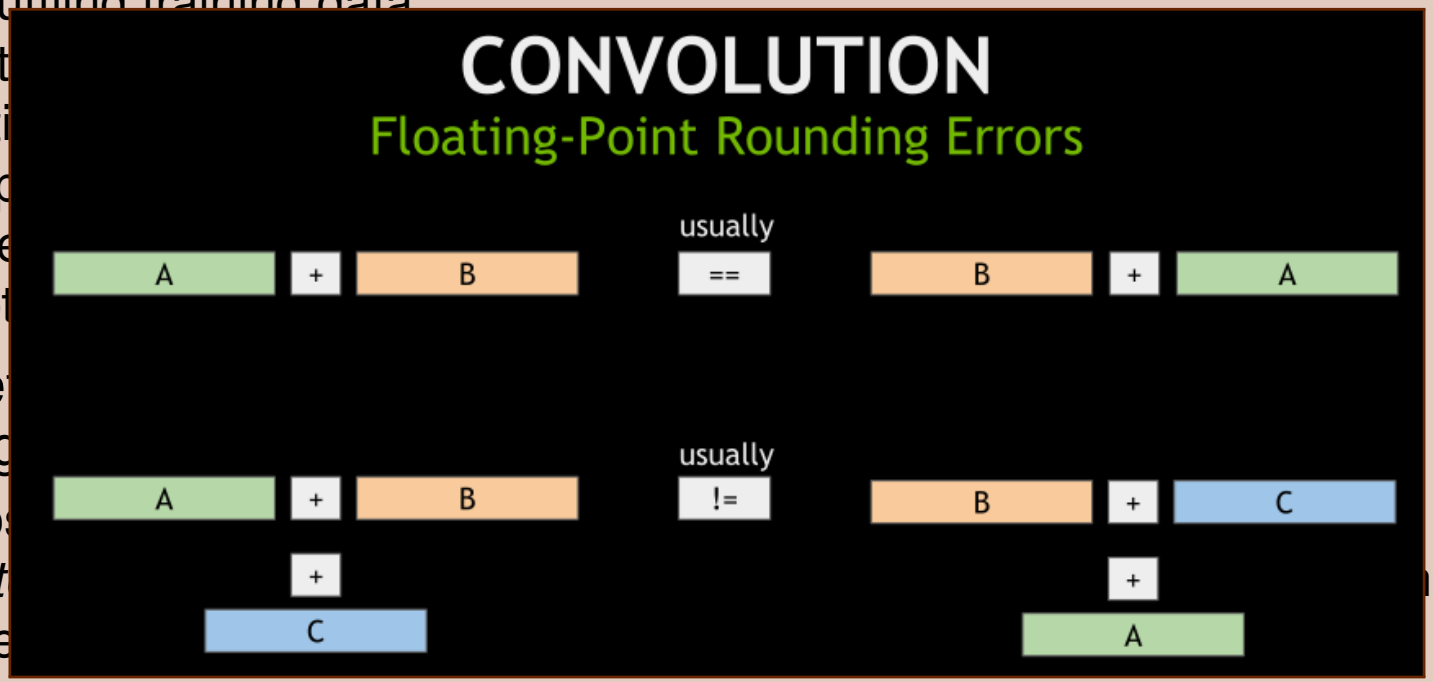

source: [NVIDIA-1]

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Reproducibility - The DL context

some practices to make DL reproducible

1/ set the **SEED** $\rightsquigarrow$ makes random generators reproducible

- tensorflow [tf-repro-1] [tf-repro-2] [tf-repro-3]
- pytorch [Pytorch-repro-1] [Pytorch-repro-2]

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tf.keras.utils.set_random_seed(<SEED>) # sets Python, NumPy and TensorFlow seed
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```

- pytorch [Pytorch-repro-1][Pytorch-repro-2]

```
import random
import numpy as np
import torch

random.seed(<SEED>)          # Sets the seed for Python built-in random module
np.random.seed(<SEED>)       # Sets the seed for NumPy random number generator

torch.manual_seed(<SEED>)    # Sets the seed for PyTorch CPU random number generator
```

```
torch.cuda.manual_seed(<SEED>)       # Sets the seed for the current GPU device
torch.cuda.manual_seed_all(<SEED>)   # Sets the seed for all available GPU devices
```

Reproducibility - The DL context

some practices to make DL reproducible

2/ Set the operations deterministic $\rightsquigarrow$ makes GPU ops deterministic at the cost of perfomence

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Reproducibility - The DL context

some practices to make DL reproducible

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```
tf.config.experimental.enable_op_determinism()
# this will make GPU ops as deterministic as possible,
#  but it will affect the overall performance
```

- pytorch [Pytorch-repro-1] [Pytorch-repro-2]

Reproducibility - The DL context

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```

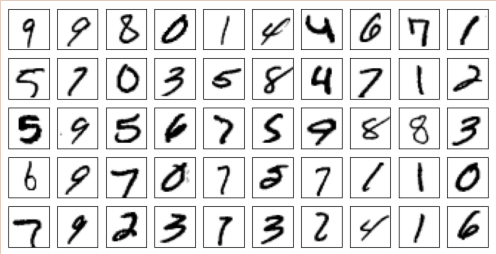
- pytorch [Pytorch-repro-1][Pytorch-repro-2]

```
# try this:
import torch.backends.cudnn
torch.backends.cudnn.deterministic = True
torch.backends.cudnn.benchmark = False
```

but it can be more tricky... seed [Pytorch-repro-2].

Reproducibility - Simple examples

A simple example: Dense NN to classify the MNIST hand-written digits



MNIST dataset: 70 000 labeled grayscale images 28×28 pixels (60000 training, 10000 validation)

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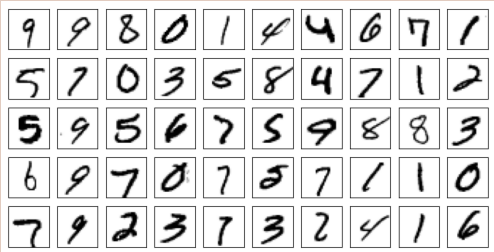

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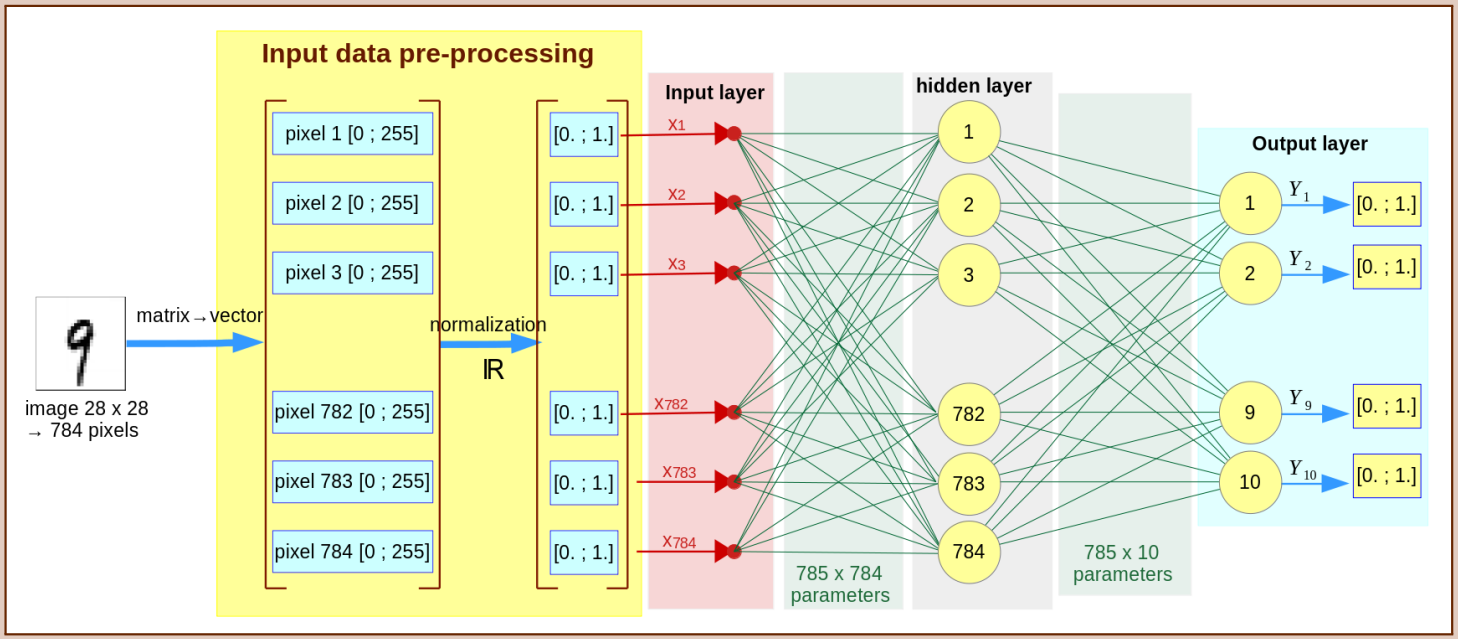

Dense NN: 784 inputs, 1 hidden layer (784 neurones, *relu*), 1 output layer (10 neurones, *softmax*)

Reproducibility - Simple examples

A simple example: Dense NN

tensorflow/keras snippet to build the model:

```
def build_DNN(seed=None):
    if seed is not None:
        ############################
        # Deterministic training  #
        ############################
        # 1/ sets the Python seed, the NumPy seed, and the TensorFlow seed:
        tf.keras.utils.set_random_seed(seed)

        # 2/ make the tf ops deterministic
        # this will make GPU ops as deterministic as possible, but it will affect
        # the overall performance:
        tf.config.experimental.enable_op_determinism()

    # 5 keras lines to build the dense network.
    model = Sequential()
    model.add(Input(shape=(NB_INPUT,), name='input'))                # INPUT layer
    model.add(Dense(NB_NEURON, activation='relu', name='c1'))        # First hidden layer
    model.add(Dense(NB_CLASS, activation='softmax', name='c2'))      # OUTPUT layer
    model.compile(loss='categorical_crossentropy',
                  optimizer='adam',
                  metrics=['accuracy'])
    return model
```

Reproducibility - Simple examples

A simple example: Dense NN **no seed fixed**

Simple experiment: write a loop where the model is built **without setting seed**, trained & evaluated once at each iteration (*epochs=1*) :

Reproducibility - Simple examples

A simple example: Dense NN **no seed fixed** $\rightsquigarrow$ **not reproducible**

Simple experiment: write a loop where the model is built **without setting seed**, trained & evaluated once at each iteration (*epochs=1*) :

```
print(get_cpu_info()['brand_raw'])
for _ in range(5):
    model = build_DNN()  # Build a new model without setting seed
    hist = model.fit(x_train, y_train, epochs=1, batch_size=16, validation_data=(x_valid, y_valid), verbose=2)
```

```
Intel(R) Xeon(R) W-1390P @ 3.50GHz
3750/3750 - 8s - 2ms/step - accuracy: 0.9448 - loss: 0.1822 - val_accuracy: 0.9582 - val_loss: 0.1349
3750/3750 - 8s - 2ms/step - accuracy: 0.9468 - loss: 0.1789 - val_accuracy: 0.9690 - val_loss: 0.0936
3750/3750 - 8s - 2ms/step - accuracy: 0.9459 - loss: 0.1800 - val_accuracy: 0.9754 - val_loss: 0.0798
3750/3750 - 8s - 2ms/step - accuracy: 0.9462 - loss: 0.1771 - val_accuracy: 0.9690 - val_loss: 0.1082
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```

$\rightsquigarrow$ Same behaviour on Google Collab platform (Xeon processor):

```
1 print(get_cpu_info()['brand_raw'])
2 for _ in range(5):
3     model = build_DNN()  # Build a new model without setting seed
4     hist = model.fit(x_train[:1000], y_train[:1000], epochs=1, batch_size=16,
5                      validation_data=(x_valid[:200], y_valid[:200]), verbose=2)
```

```
Intel(R) Xeon(R) CPU @ 2.20GHz
63/63 - 2s - 27ms/step - accuracy: 0.7410 - loss: 0.8808 - val_accuracy: 0.8550 - val_loss: 0.5447
63/63 - 2s - 27ms/step - accuracy: 0.7470 - loss: 0.8468 - val_accuracy: 0.8150 - val_loss: 0.5601
63/63 - 2s - 34ms/step - accuracy: 0.7520 - loss: 0.8321 - val_accuracy: 0.8350 - val_loss: 0.5183
63/63 - 2s - 39ms/step - accuracy: 0.7490 - loss: 0.8592 - val_accuracy: 0.8600 - val_loss: 0.4838
63/63 - 2s - 28ms/step - accuracy: 0.7360 - loss: 0.8955 - val_accuracy: 0.8150 - val_loss: 0.5690
```

Reproducibility - Simple examples

A simple example: Dense NN **no seed fixed** $\rightsquigarrow$ **not reproducible**

Non-reproducibility worsens if the dataset is reduced:

```
print(get_cpu_info()['brand_raw'])
for _ in range(5):
    model = build_DNN()  # Build a new model without setting seed
    hist = model.fit(x_train[:1000], y_train[:1000], epochs=1, batch_size=16,
                     validation_data=(x_valid[:200], y_valid[:200]), verbose=2)
```

```
Intel(R) Xeon(R) W-1390P @ 3.50GHz
63/63 - 1s - 10ms/step - accuracy: 0.7490 - loss: 0.8607 - val_accuracy: 0.8300 - val_loss: 0.5360
63/63 - 1s - 10ms/step - accuracy: 0.7510 - loss: 0.8562 - val_accuracy: 0.8300 - val_loss: 0.5765
63/63 - 1s - 10ms/step - accuracy: 0.7490 - loss: 0.8049 - val_accuracy: 0.8600 - val_loss: 0.4851
63/63 - 1s - 9ms/step - accuracy: 0.7250 - loss: 0.8943 - val_accuracy: 0.8550 - val_loss: 0.4981
63/63 - 1s - 11ms/step - accuracy: 0.7500 - loss: 0.8424 - val_accuracy: 0.8300 - val_loss: 0.5456
```

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```

Reproducibility - Simple example

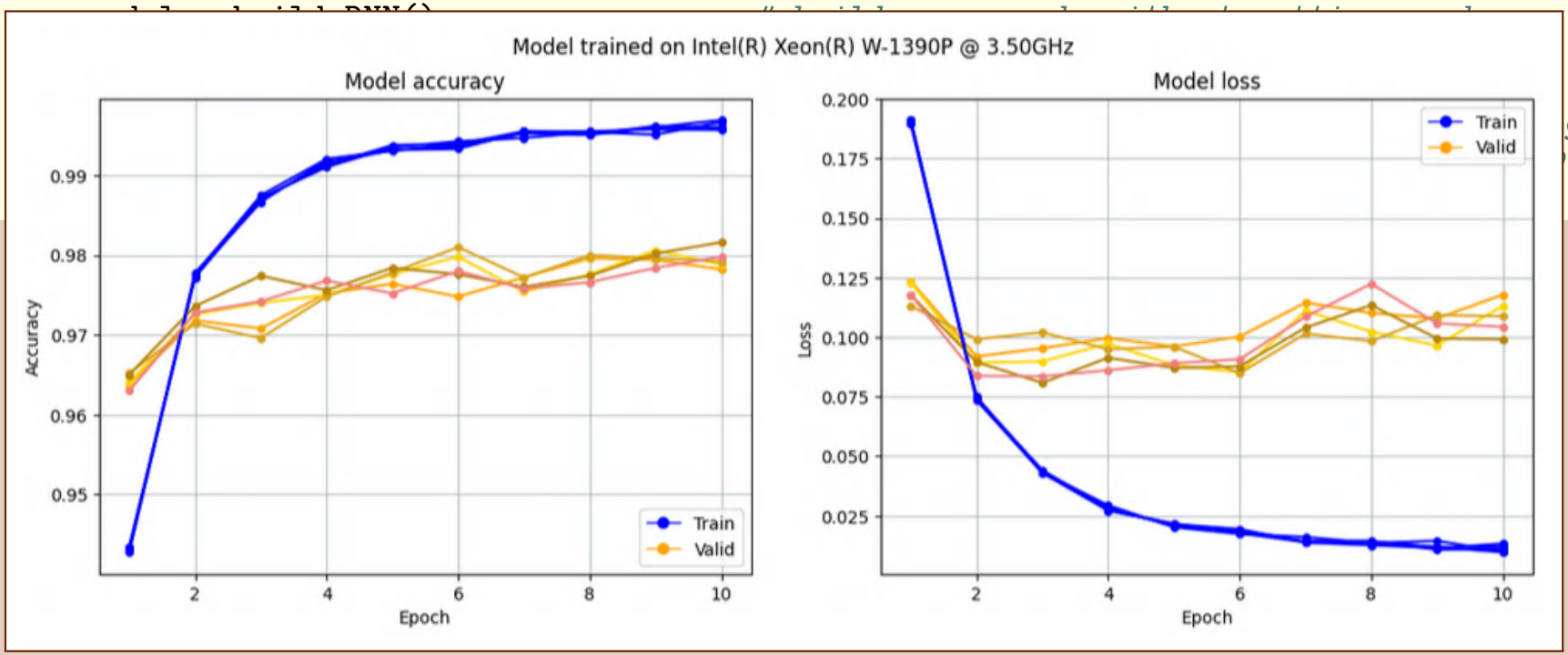
A simple example: Dense NN **no seed fixed**

```
for i in range(5):
    model = build_DNN()                    # build a new mode without setting seed
    hist  = model.fit(x_train, y_train, # images, labels
                      epochs=10,        # the total number of successive trainings
                      batch_size=32,    # input images by batch of <batche_size> images
                      validation_data=(x_valid, y_valid), # validation after each epcoh
                      verbose=0)
```

