Machine Learning II

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Introduction to Artificial Neural Networks

Berliner Hochschule für Technik

Contents

The terms *Artificial Neural Network* and *Deep Learning* are used by many interchangeably. There are small differences in the meanings, but we will not make a distinction in this course.

The course notes will use the term Artificial Neural Network with the abbreviation NN throughout.

James et al. has a Chapter called *Deep Learning* (Ch. 10), which is new to the second edition. This ML2 course doesn't follow the content in James, but there is significant overlap and the two are presented at the roughly same level of theory.

Neural Networks and Deep Learning are (probably) not new to you. Other parts of the Data Science programme concentrate more on practical aspects, constructing large NN configurations to maximise the prediction capabilities.

This course will instead concentrate on the basics and the theory behind neural networks. The subjects covered in the last five lectures of the course are:

Week No.

9) Introduction
10) Optimisation Methods
11) Mathematical and practical aspects of NNs
12) Time Series
    Christmas break
13) Image classification

Data Structure and notation

Artificial Neural Networks (NNs) can be used for both regression problems and classification problems. We'll start with *regression* because it is easier.

A data Matrix $\boldsymbol{X}$ has n rows (the elements or observations) and p columns (variables).

We conceptualise the NN as processing each observation (row) one after the other. For an arbitrary observation we will drop the row index and represent it as a p-dimensional vector $\boldsymbol{x}$.

The predicted value for the same arbitrary observation $\boldsymbol{x}$ is $f(\boldsymbol{x})$.

The outcome variable is $\boldsymbol{y}$ a vector of n observations. The observed outcome value for the arbitrary observation $\boldsymbol{x}$ is y.

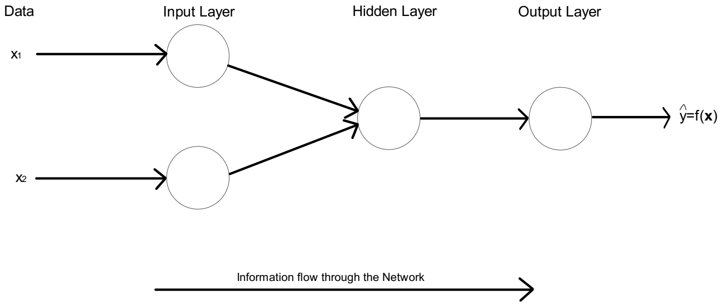
The *cost* or *loss* for one observation $\boldsymbol{x}$ is $R = (y - f(\boldsymbol{x}))^2$

When we consider all of the observations, the index $i = 1, \dots, n$ will be used.

First Neural Network

Each NN can be visualised using a network graph. A very simple NN for introductory purposes is:

Diagram 1



This NN has 3 **Layers**: an *input layer* which receives the data for observation $\boldsymbol{x}$, a *hidden layer* and an output layer whose output value is the predicted value $f(\boldsymbol{x})$, which hopefully is a value close to y.

There are two nodes in the input layer ($p{=}2$, i.e. two variables in the input data), just one node in the hidden layer and one node in the output layer.

- The hidden layer node receives a weighted sum of the data and a constant is added (called a bias).

$$z_1^{(1)} = w_{11}^{(1)} x_1 + w_{12}^{(1)} x_2 + b_1^{(1)}.$$

- This value is then transformed by a function $\sigma(\cdot)$.
- The hidden layer node outputs a value, which is called the *activation* of the node.

$$a_1^{(1)} = \sigma(z_1^{(1)}) = \sigma(w_{11}^{(1)} x_1 + w_{12}^{(1)} x_2 + b_1^{(1)})$$

- The output layer in this example receives activation from the hidden layer multiplies it by a weight $w_{11}^{(2)}$ and adds another bias.
  The result is then transformed using another function $g_1(\cdot)$:

