# Lecture 35 - Multi-Layer Perceptron and Backpropagation

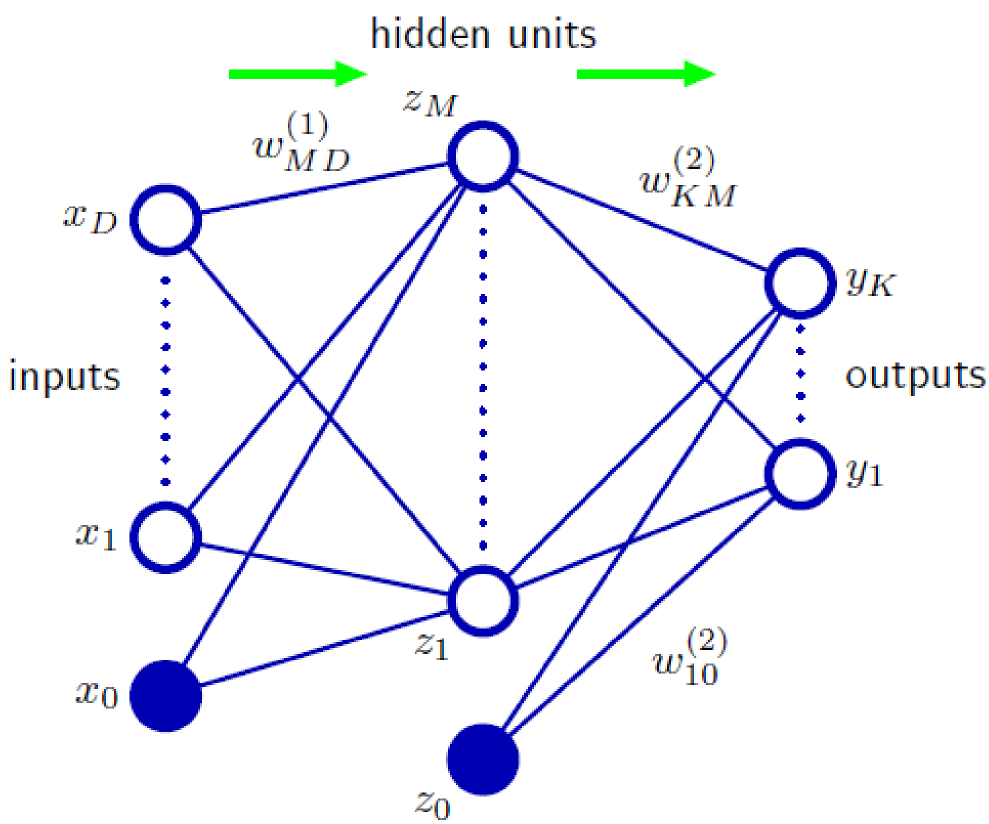
# Multi-Layer Perceptron (MLP)

A multilayer perceptron (MLP) is a class of feed-forward artificial neural network (ANN). An MLP consists of at least three layers of nodes. Except for the input nodes, each node is a neuron that uses an activation function (either linear or non-linear).

Its multiple layers and non-linear activation distinguish MLP from a linear perceptron. It can distinguish data that is not linearly separable.

In [1]:
```
from IPython.display import Image
Image('figures/mlp2.png',width=500)
```

Out[1]:




In MLPs, each neuron's output can be subject to different activation functions. The choice of the activation function is in itself a *free-parameter*.

- Which activation function would you use if you desired labels are $\{1,2,3,4,\dots,8,9\}$?
- *What each of the layers do?*
  - The first hidden layer draws boundaries
  - The second hidden layer combines the boundaries

- The third and further layers can generate arbitrarily complex shapes

# Universal Approximation Theorem

"The *Universal Approximation Theorem* states that a feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of $\mathbb{R}^N$, under mild assumptions on the activation function. The theorem thus states that simple neural networks can represent a wide variety of interesting functions when given appropriate parameters; however, it does not touch upon the algorithmic learnability of those parameters."

