HelioSPIR

Deep learning for NIR spectroscopy : overview and thoughts

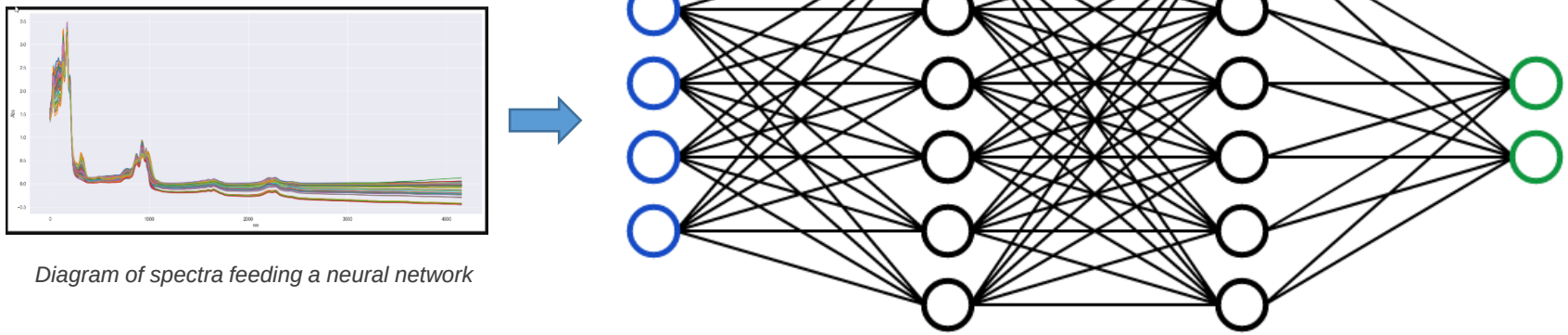

Diagram of spectra feeding a neural network

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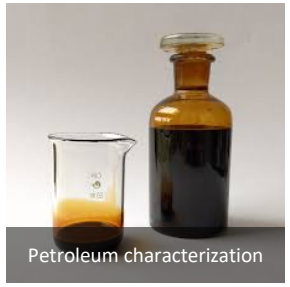
ED STIC
Sciences et technologies de l'information et de la communication

