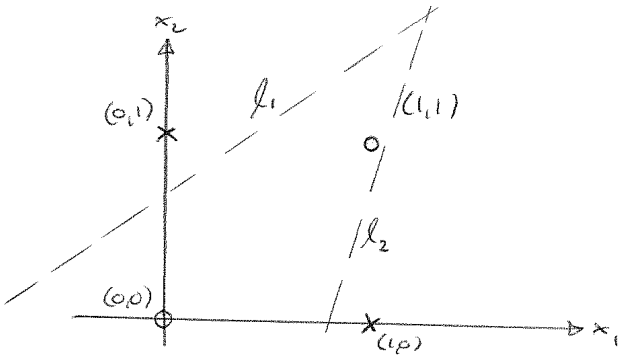
COMS 4030A

Adaptive Computation and Machine Learning

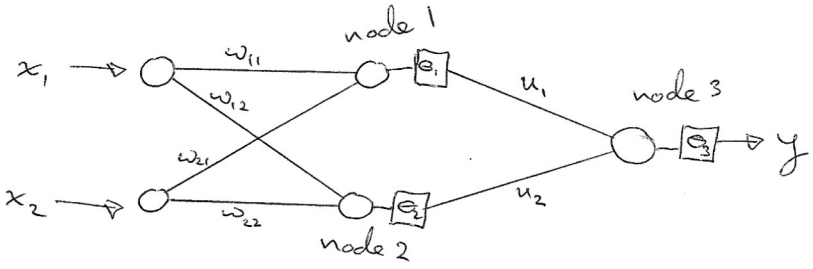
2. Neural Networks

2.1. **Multi-Layer Perceptrons.**

The dataset $D = \{((0,0),0),((0,1),1),((1,0),1),((1,1),0)\}$ is not linearly separable, i.e., it is impossible to draw a straight line in $\mathbb{R}^2$ so that all the 1's are on one side of the line and all the 0's are on the other. However, it is possible to separate the dataset using **two** straight lines, as shown below, where a $\circ$ represents a target of 0 and a $\times$ represents a target of 1.



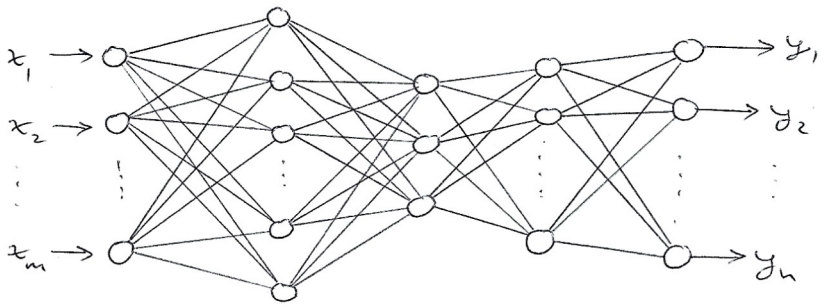
If a point lies above line ℓ_1 and above line ℓ_2 then it is a $\times$. If it lies below ℓ_1 and above ℓ_2 then it is a $\circ$; and if it lies below line ℓ_1 and below line ℓ_2 then it is a $\times$.
We can use a 2-layer perceptron to model the separation by two straight lines as follows:



We shall often use the word **node** in place of artificial neuron.
In the above figure, node 1 represents line ℓ_1, node 2 represent line ℓ_2 and node 3 decides in which region the point lies, for example, above ℓ_1 and above ℓ_2, or below ℓ_1 and above ℓ_2, etc.

EXERCISE: Try to find suitable values for w_{11}, w_{12}, w_{21}, w_{22}, u_1, u_2, θ_1, θ_2 and θ_3 so that the above 2-layer perceptron correctly outputs the data in D.

By a **multilayer perceptron** we mean a network with an input layer followed by number of layers of nodes followed by an output layer, as shown below.
Every edge has a real number **weight** assigned to it and every node has its own threshold value.