Let $\phi(\cdot)$ be a non-constant, bounded and monotonic-increasing continuous function. Let $I_{m_0}$ denote the $m_0$-dimensional unit hypercube $[0,1]^{m_0}$. The space of continuous functions on $I_{m_0}$ is denoted by $C(I_{m_0})$. Then, given any function $f \ni C(I_{m_0})$ and $\epsilon > 0$, there exists an integer $m_1$ and sets of real constants $\alpha_i, \beta_i$, and $w_{ij}$, where $i = 1, \ldots, m_1$ and $j = 1, \ldots, m_0$ such that we may define

$$F(x_1, \ldots, x_{m_0}) = \sum_{i=1}^{m_1} \alpha_i \phi\left(\sum_{j=1}^{m_0} w_{ij} x_j + b_i\right)$$

as an approximation realization of the function $f(\cdot)$, that is,

$$|F(x_1, \ldots, x_{m_0}) - f(x_1, \ldots, x_{m_0})| < \epsilon$$

for all $x_1, x_2, \ldots, x_{m_0}$ that like in the input space.

Essentially, the Universal Approximation Theorem states that a single hidden layer is sufficient for a multilayer perceptron to compute a uniform $\epsilon$ approximation to a given training set - provided you have the *right* number of neurons and the *right* activation function.

- However, this does not say that a single hidden layer is optimal with regards to learning time, generalization, etc.)
- In other words, a **feed-forward MLP with one hidden layer can approximate arbitrarily closely any function**.

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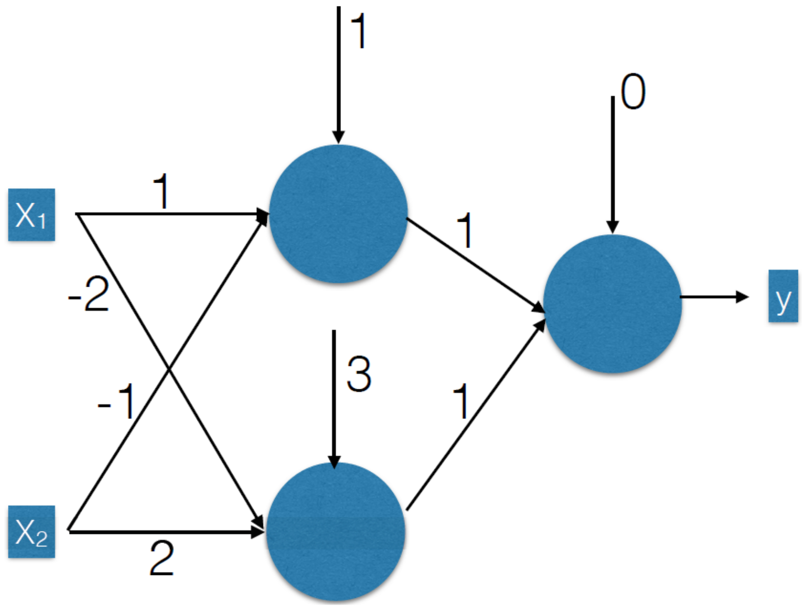
## Exercise

Suppose you had the following neural network:

In [2]:

```
Image('figures/MLP.png',width=400)
```

Out[2]:




with the activation function:

$$\phi(x) = \begin{cases} 1 & x > 0 \\ -1 & x \leq 0 \end{cases}$$

1. What is the expression of the output value $y$ in terms of the input values?

2. What is the output with the following input values?

   - $[0, 0]$
   - $[-2, -2.5]$
   - $[-5, 5]$
   - $[10, 3]$
3. What does the decision surface of this network look like graphically? Draw it out by hand.

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# Error Backpropagation

- The learning procedure involves the presentation of a set of pairs of input and output patterns, $X = \{x_i\}_{i=1}^N$ and $Y = \{y_j\}_{j=1}^M$. The system uses the input vector to produce its own output vector and then compares this with the \emph{desire output}, or \emph{target output} $t = \{t_j\}_{j=1}^M$. If there is no difference, no learning takes place. Otherwise, the weights are changed to reduce the difference. This procedure is basically the perceptron learning algorithm.