IFP Energies nouvelles

NEAR-INFRARED (NIR) SPECTROSCOPY & CHEMOMETRICS


Vegetable oil characterization


Biomass characterization

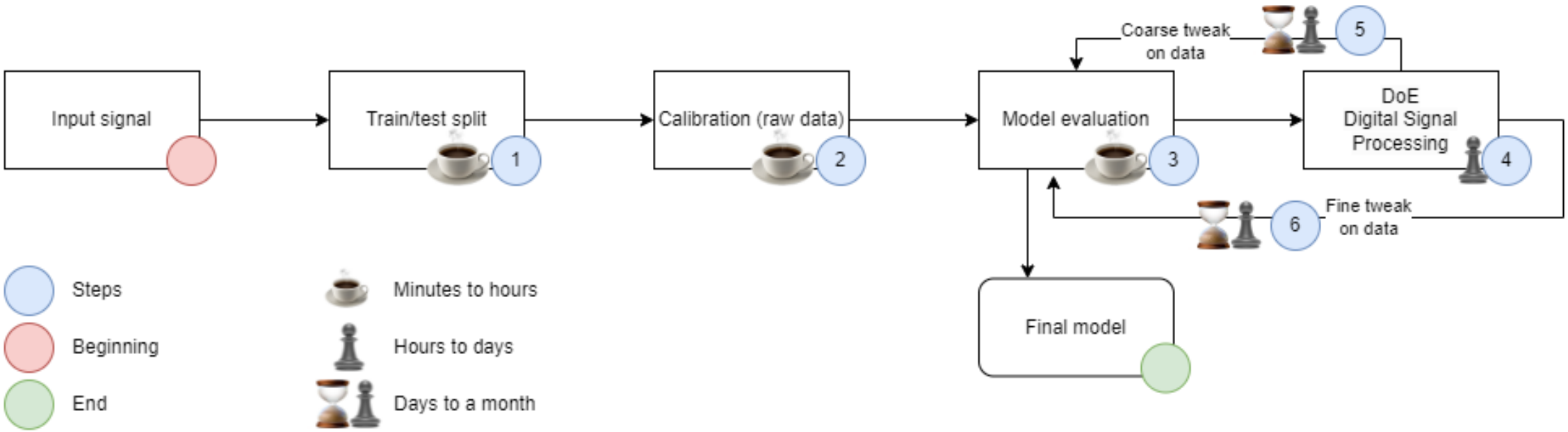

Petroleum characterization


Chemical plastic recycling characterization

APPLICATION OF NEAR-INFRARED SPECTROSCOPY IN AN ENERGY CONTEXT

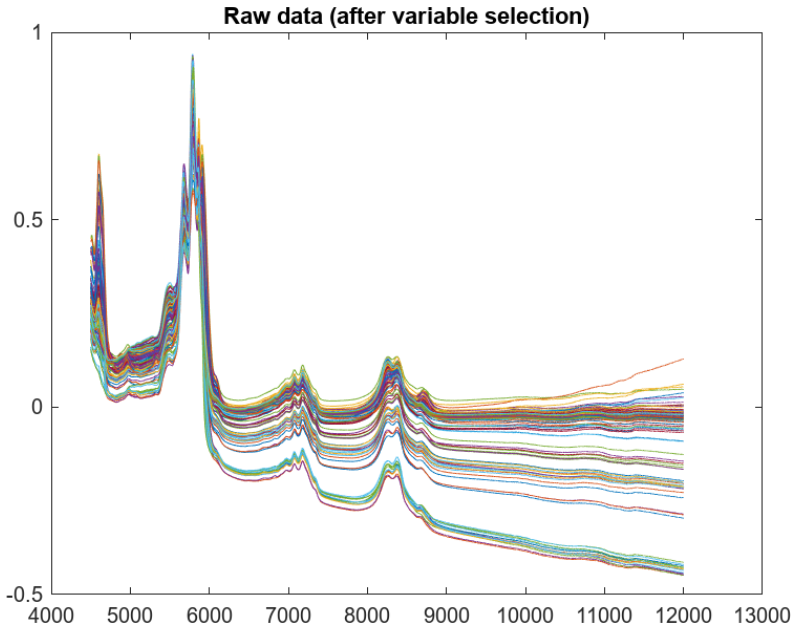
CHEMOMETRICS

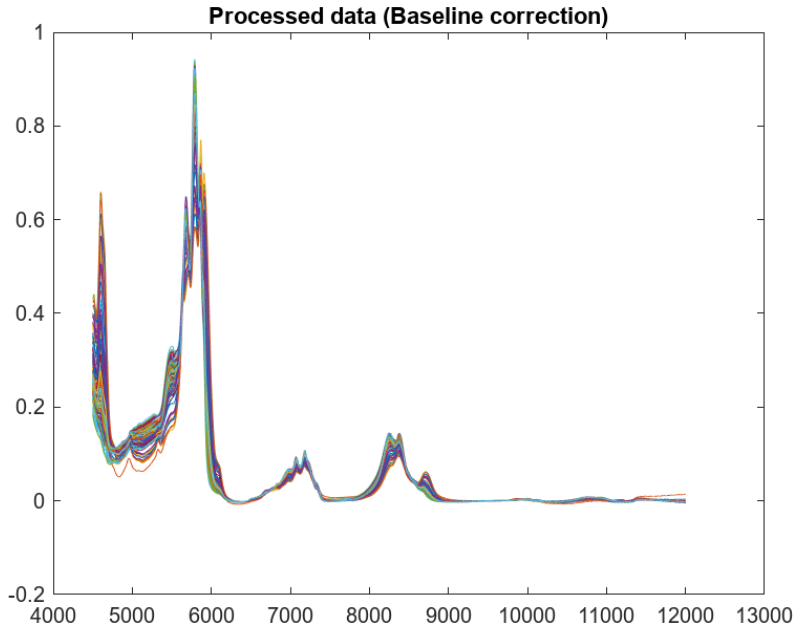
- Chemometrics use mathematical and statistical method
- Chemometrics base equation: $\boldsymbol{y = f(x) + \epsilon}$
- Typical workflow:



CHEMOMETRICS

- Chemometrics use mathematical and statistical method
- Typical chemometrics workflow
- Digital signal processing
  - Corrects spectra of unwanted analytical variability
  - Its effect





CHEMOMETRICS IS NOT ENOUGH

- PLS models used at IFPEN since more than 30 years
  - Some models have been working all this time 🥰
- But
  - It took a lot of manual time to build new models
  - Calibration spectrometers transfer is a pain point
  - With the emergence of renewable energies, we suspect our models reach their limits too quickly as they need to be often updated to respond to new scenarios…
- A new approach "*Deep learning*" is used in other fields, we want to see what it can give

WHAT IS DEEP LEARNING ?

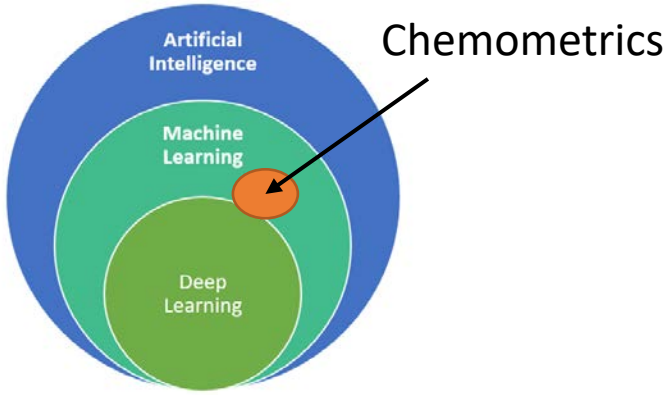


Figure 1: artificial intelligence, machine leaning and deep learning Source: Nadia BERCHANE (M2 IESCI, 2018)

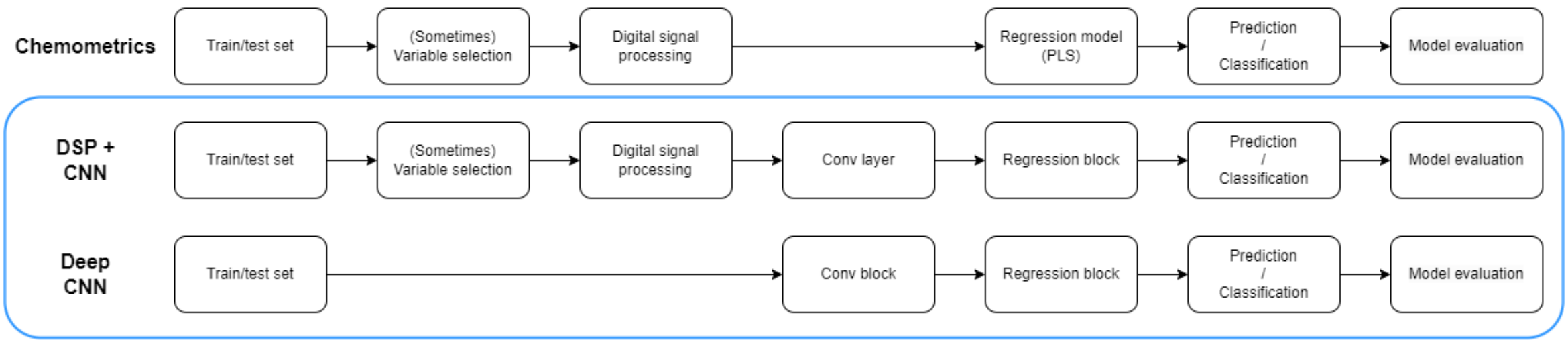
- Mostly used in computer vision, natural language processing, decision making system, etc.
- *Reminder*
  - X = *input spectral data*
  - y = *physical values to predict*
- DL base equation: $\boldsymbol{y = f(x, \theta) + \epsilon}$
  - f represent the model (a neural network)
  - θ represent model's design
  - ϵ represent error.

