

Artificial Neural Networks

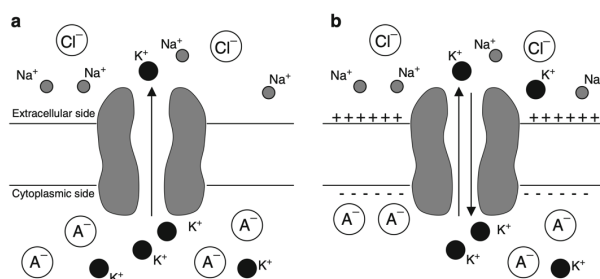
Payam Barnaghi
 Department of Brain Sciences &
 School of Convergence Science (Human and Artificial Intelligence)
 Imperial College London
 January 2026



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Hodgkin-Huxley neuron model

$$E_K = -\frac{RT}{zF} \ln \frac{[K^+]_{in}}{[K^+]_{out}} \quad (1.1)$$



This is a computational model of a biological neuron; in contrast, in ML, we are interested in modelling an **artificial neuron** that can help us to solve (machine) learning and decision-making problems.

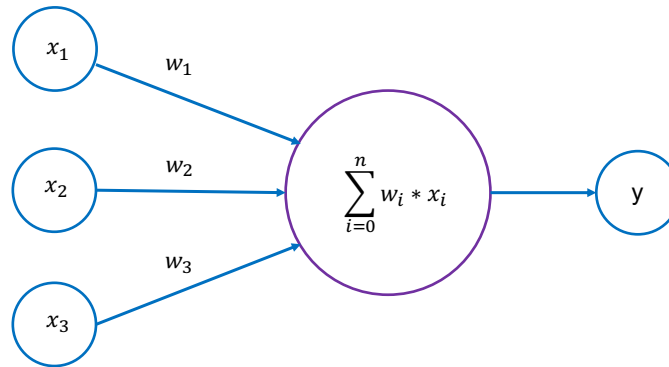
Image from: <http://www.math.pitt.edu/~bdoiron/assets/ermentrout-and-terman-ch-1.pdf>

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Artificial Neuron

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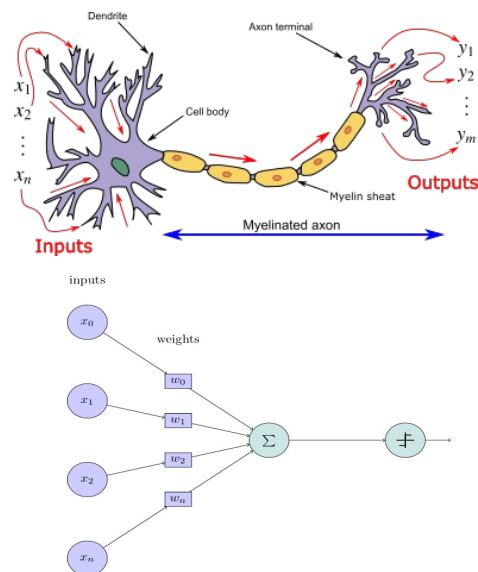


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Artificial neuron vs biological neuron

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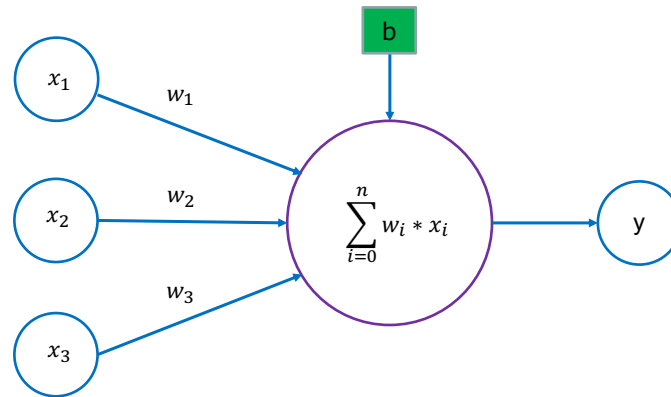


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Artificial Neuron with Bias

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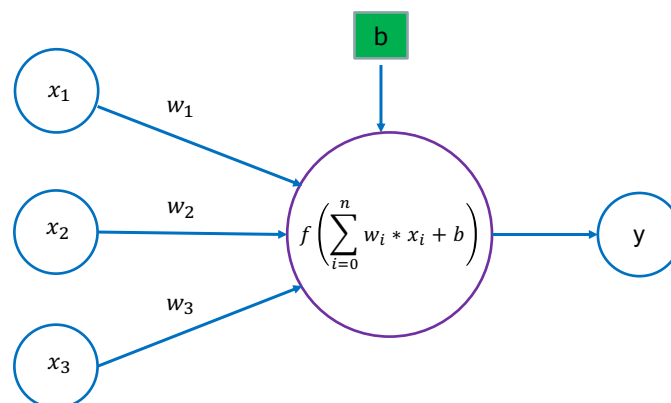


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Artificial neurons and the effect of bias

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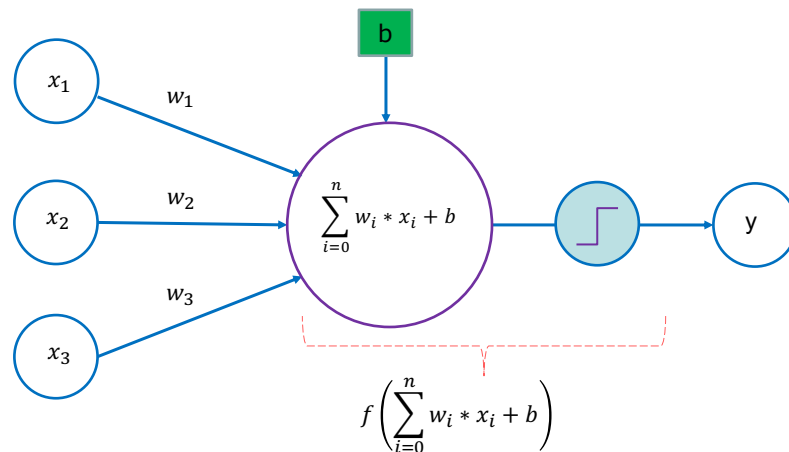


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NN with an Activation Function

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Limitations of linear models

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- Linearity implies the *weaker* assumption of *monotonicity*, i.e., that any increase in our feature must either always cause an increase in our model's output (if the corresponding weight is positive) or always cause a decrease in our model's output (if the corresponding weight is negative).
- However, this assumption is not always true or helpful in real-world applications. For individuals with a body temperature above 37°C (98.6°F), higher temperatures indicate greater risk. However, this risk does not increase linearly when, for example, the body temperature drops below 37°C or rises above 38.5°C .

