

# Méthodes avancées en exploitation de donnée (MATH80619)

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# 1 Introduction

In the first section of this paper, a literature review covers the neural networks and deep learners algorithms, focusing on different type of neural networks architecture; the purpose of adding multiple hidden layers and, ultimately, what are the challenges regarding the increase in computing time. Furthermore, in the methodology section, a list of deep learning projects are shown in order to understand some patterns and methods. Then, an exhaustive list of the R libraries allowing to build neural networks and deep learners models. Correspondingly, the advantages and disadvantages of each libraries, their capabilities as well as what you can expect when using them. To sum up, the last section will give concrete examples on how to implement the neural networks and deep learners models with these libraries, using real data.

## 2 Litterature Review

### 2.1 What is Deep Learning and why use it?

Deep learning is a subset field of articial intelligence and can be seen as a specific way of doing machine learning. Deep learning algorithms can be seen as feature representation learning. Indeed, by applying to the data multiple non-linear transformations through the use of hidden layers, deep learning models have their own trainable feature extration capability making it possible to learn specific features from the data without needing a specific human domain expert. This means that deep learning models won't require the features extraction step that is essential for classic machine learning models. However, increasing the models capacity by adding hidden layers, requires increasingly computing power and slow down the training process of the model. The choice of hyperparameters, programming languages and memory management will therefore be important criteria to take into account while building deep learning models

Since the last decade, deep learning models have shown notable predictive power and have been revolutionizing an important number of domain such as computer vision, natural language understanding, fraud detection, health and much more.

As a first glance in the subject, it is highly recommended it to read a reference from pioneers in the field ([5, Chapter 1]).

#### 2.1.1 Feed Forward Neural Network

"Deep feedforward networks, also called feedforward neural networks, or multilayer perceptrons (MLPs), are the quintessential deep learning models." [5]

FNN models are inspired from biology and by the way the human brain works. In a neural network, each neuron takes input from other neurons, processes the information and then transmits outputs to next neurons. Artificial neural networks follow the same process as each neuron will perform the weighted sum of inputs and will add a bias as a degree of freedom. It will then apply a non-linear transformation before outputting the information. Thus, the information goes forward in the network; neurons transmit information from the input layers towards the output

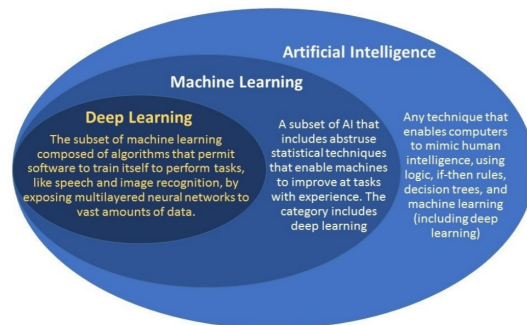


Figure 1: Artificial Intelligence vs Machine Learning vs Deep Learning

layer. It is important to know that in a feedforward neural networks (fig. 4) the neurons of a same layer are not connected to each other; they do not allow any feedback connections within a same layer. If we want to allow this process, we will be looking at recurrent neural networks.

The equation a neuron input is

$$a(x) = b + \sum_i w_i x_i \quad (1)$$

and the output

$$h(x) = g(a(x)) \quad (2)$$

where:

$x$  = the input data  
 $b$  = the bias term  
 $w$  = the weight or parameter  
 $g(\dots)$  = the activation function

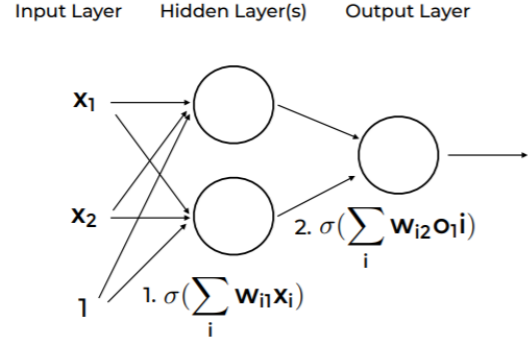


Figure 2: feedforward neural networks

Here, **the bias term  $b$**  and **the weights or parameter  $w$**  will be learned by the model in order to minimize

a cost function, through the use of the gradient descent method. Then, the network will use the backpropagation algorithm where the error is backpropagated from the output to the input layers and the bias and weights are then updated accordingly.