- θ defines model's architecture and its hyperparameters
- To minimize the error ϵ, the DL model use θ and apply an optimization algorithm to find its internal parameters.

- An architecture is composed of multiple stacked layers
- Layers have different tasks: representation, normalization, regression, …

STATE OF THE ART IN DEEP LEARNING APPLIED TO NIR ANALYSIS

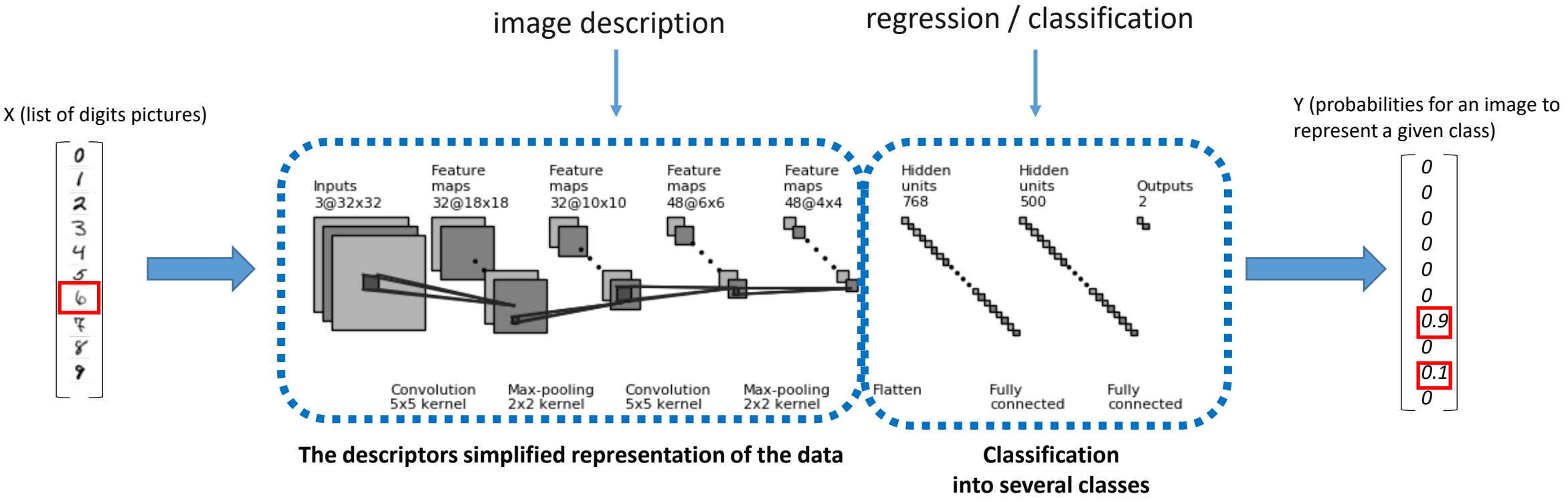
- A few try with ANNs between 2005-2010 [1,2]
- First paper of interest in 2016 [3] 👶
- According to review, 80% of DL models in NIR are CNNs [4]
- Different existing workflow:



[1] Balabin et al., Chemometrics & intelligent lab, volume 83, 2008
[2] Balabin et al., Fuel, volume 90, 2011
[3] Acquarelli et al., Analytica chimica acta, volume 954, 2016
[4] Yang et al., Analytica chimica acta, volume 1081, 2019