Reproducibility - Simple example

A simple example: Dense NN **no seed fixed $\rightsquigarrow$ not reproducible**

```
for i in range(5):
```



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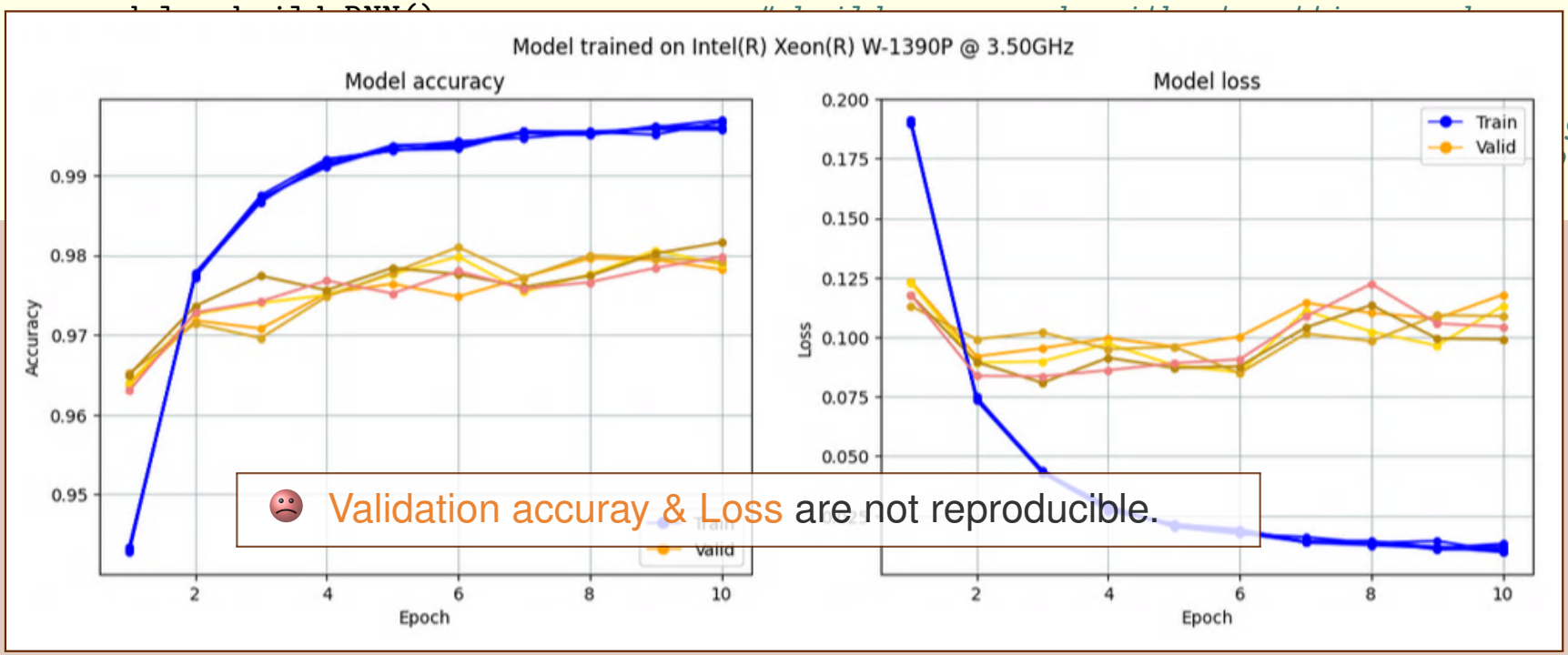

Validation accuray & Loss are not reproducible.

Reproducibility - Simple examples

A simple example: Dense NN **seed set** $\rightsquigarrow$ **reproducible**

A model is built with **seed set** at each iteration:

```
print(get_cpu_info()['brand_raw'])
for _ in range(5):
    model = build_DNN(seed=1234)  # Build a new model with seed set
    hist = model.fit(x_train, y_train, epochs=1, batch_size=16, validation_data=(x_valid, y_valid), verbose=2)
```

```
Intel(R) Xeon(R) W-1390P @ 3.50GHz
3750/3750 - 8s - 2ms/step - accuracy: 0.9457 - loss: 0.1790 - val_accuracy: 0.9688 - val_loss: 0.1067
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Reproducibility - Simple examples

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```

Reproducibility - Simple examples

A simple example: reload model structure & weights $\rightsquigarrow$ **reproducible**

The model built once with **seed set** is saved and then just re-loaded (structure & weights) at each iteration:

```
model = build_DNN(seed=1234)
model.save('models/DNN_relu_seed1234.keras')
```

```
print(get_cpu_info()['brand_raw'])
for _ in range(5):
    model = tf.keras.models.load_model('models/DNN_relu_seed1234.keras') # reload the model structure & weights
    hist = model.fit(x_train, y_train, epochs=1, batch_size=16, validation_data=(x_valid, y_valid), verbose=2)
```

```
Intel(R) Xeon(R) W-1390P @ 3.50GHz
3750/3750 - 9s - 2ms/step - accuracy: 0.9457 - loss: 0.1790 - val_accuracy: 0.9688 - val_loss: 0.1067
3750/3750 - 8s - 2ms/step - accuracy: 0.9457 - loss: 0.1790 - val_accuracy: 0.9688 - val_loss: 0.1067
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```

Reproducibility - Simple examples

A simple example: reload model structure & weights $\rightsquigarrow$ **reproducible**

The model built once with **seed set** is saved and then just re-loaded (structure & weights) at each iteration:

```
model = build_DNN(seed=1234)
model.save('models/DNN_relu_seed1234.keras')
```