Regarding the **activation function  $g(\dots)$** , the common practice is to use a ReLu (rectified linear unit) as the activation function for the neurons of the hidden layers. Regarding the neurons of the last layer, the activation function will be chosen accordingly to the task we want our model to perform:

Output type	Output Unit	Equivalent Statistical Distribution
Binary (0,1)	$\text{sigmoid}(z) = \frac{1}{1 + \exp(-z)}$	Bernoulli
Categorical (0,1,2,3,k)	$\text{softmax}(z_i) = \frac{\exp(z_i)}{\sum_r \exp(z_r)}$	Multinoulli
Continuous	Identity(a) = a	Gaussian
Multi-modal	mean, (co-)variance, components	Mixture of Gaussians

Figure 3: Activation functions: output units. HEC

A detailed explanation of the theory of feedforward neural network can be found in [5, Chapter 6]

### 2.1.2 CNN

The CNN are a modified architecture of FNN that leverage the feature engineering that used to be hand made by domain experts. This class of deep neural network are commonly used for image recognition and classification that can serve different applications such as facial recognition, document analysis and speech recognition. The original

FNN are not suited analyzing large size images since the weights increase exponentially and, at the end, don't perform very well.

A standard architecture of a CNN model is commonly represented this way: We start with an input image to which we are going to apply several kernels, a.k.a features detectors, in order to create feature maps that will form what we call a convolutional layer. A common practice is to apply the ReLu activation function to the convolutional layer output in order to increase the non linearity of the images before using the pooling method to create a pooling layer. The next step will be to combine all the pooled images from the pooling layer into one single vector, which is called flattening and will be the input of a FNN that will perform the desired task, for instance, classification. CNN parameters are trained with the backpropagation algorithm where the gradients are propagated from the output layer of the FFN to the input of the CNN in order to minimise a cost function, most of the time a categorical cross-entropy if we are performing a multi-class classification.

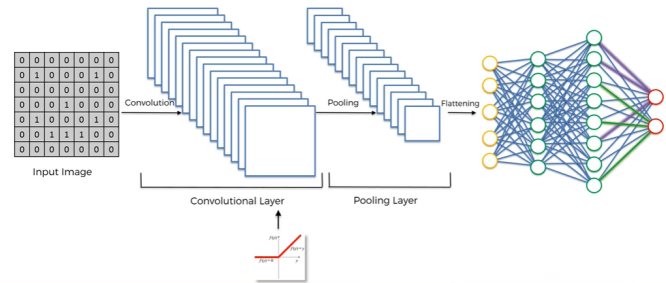
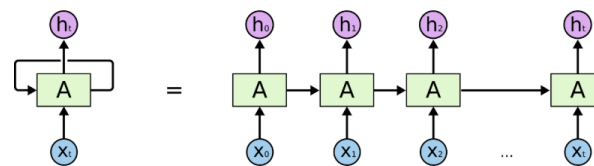


Figure 4: CNN, Deep Learning A-Z by SuperDataScience

To get a detailed explanation of convolutional neural networks we recommend to read [5, Chapter 9].

### 2.1.3 RNN

Recurrent neural networks are a more advanced type of neural networks architecture having proven state-of-art performance for solving tasks related to sequential data such as Natural Language Processing (NLP), anomaly detection and event forecasting. As a key differentiator from feedforward neural networks, is that RNNs use feedback loops connections instead of feedforward connections and get an internal memory. Indeed, that take as input each step of the sequential data as well as what they have learned over time. One of their other advantage is to be able to handle input and output sequences with different sizes. "A recurrent neural network can be thought of as multiple copies of the same network, each passing a message to a successor" Olah.



An unrolled recurrent neural network.