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Sigmoid function

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```
import math

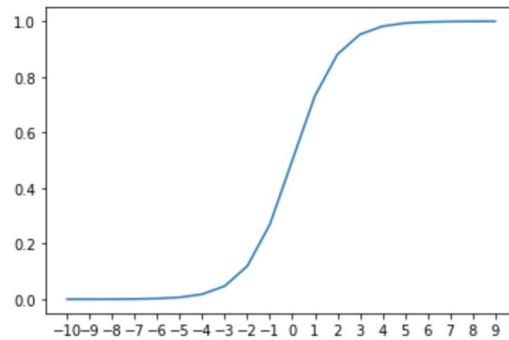
def sigmoid(x):
    return 1 / (1 + math.exp(-x))
```

✓ 0.9s

```
sigmoid(1.5)
```

✓ 0.4s

0.8175744761936437



$$\text{sigmoid}(x) = \frac{1}{1 + e^{-x}}$$

$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}$$

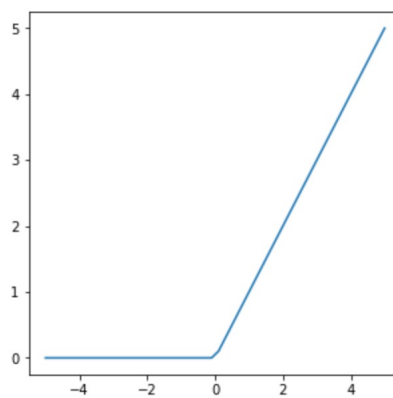
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Rectified Linear Units (ReLU)

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```
def relu(z):
    return np.maximum(0, z)
```



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ReLU

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- The half rectifying nonlinearity simulates some of the properties of biological neurons:
 - For some inputs, biological neurons are completely inactive (sparse activation).
 - For some inputs, a biological neuron's output is proportional to its inputs.
 - Most of the time, biological neurons operate in an inactive state (i.e., they have sparse activation).

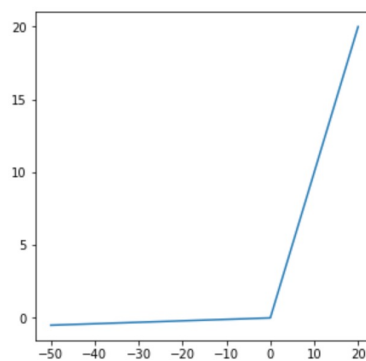
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Leaky ReLU

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```
def leaky_relu(z, alpha):  
    l = array('d')  
    for x in z:  
        if x >= 0:  
            l.append(max(0,x))  
        if x < 0:  
            l.append(alpha * min(0,x))  
    return l
```



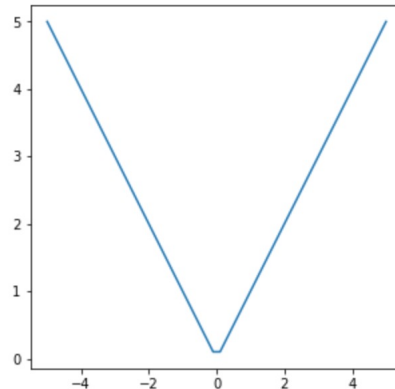
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Absolute Value Rectification

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```
def absolute_value_rectification(z):  
    alpha = -1  
    return np.maximum(0,z) + alpha * np.minimum(0,z)
```



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Nonlinearity in machine problems

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- In the past lectures, we have seen that the decision space and feature representation in most machine learning problems are not linear.
- So, the question is: how to add nonlinearity to neural network models?

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Hidden layers

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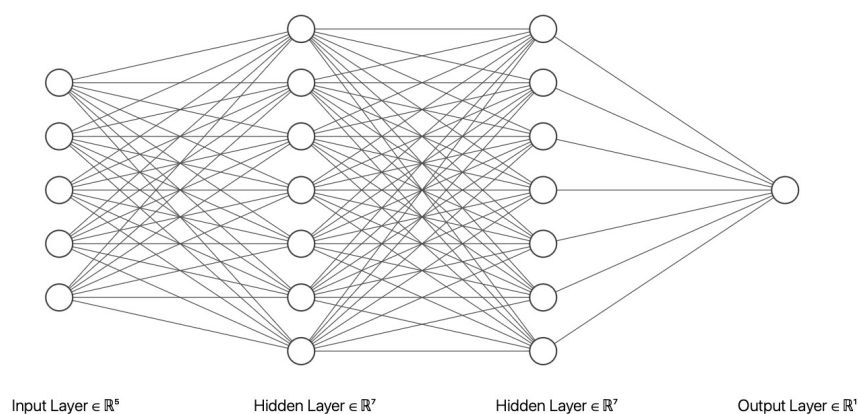
- We can overcome the limitations of linear models by also incorporating one or more hidden layers (with activation functions).
- The easiest way to do this is to stack several fully connected layers on top of each other.
- Each layer feeds into the layer above it until the model generates outputs.
- This architecture is commonly called a Multilayer Perceptron (MLP).

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Multilayer perceptron architecture

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The figure is drawn using: <https://alexlenail.me/NN-SVG/>

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MLP architecture

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- We can think of the first $L-1$ layers as our representation and the final layer as our linear predictor.

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Layers in a neural network

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- Input layer
- Hidden layers
- Output layer

- The number of hidden layers determines the depth of the network. The term “deep learning” originates from this terminology.
- The width of the network is determined by the number of nodes (dimensionality) in the hidden layer(s).