$\rightsquigarrow$ Same behaviour on Google Collab platform (Xeon processor):

```
1 model = build_DNN(seed=1234)
2 model.save('models/DNN_relu_seed1234.keras')
```

```
1 print(get_cpu_info()['brand_raw'])
2 for _ in range(5):
3     model = tf.keras.models.load_model('models/DNN_relu_seed1234.keras') # reload the model structure & weights
4     hist = model.fit(x_train, y_train, epochs=1, batch_size=16, validation_data=(x_valid, y_valid), verbose=2)
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```

Reproducibility - Simple example

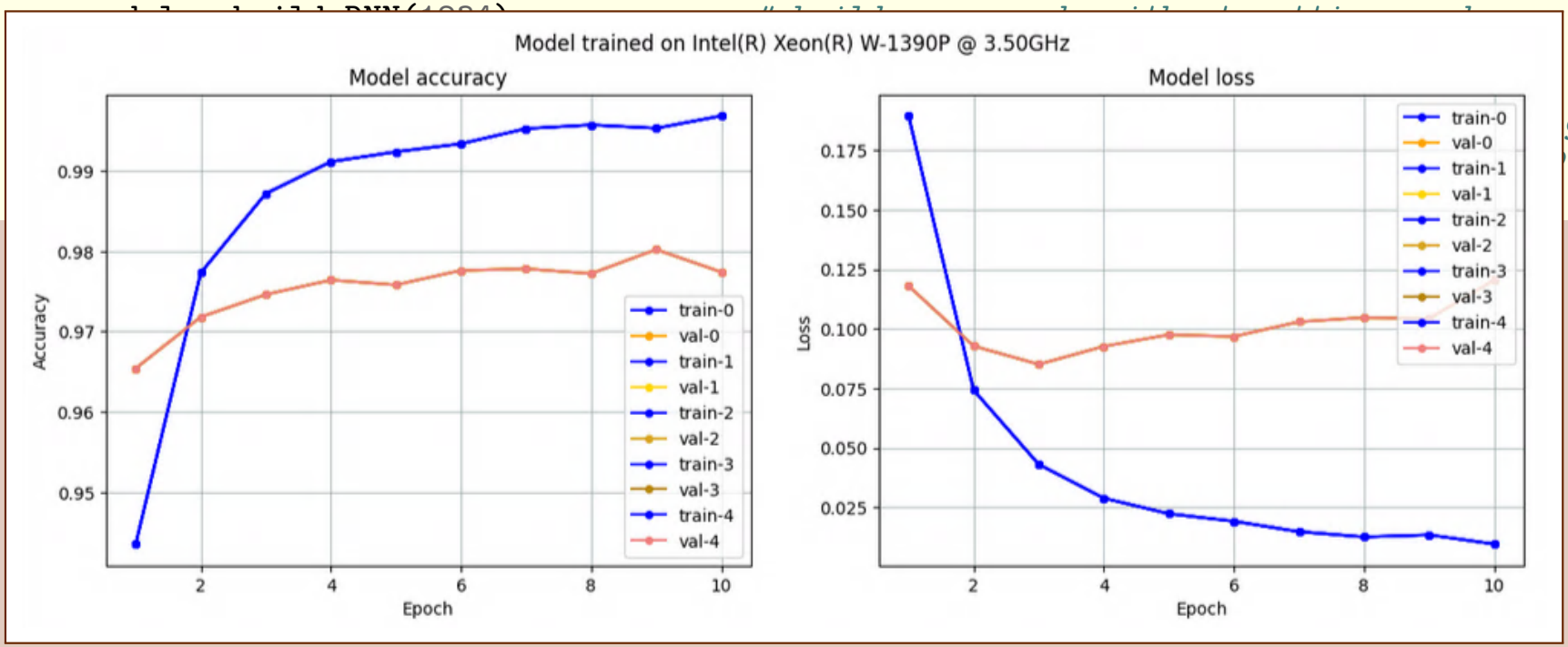
A simple example: Dense NN **seed fixed**

```
for i in range(5):
    model = build_DNN(1234)                # build a new mode without setting seed
    hist  = model.fit(x_train, y_train, # images, labels
                      epochs=10,        # the total number of successive trainings
                      batch_size=32,    # input images by batch of <batche_size> images
                      validation_data=(x_valid, y_valid), # validation after each epcoh
                      verbose=0)
```

Reproducibility - Simple example

A simple example: Dense NN **seed fixed** $\rightsquigarrow$ **reproducible**

```
for i in range(5):
```



Reproducibility - Simple example

A simple example: Dense NN **seed fixed** $\rightsquigarrow$ **reproducible**

