Back propagation in a simple neural net

October 28, 2019

Introduction

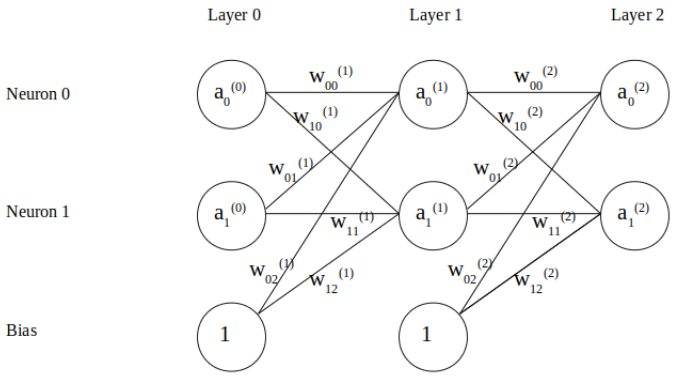
Brains are made up of neurons connected to each other. By making a mathematical model of some neurons wired together (a neural network) one can emulate some aspects of a brain.
In this note we will look at a very simple neural network in detail and show how matrices can be used to describe the processing and learning of the network.
The matrix formulation works for bigger networks as well.

The goal of this note is to look at a simple example in painstaking detail. For more background and analysis go to the links in the references at the end of the note.

The basic model

The network we will consider here consists of two input neurons (or nodes), two output neurones and a single hidden layer with two neurons.
That simple a network can only transform two input numbers, say (0.1, 0.9), to two output numbers, say (0.3, 0.4). Implementing more a complex behaviour like an AND-gate is only possible with more neurons in the hidden layer, and/or more layers.
In the Open Office Calc document *Simple_Neural_Net.ods* such a 2-2-2 network with a single hidden layer is implemented in a spreadsheet.

The layers are numbered with the input layer as (0), the hidden layer as (1) and the output layer as (2). *In this note an upper index in parenthesis refer to the layer.*
In each layer there are two neurons numbered 0 and 1 with *a lower index.*
Every neuron has a value a with indices indicating which neuron it belongs to.
For example $a_0^{(0)}$ is the value of the first (input) neuron in the first layer.



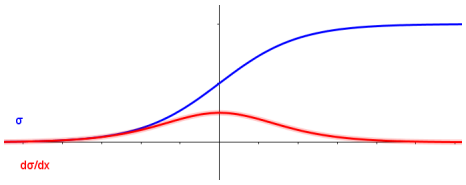
Each neuron in a layer is connected to every neuron in the previous layer (except the Input layer of course).

The weights between two layers "belongs" to the layer with the higher number and to make use of matrices easier the indices of each weight w is has the number of the end-neuron written before the number of the input neuron.
Therefore $w_{01}^{(1)}$ is the weight between the neurons with values $a_1^{(0)}$ and $a_0^{(1)}$.
A bias is added to each weighted sum in order to avoid origo ("(0, 0)") always being a minimum.
For practical reasons we use just one bias node for each layer with the value 1 and store the actual bias in the last weights in each layer.
Here $w_{02}^{(1)}$ and $w_{12}^{(1)}$ is the biases for layer (1).

The value of a neuron is a function of the weighted sum of the neuron values from previous layers.

$$a_0^{(1)} = f(\sum_{i=0}^{1} w_{0i}^{(1)} a_i^{(0)} + w_{12}^{(1)})$$

The function introduces a needed non-linearity and keeps the numbers manageable.
A lot of functions can be used, but a common choice is the sigmoid function $\sigma(x) = \dfrac{1}{(1-e^{-x})} = \dfrac{e^x}{(1-e^x)}$ with the practical derivative $\sigma'(x) = \sigma(x)(1-\sigma(x))$.



Note that the use of the sigmoid function nescessitate that the input numbers are close to zero and ascertain that the output values will be positive. One will typically operate in the interval [0; 1] on both input and output if possible.

To train the network input values are fed into the input nodes, the weighted sum is calculated for the hidden layer and then for the output layer. This is called *the forward pass*. Then the output values are compared to target values $T_0, T_1, ...$ and a *cost* is calculated.
This cost is a function of all the weights and using the derivative of the cost function with respect to each weight an adjustment to the weights can be *back propagated*.
Then the output values are compared to target values $T_0, T_1, ...$ and a *cost* is calculated. This cost is a function of all the weights and using the derivative of the cost function with respect to each weight an adjustment to the weights can be *back propagated*.