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How neuroscience has inspired this model

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- The idea of using many layers of connected neurons and networks (here, they are very structurally connected).
- The concept of using an activation function.
- There are several more advanced architectures that mimic concepts from neuroscience, such as memory-based models (e.g., LSTM) and attention-based models (e.g., Transformers).

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Forward propagation

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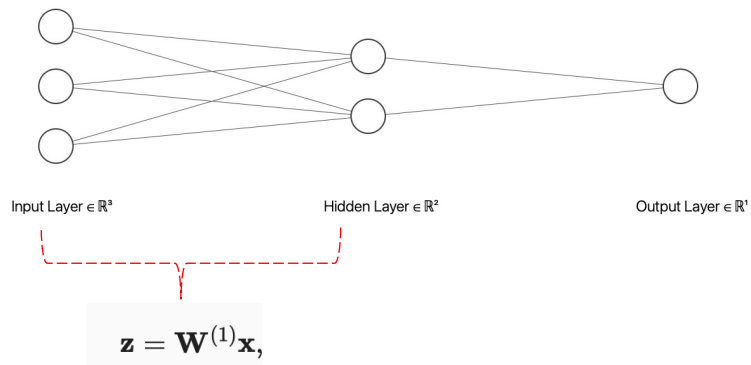
- *Forward propagation* (or *forward pass*) refers to the calculation and storage of intermediate variables (including outputs) for a neural network in order from the input layer to the output layer.
- We now work step-by-step through the mechanics of a neural network with one hidden layer.
- For the sake of simplicity, let's assume that our hidden layer does not include a bias term.

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Forward propagation – step 1

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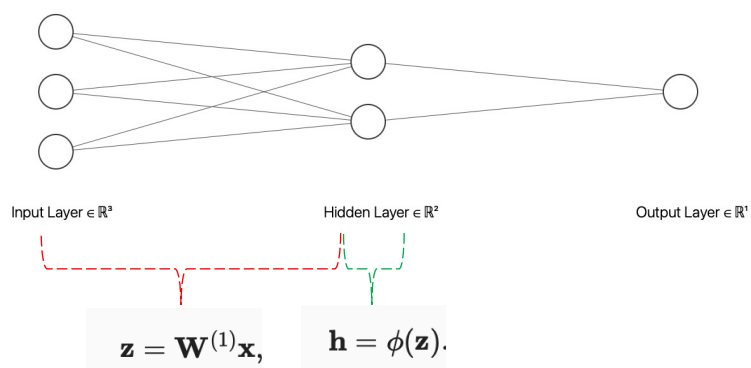


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Forward propagation – step 2

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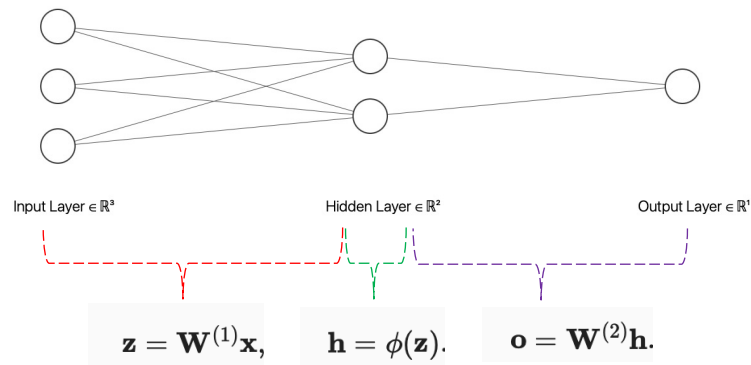


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Forward propagation – step 3

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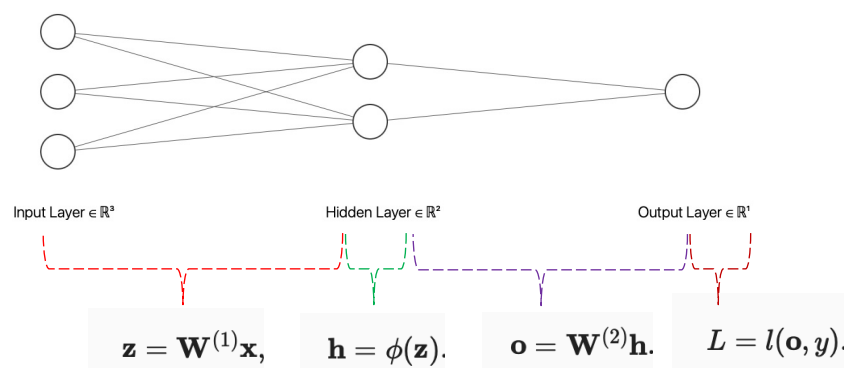


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Forward propagation – Loss function (l)

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Back propagation

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- *Backpropagation* refers to the method of calculating the gradient of neural network parameters.
- The method traverses the network in reverse order, from the output to the input layer, according to the *chain rule* from calculus.
- The algorithm stores any intermediate variables (partial derivatives) required during the calculation of the gradient with respect to some parameters.

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Training a neural network - I

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- Often, we start with random weight initialisation.
- And then go through multiple iterations applying all the training samples (forward propagation).
- Then, calculate the error or loss using a loss function.
- After that, we use the error/loss value to update the weights.
- We repeat this training iteration several times; in NN terms, each iteration of trying all the training samples in one round is called an “*epoch*”.

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Random initialisation**

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- If you are interested in the effect of initialisation parameters, see:
- <https://stackoverflow.com/questions/49433936/how-do-i-initialize-weights-in-pytorch>
- <https://pytorch.org/docs/stable/nn.init.html>
- *Understanding the difficulty of training deep feedforward neural networks, Glorot, X. & Bengio, Y. (2010)* <https://proceedings.mlr.press/v9/glorot10a/glorot10a.pdf>

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Training neural networks

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- In neural network training, forward and backward propagation depend on each other.
- In forward propagation, we traverse the computational graph in the direction of dependencies and compute all variables along the path.
- These are then used for backpropagation, where the computation order on the graph is reversed.

