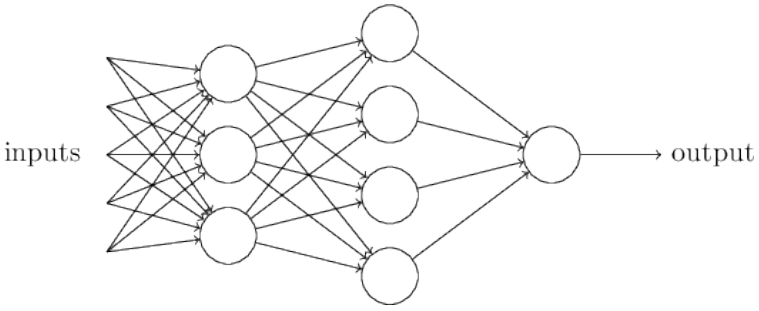
# 12 Artificial neural networks

**Artificial neural networks** (ANNs) are behind many of the "AI" successes reported in the media. **Deep learning** is to learn from data with multi-layer neural networks or deep neural networks (DNNs). It is a fast moving area, with new ideas and techniques invented every month. Some topics that are hot today may become out of fashion in 1-2 years.

We will use the online book *Neural Networks and Deep Learning* (http://neuralnetworksanddeeplearning.com) as the textbook. The original code is in Python 2.7; here is a version in Python 3.5

## 12.1 A simple feedforward neural network

The simplest neural network is a feedforward neural network (FFNN) with fully connected layers. An example is:




In this example, there are 5 input variables, $x_1, \cdots, x_5$ and an output variable, $y$, and there are two hidden layers between them. Often the input and the output are viewed as layers as well, and the above network is called a 4-layer neural network. The *nodes* are also called *neurons*. Every layer depends **only** on the previously layer. This feedforward nature allows the algorithm of backpropagation to work nicely.

In a **fully connected** layer like the figure above, every node depends on all the nodes in the previous layer, first as a linear combination of the output from the previous layer and then followed by a transformation. For example, node $i$ in layer 2 (the first hidden layer) has an input $z_i^{(2)}$ and an output $a_i^{(2)}$, where $z_i^{(2)} = \sum_{j=1}^5 w_{ij}^{(2)} x_j + b_i^{(2)}$, and

$$a_i^{(2)} = h_i^{(2)}(z_i^{(2)}) = h_i^{(2)} \left[ \sum_j w_{ij}^{(2)} x_j + b_i^{(2)} \right].$$

The parameters $w_{ij}^{(2)}$ and $b_i^{(2)}$ are called **weights** and **bias** in the NN literature. The function $h_i^{(2)}()$ is called an **activation function**. When $h(t) = I(t > 0)$, the node is also called a *perceptron*. When $h(t) = \sigma(t) = \frac{1}{1+e^{-t}} = \frac{e^t}{1+e^t}$, the *sigmoid function*, the node is called a *sigmoid neuron*. When the same activation function is used for all the nodes in a layer (which is often the case in practice), the layer is called a *perceptron layer* (when $h(t) = I(t > 0)$) or a *sigmoid layer* (when $h(t) = \sigma(t)$). This simple FFNN is sometimes called a **multilayer perceptron** (MLP) even if none of the nodes is a perceptron.

In the figure above, every node in layer 2 has 6 parameters (5 weights and 1 bias), every node in layer 3 has 4 parameters (3 weights and 1 bias), and output node in the final layer has 5 parameters (4 weights and 1 bias). Thus there are $3 \times 6 + 4 \times 4 + 1 \times 5 = 39$ parameters. If layers 2–4 are all sigmoid layers, the model is