Training a multilayer perceptron with 2 layers is far more complicated than a simple perceptron as we need to 'move' the straight lines into correct positions and at the same time learn the weights on the second layer that control the regions defined by the straight lines. If there are more layers then it becomes even more complicated.

We are going to use a learning rule based on the gradient descent method, which is an optimisation technique that makes use of the derivative of a function with respect to its variables. Note that a multilayer perceptron is a function from $\mathbb{R}^m$ to $\mathbb{R}^n$. If the weights and thresholds are considered as variables in this function, then they are adaptable as in the case of a perceptron.

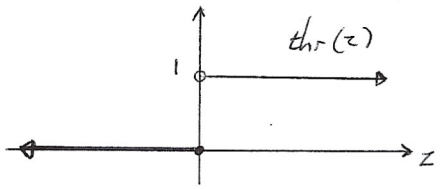
A difficulty for applying gradient descent in multilayer perceptrons is the use of 'thresholding' because this has derivative 0 and so the gradient descent method is of no use. For this reason, we will replace the threshold function with other activation functions, as discussed below.

2.2. **Activation functions.**

The thresholding function in perceptrons can be rewritten in the following way.
Instead of comparing $\sum_i x_i w_i$ with a threshold value θ, we first compute $\sum_i x_i w_i - \theta$ and then compare the result with 0. That is, we apply a **threshold** function thr, defined by:

$$thr(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{if } z \leq 0 \end{cases}$$

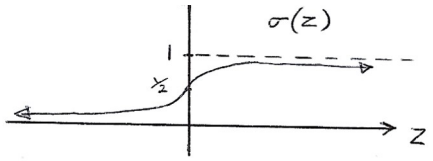
The graph of *thr* is shown below; as you can see its derivative is zero everywhere (except at $z = 0$, where it is not differentiable):



A way around the zero derivative problem is to replace *thr* with the following **sigmoid** function (sometimes called **logistic sigmoid**):

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

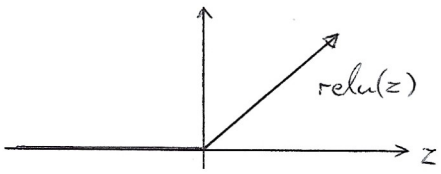
The sigmoid function is a continuous approximation to *thr*; the graph of $\sigma(z)$ looks like:



Another commonly used function is *relu*, or **rectified linear unit**, which is defined as:

$$relu(z) = \begin{cases} z & \text{if } z > 0 \\ 0 & \text{if } z \leq 0 \end{cases}$$

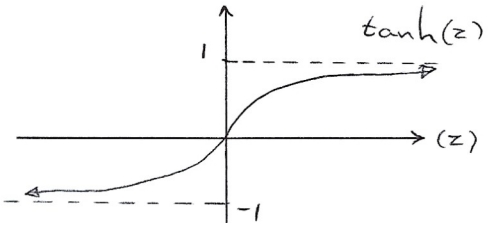
The *relu* function is also a variation of the *thr* function; the graph of *relu* looks like:



A function which is often used if you want your output scaled between -1 and 1 is the *tanh* function, or **hyperbolic tangent**, defined by:

$$tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

The graph of $tanh(z)$ looks like:



Sometimes the **linear** function *lin* is used, which is just the identity function: $lin(z) = z$.

We use the term **activation function** for functions like σ, *relu*, *tanh* and *lin*.
We use the symbol g to represent an arbitrary activation function.
The above activation functions are not the only possible ones. There are variants of the above functions which are often used, as well as completely different types of activation function.

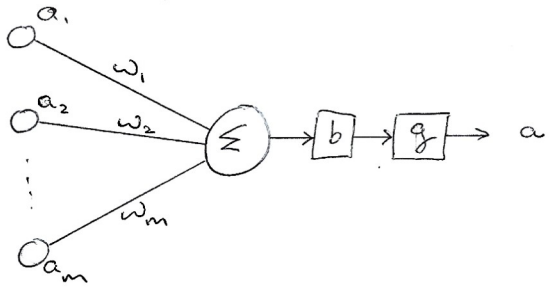
2.3. **Activation value of a node.**

We describe here the new structure of nodes, or artificial neurons, and how to compute the activation value of a node.