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Training a neural network - I

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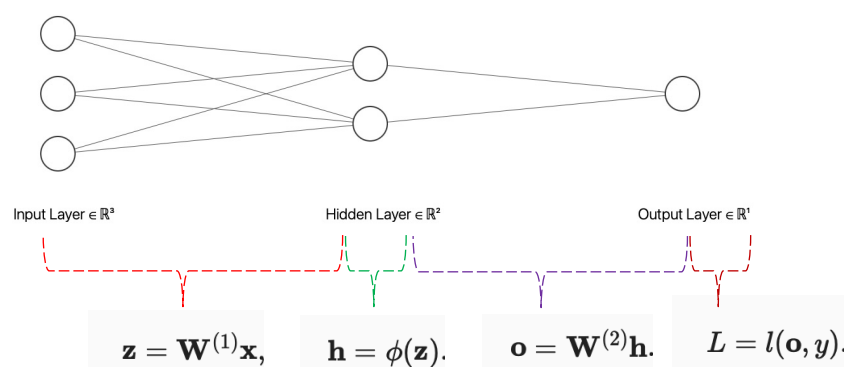
- Now, the question is how to update the weights to optimise the model and reduce error/loss.
- We need a way to calculate the intermediate values for backpropagation and weight updates.
- We need a hyperparameter to control the rate of change. This is often done by a hyperparameter called “*learning rate*”.

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Forward propagation – Loss function (I)

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Gradient in neural network

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- Or more precisely, the gradient of neural network parameters.
- In backpropagation, we need to calculate the partial derivatives of variables with respect to some parameters.

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Derivatives and Differentiation*

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- A *derivative* is the rate of change in a function with respect to changes in its arguments.
- Derivatives can tell us how rapidly a loss function would increase or decrease if we *increase* or *decrease* each parameter by an infinitesimally small amount.

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}.$$

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**** Example: Calculate the derivative of $f(x) = x^2$**

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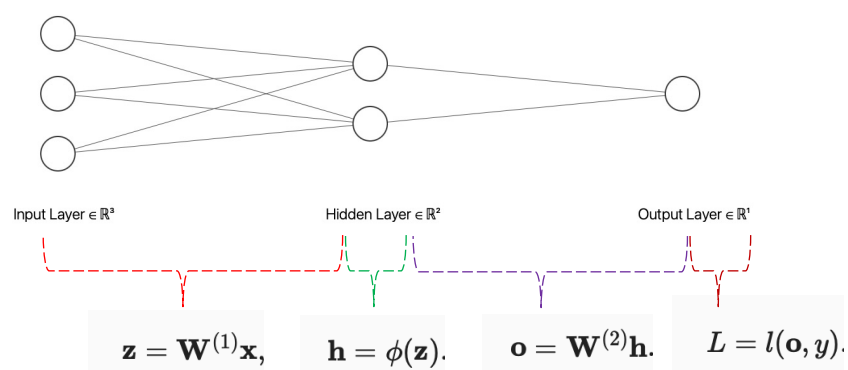
$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}.$$

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Example - I

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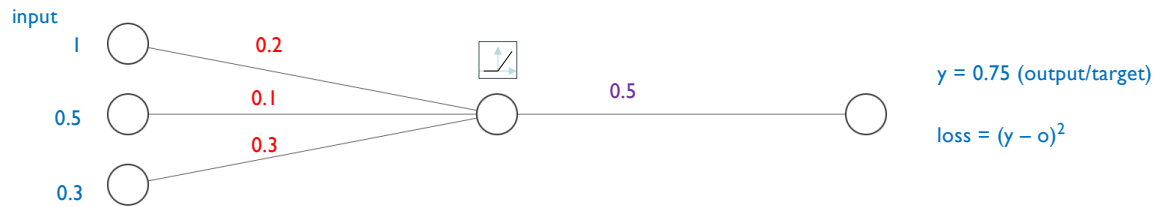


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Example - 2

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$$z = (1 \times 0.2) + (0.5 \times 0.1) + (0.3 \times 0.3) = 0.34$$

$$h = \varphi(z) = \text{ReLU}(z) = \text{ReLU}(0.34) = \max(0, 0.34) = 0.34$$

$$o = 0.34 \times 0.5 = 0.17$$

$$l = (0.75 - 0.17)^2 = 0.3364$$

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Gradient of the loss function*

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- Taking the gradient with *regards to* \hat{y}

$$\frac{\partial L}{\partial \hat{y}}$$

$$L = (y - \hat{y})^2$$

Applying the chain rule:

$$\frac{\partial}{\partial \hat{y}} (y - \hat{y})^2 = 2(y - \hat{y}) \cdot \frac{\partial (y - \hat{y})}{\partial \hat{y}}$$

considering: $\frac{\partial (y - \hat{y})}{\partial \hat{y}} = -1$

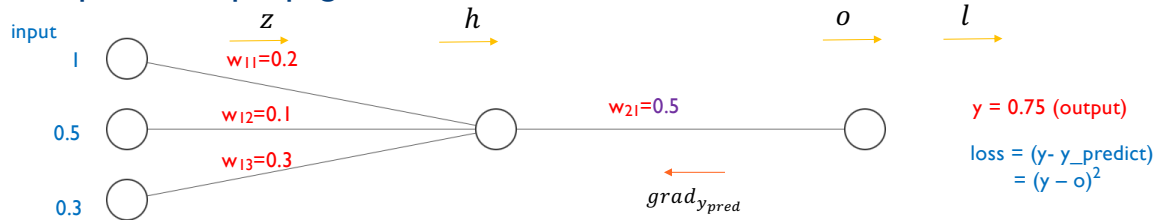
Then:

$$\frac{\partial L}{\partial \hat{y}} = 2(y - \hat{y})(-1) = -2(y - \hat{y})$$

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Example – backpropagation



$$z = (1 \times 0.2) + (0.5 \times 0.1) + (0.3 \times 0.3) = 0.34$$

$$h = \varphi(z) = \text{ReLU}(z) = \text{ReLU}(0.34) = \max(0, 0.34) = 0.34$$

$$o = 0.34 \times 0.5 = 0.17$$

$$l = (0.75 - 0.17)^2 = 0.3364$$

$$grad_{y_{\text{pred}}} = -2 \times (y - y_{\text{pred}}) = -2 \times (y - o) = -2 \times (0.75 - 0.17) = -1.16$$