CONVOLUTION DEEP NETWORK (CNN) FOR COMPUTER VISION

A classic CNN architecture [1]

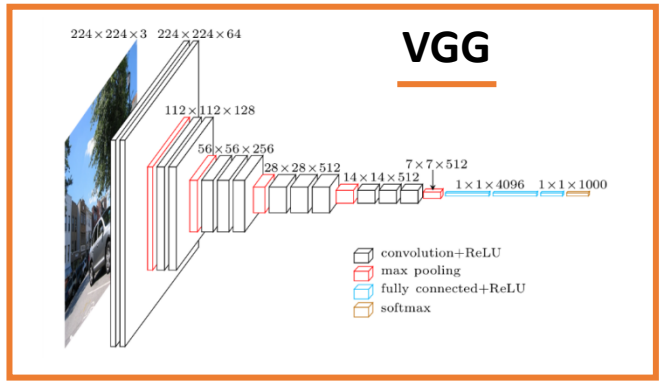


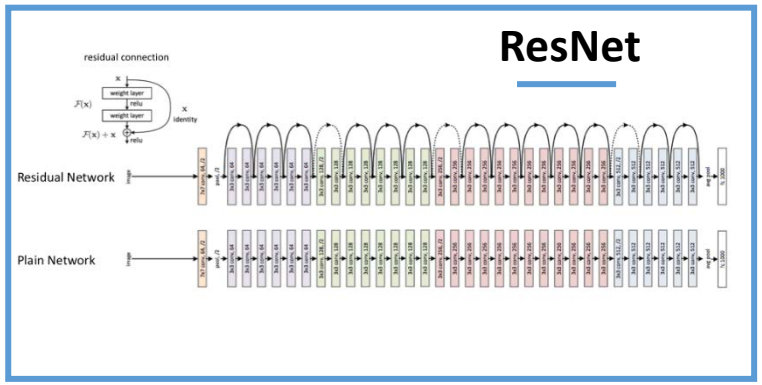
[1] LeCun et al., IEEE, volume 86, 1998

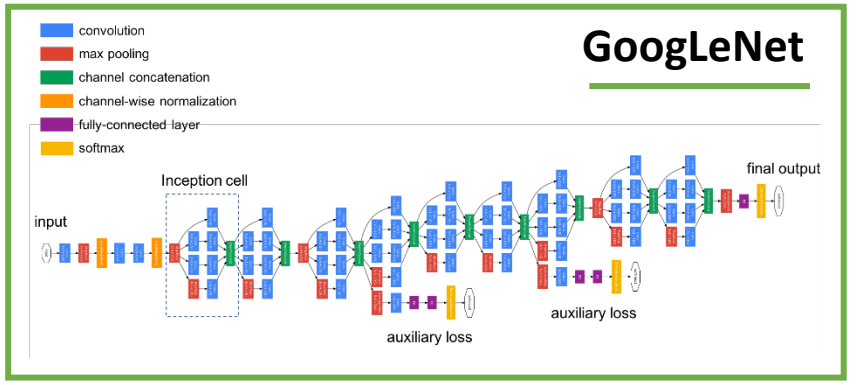
Source : draw_convnet Python script

CNN IN NIR

- Most of DL on NIR is applied to agri-food
- We can use this knowledge to adapt it to our problems
  How to? To which answer will we respond ?
- Reference architecture exist in computer vision, signal processing, etc.
- Review [1] propose to use ref. archi. as base