Every node has a **bias** value b (where b can be positive or negative).
The bias replaces the $-\theta$ term in the expression $\sum_i x_i w_i - \theta$.
b plays a similar role to θ, but we prefer to work with $+b$ rather than $-\theta$.

Every node has an **activation function**, say g.
Usually, g is one of the following: σ, *relu*, *tanh* or *lin*.

At every node, the **activation value** at that node is computed as follows.
Consider all nodes that have an edge connecting to this node. Let $a_1, \ldots, a_m$ be the activation values at those nodes (or input values of they are input nodes), and let $w_1, \ldots, w_m$ be the weights of the corresponding edges, as in the figure below.



The **activation value**, or output, of the node is calculated as follows

1) calculate the following sum: $\sum a_i w_i$

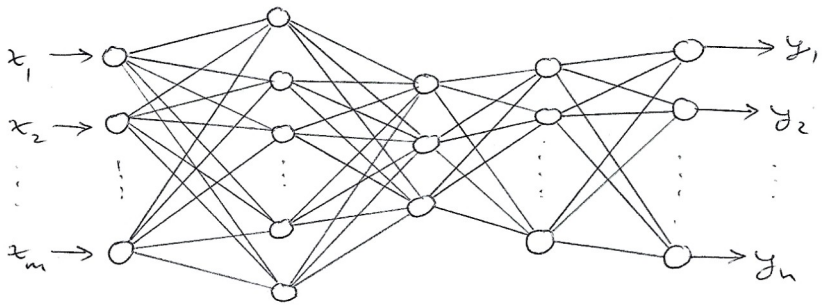
2) add the **bias** value of the node: $\sum a_i w_i + b$

3) apply the **activation function**: $g\left(\sum a_i w_i + b\right)$.

The activation value of the node is then $a = g\left(\sum a_i w_i + b\right)$.

2.4. **Neural Networks.**

An (artificial) **neural network** is network consisting of nodes and edges; the nodes are usually organised into layers with edges connecting nodes in consecutive layers, as shown below. The first layer is called the input layer, which is followed by a number of layers of nodes, with the last layer called the output layer.

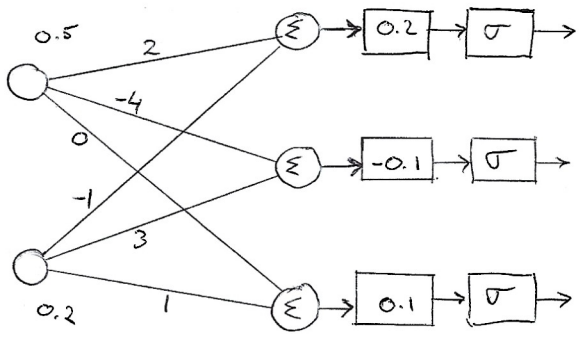


The middle layers are usually called **hidden layers**.
Every edge has a real number **weight** assigned to it.
Every node has its own **bias value** and **activation function**. Usually, all the nodes within a given layer use the same activation function; however, different layers can use different activation functions.
In the above figure, every node in a layer has an edge to every node in the next layer – in such a case, we say that the neural network is **fully connected**.

The weights of the edges between one layer and the next are usually represented by a matrix and the bias values of the nodes in a layer are represented by a list.

Example: In this example we show how the activation values of a layer of nodes in a neural network are computed. The following figure represents two consecutive layers within a neural

network. The weights of each edge are shown in the figure and the bias values of nodes in the second layer are shown in the square boxes. The activation value at each node is the sigmoid function σ. Suppose that 0.5 and 0.2 are the activation values of the two nodes in the left layer.