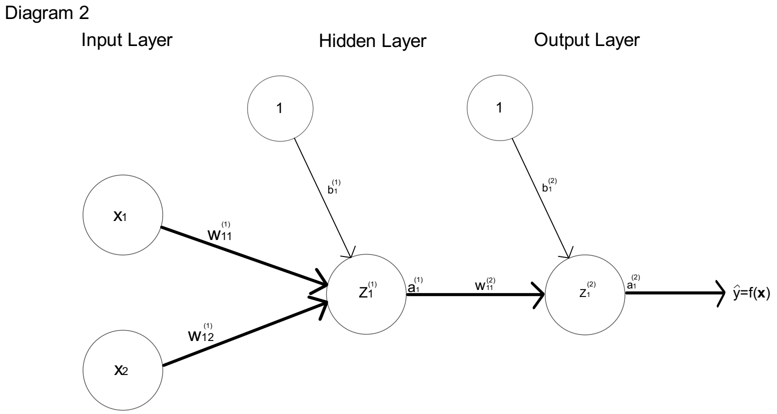
$$a_1^{(2)} = g_1(w_{11}^{(2)} a_1^{(1)} + b_1^{(2)}).$$

- The fitted/predicted value is the activation at the output layer.

$$f(\boldsymbol{x}) = a_1^{(2)}$$

- The superscript $^{(\cdot)}$ indicates which layer we are dealing with. The zero-th layer is the input layer. The last layer L is the output layer and all layers in between are hidden layers.

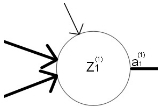
The NN can now be graphically represented with coefficients.

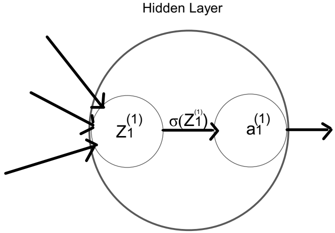


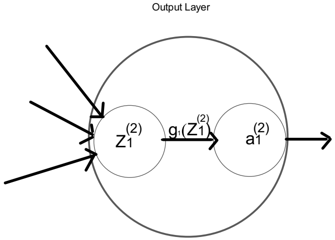
Note the order of the $w_{st}^{(\cdot)}$ weights, which corresponds to "from node t to node s". The reason for this ordering is that it keeps the notation for matrix multiplication simpler.

Each hidden and output layer node is represented as one circle, but carries out two transformations, which could be represented by two circles.

Diagram 3







$\sigma(\ )$ is the activation function

A common activation function $\sigma(\cdot)$ is the sigmoid or inverse logistic function

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

In early neural networks, the activation function was the so called *heaviside* function

$$\sigma(v) = \begin{cases} 1 & \text{for } v > 0 \\ 0 & \text{for } v \leqslant 0. \end{cases}$$

The node is “activated” if the combination of the inputs exceed the threshold zero. This is a simple model for how neurons in the brain function, hence the name artificial neural network.

For regression the identity function is often used as the output function

$$g_1(v) = v.$$

A simple numerical example

Let $x_1 = 4, x_2 = 7$ and $y = 4.1$.

The weights for the first node are $w_{11}^{(1)} = 0.1, w_{12}^{(1)} = 0.2$ and $b_1^{(1)} = 1.2$
The weights for the second node (output layer) are $w_{11}^{(2)} = 0.5$ and $b_1^{(2)} = 3.5$

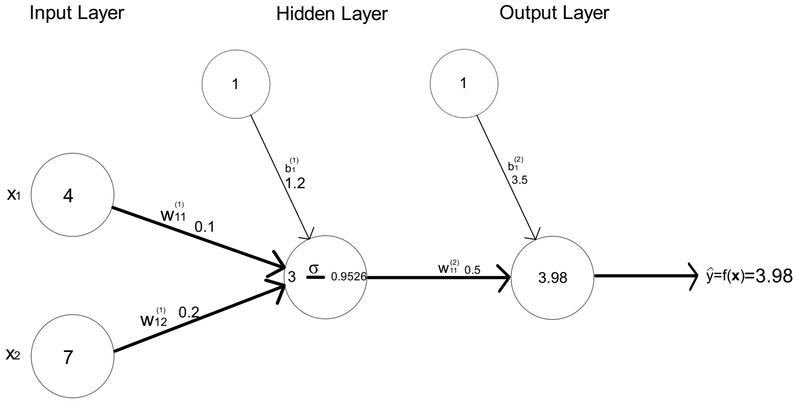
The activation function is the sigmoid function, and their output function is the identity function.