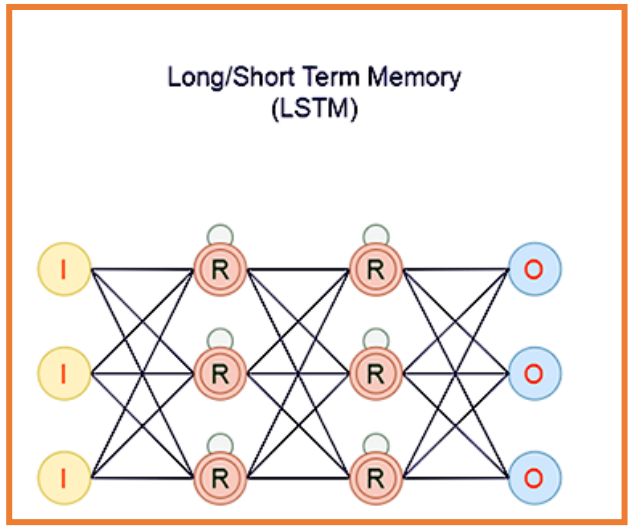


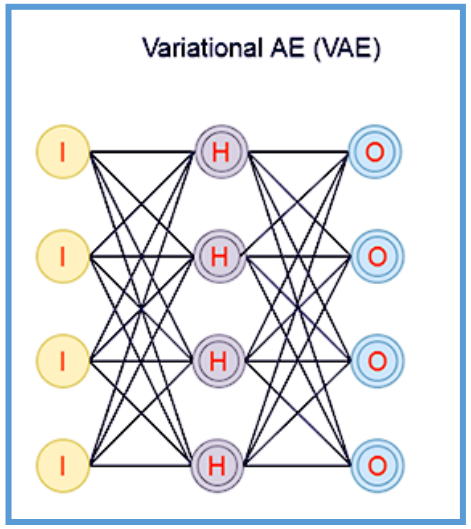
- A model based on GoogLeNet were applied in NIR and works very well [2]

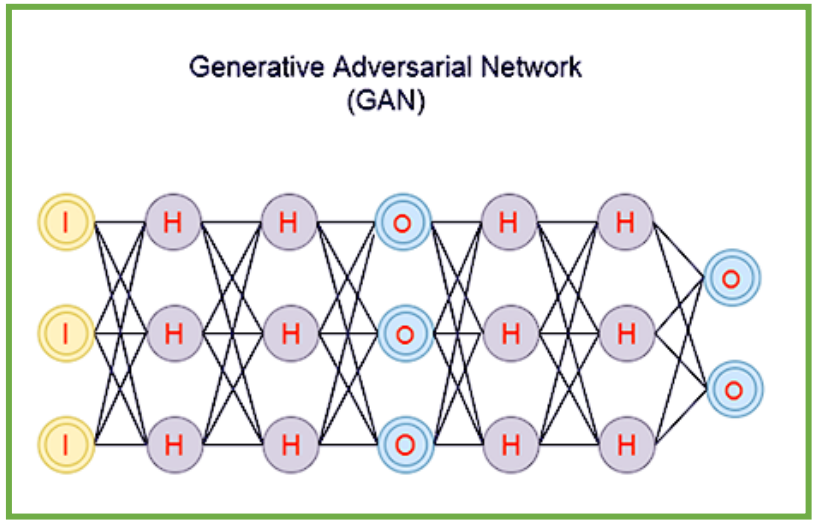
[1] Yang et al., Analytica chimica acta, volume 1081, 2019
[2] Zhang et al., Analytica chimica acta, volume 1058, 2019

OTHER NETWORKS TYPE USED FOR NIR ANALYSIS

- LSTM used to study manure on food analysis [1]
- VAE used to study the aging of chemical product in water pipe [2]
- GAN used to improve dataset to predict gasoline properties [3]