$$\begin{aligned}
f(x_1, \ldots, x_5) &= \sigma \left[ w_1^{(4)} a_1^{(3)} + w_2^{(4)} a_2^{(3)} + w_3^{(4)} a_3^{(3)} + w_4^{(4)} a_4^{(3)} + b^{(4)} \right], \text{ where} \\
a_k^{(3)} &= \sigma \left[ w_{k1}^{(3)} a_1^{(2)} + w_{k2}^{(3)} a_2^{(2)} + w_{k3}^{(3)} a_3^{(2)} + b_k^{(3)} \right] \quad (k = 1, 2, 3, 4) \\
a_k^{(2)} &= \sigma \left[ w_{k1}^{(2)} x_1 + w_{k2}^{(2)} x_2 + w_{k3}^{(2)} x_3 + w_{k4}^{(2)} x_4 + w_{k5}^{(2)} x_5 + b_k^{(2)} \right] \quad (k = 1, 2, 3).
\end{aligned}$$

To fit the model, we estimate these 39 parameters under an optimization criterion (e.g., minimizing a total cost). The model can quickly become very complex with additional nodes or layers.

If the outcome is continuous, a commonly used cost function is the squared error loss, for which the total cost is $C = \sum_i (y_i - f(x_{i1}, \ldots, x_{ip}))^2$. We do not have a closed-form solution and have to rely on numerical algorithms to minimize $C$. When the sample size is large, it can be computationally expensive to use 2nd-order approximations such as the Newton–Raphson algorithm. In ANN, we often rely on the 1st-order approximation algorithm called the **gradient descent** or its stochastic version, the **stochastic gradient descent** (details below).

## 12.2 Tensorflow and Keras

A **tensor** is another name for an array. Arrays are a basic data type in programming. A matrix is effectively a 2-dimensional array. A vector is effectively a 1-dimensional array. A single number (sometimes called a *scalar*) is effectively a 0-dimentional array, although most computer languages do not treat a scalar as an array. All these can be viewed as tensors.

The **rank** of a tensor is the number of dimensions, and the **shape** of a tensor is the dimensions. For example, a rank 2 tensor with shape $[3, 5]$ is effectively a $3 \times 5$ matrix; a rank 0 tensor is a scalar and it has an empty shape; a rank 1 tensor with shape $[8]$ is effectively a vector of length 8. In TensorFlow we may see a rank 4 tensor with shape $[1, 1, 100, 1]$, which is just a vector of length 100 masqueraded as a 4-dimensional array. Below I use the `array()` function in R to show what arrays look like:

```
array(1:6, c(2,3))  ## same as matrix(1:6, c(2,3))
array(1:6, c(6))
array(1:18, c(2,3,3))
array(1:6, c(1,1,6,1))
```

In ANNs, operations can be formulated as a flow of tensors. For example, in the FFNN model above, the flow is from a tensor of length 5 to a tensor of length 3, and then to a tensor of length 4, and then to a tensor of length 1.

**TensorFlow** is a neural network package from Google. It has some competitors out there: **PyTorch** and **Caffe2** from Facebook, **MXNet** from Amazon, **CNTK** from Microsoft, **H2O**, etc.

**Keras** is a front end for TensorFlow. It uses simpler syntax when fitting standard neural network models. It is available in Python and R (https://keras.rstudio.com/). To install the Python version in Anaconda, use `conda install keras`. The installation of the R version has two steps:

```
install.packages("keras")      ## install a few necessary R packages first
keras::install_keras("conda")  ## install necessary conda/tensorflow packages outside R
```

Notes: (1) The second step is not needed if you have installed TF packages in anaconda. (2) If you use the second step, `install_keras("conda")`, it first installs a few necessary conda packages, then creates a conda environment and installs TF packages into the environment. In Windows, Anaconda 3.x is required. (3) When Keras is loaded with `library(keras)`, by default the backend is "tensorflow" and the implementation is "keras". Use `use_backend()` and `use_implementation()` to change them if needed. All backend API functions have a `k_` prefix. In Linux, the configuration file is `$HOME/.keras/keras.json`, and all example datasets downloaded with `datasets_*()` are in `$HOME/.keras/datasets/`.