The weighted inputs are $z_1^{(1)} = 0.1 \times 4 + 0.2 \times 7 + 1.2 = 3.$
The activation of the hidden layer node is $a_1^{(1)} = \sigma(3) = \dfrac{1}{1 + e^{-3}} = 0.9526$

The output is then $a_1^{(2)} = g_1(0.5 \times 0.9526 + 3.5) = 3.976$

A simple numerical example:

Diagram 4



It is important to note that all the weights and biases are the parameters of the NN model.

These values are applied to *every observation* in the (training) data set.

If the second observation were $x_1 = 3, x_2 = -1$ and $y = 4.1$.
The above model for the second observation gives:

$$\begin{aligned} z_1^{(1)} &= 1.3. \\ a_1^{(1)} &= 0.7858 \\ a_1^{(2)} &= 3.892, \end{aligned}$$

so 3.892 is the second fitted value.

Fitting

As with all machine learning methods we need to fit or train the model to the data.
This is done in the usual way by minimising the loss function, which for NN-regression is the sum of squared errors SSE over the training set.

$$SSE = \sum_{i \in Tr} R_i = \sum_{i \in Tr} (y_i - f(\boldsymbol{x_i}))^2$$

Where *Tr* is the training data set.

The minimisation is done over all parameters $w_{11}^{(1)}$, $w_{12}^{(1)}$, $b_1^{(1)}$, $w_{11}^{(2)}$ and $b_1^{(2)}$.

Note that the number of nodes in each layer and the activation/output function are hyperparameters chosen by the user and are not part of the minimisation.

Training, validation and test data

Today we are only considering the most simple neural networks. In practice the the NN model can be extended in many ways e.g more nodes in the first hidden layer, more hidden layers, different choice of activation and output functions. The complexity of these models means that it is very easy to fit the data very well with the result that the prediction for future data is poor.

It is particularly important that the data are split into training and validation data sets. Very often we want a final assessment for the accuracy of model, in which case a test data set is needed as well.

The minimisation of the parameters $w_{11}^{(1)}$, $w_{12}^{(1)}$, $b_1^{(1)}$, $w_{11}^{(2)}$ and $b_1^{(2)}$ for a fixed model design is done using the training data.

If you want to make a choice about hyperparameters, such as how many nodes to fit in the first hidden layer, this is done by fitting each model on the training data, and choosing the hyperparameters that minimise the MSE of the **validation data**.

Reporting benchmark statistics (such as the accuracy rate of a classifier) or comparing different machine learning methods must be done using “clean data” i.e. the **test data**.

Note that if the data are only split into two data sets, then data on which the model is validated are often called the test data!

Scaling

Although not totally necessary, fitting a neural network is much faster if the data are scaled (also called normalised) first.

Each variable is scaled by subtracting that variable's *training data* mean and dividing by that variable's *training data* standard deviation.

There are two common methods of scaling.

The first is standardisation, i.e. mean & sd scaling: for variable x_j

$$x'_{ij} = \frac{x_{ij} - \overline{x}_j}{s_j} \qquad \text{with } \overline{x}_j = \frac{1}{|Tr|}\sum_{i \in Tr} x_{ij} \qquad \text{and } s_j = \frac{1}{|Tr| - 1}\sum_{i \in Tr}(x_{ij} - \overline{x}_j)^2$$

The second is normalisation to the intervall $[0, 1]$:

$$x'_{ij} = \frac{x_{ij} - \min\{x_j\}}{\max\{x_j\} - \min\{x_j\}}$$

The output variable (for regression) is also scaled using the same method.