```
for i in range(5):
```

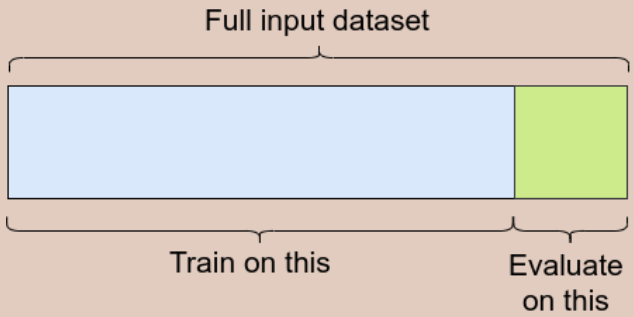
Accuracy & loss for training and validation perfectly reproducible.

Training & Evaluation strategy

Validation techniques are essential for assessing how well a model generalizes to unseen data.

Split the input Dataset

Common practice: Simple hold-out validation split



Input Dataset $\rightsquigarrow$ **Train** and **Valid** (test) datasets

Training & Evaluation strategy

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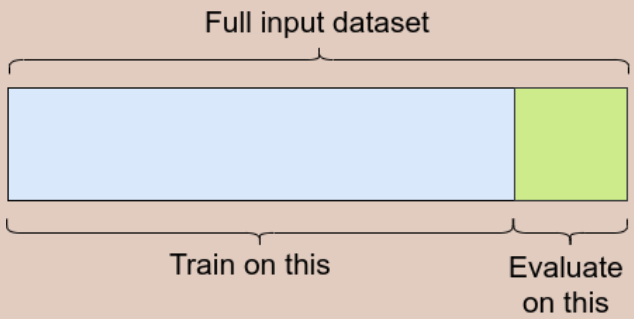
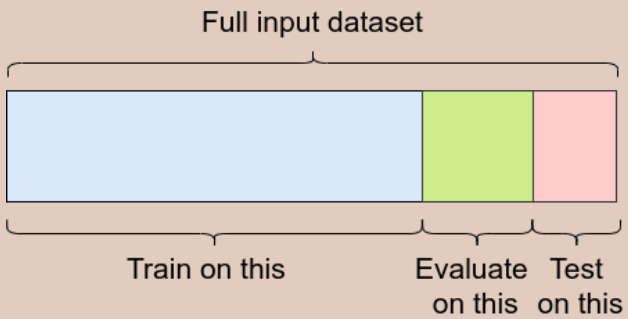


Input Dataset $\rightsquigarrow$ **Train** and **Valid** (test) datasets

State of the art: Train/Validation/Test



Input Dataset $\rightsquigarrow$ **Train**, **Valid** and **test** datasets.

Training & Evaluation strategy

Split the input Dataset

Random Split: most used method
unless dealing with ordered data like time-series

- **Training Dataset**
- **Validation Dataset**

- **Test Dataset**

Training & Evaluation strategy

Split the input Dataset

Random Split: most used method
unless dealing with ordered data like time-series

- **Training Dataset** $\rightsquigarrow$ to train the model
- **Validation Dataset**
- **Test Dataset**

Training & Evaluation strategy

Split the input Dataset

Random Split: most used method
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- **Training Dataset** $\rightsquigarrow$ to train the model
- **Validation Dataset** $\rightsquigarrow$ to get unbiased evaluation (loss function...) of the model during training , used to tune:
  - **model hyper-parameters**: nb layers, nb neurons/layer, activation function/layer, optimisation algorithm...
  - **training hyper-parmeters**: split ratio, batch size, nb epochs, learning rate
  - But training and validation dataset are known to the trained DL model
- **Test Dataset**

Training & Evaluation strategy

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  - **training hyper-parmeters**: split ratio, batch size, nb epochs, learning rate
  - But training and validation dataset are known to the trained DL model
- **Test Dataset** completly new to the model $\rightsquigarrow$ to get performance of the trained model.

Training & Evaluation strategy

Split the input Dataset: different strategies

- **Random Splitting**
  - Randomly shuffle dataset and assign samples to train, valid or test sets according to given ratios
  - Supervised Learning $\rightsquigarrow$ may not be indicated with *imbalanced dataset* (some classes have significantly fewer items than others)
- **Stratified Splitting** (Supervised Learning)
  - The dataset is divided while preserving the relative proportions of each class across the subsets

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- For example : scikit train_test_split function $\rightsquigarrow$ random & stratified split.

Training & Evaluation strategy

Split the input Dataset: strategies

- **K-fold Cross-Validation** K-Fold CV
- **Stratified K-Fold Cross-Validation**
- And yet other strategies depending on the dataset...

Training & Evaluation strategy

Split the input Dataset: strategies

- **K-fold Cross-Validation** K-Fold CV
  - Recommended with small datasets
  - One of the ways to reduce training overfit
  - Shuffle then split the input dataset into K (often 10) partitions (*folds*)
  - Loop over K:
    fold $k \rightsquigarrow$ validation and the $k-1$ remaining folds $\rightsquigarrow$ training
    At the end, compute average metrics (val loss, val accuracy...) over k
- **Stratified K-Fold Cross-Validation**
- And yet other strategies depending on the dataset...

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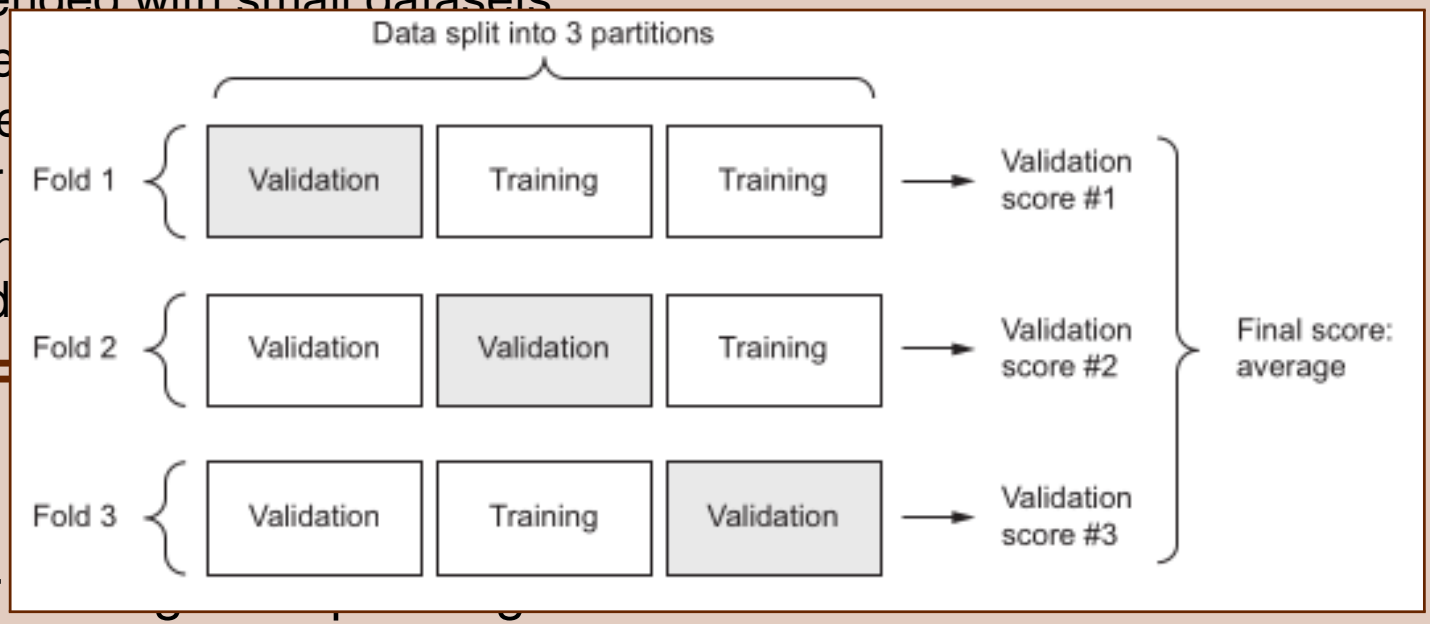

source: [DL4] p. 99

Training & Evaluation strategy

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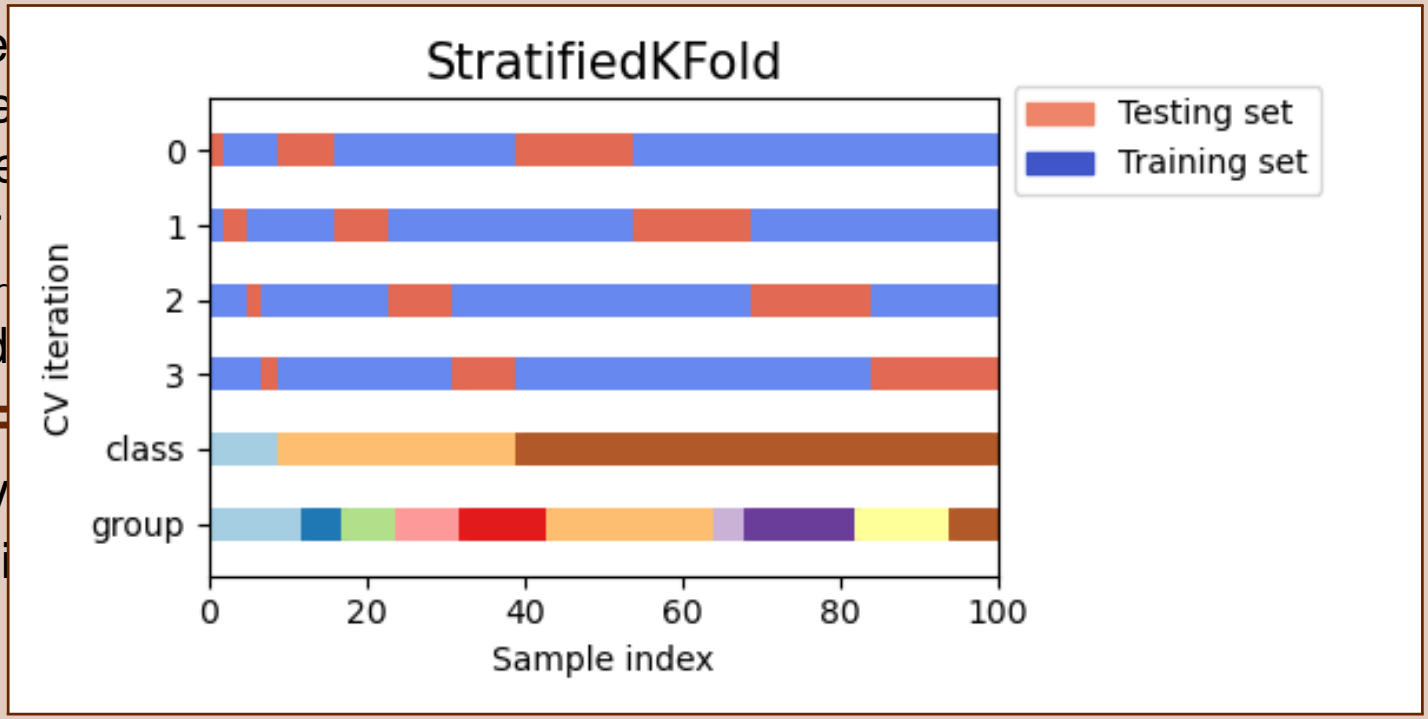

source: scikit-learn Cross-validation pages

Training & Evaluation strategy

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- And yet other strategies depending on the dataset...
  - Exple Python : scikit KFold function $\rightsquigarrow$ random, stratified, grouped...

Training & Evaluation strategy

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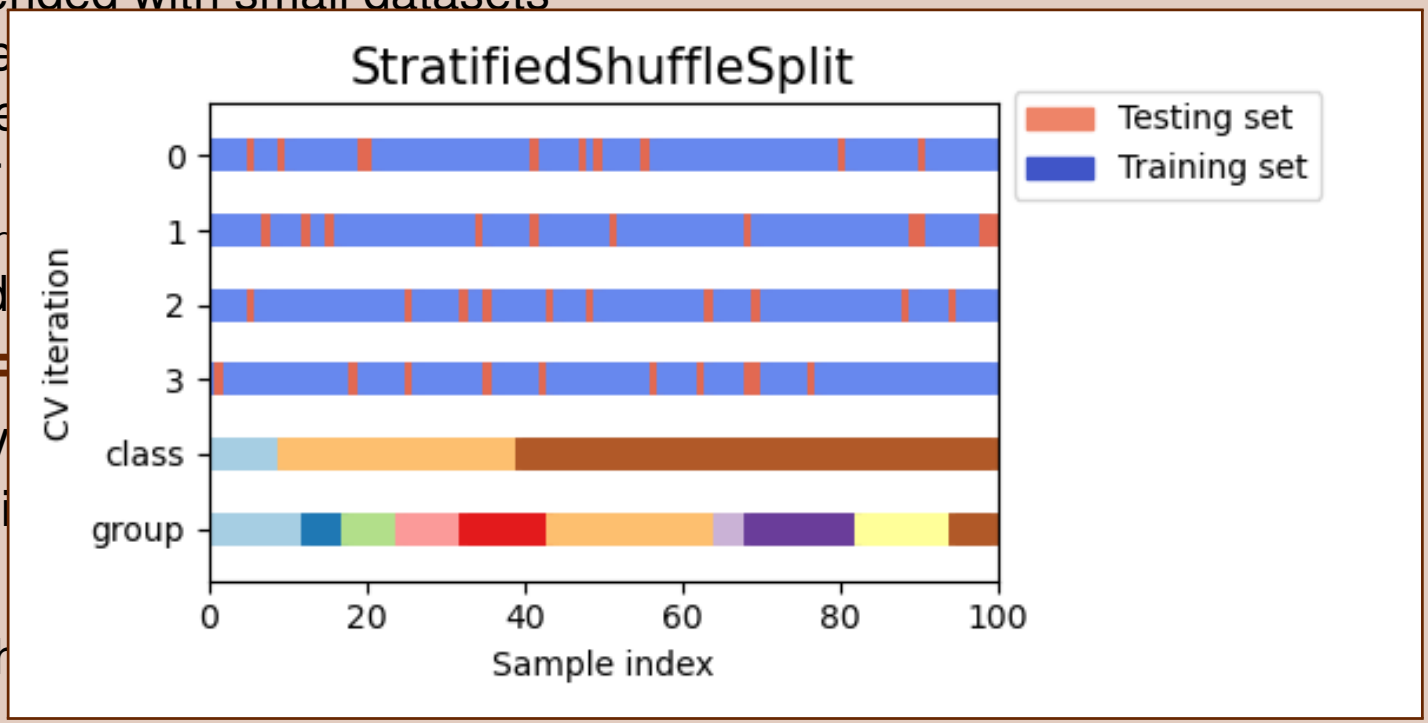

source: [DL4] p. 99

Hyper parameters

The training **Hyper-Parameters**

- Have a determinant influence on:
  - the whole training process
  - the performance of the trained network
- **Many** hyper-parameters are involved in the training of a Neural Network
  - Some are *well known* and clearly visible in the computer code:
    - the `ratios` used to split the input Dataset into train/valid/test sets
    - `epochs` $\rightsquigarrow$ the number of epochs
    - `batch_size` $\rightsquigarrow$ the size of the mini-batch
    - `learning_rate` $\rightsquigarrow$ the learning rate of the optimizer (SGD, ADAM...)
  - Some are less *highlighted* in published papers &tutos

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    - `learn`[illegible]te of the optimizer (SGD, ADAM...)
  - Some are [illegible]hed papers &tutos

well known