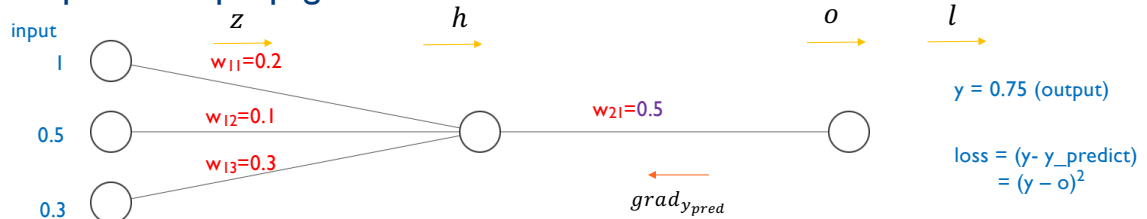
$$\frac{\partial L}{\partial w_{21}} = h \times \frac{\partial L}{\partial o} = 0.34 \times (-1.16) = -0.3944$$

$$grad_h = w_{21} \times \frac{\partial L}{\partial o} = 0.5 \times (-1.16) = -0.58$$

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Example – backpropagation



$$z = (1 \times 0.2) + (0.5 \times 0.1) + (0.3 \times 0.3) = 0.34$$

$$h = \varphi(z) = \text{ReLU}(z) = \text{ReLU}(0.34) = \max(0, 0.34) = 0.34$$

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$$grad_{y_{\text{pred}}} = -2 \times (y - y_{\text{pred}}) = -2 \times (y - o) = -2 \times (0.75 - 0.17) = -1.16$$

$$\frac{\partial L}{\partial w_{21}} = h \times \frac{\partial L}{\partial o} = 0.34 \times (-1.16) = -0.3944$$

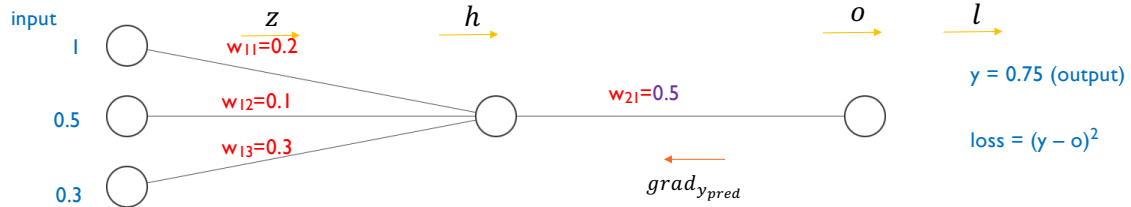
$$\frac{\partial L}{\partial w_{11}} = x_1 \times \frac{\partial L}{\partial z} = x_1 \times grad_h = 0.2 \times -0.3944 = -0.07888$$

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Example – backpropagation

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$$z = (1 \times 0.2) + (0.5 \times 0.1) + (0.3 \times 0.3) = 0.34$$

$$h = \varphi(z) = ReLU(z) = ReLU(0.34) = \max(0, 0.34) = 0.34$$

$$o = 0.34 \times 0.5 = 0.17$$

$$l = (0.75 - 0.17)^2 = 0.3364$$

$$grad_{y_{pred}} = -2 \times (y - y_{pred}) = -2 \times (y - o) = -2 \times (0.75 - 0.17) = -1.16$$

$$\frac{\partial L}{\partial w_{21}} = h \times \frac{\partial L}{\partial o} = 0.34 \times (-1.16) = -0.3944$$

$$\frac{\partial L}{\partial w_{11}} = x_1 \times \frac{\partial L}{\partial z} = x_1 \times grad_h = 1 \times -0.3944 = -0.3944$$

$$w_{11} = w_{11} - grad_w_{11};$$

$$w_{12} = w_{12} - grad_w_{12};$$

$$w_{11} = w_{11} - grad_w_{11}$$

$$w_{11} = 0.2 - (-0.07888)$$

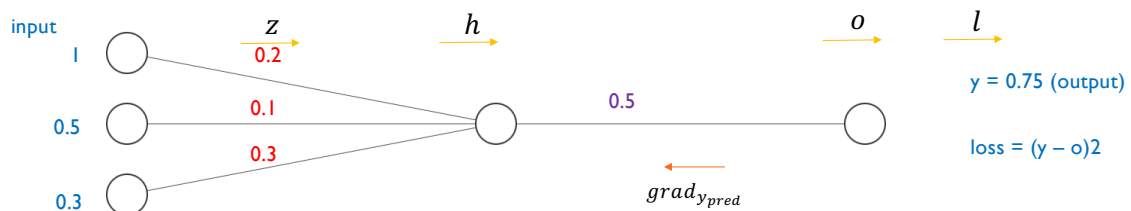
$$= 0.27888$$

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Example – backpropagation

IMPERIAL



$$z = (1 \times 0.2) + (0.5 \times 0.1) + (0.3 \times 0.3) = 0.34$$

$$h = \varphi(z) = ReLU(z) = ReLU(0.34) = \max(0, 0.34) = 0.34$$

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$$grad_{y_{pred}} = -2 \times (y - y_{pred}) = -2 \times (y - o) = -2 \times (0.75 - 0.17) = -1.16$$

$$\frac{\partial L}{\partial w_{21}} = h \times \frac{\partial L}{\partial o} = 0.34 \times (-1.16) = -0.3944$$

$$\frac{\partial L}{\partial w_{11}} = x_1 \times \frac{\partial L}{\partial z} = x_1 \times grad_h = 1 \times -0.3944 = -0.3944$$

$$w_{11} = w_{11} - grad_w_{11}$$

$$w_{11} = 0.2 - (-0.07888)$$

$$= 0.27888$$

$$w_{11} = w_{11} - (learning_rate \times grad_w_{11})$$

$$w_{12} = w_{12} - (learning_rate \times grad_w_{12})$$

$$w_{13} = w_{13} - (learning_rate \times grad_w_{13})$$

$$w_{21} = w_{21} - (learning_rate \times grad_w_{21})$$

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Learning rate

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- The learning rate is a hyperparameter that controls the change in weights in neural networks based on the gradient.
- The learning rate scales the magnitude of weight updates.
- For example:

$$w1 = w1 - (\text{learning_rate} * \text{grad_w1})$$

$$w2 = w2 - (\text{learning_rate} * \text{grad_w2})$$

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How to choose a learning rate