Forward pass

In the forward pass the values of each neuron is calculated by applying the sigmoid function to the weighted sum of input for each layer:

$$a_0^{(1)} = \sigma(w_{00}^{(1)} a_0^{(0)} + w_{01}^{(1)} a_1^{(0)} + w_{02}^{(1)}) \quad (1)$$
$$a_1^{(1)} = \sigma(w_{10}^{(1)} a_0^{(0)} + w_{11}^{(1)} a_1^{(0)} + w_{12}^{(1)}) \quad (2)$$

$$a_0^{(2)} = \sigma(w_{00}^{(2)} a_0^{(1)} + w_{01}^{(2)} a_1^{(1)} + w_{02}^{(2)}) \quad (3)$$
$$a_1^{(2)} = \sigma(w_{10}^{(2)} a_0^{(1)} + w_{11}^{(2)} a_1^{(1)} + w_{12}^{(2)}) \quad (4)$$

Or in matrix notation (see appendix A for the basic rules concerning matrices):

$$\vec{a}^{(1)} = \begin{pmatrix} a_0^{(1)} \\ a_1^{(1)} \end{pmatrix} = \sigma\left(\begin{pmatrix} w_{00}^{(1)}a_0^{(0)} + w_{01}^{(1)}a_1^{(0)} + w_{02}^{(1)} \\ w_{10}^{(1)}a_0^{(0)} + w_{11}^{(1)}a_1^{(0)} + w_{12}^{(1)} \end{pmatrix}\right) = \sigma\left((a_0^{(0)}a_1^{(0)}1)\begin{pmatrix} w_{00}^{(1)} & w_{10}^{(1)} \\ w_{01}^{(1)} & w_{11}^{(1)} \\ w_{02}^{(1)} & w_{12}^{(1)} \end{pmatrix}\right) = \sigma(\vec{A}^{(0)}W^{(1)})$$

In the same way

$$\vec{a}^{(2)} = \sigma(\vec{A}^{(1)}W^{(2)})$$

Note that $\vec{a}^{(1)} = \binom{a_0^{(1)}}{a_1^{(1)}}$ and $\vec{A}^{(1)} = (a_0^{(1)}a_1^{(1)}1)$ both contain the values for the nodes in layer (1).
$\vec{A}^{(1)}$ is needed to include the biases in some calculations.

Back propagation

To train the network we need a measure of how far the output values $\vec{a}^{(2)}$ are from the target values $\vec{T}$. As mentioned before this measure is called *the cost function*.
We define the cost as the difference between output values and target values. To avoid negative numbers we square the difference before we sum up the differnces.
And as the cost is just a number we want to minimize, we can multiply with $\frac{1}{2}$ to simplify the derivative.

In this case the cost function will be

$$C = \frac{1}{2}(a_0^{(2)} - T_0)^2 + \frac{1}{2}(a_1^{(2)} - T_1)^2$$

or using (3) and (4)

$$\begin{aligned} C = \frac{1}{2}(\sigma(w_{00}^{(2)}a_0^{(1)} + w_{01}^{(2)}a_1^{(1)} + w_{02}^{(2)}) - T_0)^2 + \\ \frac{1}{2}(\sigma(w_{10}^{(2)}a_0^{(1)} + w_{11}^{(2)}a_1^{(1)} + w_{12}^{(2)}) - T_1)^2 \end{aligned} \tag{5}$$

To minimize the cost we find the derivative of C with respect to each weight in layer (2).
This derivative can be subtracted from the relevant weights in order to get a better cost value after the next forward pass.

Note that the derivative of *all* weights in *all* layers have to be calculated before *any* weight is changed.

Let's start by finding $\frac{dC}{dw_{00}^{(2)}}$
Only the first term of C in equation (5) include $w_{00}^{(2)}$.