Figure 5: RNN, Understanding LSTM Networks by Olah

To get a detailed explanation of the theory of recurrent neural networks we recommend to read [5, Chapter 10]. We also recommend reading this blog post <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

## 2.2 How to integrate Deep Learning in R

The integration of Deep learning in R can be separate in two part ; (1) The API integration and (2) the standalone R packages.

1. The API will give the possibility to control externally through R an existing installation. In other words, a software translator for a already known software installation. This approach is not always trivial to install nor to manipulate but in long term will probably give the best flexibility in terms of Deep Learning projects.
2. The standalone R packages will be packages that require no third party software in order to create the deep learning projects. This approach is relatively fast to install but is restraining in terms deep learning architecture.

A list of the available resources with installation and examples tutorials can be found in section ?? and ?? .

## 3 Methodology

This section is divided in two; the dataset description and the benchmark type. The dataset description is mostly to describe what dataset is going to be use for the different type of deep learning algorithms. The second section will describe two indicators in order to compare results of similar algorithms. The first indicator is mostly about a simple accuracy base on the same training and validation dataset and second indicator is about the time it took to execute the same task on differents ressources.

### 3.1 Dataset

#### 3.1.1 FNN

For the FNN, the training data will be the well known *Iris* dataset. It contains four covariables and one categorical target variable.

```
library(datasets)
data(iris)
```

#### 3.1.2 CNN

For the CNN, the training data will also be a well known dataset called CIFAR-10. The CIFAR-10 dataset consists of 60000 32x32 colour images in 10 classes, with 6000 images per class. The easiest way in R to download this package is using the Keras API. The training dataset has 50 000 images in three color (Red-Green-Blue) that are 32 pixels by 32 pixels. The testing dataset has a total of 10 000 images

```
library(keras)
cifar10 = dataset_cifar10()
```

#### 3.1.3 RNN

The dataset use to test an RNN is the IMDB Movie reviews sentiment classification. This pack

```
imdb = dataset_imdb( path = "imdb.npz", num_words = NULL, skip_top = 0L, maxlen = NULL,
  seed = 113L, start_char = 1L, oov_char = 2L, index_from = 3L)
```

## 4 Available resources

Like explain earlier this section will be divided in two in order to really differentiate the R packages standalone of the ressources that add an application interface.

## 4.1 R packages

4.1.0. à voir si on a encore de la place pour mettre un tableau récapitulatif

### 4.1.1 Neuralnet package

**Keyword:** FNN; Deep FNN

**Description** According to its CRAN description, the package allows the "training of neural networks using the backpropagation, resilient backpropagation with (Riedmiller, 1994) or without weight backtracking (Riedmiller, 1993) or the modified globally convergent version by Anastasiadis et al. (2005). The package allows flexible settings through custom-choice of error and activation function. Furthermore, the calculation of generalized weights (Intrator O & Intrator N, 1993) is implemented." This package uses C/C++ in backend.

#### Usage

```
neuralnet(formula, data, hidden = 1, threshold = 0.01,
  stepmax = 1e+05, rep = 1, startweights = NULL,
  learningrate.limit = NULL, learningrate.factor = list(minus = 0.5,
  plus = 1.2), learningrate = NULL, lifesign = "none",
  lifesign.step = 1000, algorithm = "rprop+", err.fct = "sse",
  act.fct = "logistic", linear.output = TRUE, exclude = NULL,
  constant.weights = NULL, likelihood = FALSE)
```

Figure 6: Package neuralnet, CRAN

#### Pros

- Very easy to use and to build a quick FFN and deep FNN model.
- Allows to use several types of backpropagation algorithms. By default, the resilient backpropagation algorithm is used "rprop+" instead of regular backpropagation which is an algorithm not very used in practice as it is more tricky to implement. We can however decided to change the rprop+ for a standard backpropagation by changing for **algorithm = "backprop"**.
- Several hidden layers and neurons per layer can be added. By default, the algorithm uses only 1 hidden layer with 1 neuron, but it can be increased by addind the command line: **hidden = c(5,2)** to get 2 hidden layers of 5 neurons.
- Allows to easily plot and visualize the model and its parameters with the command line: **plot(model)**.