We now define the model in the last section. The order of the statements is very important. Note the use of pipes with `%>%`. The function `layer_dense()` is to specify a fully-connected layer.

```
library(keras)

model = keras_model_sequential()    ## initialize the keras model object
model %>%                           ## define the layers
  layer_dense(units=3, activation="sigmoid", input_shape=c(5)) %>%
  layer_dense(units=4, activation="sigmoid") %>%
  layer_dense(units=1, activation="sigmoid")

summary(model)                    ## summary of model structure
```

The equivalent Python code is

```
from keras.models import Sequential
from keras.layers import Dense, Dropout

model = Sequential()
model.add(Dense(3, activation='sigmoid', input_shape=(5,)))
model.add(Dense(4, activation='sigmoid'))
model.add(Dense(1, activation='sigmoid'))
model.summary()
```

## 12.3 Commonly used activation functions

**Sigmoid**: $\sigma(x) = (1 + e^{-x})^{-1} \in (0, 1)$

- $\sigma'(x) = \sigma(x)(1 - \sigma(x))$. It was a popular choice a few years ago.

**Hyperbolic tangent**: $\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1} = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(2x) - 1 \in (-1, 1)$

- $\tanh'(x) = (1 + \tanh(x))(1 - \tanh(x))$.

**ReLU** (rectified linear unit): $h(x) = x_+ = \max\{0, x\}$

- It is a popular choice nowadays.

**Leaky ReLU**: $h(x) = x_+ + ax_-$, where $x_- = \min\{0, x\}$ and $a > 0$ but $a$ very close to zero

**Perceptron**: $h(x) = I(x \geq 0) \in \{0, 1\}$

**Identity**: $h(x) = x$. The corresponding neuron is called a *linear neuron*.

A **softmax layer** is often used for the output layer when the outcome is multinomial. For example, for the MNIST dataset, the output has $K = 10$ categories. The activation function for the output layer is a softmax function

$$(z_1, \cdots, z_K) \to (a_1, \ldots, a_K) = \left( \frac{\exp(z_1)}{\sum_k \exp(z_k)}, \cdots, \frac{\exp(z_K)}{\sum_k \exp(z_k)} \right),$$

where $(z_1, \cdots, z_K)$ are the input to the $K$ nodes and they are linear combinations of the output from the previous layer. This definition ensures that final output $(a_1, \ldots, a_K)$ is a multinomial probability distribution with $\sum_k a_k = 1$.

## 12.4 Commonly used cost functions

Ideally, the cost function should be chosen to reflect the real cost. But often a mathematically convenient cost is chosen. For example, for MNIST data, classification accuracy is the ultimate goal, but often the softmax output layer coupled with the negative log-likelihood cost is used to avoid slow learning at the output layer. It is possible that while the cost for the training set is being driven down, the cost for the test data can be ascending but the test data classification accuracy is being improved (an example in NNDL Chapter 3).

**Quadratic cost** (squared error): $C(y, a) = \frac{1}{2}\|y - a\|^2$; $\nabla_a C = \frac{\partial C}{\partial a} = a - y$

**Negative log-likelihood**: $-\ln L$.

**Cross-entropy** for $0 \leq y \leq 1$: $C(y, a) = -[y \ln a + (1 - y)\ln(1 - a)]$ with $a \in (0, 1)$; $\nabla_a C = \frac{a-y}{a(1-a)}$. In back-propagation, if $H = \sigma$, then $\delta^L = a^L - y$.

**Cross-entropy** for multinomial $y$ (a vector with one element 1 and others 0): $C(y, a) = -\ln(y'a)$, where $a$ is a multinomial probability distribution. This is negative multinomial log-likelihood.

**Total cost**: $C = \frac{1}{n}\sum_i C(y_i, a_i)$, where $y_i$ is the outcome for observation $i$ and $a_i$ is a predicted value given $x_i$.