This term is a composite function $f \circ g \circ h(w_{00}^{(2)}, w_{01}^{(2)}, w_{02}^{(2)}, w_{10}^{(2)}, w_{11}^{(2)}, w_{12}^{(2)})$ where f, g and h and their derivatives are

$$f(\sigma) = \frac{1}{2}(\sigma - T_0)^2 \qquad \frac{df}{d\sigma} = (\sigma - T_0)$$

$$g(h) = \sigma(h) \qquad \frac{dg}{dh} = \frac{d\sigma}{dh} = \sigma(h)(1 - \sigma(h))$$

$$h(w_{00}^{(2)}, w_{01}^{(2)}, w_{02}^{(2)}) = w_{00}^{(2)}a_0^{(1)} + w_{01}^{(2)}a_1^{(1)} + w_{02}^{(2)} \qquad \frac{dh}{dw_{00}^{(2)}} = a_0^{(1)}$$

By using (3) we note that

$$(\sigma - T_0) = (a_0^{(2)} - T_0)$$

and

$$\sigma(h)(1 - \sigma(h)) = a_0^{(2)}(1 - a_0^{(2)})$$

The chain rule

$$\frac{dC}{dw_{00}^{(2)}} = \frac{df}{d\sigma}\ \frac{d\sigma}{dh}\ \frac{dh}{dw_{00}^{(2)}}$$

then gives us $\frac{dC}{dw_{00}^{(2)}} = (a_0^{(2)} - T_0)\ a_0^{(2)}(1 - a_0^{(2)})\ a_0^{(1)}$, the first entry in the change matrix.

The rest is found in a similar manner:

$$\begin{pmatrix} \frac{dC}{dw_{00}^{(2)}} & \frac{dC}{dw_{01}^{(2)}} & \frac{dC}{dw_{02}^{(2)}} \\ \\ \frac{dC}{dw_{10}^{(2)}} & \frac{dC}{dw_{11}^{(2)}} & \frac{dC}{dw_{12}^{(2)}} \end{pmatrix} =$$

$$\begin{pmatrix} (a_0^{(2)} - T_0)a_0^{(2)}(1 - a_0^{(2)})a_0^{(1)} & (a_0^{(2)} - T_0)a_0^{(2)}(1 - a_0^{(2)})a_1^{(1)} & (a_0^{(2)} - T_0)a_0^{(2)}(1 - a_0^{(2)})1 \\ \\ (a_1^{(2)} - T_1)a_1^{(2)}(1 - a_1^{(2)})a_0^{(1)} & (a_1^{(2)} - T_1)a_1^{(2)}(1 - a_1^{(2)})a_1^{(1)} & (a_1^{(2)} - T_1)a_1^{(2)}(1 - a_1^{(2)})1 \end{pmatrix}$$

We note that each entry in the upper row contains $\delta_0^{(2)} = (a_0^{(2)} - T_0)a_0^{(2)}(1 - a_0^{(2)})$ and that each entry in the lower row contains $\delta_1^{(2)} = (a_1^{(2)} - T_1)a_1^{(2)}(1 - a_1^{(2)})$.

Therefore the *transposed* change matrix for layer (2) is

$$\frac{dC}{dW^{(2)}}^T = \begin{pmatrix} \frac{dC}{dw_{00}^{(2)}} & \frac{dC}{dw_{01}^{(2)}} & \frac{dC}{dw_{02}^{(2)}} \\ \\ \frac{dC}{dw_{10}^{(2)}} & \frac{dC}{dw_{11}^{(2)}} & \frac{dC}{dw_{12}^{(2)}} \end{pmatrix} = \begin{pmatrix} \delta_0^{(2)}a_0^{(1)} & \delta_0^{(2)}a_1^{(1)} & \delta_0^{(2)} \cdot 1 \\ \\ \delta_1^{(2)}a_0^{(1)} & \delta_1^{(2)}a_1^{(1)} & \delta_1^{(2)} \cdot 1 \end{pmatrix} = \delta^{(2)}A^{(1)}$$

where $\delta^{(2)} = \binom{\delta_0^{(2)}}{\delta_1^{(2)}}$ and we had $A^{(1)} = (a_0^{(1)}a_1^{(1)}1)$.
After all change matrices is found the change is applied to all weights.
For layer (2) this will be

$$W^{(2)} = W^{(2)} - \gamma \cdot \frac{dC}{dW^{(2)}}$$

where γ is a number between 0 and 1 called the *learning rate*. A good start value for γ is usually 0.5
Remember to transpose the change matrix before subtracting it from the weight matrix.