#### Cons

- One of the disadvantage of this package is that it requires some data preprocessing as it only works with numeric inputs. Therefore, factor variables will need to be transformed into dummies during the preprocessing phase.
- The package doesn't provide built-in normalization functions. Therefore, it is recommended to manually normalize the data before using them as input in the neural networks in order to reduce the number of iteration of the algorithm.

### 4.1.2 nnet package

**Keyword:** FNN

**Description** This package comes from the CRAN platform and allows to build and fit "FNN with a single hidden layer and multinomial log-linear models". This package uses C/C++ in backend.

```
nnet(x, y, weights, size, Wts, mask,
     linout = FALSE, entropy = FALSE, softmax = FALSE,
     censored = FALSE, skip = FALSE, rang = 0.7, decay = 0,
     maxit = 100, Hess = FALSE, trace = TRUE, MaxNWts = 1000,
     abstol = 1.0e-4, reltol = 1.0e-8, ...)
```

Figure 7: Package nnet, CRAN

#### Pros

- One of the easiest R package to build a quick FNN model.

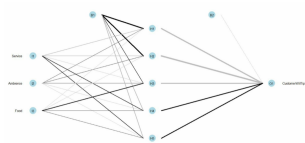
#### Cons

- It does not offer a lot of flexibility, and can only apply logistic sigmoid function for the hidden layer activation and cannot use tanH and ReLu.
- This package does not allow to use more than one hidden layer, and does not have any feature to find the optimal number of neurones in the hidden layer. It is up to the analyst to build a loop to test by cross-validation, for example, the optimal hyperparameter values.
- Cannot use classical backpropagation algorithm to train the network. It only uses the BFGS (Broyden-Fletcher-Goldfarb-Shanno) which is a Quasi-Newton method and therefore increases the number of computation to reach a local optima. However, applied on a small dataset with a model having only one hidden layer does not seem to be a problem.
- Does not have any function to plot the model.

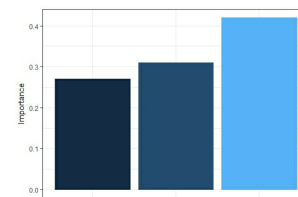
### 4.1.3 NeuralNetTools package

**Keywords:** Visualization; Variable importance; Sensitivity

**Description** This package is a complement to R's neural networks packages as it allows to visualize and perform analysis on neural network models. "Functions are available for plotting, quantifying variable importance, conducting a sensitivity analysis, and obtaining a simple list of model weights."



(a) NeuralNetTools, plotnet function



(b) NeuralNetToolsm Input variables importance

Figure 8: Embedding dimension hyper parameter

**Pros**

- Very easy to plot your neural network models with the function **plotnet(model)**.
- Visualize the input variables importance to the output prediction with the Garson and Olden algorithm.
- Perform sensitivity analysis on your neural networks model using the Lek profile method.
- Works with the models built from different packages: **caret**, **neuralnet**, **nnet**, **RSNNS**
- Can plot neural networks with pruned connections from the RSNSS package.

**Cons**

- Does not provide any function for neural network model development.
- Is not optimized to visualize large neural networks models.

**4.1.4 Deepnet package**

**Keywords:** FNN; RBM; DBN; Autoencoder

**Description** This package is available on the CRAN platform and has been written specifically for R. It allows "implement some deep learning architectures and neural network algorithms, including backpropagation, Restricted Boltzmann Machine (RBM), Deep Belief Network (DBN) and Deep autoencoder".

```
nn.train(x, y, initW = NULL, initB = NULL, hidden = c(10), activationfun = "sigm",
        learningrate = 0.8, momentum = 0.5, learningrate_scale = 1, output = "sigm",
        numepochs = 3, batchsize = 100, hidden_dropout = 0, visible_dropout = 0)
```

Figure 9: Package deepnet, CRAN

**Pros**

- Allows to load benchmark datasets such as MNIST with the function `load.mnist(dir)`
- Allows to initialize the weights of a FNN with the Deep Belief Network algorithm (`dbn.dnn.train()`) or Stacked AutoEncoder algorithm (`sae.dnn.train()`).
- Allows to have an estimation of the probabilistic distribution of a dataset through the use of the Restricted Boltzmann machine algorithm.
- Have more activation functions than the other R packages. Hidden Layers activation function can be linear, sigmoid or tanh. The output activation function can be linear, sigmoid or softmax.