```
fit(
    x=None,
    y=None,
    batch_size=None,
    epochs=1,
    verbose='auto',
    callbacks=None,
    validation_split=0.0,
    validation_data=None,
    shuffle=True,
    class_weight=None,
    sample_weight=None,
    initial_epoch=0,
    steps_per_epoch=None,
    validation_steps=None,
    validation_batch_size=None,
    validation_freq=1
)
```

tensorflow model fit

Hyper parameters

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    - `learn` te of the optimizer (SGD, ADAM...)
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well known

```
tf.keras.optimizers.Adam(
    learning_rate=0.001,
    beta_1=0.9,
    beta_2=0.999,
    epsilon=1e-07,
    amsgrad=False,
    weight_decay=None,
    clipnorm=None,
    clipvalue=None,
    global_clipnorm=None,
    use_ema=False,
    ema_momentum=0.99,
    ema_overwrite_frequency=None,
    loss_scale_factor=None,
    gradient_accumulation_steps=None,
    name='adam',
    **kwargs
)
```

tensorflow optimizers Adam

Hyper parameters

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    - the ra Dataset into train/valid/test sets
    - epoch
    - batch i-batch
    - learn te of the optimizer (SGD, ADAM...)
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well known

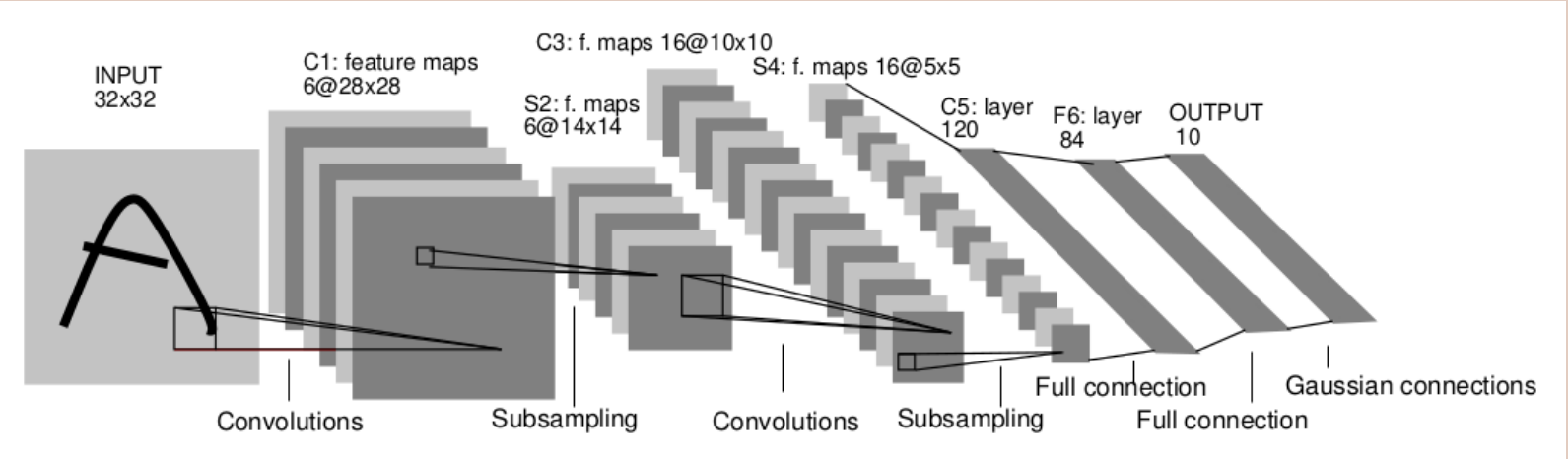
```
tf.keras.optimizers.SGD(
    learning_rate=0.01,
    momentum=0.0,
    nesterov=False,
    weight_decay=None,
    clipnorm=None,
    clipvalue=None,
    global_clipnorm=None,
    use_ema=False,
    ema_momentum=0.99,
    ema_overwrite_frequency=None,
    loss_scale_factor=None,
    gradient_accumulation_steps=None,
    name='SGD',
    **kwargs
)
```

tensorflow optimizers SGD

Hyper parameters

The **batch_size** hyper-parameter

- Exemple: MNISTdataset, CNN model LeNet5 build with SEED set



LeNet5 from LeCun

Hyper parameters

The **batch_size** hyper-parameter

- Example: MNIST dataset, CNN model LeNet5 build with SEED set
- 6 trainings with `batch_size` in (16, 32, 64, 128, 256, 512, 1024)

Hyper parameters

The **batch_size** hyper-parameter

- Example: MNIST dataset, CNN model LeNet5 build with SEED set
- 6 trainings with `batch_size` in (16, 32, 64, 128, 256, 512, 1024)

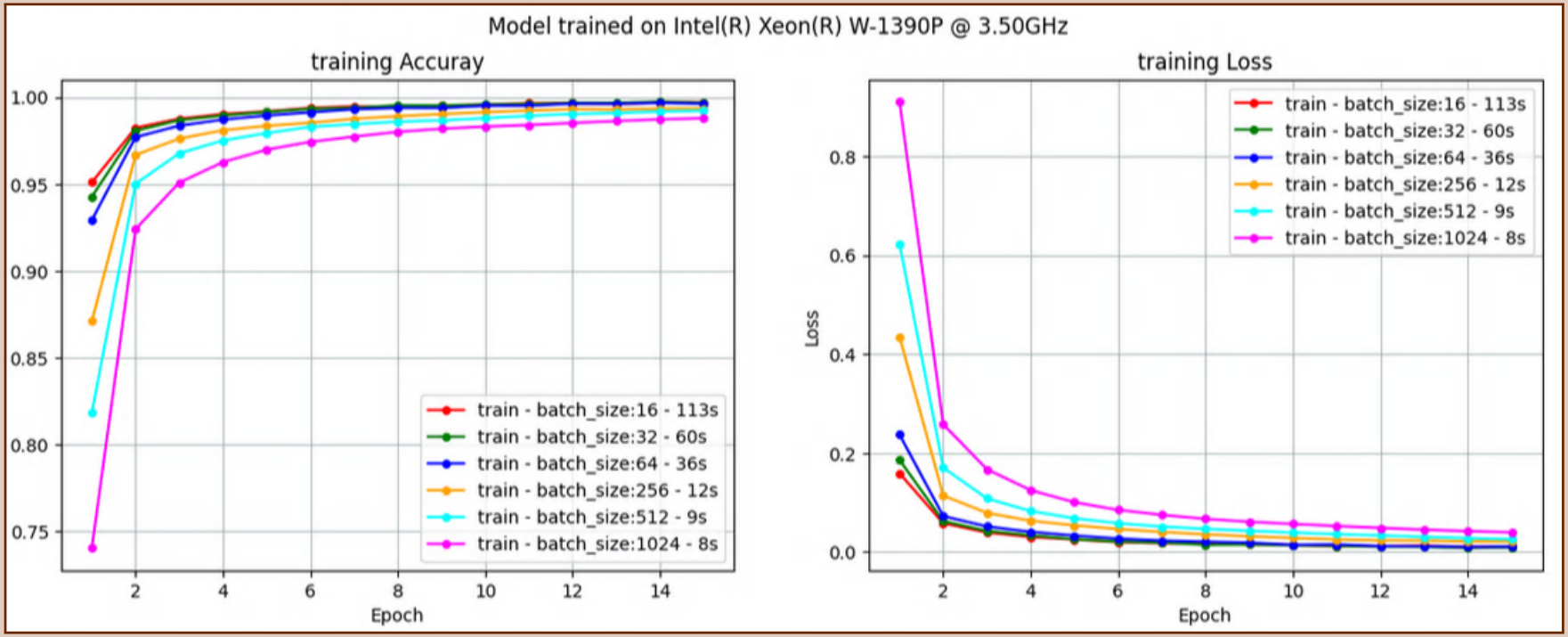
tensorflow/keras snippet:

```
nb_epoch = 15
for bs in (16, 32, 64, 256, 512, 1024):
    print(f'batch_size={bs}, {SEED=}')
    ...
    # Build a new model at each lopp lap, with seed set:
    model = build_CNN(IM_SHAPE, seed=SEED)

    hist = model.fit(x_train, y_train, # images, labels
                     epochs=nb_epoch,  # the total number of successive trainings
                     batch_size=bs,    # split the train dataset in multiple batches
                     validation_data=(x_valid, y_valid),
                     verbose=0)
    ...
```

Hyper parameters

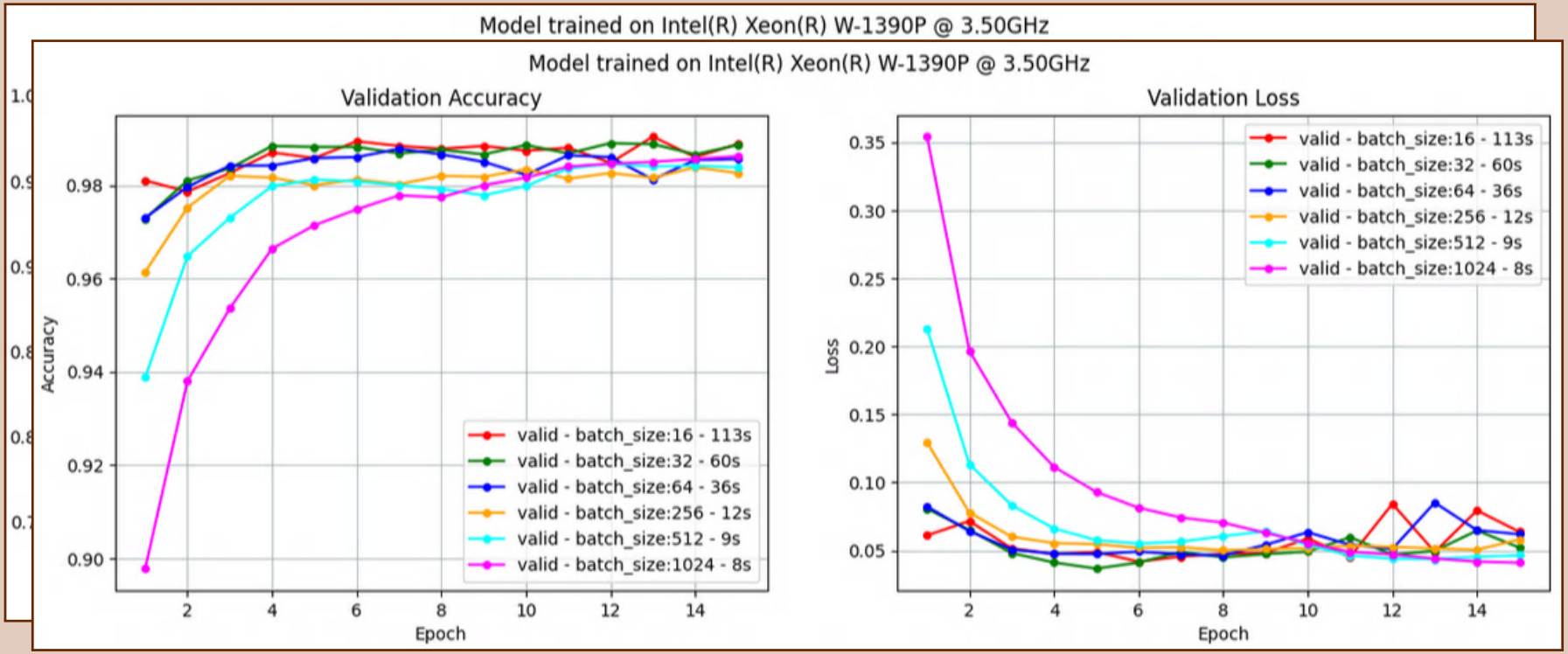
The **batch_size** hyper-parameter



- Training metrics (accuray & loss) $\rightsquigarrow$ right shape but not relevant.
- Validation metrics $\rightsquigarrow$ interesting minimum loss for `batch_size`=32 at `epoch`=5

Hyper parameters

The **batch_size** hyper-parameter



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Hyper parameters

The **patience** hyper-parameter in the **EarlyStopping** algorithm

- Given the previous Validation Loss curves, it should be wise to stop the training for `batch_size`=32 at `epoch`=5 because the validation loss increases.
- tensorflow & PyTorch offer such mecanism known as **Early Stopping**

Hyper parameters

The **patience** hyper-parameter in the **EarlyStopping** algorithm

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- tensorflow & PyTorch offer such mecanism known as **Early Stopping**

tensorflow/keras snippet: using `EarlyStopping` *callback* to stop the training

```
for bs in (16, 32, 64, 256, 512, 1024):
    ...
    # Build a new model at each lopp lap, with seed set:
    model = build_CNN(IM_SHAPE, seed=SEED)
    callbacks_list = [
        EarlyStopping(monitor='val_loss',  # The parameter to monitor
                      patience=1,          # accept that 'val_loss' increases 1 time
                      restore_best_weights=True, # important !!!
                      verbose=1) ]
    hist = model.fit(x_train, y_train, # images, labels
                     epochs=nb_epoch,  # the total number of successive trainings
                     batch_size=bs,    # split the train dataset in multiple batches
                     validation_data=(x_valid, y_valid),
                     verbose=0,
                     callbacks = callbacks_list)
```

Hyper parameters

The **patience** hyper-parameter in the **EarlyStopping** algorithm