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- There are various ways to choose and optimise the learning rate.
- A simple approach is to start with a relatively large value (e.g. 0.01 or 0.1) and then (exponentially) reduce it over iterations.
- With dynamic learning rates, if the learning rate decreases too rapidly, it can affect network convergence (i.e., finding an optimal solution).
- If (a large) learning rate changes too slowly, the network may fail to converge to a good enough solution since noise (noise in samples that causes noisy gradients) could keep on driving the network away from an optimal solution.

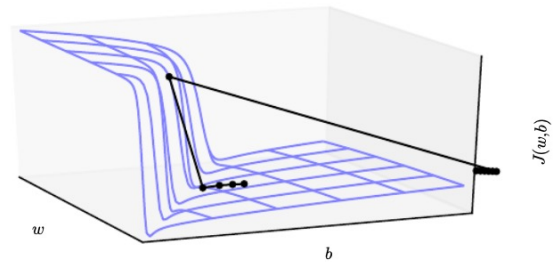
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Exploding and vanishing gradients*

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- The objective function for highly nonlinear deep neural networks or recurrent neural networks often contains sharp nonlinearities in parameter space resulting from the multiplication of several parameters.
- These nonlinearities give rise to very high derivatives in some places.
- When the parameters get close to such a cliff region, a gradient descent update can catapult the parameters very far, possibly losing most of the optimisation work that has been done.



Source: Adapted from Goodfellow et al., Deep Learning, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>
Original figure from (Pascanu et al., 2013)

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Momentum

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- While stochastic gradient descent remains a popular optimisation strategy, learning with it can sometimes be slow. The momentum method (Polyak, 1964) was designed to accelerate learning.
- The momentum algorithm accumulates an exponentially decaying moving average of past gradients and continues moving in that direction.
- Formally, the momentum algorithm introduces a variable \mathcal{V} that plays the role of velocity: it specifies the direction and speed at which the parameters move through parameter space.

Goodfellow et al., Deep Learning, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>

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SGD*

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Algorithm 8.1 Stochastic gradient descent (SGD) update**Require:** Learning rate schedule $\epsilon_1, \epsilon_2, \dots$ **Require:** Initial parameter θ $k \leftarrow 1$ **while** stopping criterion not met **do**Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.Compute gradient estimate: $\hat{\mathbf{g}} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$ Apply update: $\theta \leftarrow \theta - \epsilon_k \hat{\mathbf{g}}$ $k \leftarrow k + 1$ **end while**Source: Goodfellow et al., Deep Learning, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>

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SGD with momentum

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Algorithm 8.2 Stochastic gradient descent (SGD) with momentum**Require:** Learning rate ϵ , momentum parameter α **Require:** Initial parameter θ , initial velocity \mathbf{v} **while** stopping criterion not met **do**Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.Compute gradient estimate: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$.Compute velocity update: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$.Apply update: $\theta \leftarrow \theta + \mathbf{v}$.**end while**Source: Goodfellow et al., Deep Learning, <https://www.deeplearningbook.org/contents/optimization.html>

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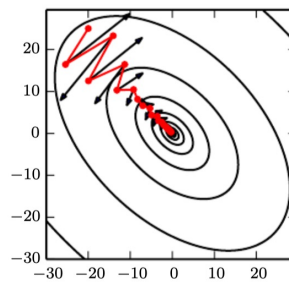
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Momentum*

IMPERIAL

- If $\alpha = 0$, the momentum acts like a normal gradient descent:

An example with a non-zero α :



Source: Goodfellow *et al.*, *deep Learning*, <https://www.deeplearningbook.org/contents/optimization.html>

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Algorithms with adaptive learning rate

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- The **AdaGrad** algorithm adapts the learning rates of all model parameters by scaling them inversely proportional to the square root of the sum of the historical squared gradients (Duchi et al., 2011).

Source: Adapted from Goodfellow et al., *Deep Learning*, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>

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RMSPProp

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- The **RMSPProp** algorithm (Hinton, 2012) modifies AdaGrad to perform better in the nonconvex setting by replacing gradient accumulation with an exponentially weighted moving average.
- AdaGrad shrinks the learning rate according to the entire history of the squared gradient and may have made the learning rate too small before arriving at such a convex structure.
- RMSPProp uses an exponentially decaying average to discard history from the distant past, allowing it to converge rapidly.
- It has a decay rate parameter.

Source: Adapted from Goodfellow et al., Deep Learning, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>

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Adam

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- Adam (Kingma and Ba, 2014) is another adaptive learning rate optimisation algorithm.
- The name “Adam” derives from the phrase “ADaptive Moments.”
- In Adam, momentum is incorporated directly as an estimate of the first-order moment (with exponential weighting) of the gradient.
- The simplest way to add momentum to RMSPProp is to apply it to the rescaled gradients.
- Adam includes bias corrections to the estimates of both the first-order moments (the momentum term) and the (uncentered) second-order moments to account for their initialisation at the origin.

Source: Adapted from Goodfellow et al., Deep Learning, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>

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Adam*

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Adam uses exponential weighted moving averages (also known as leaky averaging) to obtain an estimate of both the momentum and the second moment of the gradient.