**Cons**

- Does not support the ReLu activation function for hidden layers.
- Not the fastest package due to its implementation in R.
- Does not provide a lot of hyperparameters tuning options, and is not user-friendly.



#### 4.1.5 brnn package

**Keywords:** Bayesian Regularization; FNN

**Description** This package available on the platform CRAN, allows to perform "Baeyesian regularized neural networks including both additive and dominance effects, and allows to takes advantage of multicore architectures via a parallel computing approach using openMP for the computations". (Pérez-Rodriguez, ...)

```
brnn(x,y,neurons=2,normalize=TRUE,epochs=1000,mu=0.005,mu_dec=0.1,
mu_inc=10,mu_max=1e10,min_grad=1e-10,change = 0.001,cores=1,
verbose=FALSE,Monte_Carlo = FALSE,tol = 1e-06, samples = 40,...)
```

Figure 10: Package nnet, CRAN

#### Pros

- Allows to add Additive and Dominance effects in the neural networks models.
- Take advantage of multicore processors (only for UNIX-like systems).
- Allows to use a Gauss-Newton algorithm for optimization.
- The package is able to assign initial weights by using the Nguyen and Widrow algorithm.
- Include an algorithm to deal with ordinal data by using the function **brnn\_ordinal(x, ...)**
- It has a function to normalize and unnormalized the data.

#### Cons

- Cannot use the classic backpropagation algorithm for optimization.
- The package fits a two layers neural networks and it is not possible to increase the number of hidden layers.

#### 4.1.6 rnn package

**Keywords: RNN Installation:** You will need to install the diges package first through the function **install.packages(digest)** in order to download the rnn package.

**Description** Available from the CRAN platform, this package allows the "implementation of a Recurrent Neural Network architectures in native R, including Long-Short Term Memory (LSTM), Gated Recurrent Unit (GRU) and vanilla RNN.

```
trainr(Y, X, model = NULL, learningrate, learningrate_decay = 1,
momentum = 0, hidden_dim = c(10), network_type = "rnn",
numepochs = 1, sigmoid = c("logistic", "Gompertz", "tanh"),
use_bias = F, batch_size = 1, seq_to_seq_unsync = F,
update_rule = "sgd", epoch_function = c(epoch_print,
epoch_annealing), loss_function = loss_L1, ...)
```

Figure 11: Package rnn, CRAN

**Pros**

- Allows to run a demonstration of how RNN models work by using predefined values and allowing the user to see the impact of a changes in the model's hyperparameters by using the function `run.rnn_demo()`
- Allows to plot the model's errors through all epochs.
- Allows to use LSTM and GRU models.

**Cons**

- Uses R native, therefore it might not be the best package in terms of time computation.

**4.2 API packages****4.2.1 Keras**

**Keywords:** FNN, CNN, RNN

**Description** This API is really popular in the Python world because it acts like a wrapper of more popular libraries. It might become hard to follow but Keras has multiple backends such as Tensorflow, Theano and MXNET. The *Keras* [2] is mostly use to link the wrapper tool with R. The most useful reference one can get for this workflow is written by two major players ; *Keras* creator and *RStudio* creator. It explains in detail the best practices in order to use *Keras* in R [4].

**Pros**

- Give a lot of flexibility since can basically be use to create all type of deep learning algorithms.
- Easy and fast prototyping
- Construct models exactly the same way as in python with a minimalist philosophy.
- Give the possibility to save everything on the workspace (model, training history, etc.)

**Cons**

- It is an encapsulation of a program inside a python environment.
- For some, it might be to high level and limit the customization.
- It can only work on top Tensorflow, CNTK and Theano backend.