When scaling or unscaling the validation/test data, you use the same min/max/mean/sd **as used on the training data**. You will get worse results if you do not do this.

We will usually assume the data x_{ij} has already been scaled and omit the '.

In the previous very simple example we already have 5 parameters to vary in order to minimise the SSE. This is a five dimensional **function minimisation** problem. We can use any function minimisation algorithm to search for the best values for the 5 parameters.

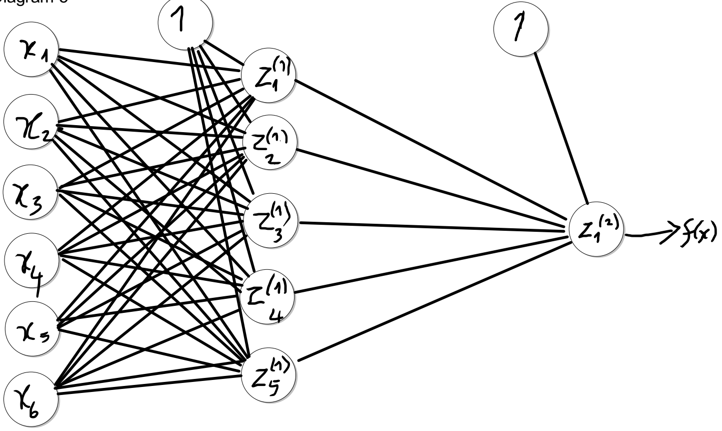
In this week's workshop, you will use a very simple minimisation routine so that you can learn the mathematical principles of the NN Model.

This minimisation routine converges very slowly.

Next week we will take a closer look at better minimisation algorithms. The "basic" algorithm for NNs is the steepest descent algorithm using *back propagation*. Recently other minimisation algorithms have been developed but most are based around speeding up the steepest descent/back propagation method.

There is never just one node in the hidden layer. Even with small data sets it is common to use $M = 5$ to 20 nodes.
Example and notation for one hidden layer with $M = 5$ units and $p = 6$.

Diagram 5



Each edge has a weight, and there is a bias for each Node in the first and second layer.
The general number of parameters (for a model with one hidden Layer) is

$$(p+1)M + (M+1) = (p+2)M + 1.$$

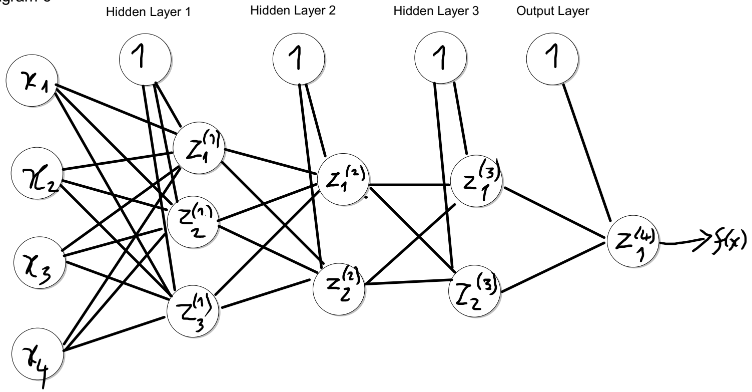
The network on the last slide has 41 edges. Each edge has a weight which needs to be optimised!

Fitting a neural network requires many settings to be tweaked. The aim is to find a combination which gives a good output, like being the sound engineer setting up a mixing desk before a concert!

Multiple hidden layers

Instead of adding more nodes to one hidden layer, we can add more hidden layers. Example: 3 hidden layers $L{=}4$, $M_1{=}3$ $M_2{=}2$,$M_3{=}2$ and $p{=}4$.