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Adam**

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Algorithm 8.7 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)

Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$. (Suggested defaults: 0.9 and 0.999 respectively)

Require: Small constant δ used for numerical stabilization (Suggested default: 10^{-8})

Require: Initial parameters θ

Initialize 1st and 2nd moment variables $\mathbf{s} = \mathbf{0}$, $\mathbf{r} = \mathbf{0}$

Initialize time step $t = 0$

while stopping criterion not met **do**

Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

$t \leftarrow t + 1$

Update biased first moment estimate: $\mathbf{s} \leftarrow \rho_1 \mathbf{s} + (1 - \rho_1) \mathbf{g}$

Update biased second moment estimate: $\mathbf{r} \leftarrow \rho_2 \mathbf{r} + (1 - \rho_2) \mathbf{g} \odot \mathbf{g}$

Correct bias in first moment: $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \rho_1^t}$

Correct bias in second moment: $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1 - \rho_2^t}$

Compute update: $\Delta \theta = -\epsilon \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}} + \delta}}$ (operations applied element-wise)

Apply update: $\theta \leftarrow \theta + \Delta \theta$

end while

Source: Adapted from Goodfellow et al., Deep Learning, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>

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Adam**

Same as the previous slide with just different notations to show the variables and parameters.

ADAM

```
CLASS torch.optim.Adam(params, lr=0.001, betas=(0.9, 0.999), eps=1e-08, weight_decay=0,
                        amsgrad=False, *, foreach=None, maximize=False, capturable=False, differentiable=False,
                        fused=False) [SOURCE]
```

Implements Adam algorithm.

```
input :  $\gamma$  (lr),  $\beta_1, \beta_2$  (betas),  $\theta_0$  (params),  $f(\theta)$  (objective)
         $\lambda$  (weight decay), amsgrad, maximize
initialize :  $m_0 \leftarrow 0$  (first moment),  $v_0 \leftarrow 0$  (second moment),  $\bar{v}_0^{max} \leftarrow 0$ 

for  $t = 1$  to ... do
    if maximize :
         $g_t \leftarrow -\nabla_{\theta} f_t(\theta_{t-1})$ 
    else
         $g_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1})$ 
    if  $\lambda \neq 0$ 
         $g_t \leftarrow g_t + \lambda \theta_{t-1}$ 
     $m_t \leftarrow \beta_1 m_{t-1} + (1 - \beta_1) g_t$ 
     $v_t \leftarrow \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$ 
     $\bar{m}_t \leftarrow m_t / (1 - \beta_1^t)$ 
     $\bar{v}_t \leftarrow v_t / (1 - \beta_2^t)$ 
    if amsgrad
         $\bar{v}_t^{max} \leftarrow \max(\bar{v}_t^{max}, \bar{v}_t)$ 
     $\theta_t \leftarrow \theta_{t-1} - \gamma \bar{m}_t / (\sqrt{\bar{v}_t^{max}} + \epsilon)$ 
    else
         $\theta_t \leftarrow \theta_{t-1} - \gamma \bar{m}_t / (\sqrt{\bar{v}_t} + \epsilon)$ 

return  $\theta_t$ 
```

See: <https://pytorch.org/docs/stable/generated/torch.optim.Adam.html>

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How to choose the number of hidden layers

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- This depends on the complexity of the data and the decision boundaries (i.e. how separable the data is).
- This could also depend on the number of features/dimensions.
- A very basic recommendation is that 2 to 3 hidden layers be used for less complex problems, and 3 to 5 hidden layers be used for more complex problems.
- Several deep learning architectures use more layers. The more layers you add, the more hyperparameters you need to train and optimise. This complexity would impact your network's convergence (and overfitting).
- The number of neurons in hidden layers is also important (width) of the network.

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Dropouts

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- Dropout is a regularisation technique to reduce the risk of overfitting in neural networks.
- In neural networks, it refers to temporarily dropping input and hidden layer nodes.
- This creates a new temporary architecture by randomly dropping a percentage of nodes during the training process.

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Dropout – philosophy

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- A key idea behind applying dropout is that training a neural network by adding a stochastic behaviour and making predictions, and averaging over multiple stochastic decisions simulates a form of bagging with parameter sharing.
- In Bagging (i.e., bootstrap aggregation), several models are combined to reduce the generalisation error.
- The idea of Bagging is to train multiple models separately and then use all the models to vote on the output for the test example.

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Dropouts – practical notes

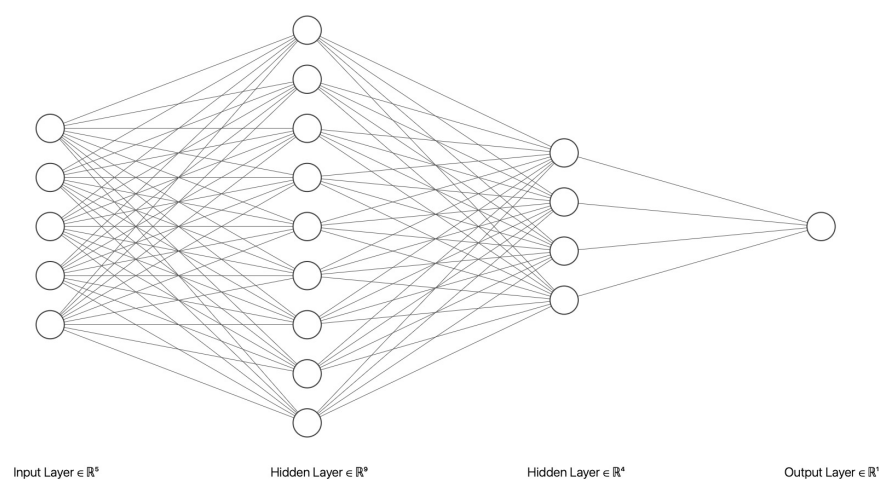
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- When the training sample is very small, the dropout method is not very effective.
- When additional unlabeled samples are available, unsupervised feature learning can improve performance better than dropout.

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Example

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Open discussion

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You're training an MLP to predict stroke risk from patient data (age, blood pressure, imaging features). The network has multiple hidden layers and uses ReLU activations.