The activation values at the three nodes in the second layer are obtained as follows:
(Node 1 is the top node in the figure and node 3 is the bottom node.)
node 1: $(0.5)(2) + (0.2)(-1) = 0.8 \ \rightarrow$ (add bias) $0.8 + 0.2 = 1 \ \rightarrow \ \sigma(1) = 0.731$
node 2: $(0.5)(-4)+(0.2)(3) = -1.4 \ \rightarrow$ (add bias) $-1.4+(-0.1) = -1.5 \ \rightarrow \ \sigma(-1.5) = 0.182$
node 3: $(0.5)(0) + (0.2)(1) = 0.2 \ \rightarrow$ (add bias) $0.2 + 0.1 = 0.3 \ \rightarrow \ \sigma(0.3) = 0.574$
Thus, the activation values at the three nodes are given by $(0.731, 0.182, 0.574)$.

Next, we show how to compute the same activation values if we represent the weights by a matrix. Set

$$W = \begin{bmatrix} 2 & -4 & 0 \\ -1 & 3 & 1 \end{bmatrix}.$$

Then W contains all the weights of the edges between the two layers in the figure above. Using the notation $W = [w_{ij}]$, the entry w_{ij} is the weight of the edge between node i in the left layer and node j in the right layer.
We can write the bias values as $\boldsymbol{b} = (0.2, -0.1, 0.1)$.
If we write the activation values of the nodes in the left layer as $\boldsymbol{a} = (0.5, 0.2)$, then the activation values at the right layer are computed as follows:

$$\boldsymbol{a}W = (0.5, 0.2) \begin{bmatrix} 2 & -4 & 0 \\ -1 & 3 & 1 \end{bmatrix} = (0.8, -1.4, 0.2).$$

Next, add the bias:

$$\boldsymbol{a}W + \boldsymbol{b} = (0.8, -1.4, 0.2) + (0.2, -0.1, 0.1) = (1, -1.5, 0.3).$$

Lastly, apply the activation function:

$$\sigma(\boldsymbol{a}W + \boldsymbol{b}) = \sigma(1, -1.5, 0.3) = (\sigma(1), \sigma(-1.5), \sigma(0.3)) = (0.731, 0.182, 0.574).$$

2.5. **Feedforward Step.**

Given a neural network and a list of input values to the network, we can compute the corresponding list of output values. This computation is called the **feedforward step**, or **forward propagation**. The computation proceeds layer-by-layer.

We refer to the input layer as layer 0 and denote the list of input values by $\boldsymbol{a}_0$.
Let W_1 be the matrix of edge weights between the input nodes and the first hidden layer, i.e., layer 1, let $\boldsymbol{b}_1$ be the list of bias values of the nodes in layer 1, and let g_1 be the activation function at layer 1. Then the activation values at layer 1 are computed as follows.
First, we multiply $\boldsymbol{a}_0$ with the matrix of weights W_1, then add the bias values $\boldsymbol{b}_1$, and then apply the activation function g_1 to obtain the activation values at layer 1, which we call $\boldsymbol{a}_1$:

$$\boldsymbol{a}_0 \longrightarrow \boldsymbol{a}_0W_1 \longrightarrow \boldsymbol{a}_0W_1 + \boldsymbol{b}_1 \longrightarrow g_1(\boldsymbol{a}_0W_1 + \boldsymbol{b}_1) = \boldsymbol{a}_1$$

The values in $\boldsymbol{a}_1$ are the input into the next layer and the pattern repeats with the next layer's weights, biases and activation function. The general pattern is as follows.
Let W_k be the matrix of weights between layer $k-1$ and layer k, let $\boldsymbol{b}_k$ be the list of bias values at layer k, and g_k the activation function at layer k. If $\boldsymbol{a}_{k-1}$ are the activation values at layer $k-1$, then the activation values at layer k, that is $\boldsymbol{a}_k$, are calculated as follows:

$$\boldsymbol{a}_{k-1} \longrightarrow \boldsymbol{a}_{k-1}W_k \longrightarrow \boldsymbol{a}_{k-1}W_k + \boldsymbol{b}_k \longrightarrow g_k(\boldsymbol{a}_{k-1}W_k + \boldsymbol{b}_k) = \boldsymbol{a}_k$$

The list of activation values at the final layer is the output of the network.