To find how much each weight in layer (1) have to change we can use (1) and (2) in (5)

$$\begin{aligned} C = \frac{1}{2}\left(\sigma\left(w_{00}^{(2)}\sigma(w_{00}^{(1)}a_0^{(0)} + w_{01}^{(1)}a_1^{(0)} + w_{02}^{(1)}) + w_{01}^{(2)}\sigma(w_{10}^{(1)}a_0^{(0)} + w_{11}^{(1)}a_1^{(0)} + w_{12}^{(1)}) + w_{02}^{(2)}\right) - T_0\right)^2 + \\ \frac{1}{2}\left(\sigma\left(w_{10}^{(2)}\sigma(w_{00}^{(1)}a_0^{(0)} + w_{01}^{(1)}a_0^{(0)} + w_{02}^{(1)}) + w_{11}^{(2)}\sigma(w_{10}^{(1)}a_0^{(0)} + w_{11}^{(1)}a_1^{(0)} + w_{12}^{(1)}) + w_{12}^{(2)}\right) - T_1\right)^2 \end{aligned} \tag{6}$$

We want to find $\frac{dC}{dw_{00}^{(1)}}$ and note that $dw_{00}^{(1)}$ occur in both terms of (6). The composite function is a little more complicated, but nothing new happens.

A little work will show that

$$\frac{dC}{dw_{00}^{(1)}} = (a_0^{(2)} - T_0)\ a_0^{(2)}(1 - a_0^{(2)})w_{00}^{(2)}\ a_0^{(1)}(1 - a_0^{(1)})\ a_0^{(0)} + (a_1^{(2)} - T_1)\ a_1^{(2)}(1 - a_1^{(2)})w_{10}^{(2)}\ a_0^{(1)}(1 - a_0^{(1)})\ a_0^{(0)}$$

$$\frac{dC}{dw_{01}^{(1)}} = (a_0^{(2)} - T_0)\ a_0^{(2)}(1 - a_0^{(2)})w_{00}^{(2)}\ a_0^{(1)}(1 - a_0^{(1)})\ a_1^{(0)} + (a_1^{(2)} - T_1)\ a_1^{(2)}(1 - a_1^{(2)})w_{10}^{(2)}\ a_0^{(1)}(1 - a_0^{(1)})\ a_1^{(0)}$$

$$\frac{dC}{dw_{02}^{(1)}} = (a_0^{(2)} - T_0)\ a_0^{(2)}(1 - a_0^{(2)})w_{00}^{(2)}\ a_0^{(1)}(1 - a_0^{(1)}) \cdot 1 + (a_1^{(2)} - T_1)\ a_1^{(2)}(1 - a_1^{(2)})w_{10}^{(2)}\ a_0^{(1)}(1 - a_0^{(1)}) \cdot 1$$

$$\frac{dC}{dw_{10}^{(1)}} = (a_0^{(2)} - T_0)\ a_0^{(2)}(1-a_0^{(2)})w_{01}^{(2)}\ a_1^{(1)}(1-a_1^{(1)})\ a_0^{(0)} + (a_1^{(2)} - T_1)\ a_1^{(2)}(1-a_1^{(2)})w_{11}^{(2)}\ a_1^{(1)}(1-a_1^{(1)})\ a_0^{(0)}$$

$$\frac{dC}{dw_{11}^{(1)}} = (a_0^{(2)} - T_0)\ a_1^{(2)}(1-a_1^{(2)})w_{01}^{(2)}\ a_0^{(1)}(1-a_1^{(1)})\ a_1^{(0)} + (a_1^{(2)} - T_1)\ a_1^{(2)}(1-a_1^{(2)})w_{11}^{(2)}\ a_1^{(1)}(1-a_1^{(1)})\ a_1^{(0)}$$

$$\frac{dC}{dw_{12}^{(1)}} = (a_0^{(2)} - T_0)\ a_0^{(2)}(1-a_0^{(2)})w_{01}^{(2)}\ a_1^{(1)}(1-a_1^{(1)}) \cdot 1 + (a_1^{(2)} - T_1)\ a_1^{(2)}(1-a_1^{(2)})w_{11}^{(2)}\ a_1^{(1)}(1-a_1^{(1)}) \cdot 1$$

If we again use $\delta_0^{(2)} = (a_0^{(2)} - T_0)a_0^{(2)}(1-a_0^{(2)})$ and $\delta_1^{(2)} = (a_1^{(2)} - T_1)a_1^{(2)}(1-a_1^{(2)})$ we can write

$$\frac{dC}{dw_{00}^{(1)}} = \delta_0^{(2)} w_{00}^{(2)}\ a_0^{(1)}(1-a_0^{(1)})a_0^{(0)} + \delta_1^{(2)} w_{10}^{(2)}\ a_0^{(1)}(1-a_0^{(1)})a_0^{(0)}$$

and by letting $\delta_0^{(1)} = a_0^{(1)}(1-a_0^{(1)})\sum_{i=0}^{1}\delta_i^{(2)}w_{i0}^{(2)}$ we have $\frac{dC}{dw_{00}^{(1)}} = \delta_0^{(1)}a_0^{(0)}$