- **Gradient Flow:**
 - How do optimisers like **SGD**, **Momentum**, and **Adam** affect convergence speed and stability in deep MLPs?
 - What happens if gradients vanish or explode during training?
- **Learning Rate Scheduling:**
 - Why is a fixed learning rate problematic for MLPs?
 - How do adaptive methods (Adam, RMSProp) compare to scheduled decay?
- **Regularisation and Generalisation:**
 - How do dropout and weight decay interact with optimiser behaviour?
 - Can an optimiser compensate for poor regularisation choices?

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Review questions

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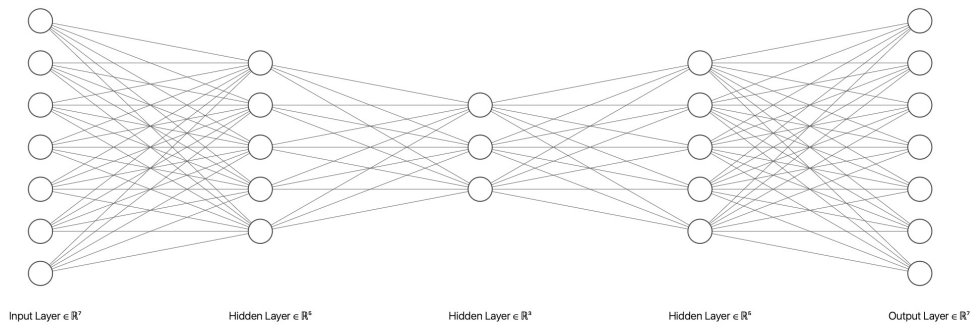
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Q1

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– What could be the purpose of a NN architecture like this?



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Q2

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– Which of these will not improve the convergence of a neural network model?

- Adaptive learning rate
- Data normalisation
- Using an optimiser method
- Initialising all the weights to zero (zero initialisation)

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Acknowledgments

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- Some of the slides are adapted from Dive into Deep Learning by Aston Zhang *et al.*, <https://d2l.ai/index.html>

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If you have any questions

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- Please feel free to arrange a meeting or email (p.barnaghi@imperial.ac.uk).
- My office: 928, Sir Michael Uren Research Hub, White City Campus.

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Further reading

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Derivative of Sigmoid function

$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}.$$

$$\frac{d}{dx} \text{sigmoid}(x) = \frac{\exp(-x)}{(1 + \exp(-x))^2} = \text{sigmoid}(x) (1 - \text{sigmoid}(x)).$$

If you are interested in the proof of how this is derived, see:

Lin (2019, Jan. 12). Data science: Data science tutorials.

<https://hausetutorials.netlify.app/posts/2019-12-01-neural-networks-deriving-the-sigmoid-derivative/>

For more information on e^x derivative, see:

<http://www.intuitive-calculus.com/derivative-of-e-x.html>

Source for the formula: Dive into Deep Learning by Aston Zhang et al., <https://d2l.ai/index.html>

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Gradient of ReLU

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$$\text{gradient of ReLU} = \frac{\partial \text{ReLU}(x)}{\partial x} = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases}$$

For other gradients and an excellent summary, you can refer to the blog post by by Andrew Wood at:

https://aew61.github.io/blog/artificial_neural_networks/l_background/l_b_activation_functions_and_derivatives.html

Source for the formula: Dive into Deep Learning by Aston Zhang et al., <https://d2l.ai/index.html>

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Random initialisation**

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- *Pytorch* return the recommended gain value for the given nonlinearity function.
- According to the method described in *Understanding the difficulty of training deep feedforward neural networks*, Glorot, X. & Bengio, Y. (2010), using a uniform distribution. The resulting tensor will have values sampled from $U(-a, a)$ where (also known as Glorot initialisation):

$$a = \text{gain} \times \sqrt{\frac{6}{\text{fan_in} + \text{fan_out}}}$$

fan_in and *fan_out*:

<https://stackoverflow.com/questions/42670274/how-to-calculate-fan-in-and-fan-out-in-xavier-initialization-for-neural-networks>

Source: <https://pytorch.org/docs/stable/nn.init.html>

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Newton's method**

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- Newton's method is an optimisation scheme based on using a second-order Taylor series expansion to approximate $J(\theta)$ near some point θ_0 ignoring derivatives a of higher order:

$$J(\theta) \approx J(\theta_0) + (\theta - \theta_0)^\top \nabla_{\theta} J(\theta_0) + \frac{1}{2}(\theta - \theta_0)^\top \mathbf{H}(\theta - \theta_0)$$

- Where H is the *Hessian* of J with respect to θ evaluated at θ_0 If we then solve for the critical point of this function, we obtain the Newton parameter update rule:

$$\theta^* = \theta_0 - \mathbf{H}^{-1} \nabla_{\theta} J(\theta_0)$$

Source: Adapted from Goodfellow et al., deep Learning, <https://www.deeplearningbook.org/contents/optimization.html>
For more information see Chapter 8 of Goodfellow et al.'s book.

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Newton's method – the algorithm

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- If the objective function is convex but not quadratic (there are higher-order terms), this update can be iterated, yielding the training algorithm associated with Newton's method, given in algorithm

Algorithm 8.8 Newton's method with objective $J(\theta) = \frac{1}{m} \sum_{i=1}^m L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

Require: Initial parameter θ_0

Require: Training set of m examples

while stopping criterion not met **do**

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

 Compute Hessian: $\mathbf{H} \leftarrow \frac{1}{m} \nabla_{\theta}^2 \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

 Compute Hessian inverse: \mathbf{H}^{-1}

 Compute update: $\Delta\theta = -\mathbf{H}^{-1} \mathbf{g}$

 Apply update: $\theta = \theta + \Delta\theta$

end while

Source: Adapted from Goodfellow et al., Deep Learning, MIT Press, <https://www.deeplearningbook.org/contents/optimization.html>

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The *Hessian* Matrix (H)

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– For more information on the Hessian matrix and how to derive it, see:

<https://www.khanacademy.org/math/multivariable-calculus/applications-of-multivariable-derivatives/quadratic-approximations/a/the-hessian>

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