Example: Consider a neural network with two input nodes, one hidden layer with 3 nodes and 2 output nodes, that uses the sigmoid activation function σ at each node (so $g_1 = \sigma$ and $g_2 = \sigma$). Let the weights between the input layer and the hidden layer (layer 1) be given by W_1 and let the bias values at layer 1 be given by $\boldsymbol{b}_1$:

$$W_1 = \begin{bmatrix} 2 & 1 & -1 \\ -2 & -4 & 1 \end{bmatrix}, \quad \boldsymbol{b}_1 = (1, -1, 2).$$

Let the weights between the hidden layer and the output layer (layer 2) be given by W_2 and the bias values at the output layer (layer 2) be given by $\boldsymbol{b}_2$:

$$W_2 = \begin{bmatrix} -2 & 3 \\ 3 & -1 \\ 5 & 0 \end{bmatrix}, \quad \boldsymbol{b}_2 = (0, -1).$$

Suppose the input $(2, 1)$ is fed into the network.

The output of the network is calculated as follows.

Set $\boldsymbol{a}_0 = (2, 1)$ and calculate:

$$\boldsymbol{a}_0 W_1 = (2, 1) \begin{bmatrix} 2 & 1 & -1 \\ -2 & -4 & 1 \end{bmatrix} = (2, -2, -1).$$

Then add the bias values in $\boldsymbol{b}_1$:

$$(2, -2, -1) + (1, -1, 2) = (3, -3, 1).$$

Then apply the activation function g_1 to get:

$$g_1(3, -3, 1) = \sigma(3, -3, 1) = (\sigma(3), \sigma(-3), \sigma(1)) = (0.953, 0.047, 0.731).$$

Thus, $\boldsymbol{a}_1 = (0.953, 0.047, 0.731)$ is the list of activation values at layer 1, which forms the input into layer 2. To get the activation values at layer 2, first compute:

$$\boldsymbol{a}_1 W_2 = (0.953, 0.047, 0.731) \begin{bmatrix} -2 & 3 \\ 3 & -1 \\ 5 & 0 \end{bmatrix} = (1.89, 2.812).$$

Then add the bias values in $\boldsymbol{b}_2$:

$$(1.89, 2.812) + (0, -1) = (1.89, 1.812).$$

Then apply the activation function g_2 to get:

$$g_2(1.89, 1.812) = \sigma(1.89, 1.812) = (\sigma(1.89), \sigma(1.812)) = (0.869, 0.860).$$

Thus, if $(2, 1)$ is input into the network, then the output obtained is $(0.869, 0.860)$.

EXERCISES

(1) Consider a network with 4 input nodes, one hidden layer with 4 nodes and 2 output nodes. The weights between layer 0 and layer 1, and the biases at layer 1 are given by:

$$W_1 = \begin{bmatrix} 4 & -5 & 0 & 1 \\ -3 & 6 & -1 & 2 \\ 0 & 1 & 1 & -2 \\ 2 & 0 & -3 & 4 \end{bmatrix}, \qquad \boldsymbol{b}_1 = (1, -2, 0, -1).$$

The weights between layer 1 and layer 2, and the biases at layer 2 are given by:

$$W_2 = \begin{bmatrix} -2 & 1 \\ -1 & 0 \\ 1 & -3 \\ 5 & -1 \end{bmatrix}, \qquad \boldsymbol{b}_2 = (-2, 2).$$

(a) Using the sigmoid activation function σ at each node, calculate the output from the network for the following inputs:

(i) $(1, 0, 2, -3)$

(ii) $(-2, 3, 1, 0)$

(iii) $(1, 0, 1, 1)$

(b) Using the activation function *relu* at each node, calculate the output from the network with same inputs as above.