**4.2.2 Tensorflow**

**Keywords:** FNN, CNN, RNN

**Description** This library was created by Google and written in *C++* and python. It is pretty well known in the python enviromnent. Recently, a R package was created to interface this popular library [3]. "TensorFlow" was originally developed by researchers and engineers working on the Google Brain Team within Google's Machine Intelligence research organization for the purposes of conducting machine learning and deep neural networks research."

**Pros**

- Well documented with a lot of tutorials online.
- Pre trained models accessible

**Cons**

- Struggles with poor results for speed.
- Not a trivial since it is consider a low-level coding

**4.2.3 MXNet**

**Keywords:** FNN, CNN, RNN

**Description** MXNet is a DL framework open source created by Apache. The framework is mostly backed by Intel, Microsoft and MIT. There is a manual[6] but itsn't part of the CRAN database.

**Pros**

- Allows the use of multiple CPU and multiple GPU, but it requires to download the package Rtools and a c++ compiler.
- Very easy to use and has a flexible implementation of diffenent neural networks architectures and models.
- The models can be built layer per layer.
- Provide details and information about the learning progress during the training phase.

**Cons**

- It has a smaller community compared to other popular framework.
- A package more use in the industrial projects and not so much in the research community.

**4.2.4 rTorch**

The rTorch CRAN package is to interface the popular open source machine learning library PyTorch[1]. The PyTorch was developed by Facebook AI Research lab (FAIR) and all the original features are available in rTorch.

**Description****Pros**

- Multiple pre-trained model available
- Simple and easy to use

**Cons**

- It is an encapsulation of a program inside a python environment.

### 4.2.5 H2o

**Description** H2o is a "scalable open source machine learning platform that offers parallelized implementations of many supervised, unsupervised and fully automatic machine learning algorithms on clusters". This package allows to run H2o via its REST API through R and offers several advantages such as the ability to know the computation time remaining when running a model.

```
dl_fit3 <- h2o.deeplearning(x = x,
  y = y,
  training_frame = train,
  model_id = "dl_fit3",
  epochs = 50,
  hidden = c(20,20),
  nfolds = 3,
  score_interval = 1,
  stopping_rounds = 5,
  stopping_metric = "misclassification",
  stopping_tolerance = 1e-3,
  seed = 1)
#used for early stopping
#used for early stopping
#used for early stopping
#used for early stopping
```

Figure 12: H2o package

#### Pros

- Very easy to use and includes a cross-validation feature and functions for grid search in order to optimize the model's hyperparameters.
- 
- Allows the use of multiple CPU.
- Provide an adaptive learning rate (ADADELTA) which improves the optimization process by having a different learning rate for each neuron.
- Provide details and information about the learning progress during the training phase.

#### Cons

- Requires the latest version of Java.

## 5 Examples

In order to give concrete deep learning examples, four resources were selected for tutorials; Keras using Tensorflow backend, H2O, rTorch and MXNET.

### 5.1 Keras

#### 5.1.1 Installation

First step, is the installation and download of the Keras files from GitHub :

```
devtools::install_github("rstudio/keras")
```

Then, we need to to install the package and import in the project :

```
library(keras)
install_keras()
```

When the *"Installation complete."* message appear you have a complete installation with CPU configure on the TensorFlow backend. If you want to take advantage of your GPU (Ensure that you have the hardware prerequisites) you will need to execute a different command as follows:

```
install_keras(tensorflow = "gpu")
```

### 5.1.2 FNN

### 5.1.3 CNN

### 5.1.4 RNN

## 5.2 H2O

### 5.2.1 Installation

```
install.packages("h2o")
library(h2o)
```

**Prerequisites to launch H2o**, 64 bit Java 6+ if you want to open a h2o model that s more than 1 GB.

### 5.2.2 FNN

### 5.2.3 CNN

### 5.2.4 RNN

## 5.3 rTorch

### 5.3.1 Installation

### 5.3.2 FNN

### 5.3.3 CNN

### 5.3.4 RNN

## 5.4 MXNET

### 5.4.1 Installation

### 5.4.2 FNN

### 5.4.3 CNN

### 5.4.4 RNN

## 6 Discussion

## References

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