With $\delta_1^{(1)} = a_1^{(1)}(1-a_1^{(1)})\sum_{i=0}^{1}\delta_i^{(2)}w_{i1}^{(2)}$ the transposed change matrix for layer (1) is

$$\frac{dC}{dW^{(1)}} = \begin{pmatrix} \frac{dC}{dw_{00}^{(1)}} & \frac{dC}{dw_{01}^{(1)}} & \frac{dC}{dw_{02}^{(1)}} \\ \\ \frac{dC}{dw_{10}^{(1)}} & \frac{dC}{dw_{11}^{(1)}} & \frac{dC}{dw_{12}^{(1)}} \end{pmatrix} = \begin{pmatrix} \delta_0^{(1)}a_0^{(0} & \delta_0^{(1)}a_1^{(0)} & \delta_0^{(1)} \cdot 1 \\ \\ \delta_1^{(1)}a_0^{(0)} & \delta_1^{(1)}a_1^{(0)} & \delta_1^{(2)} \cdot 1 \end{pmatrix} = \delta^{(1)}A^{(0)}$$

where $\delta^{(1)} = \binom{\delta_0^{(1)}}{\delta_1^{(1)}}$ and $A^{(0)} = (a_0^{(0)}a_1^{(0)}1)$.

By introducing the matrices

$$c = \begin{pmatrix} a_0^{(2)} - T_0 \\ a_1^{(2)} - T_1 \end{pmatrix} \qquad\qquad w_2 = \begin{pmatrix} w_{00}^{(2)} & w_{01}^{(2)} \\ w_{10}^{(2)} & w_{11}^{(2)} \end{pmatrix}$$

$$D^{(2)} = \begin{pmatrix} a_0^{(2)}(1-a_0^{(2)}) & 0 \\ 0 & a_1^{(2)}(1-a_1^{(2)}) \end{pmatrix} \qquad D^{(1)} = \begin{pmatrix} a_0^{(1)}(1-a_0^{(1)}) & 0 \\ 0 & a_0^{(1)}(1-a_0^{(1)}) \end{pmatrix}$$

we can write $\delta^{(2)} = \begin{pmatrix} \delta_0^{(2)} \\ \delta_1^{(2)} \end{pmatrix} = D^{(2)} \cdot c = \begin{pmatrix} a_0^{(2)}(1-a_0^{(2)}) & 0 \\ 0 & a_1^{(2)}(1-a_1^{(2)}) \end{pmatrix} \begin{pmatrix} a_0^{(2)} - T_0 \\ a_1^{(2)} - T_1 \end{pmatrix} = \begin{pmatrix} (a_0^{(2)} - T_0)a_0^{(2)}(1-a_0^{(2)}) \\ (a_1^{(2)} - T_1)a_1^{(2)}(1-a_1^{(2)}) \end{pmatrix}$

Then

$$D^{(1)}w^{(2)}\delta^{(2)} = \begin{pmatrix} a_0^{(1)}(1-a_0^{(1)}) & 0 \\ 0 & a_1^{(1)}(1-a_1^{(1)}) \end{pmatrix} \begin{pmatrix} w_{00}^{(2)} & w_{01}^{(2)} \\ w_{10}^{(2)} & w_{11}^{(2)} \end{pmatrix} \begin{pmatrix} \delta_0^{(2)} \\ \delta_1^{(2)} \end{pmatrix}$$

$$= \begin{pmatrix} w_{00}^{(2)}a_0^{(1)}(1-a_0^{(1)}) & w_{10}^{(2)}a_0^{(1)}(1-a_0^{(1)}) \\ w_{01}^{(2)}a_1^{(1)}(1-a_1^{(1)}) & w_{11}^{(2)}a_1^{(1)}(1-a_1^{(1)}) \end{pmatrix} \begin{pmatrix} \delta_0^{(2)} \\ \delta_1^{(2)} \end{pmatrix} = \begin{pmatrix} \delta_0^{(2)}w_{00}^{(2)}a_0^{(1)}(1-a_0^{(1)}) + \delta_1^{(2)}w_{10}^{(2)}a_0^{(1)}(1-a_0^{(1)}) \\ \delta_0^{(2)}w_{01}^{(2)}a_1^{(1)}(1-a_1^{(1)}) + \delta_1^{(2)}w_{11}^{(2)}a_1^{(1)}(1-a_1^{(1)}) \end{pmatrix} = \begin{pmatrix} \delta_0^{(1)} \\ \delta_1^{(1)} \end{pmatrix} = \delta^{(1)}$$