[1] Tan et al., Spectrochimica acta., volume 283, 2022

[2] Grossuti et al., Journal of physical chemistry, volume 13, 2022

[3] He et al., Italian Association of Chemical Engineering, volume 81, 2020

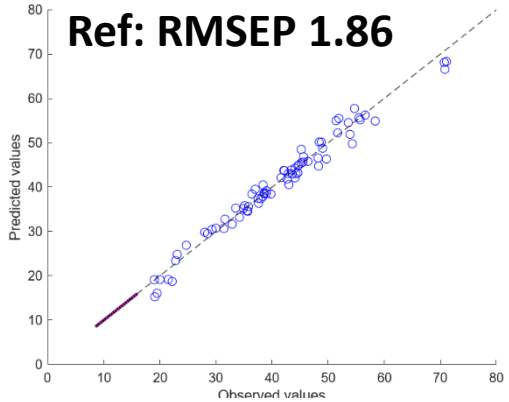
RESULTS & DISCUSSION

RESULTS

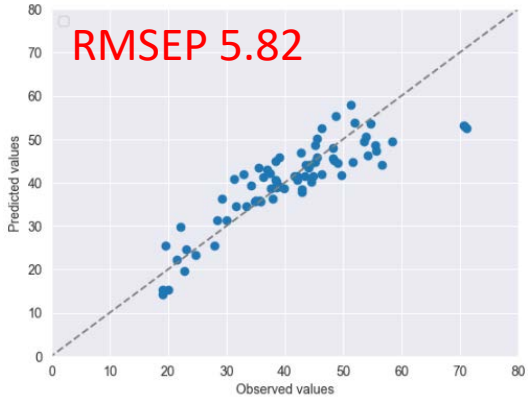
- We developed a Chemometric model, it has similar performance to IFPEN reference
- Several DL models (CNNs) tested
- Mastering DL design ($\boldsymbol{\theta}$) is complex. It's not magical!

CHEMOMETRICS

DEEP LEARNING



✅ BUT 🤔



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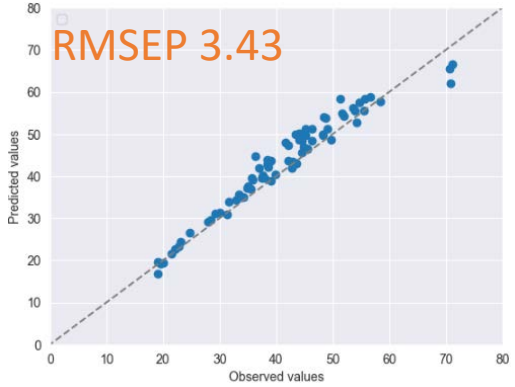
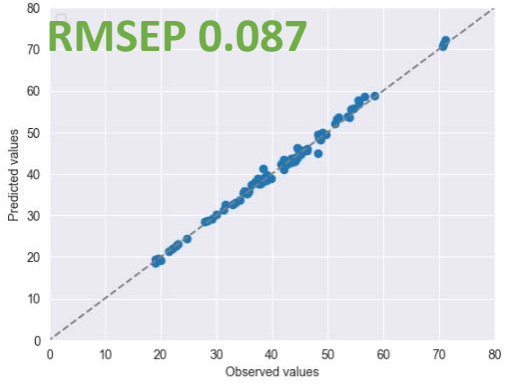


🤔 💡



🤩 ✅

TIME

CONTEXT | PROBLEM | LITTERATURE | RESULTS

RESULTS & DISCUSSION

- We developed a Chemometric model, it has similar performance to IFPEN reference
- Several DL design tested
- Mastering DL design ($\boldsymbol{\theta}$) is complex. It is not magical!
- Implementation of neural networks is hard: they fail silently…

- Building an efficient network :
  - Using good metrics (RMSEC, RMSEP, R2, training plot, error plot & parity plot)
  - Having (mainly) experience
- Process I used
  - Copy/paste code from working network on similar dataset
  - Iterate over hyperparameters (loss functions, activation, representations, scaling, initializer & optimizer)
  - Start with a reference architecture, then try variations to see if it's worth converging from it.

THANK YOU FOR YOUR TIME, HAVE A GREAT DAY ;)