(c) Using *relu* at the hidden layer and σ at the output layer, calculate the output from the network with same inputs as above.

(2) Consider a network with 2 input nodes, 3 nodes in the first hidden layer, 3 nodes in the second hidden layer and 2 output nodes. The weights between the respective layers are given by the following matrices:

$$W_1 = \begin{bmatrix} 1 & -1 & 0 \\ -2 & 4 & -1 \end{bmatrix} \quad W_2 = \begin{bmatrix} 2 & 0 & -1 \\ 1 & -2 & -3 \\ 5 & 0 & 0 \end{bmatrix} \quad W_3 = \begin{bmatrix} 0 & 2 \\ -1 & -1 \\ 4 & -3 \end{bmatrix}$$

The bias values at the two hidden layers and output layer are given by:

$$\boldsymbol{b}_1 = (0, -3, 2), \quad \boldsymbol{b}_2 = (3, 3, -1), \quad \boldsymbol{b}_3 = (0, 1).$$

(a) Using the *relu* activation function at each node, calculate the output from the network for the following inputs:

(i) $(1, -1)$

(ii) $(3, -2)$

(b) Using the sigmoid activation function σ at each node, calculate the output from the network with same inputs as above.

2.6. **Structuring the output.**

Suppose we are given a dataset with inputs and corresponding targets as in the tables below:

$$\begin{array}{cccc} x_1 & x_2 & \cdots & x_m \end{array} \qquad t$$

$$\begin{bmatrix} 1 & 2 & \cdots & -3 \\ -3 & -2 & \cdots & 5 \\ 0 & 1 & \cdots & -7 \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \qquad \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

Each input is an m-tuple $(x_1, \ldots, x_m) \in \mathbb{R}^m$ and each target value is a classification of the input into either 0 or 1, i.e., $t \in \{0, 1\}$.

A possible structure of a neural network for such a dataset would have m input nodes, then some hidden layers, followed by an output layer with 1 output node.
The number of hidden layers and the number of nodes in each hidden layer, as well as the activation functions at each hidden layer, would be chosen by the user.
For the output node, we could use a sigmoid activation function, which means that the output for a given input is a value between 0 and 1.
Then we need to interpret the output as either class 0 or class 1, which we can do as follows:

if $0 \leq y \leq \frac{1}{2}$, then the classification is 0,
if $\frac{1}{2} < y \leq 1$, then the classification is 1.

Another way to structure the output is to have two output nodes, where the first output node corresponds to an output of 0, and the second node corresponds to an output of 1. To do that,

we need to change the target table as follows:

$$\begin{matrix} x_1 & x_2 & \cdots & x_m \end{matrix} \qquad \begin{matrix} t_1 & t_2 \end{matrix}$$

$$\begin{bmatrix} 1 & 2 & \cdots & -3 \\ -3 & -2 & \cdots & 5 \\ 0 & 1 & \cdots & -7 \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \qquad \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ \vdots & \end{bmatrix}$$

The original 0's were changed to $(1, 0)$ and the original 1's were change to $(0, 1)$.
If we use sigmoid activation functions at the two output nodes, then the output of the two nodes would be a pair of values, say (y_1, y_2), in the range 0 to 1. The node which fires more strongly determines the classification:

if $y_1 \geq y_2$, i.e., y_1 fires more strongly than y_2, then we assign classification 0;
if $y_1 < y_2$, i.e., y_2 fires more strongly than y_1, then we assign classification 1.

For the next example, suppose we are given a dataset with inputs and corresponding targets as in the tables below:

$$\begin{matrix} x_1 & x_2 & \cdots & x_m \end{matrix} \qquad \begin{matrix} t \end{matrix}$$

$$\begin{bmatrix} -3 & 4 & \cdots & -1 \\ 2 & -1.5 & \cdots & 6.7 \\ 0.5 & -1 & \cdots & -3 \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \qquad \begin{bmatrix} a \\ b \\ c \\ \vdots \end{bmatrix}$$

Each input is an m-tuple $(x_1, \ldots, x_m) \in \mathbb{R}^m$ and each target value is a classification of the input into either a, b, or c, i.e., $t \in \{a, b, c\}$.