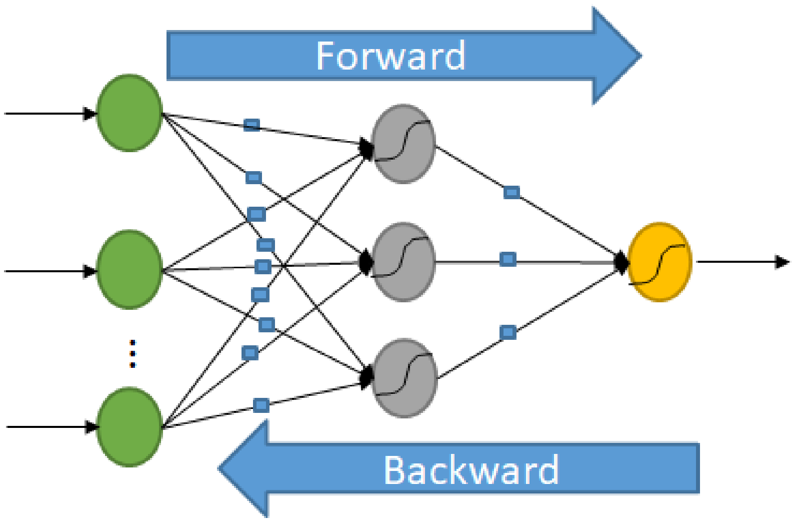
- This procedure can be *automated* by the machine itself, without any outside help, if we provide some **feedback** to the machine on how it is doing. The feedback comes in the form of the definition of an *error criterion* or *objective function* that must be *minimized* (e.g. Mean Squared Error). For each training pattern we can define an error ($\epsilon_k$) between the desired response ($d_k$) and the actual output ($y_k$). Note that when the error is zero, the machine output is equal to the desired response. This learning mechanism is called **(error) backpropagation** (or **BP**).

- The backpropagation algorithm consists of two phases:

    - **Forward phase:** computes the *functional signal*, feed-forward propagation of input pattern signals through the network.
        - **Backward phase:** computes the *error signal*, propagates the error backwards through the network starting at the output units (where the error is the difference between desired and predicted output values).

In [3]:
```
Image('figures/ForwardBackward.png',width=400)
```

Out[3]:




- **Objective function/Error Criterion:** there are many possible definitions of the error, but commonly in neuro-computing one uses the error variance (or power):

$$J(w) = \frac{1}{2}\sum_{k=1}^{N}\epsilon^2 = \frac{1}{2}\sum_{k=1}^{N}(d_k - y_k)^2 = \frac{1}{2}\sum_{k=1}^{N}(d_k - w^T x_k)^2$$

- Now we need to define an **adaptive learning** algorithm. Backpropagation commonly uses the gradient descent as the adaptive learning algorithm.

- **Adaptive Learning Algorithm:** there are many learning algorithms, the most common is the method of Gradient/Steepest Descent.

    - Move in direction opposite to the gradient, $\nabla J(\mathbf{w})$, vector (**gradient descent**):

$$w^{(n+1)} = w^{(n)} + \Delta w^{(n)}$$

This is known as the **error correction rule**. We define:

$$\Delta w^{(n)} = w^{(n)} - w^{(n-1)}$$
$$\Delta w^{(n)} = -\eta \nabla J(w^{(n)})$$

where $\eta$ is the learning rate.

## Backpropagation of the Error for the Output Layer

There are many approaches to train a neural network. One of the most commonly used is the **Error Backpropagation Algorithm**.

Let's first consider the output layer:

- Given a training set, $\{x_n, d_n\}_{n=1}^N$, we want to find the parameters of our network that minimizes the squared error:

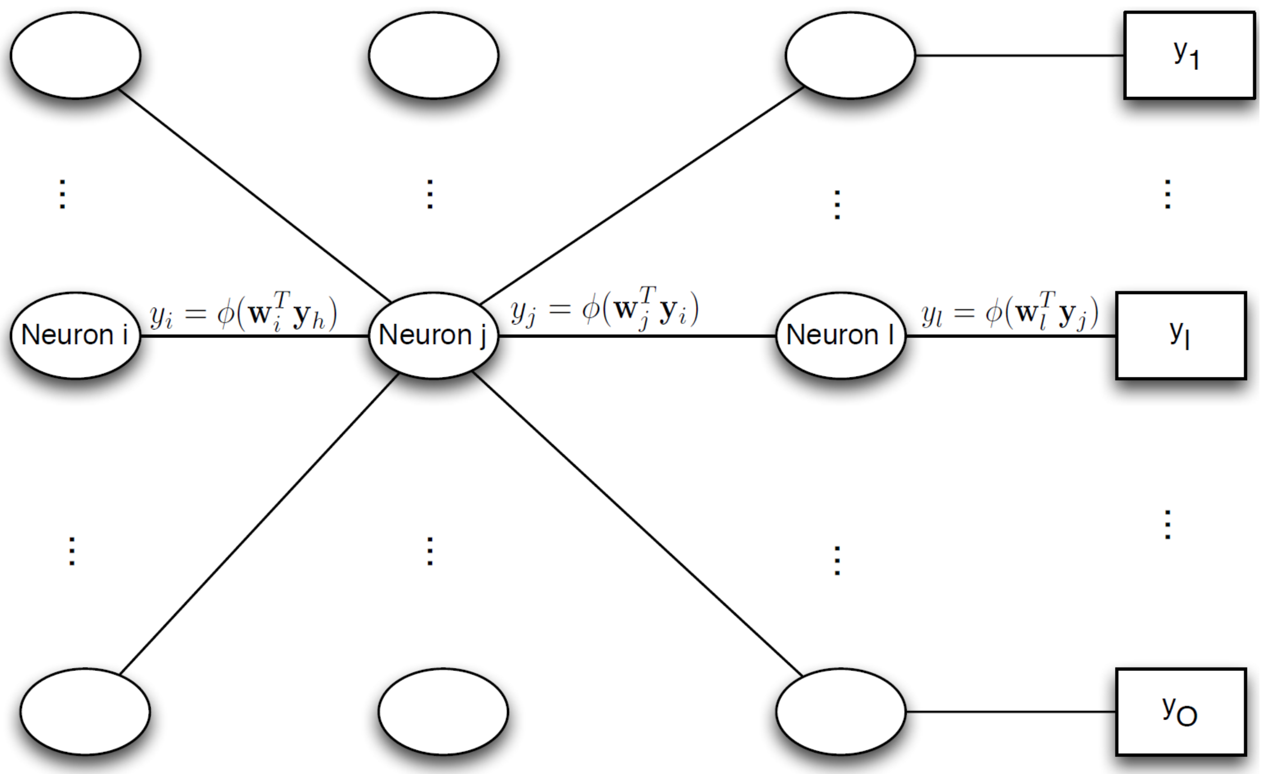
$$J(w) = \frac{1}{2}\sum_{l=1}^{N}(d_l - y_l)^2$$