```
batch_size=16, SEED=1234 Epoch 2: early stopping
Restoring model weights from the end of the best epoch: 1.
 Train Elapsed time 17s -> 00:00:17
batch_size=32, SEED=1234 Epoch 6: early stopping
Restoring model weights from the end of the best epoch: 5.
 Train Elapsed time 27s -> 00:00:27
batch_size=64, SEED=1234 Epoch 6: early stopping
Restoring model weights from the end of the best epoch: 5.
 Train Elapsed time 15s -> 00:00:15
batch_size=256, SEED=1234 Epoch 7: early stopping
Restoring model weights from the end of the best epoch: 6.
 Train Elapsed time 6s -> 00:00:06
batch_size=512, SEED=1234 Epoch 7: early stopping
Restoring model weights from the end of the best epoch: 6.
 Train Elapsed time 5s -> 00:00:05
batch_size=1024, SEED=1234 Restoring model weights from the end of the best epoch: 15.
 Train Elapsed time 7s -> 00:00:07
```

- Training for `batch_size`=32 stopped at `epoch`=6 (model is saved for `epoch`=5)

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The **patience** hyper-parameter in the **EarlyStopping** algorithm

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batch_size=16, SEED=1234 Epoch 2: early stopping
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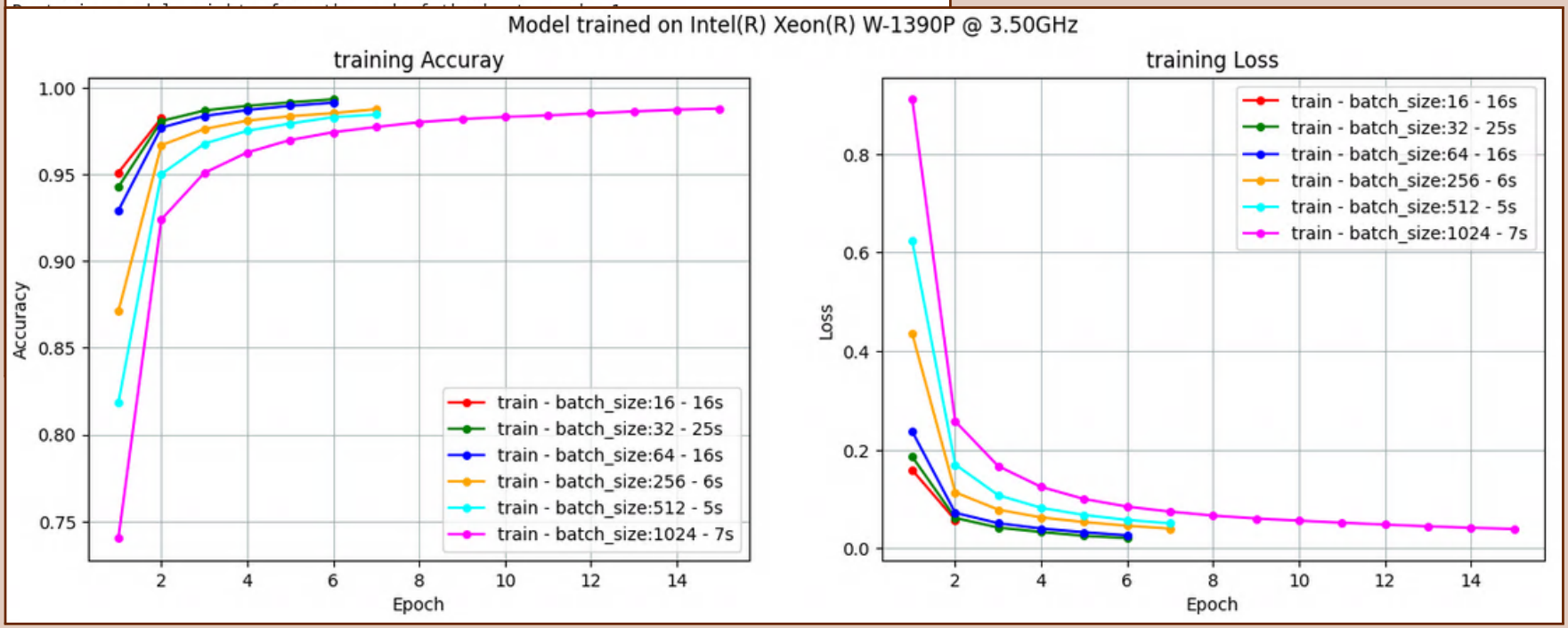

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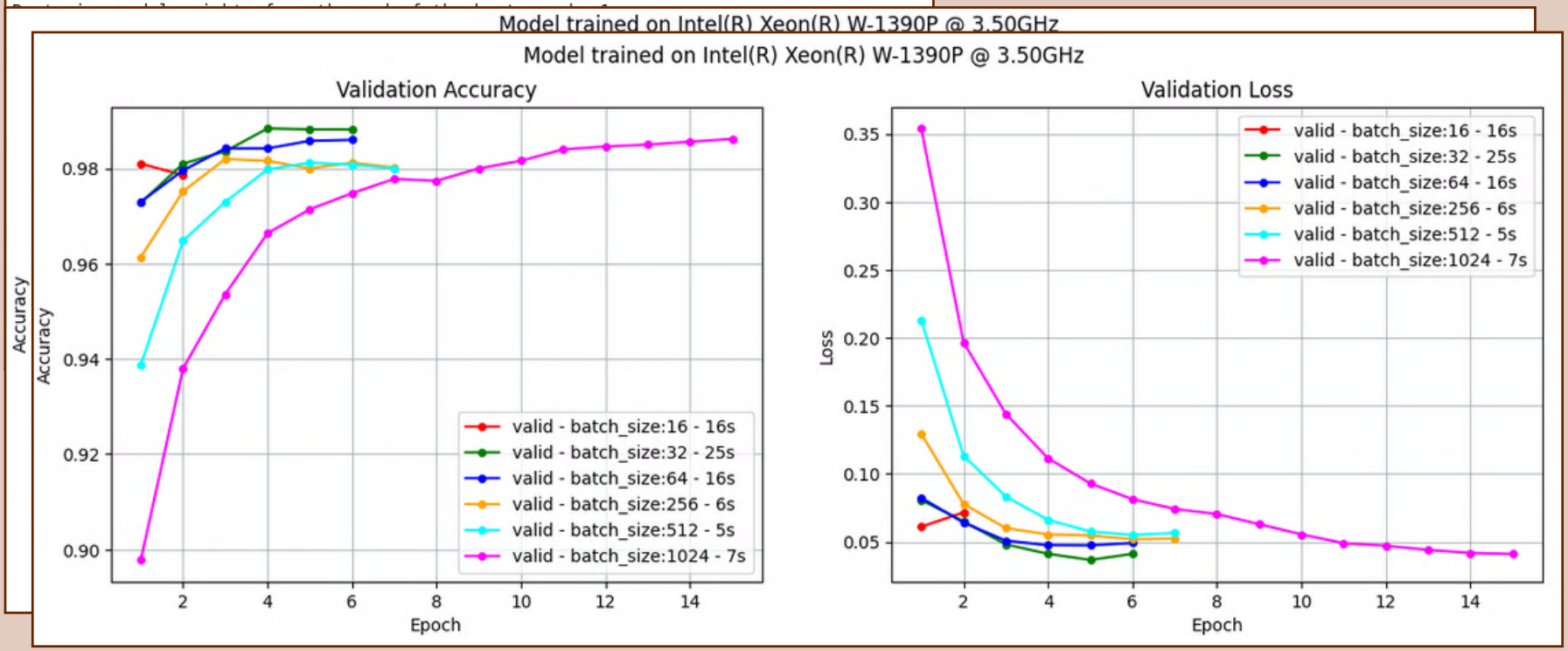

- Training for `batch_size`=32 stopped at `epoch`=6 (model is saved for `epoch`=5)

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The **patience** hyper-parameter in the **EarlyStopping** algorithm

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batch_size:  32 time:25s  test_acc: 0.990 test_loss:0.035
batch_size:  64 time:16s  test_acc: 0.986 test_loss:0.044
batch_size: 256 time:6s   test_acc: 0.983 test_loss:0.050
batch_size: 512 time:5s   test_acc: 0.981 test_loss:0.054
batch_size:1024 time:7s   test_acc: 0.987 test_loss:0.040
```

- The model perfomance for `batch_size`=32 at `epoch`=5 has the best score when tested with the **test Dataset**.
- The training elapsed time is now only 25 sec.
- The whole notebook is reproducible.

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Sharing reproducible DL training

Use a **Python Virtual Environment** (PVE)

- A PVE defines a dedicated file tree where to store the Python modules & tools of a DL project
- Ensures that different projects do not interfere with each other
- Isolate project dependencies
- Protects the Python modules from system updates or from modules updates in other projects
- Provides tools to easily delete/duplicate/reproduce it
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- Use a dedicated PVE for each DL project, even if small project

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Use a tool to manage your DL projects & PVEs

- Minimalist: `venv`, `virtualenv`...
- More efficient: `conda`, `poetry`...
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  - From the Web page of `uv`:
  - A single tool to replace pip, pipx, poetry, pyenv, virtualenv...
  - 10-100x faster than pip !
  - Provides comprehensive project management, with a universal lockfile.
  - Installs and manages Python versions.
  - Includes a pip-compatible interface for a performance boost with a familiar CLI.
  - Disk-space efficient, with a global cache for dependency deduplication.
  - Supports macOS, Linux, and Windows....

Sharing reproducible DL training

Use an **Integrated Developpment Environment** (IDE) **aware** of PVE

- VSCode
- PyCharm
- Atom
- PyDev
- Jupyter notebook
- Jupyter Lab
- ...

Sharing reproducible DL training

Use a **versionning** tool

- To keep track of **code** and **data** versions
- To share **code** and **data**
- Example: **git** repository for code and data (< 5 GB)
  - Maintain the repository !
  - If your data files are too big, use the **Git Large File** (GLF) extension to version the data with Git.

Thank you for your attention.

Bibliography I

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Reproducibility

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Interpretable Machine learning (IML)

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