To summarise

$$\frac{dC}{dW^{(1)}} = \delta^{(1)}A^{(0)} = D^{(1)}w^{(2)}\delta^{(2)}A^{(0)}$$

and

$$\frac{dC}{dW^{(2)}} = \delta^{(2)}A^{(1)}$$

δ is sometimes called the "error" because it tell us how much the weights have to change, and part of δ is the difference between the output and the target $(a_0^{(2)} - T_0)$.

We also see that neurons with high values of a contribute more to the change matrix, kind of like more active neurons in a biological network tend to reinforce learning in the network.

Bigger networks

When we add neurons to a layer nothing changes if we use matrix notation, except for the size of the matrices. If we introduce new layers the changes to the forward pass is trivia and the back propagation between each layer is done as before; we just find the new δ's as

$$\delta^{(i)} = D^{(i)} w^{(i+1)} \delta^{(i+1)}$$

A note for implementation:

When the network becomes bigger multiplying matrices like $D^{(1)}$ will eat up unnecessary computer cycles due to the many zeroes in diagonal matrices.
This can be avoided by using the lesser known Hadamard product $\odot$.
(`https://en.wikipedia.org/wiki/Hadamard_product_(matrices)`)

Instead of

$$\begin{pmatrix} a_0^{(2)}(1-a_0^{(2)}) & 0 \\ 0 & a_1^{(2)}(1-a_1^{(2)}) \end{pmatrix} \begin{pmatrix} a_0^{(2)} - T_0 \\ a_1^{(2)} - T_1 \end{pmatrix} = \begin{pmatrix} (a_0^{(2)} - T_0)a_0^{(2)}(1-a_0^{(2)}) \\ (a_1^{(2)} - T_1)a_1^{(2)}(1-a_1^{(2)}) \end{pmatrix}$$

we would write

$$\begin{pmatrix} a_0^{(2)}(1-a_0^{(2)}) \\ a_1^{(2)}(1-a_1^{(2)}) \end{pmatrix} \odot \begin{pmatrix} a_0^{(2)} - T_0 \\ a_1^{(2)} - T_1 \end{pmatrix} = \begin{pmatrix} (a_0^{(2)} - T_0)a_0^{(2)}(1-a_0^{(2)}) \\ (a_1^{(2)} - T_1)a_1^{(2)}(1-a_1^{(2)}) \end{pmatrix}$$

This saves both memory and processing time.

References:

Youtube video:
3BLUE1BROWN SERIES S3 A1
But what is a Neural Network? — Deep learning, chapter 1 `https://www.youtube.com/watch?v=aircAruvnKk`

Blogs/papers:
`https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/`
`https://page.mi.fu-berlin.de/rojas/neural/chapter/K7.pdf`
`http://neuralnetworksanddeeplearning.com/chap2.html`
`http://cs231n.stanford.edu/handouts/linear-backprop.pdf`
`https://sudeepraja.github.io/Neural/`

Appendix A: Matrices, basic rules

• A matrix with 3 rows and 2 columns is called a 3×2 matrix.

Example: A 3×2 *matrix and a* 1×3 *matrix*

$$\begin{pmatrix} * & * \\ * & * \\ * & * \end{pmatrix} \qquad\qquad \begin{pmatrix} * & * & * \end{pmatrix}$$

• Multiplication of a $k \times m$ matrix with a $m \times n$ matrix yields a $k \times n$ matrix.
One simply multiply each entry in the rows in the first matrix with each colum in the second matrix and sum up the result.

Example: A 3×2 *matrix times* 1×2 *matrix resulting in a* 3×2 *matrix*

$$\begin{pmatrix} g & h \\ i & j \\ k & l \end{pmatrix} \begin{pmatrix} a & b \\ d & e \end{pmatrix} = \begin{pmatrix} ag + dh & bg + eh \\ ai + dj & bi + ej \\ ak + dl & bk + el \end{pmatrix}$$

• A matrix can be multiplied by a vector and the result is a vector of the same size.

Example: A 2×2 *matrix times a vector resulting in a vector*

$$\begin{pmatrix} a & b \\ d & e \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} af + bg \\ df + eg \end{pmatrix}$$