Diagram 6



The output layer

So far we have used one output node with:

$$a_1^{(L)} = g_1\left(\sum_{j=1}^{M_{L-1}} w_{1j}^{(L)} a_j^{(L-1)} + b_1^{(L)}\right).$$

The outcome variable can be multidimensional in which case there are as many output nodes as there are dimensions in y.

Example: if the outcome variable consists of the two standard blood pressure measurements, systolic and diastolic, then a NN predicting these outcomes requires two output nodes

$$a_1^{(L)} = g_1\left(\sum_{j=1}^{M_{L-1}} w_{1j}^{(L)} a_j^{(L-1)} + b_1^{(L)}\right) \text{ and } a_2^{(L)} = g_2\left(\sum_{j=1}^{M_{L-1}} w_{2j}^{(L)} a_j^{(L-1)} + b_2^{(L)}\right).$$

The predictor function is an $\mathbb{R}^p \to \mathbb{R}^2$ function $f(\boldsymbol{x}) = (a_1^{(L)}, a_2^{(L)})$.

Neural network classifiers

Classification NNs have the same configuration for the input and hidden layers, but the output layer takes account of the fact that the output variable takes one of K values.

Examples:

- Binary classifier ($K=2$), $y \in \{\text{Yes}, \text{No}\}$ usually internally coded as $\{0, 1\}$.
- $K=3$ classifier: Iris dataset.
- $K=10$ classifier: handwritten digits 0 to 9.
- $K=62$ classifier: handwritten upper case letters, lower case letters and digits 0 to 9.

In K-class classification there are K output nodes one for each class.

In NN-regression we used the identity function at the output layer.

For NN-classifiers the usual output function is the sigmoid function, so

$$g_k(v) = \sigma(v)$$

The activation of each output node is

$$a_k^{(L)} = \sigma\left(\sum_{j=1}^{M_{L-1}} w_{kj}^{(L)} a_j^{(L-1)} + b_1^{(L)}\right)$$

The activation is a number between 0 and 1.

The K activations are numbers between 0 and 1 but how do we obtain our prediction?

The answer depends on what we actually want.

The *predicted value* is the class number k with the largest activation value.

$$f(\boldsymbol{x}) = \arg\max_k \{a_k^{(L)}\}$$

If instead we want to predict the probabilities for each class $\pi_k(\boldsymbol{x})$, we need to standardise the activations, because they do not add up to one.

$$\pi_k(\boldsymbol{x}) = \frac{a_k^{(L)}}{\sum_{k=1}^{K} a_k^{(L)}}$$

Loss function for classification

To fit the NN classifier we minimise a loss function, comparing the K output values $a_k^{(L)}$ with the one observed value y.

To do this we redefine y as a K-dimensional binary vector.

Eg.
In the Iris dataset the 60th observation has species *versicolor* from the classes *setosa*, *versicolor* and *virginica*.

For a NN we redefine y_{60} as the 3-dim. binary vector $y_{60} = (0, 1, 0)$.

As with NN-regression, we can use the squared error loss for the loss in the i-th observation: $R_i = \sum_{k=1}^{K} (\pi_k(\boldsymbol{x}_i) - y_{ik})^2$

For classification the so called cross-entropy or deviance is used as the loss function more often than the squared error loss:

$$R_i = -\sum_{k=1}^{K} y_{ik} \log(\pi_k(\boldsymbol{x_i})).$$

By using the continuous values of $\pi_k(\cdot)$ rather than the binary predicted values, the loss function is continuous, making it much easier to minimise using numerical methods.

Workshop

We will use R-Code to create and optimise neural networks, both a regression NN and a classifier with $K=3$. The aim is to understand the mathematical aspects of the NN and the concept of minimising the loss function

A source file and simulated data sets are provided. The neural network is fitted using user defined R-functions called `NN`, `NN2` and `NN3`.

You will need to fill in some of the gaps in the code.

The minimising routine is explained in the worksheet. It is easy to code but the convergence is very slow. Nevertheless, the fit can be surprisingly good considering that only a very small NN is fitted.