- In order to use gradient descent, we need to compute the analytic form of the gradient, $\frac{\partial J}{\partial w_{lj}}$.

In [3]:

```
Image('figures/HiddenLayer.png',width=700)
```

Out[3]:




**Chain Rule** Given a labelled training set, $\{x_n, d_n\}_{n=1}^N$, consider the objetive function

$$J(w) = \frac{1}{2}\sum_{l=1}^{N} e_l^2$$

where $w$ are the parameters to be estimated and $\forall l$:

$$\begin{aligned} e_l &= d_l - y_l \\ y_l &= \phi(v_l), \phi(\bullet) \text{ is an activation function} \\ v_l &= w^T x_j \text{ (note that } x_j \in \mathbb{R}^{D+1}) \end{aligned}$$

Using the Chain Rule, we find:

$$\frac{\partial J}{\partial w_{lj}} = \frac{\partial J}{\partial e_l}\frac{\partial e_l}{\partial y_l}\frac{\partial y_l}{\partial v_l}\frac{\partial v_l}{\partial w_{lj}}$$

where

$$\frac{\partial J}{\partial e_l} = \frac{1}{2}2e_l = e_l = d_l - y_l$$

$$\frac{\partial e_l}{\partial y_l} = -1$$

$$\frac{\partial y_l}{\partial v_l} = \frac{\partial \phi(v_l)}{\partial v_l} = \phi'(v_l)$$

$$\frac{\partial v_l}{\partial w_{lj}} = x_j$$

Therefore

$$\frac{\partial J}{\partial w_{lj}} = e_l(-1)\phi'(v_l)x_j$$

- If activation function is the sigmoid, $\phi(x) = \frac{1}{1+e^{-x}}$, then $\phi'(x) = \phi(x)(1-\phi(x))$
- If activation function is the hyperbolic tangent (tanh), $\phi(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$, then $\phi'(x) = 1 - \phi(x)^2$
- If activation function is the ReLU, $\phi(x) = \begin{cases} 0, & x \leq 0 \\ x, & x > 0 \end{cases}$, then $\phi'(x) = \begin{cases} 0, & x \leq 0 \\ 1, & x > 0 \end{cases}$

Now that we have the gradient, how do we use this to update the output layer weights in our MLP?

$$w_{lj}^{(t+1)} = w_{lj}^{(t)} - \eta\frac{\partial J}{\partial w_{lj}} = w_{lj}^{(t)} + \eta e_i \phi'(v_l)x_j$$

- How will this update equation (for the output layer) change if the network is a multilayer perceptron with hidden units?
- Can you write this in vector form to update all weights simultaneously?
- Next, the hidden layers...

## Recommended Reading

"Learning representations by back-propagating errors" by David E. Rumelhart, Geoffrey E. Hinton, and Ronald J. Williams. Nature 323 (6088): 533–536, 8, October 1986.