In this case, if we use a single output node with a sigmoid activation function in the output layer then, to interpret the output value y, we need some sort of rules, such as:
if $0 \leq y \leq \frac{1}{3}$, then classify as a,
if $\frac{1}{3} < y \leq \frac{2}{3}$, then classify as b,
if $\frac{2}{3} < y \leq 1$, then classify as c.

This method can create dependencies between the different classification classes.
A better method is to have 3 output nodes in the output layer and change the target values as follows:

each target a is replaced by target $(1, 0, 0)$
each target b is replaced by target $(0, 1, 0)$
each target c is replaced by target $(0, 0, 1)$.

Thus, our dataset looks like:

$$\begin{matrix} x_1 & x_2 & \cdots & x_m \end{matrix} \qquad \begin{matrix} t_1 & t_2 & t_3 \end{matrix}$$
$$\begin{bmatrix} -3 & 4 & \cdots & -1 \\ 2 & -1.5 & \cdots & 6.7 \\ 0.5 & -1 & \cdots & -3 \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \vdots & \vdots & \vdots \end{bmatrix}$$

We still need to decide how to interpret the output of the network. We can think of the three output nodes as corresponding to the three classifications. The node that fires the strongest, i.e., the node with the maximum output value, determines the classification. For example, $(0.9, 0.2, 0.1)$ gives a classification of a, $(0.6, 0.7, 0.1)$ gives a classification of b, while $(0.3, 0.4, 0.9)$ gives a classification of c. We may need some extra rules for special cases such as if we need to break a tie, as in $(0.5, 0.5, 0.1)$.

Creating targets in the above way is called a **one-hot encoding** of the data.
It can be applied regardless of how many output classifications there are; we add an output node for each possible classification.

2.7. **Regression with Neural Networks.**

Suppose our dataset is of the following type:

$$\begin{matrix} x_1 & x_2 & \cdots & x_m \end{matrix} \qquad t$$
$$\begin{bmatrix} -1 & 3 & \cdots & -4 \\ 5 & -1 & \cdots & 6 \\ 1 & 0 & \cdots & -7 \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \quad \begin{bmatrix} 3.6 \\ 2.7 \\ -4.1 \\ \vdots \end{bmatrix}$$

In this case, the targets are not classification values but real numbers, and the goal is not to separate data into classes but to find a network that acts as a function approximator to the above data. This is called a **regression** problem, or a curve-fitting problem.

One way to deal with real values is to use a single output node and to use the linear activation function *lin* at the output node. Then the output can take on any real number because the weights leading to the output node can be any numbers. If the dataset has two or more real-valued targets, then we use that many output nodes, each with linear activation function.
(If the outputs are all in the range $[0, 1]$, then the sigmoid activation function could also be used; if they are in the range $[-1, 1]$, then a *tanh* activation function could be used.)

Lastly, we mention the following theoretical result which provides information on what types of functions a neural network can approximate.

Universal Approximation Theorem
Any continuous real-valued function on a closed and bounded subset of $\mathbb{R}^m$ *can be approximated to any desired nonzero error by a neural network with one hidden layer that uses a sigmoid (or similar) activation function at the hidden nodes and a linear activation function at the output node.*

The above result states that basically any continuous function, as long as it's defined on a closed and bounded region of $\mathbb{R}^m$, can be approximated with arbitrarily small error by a neural network. In addition, the network requires only one hidden layer. However, note that the number of nodes in the hidden layer is not specified and it can be huge. The use of additional hidden layers reduces the total number of nodes required but, as we shall see, the more layers there are, the more difficult it is to train the network.