CEE 616: Probabilistic Machine Learning
M3 Deep Neural Networks:
Neural Networks for Structured Data I

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Outline

Neural networks

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- Also known as a **multilayer perception** (MLP)
- When L is large, this is termed a **deep neural network** (DNN)

Biological neuron

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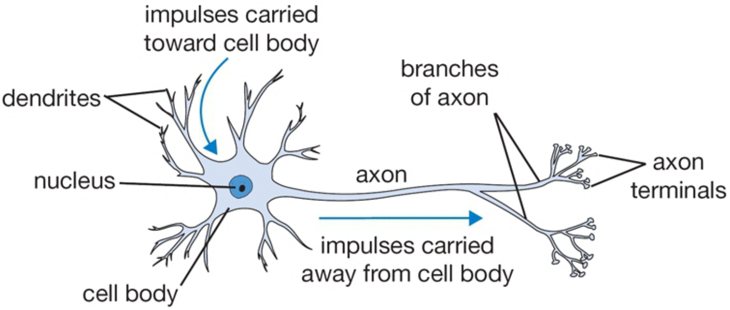

Figure: Biological neuron (Source: `https://cs231n.github.io/neural-networks-1/`)

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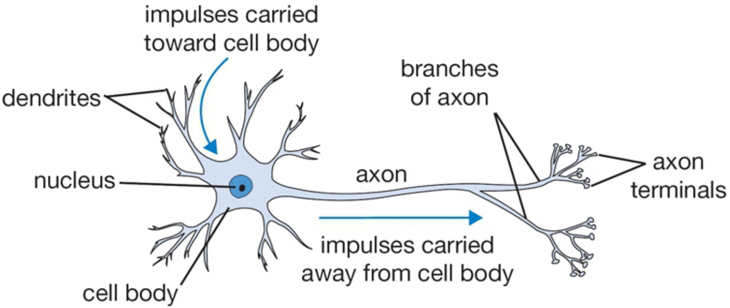

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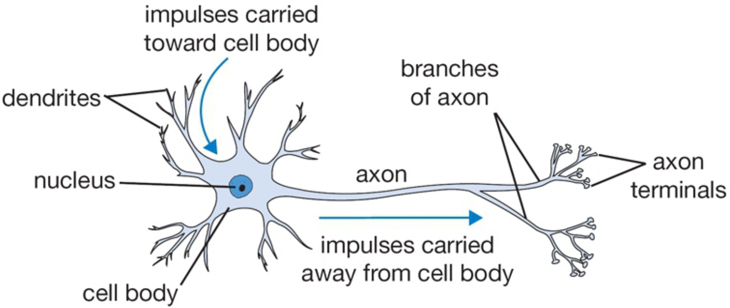

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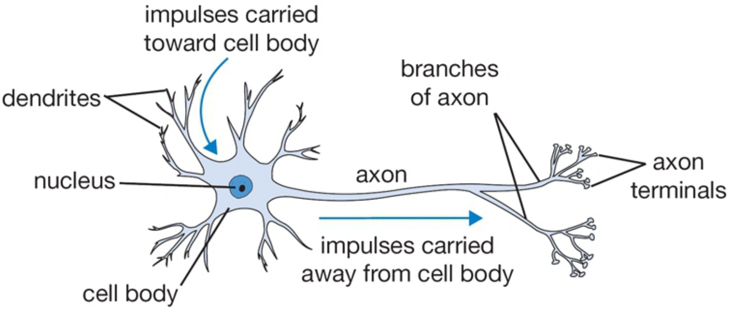

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- The axon in turn connects to other neurons via synapses

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- The output neurons have no activation function. Instead, they perform a final transformation of outputs from the penultimate layer

Computational neuron model

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axon from a neuron

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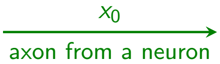

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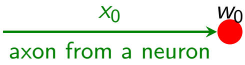

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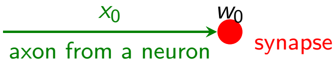

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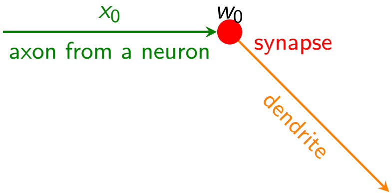

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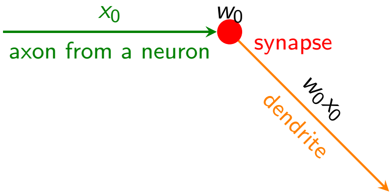

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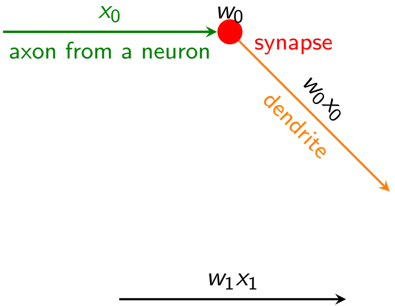

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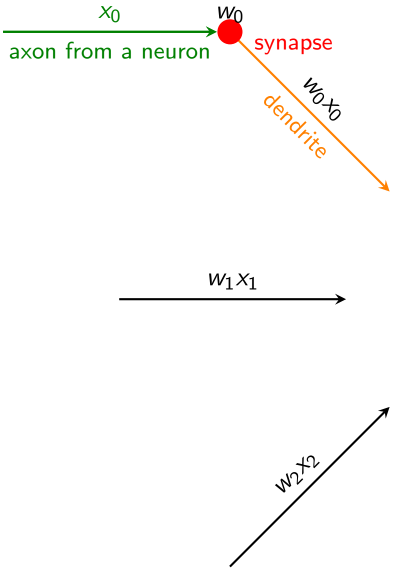

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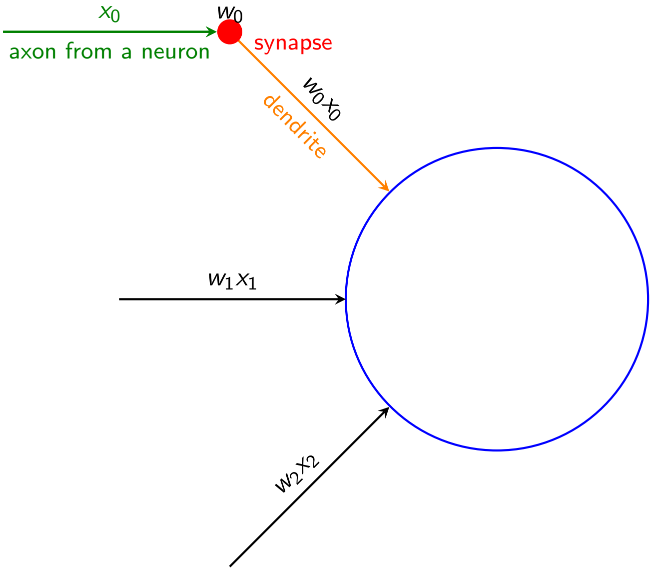

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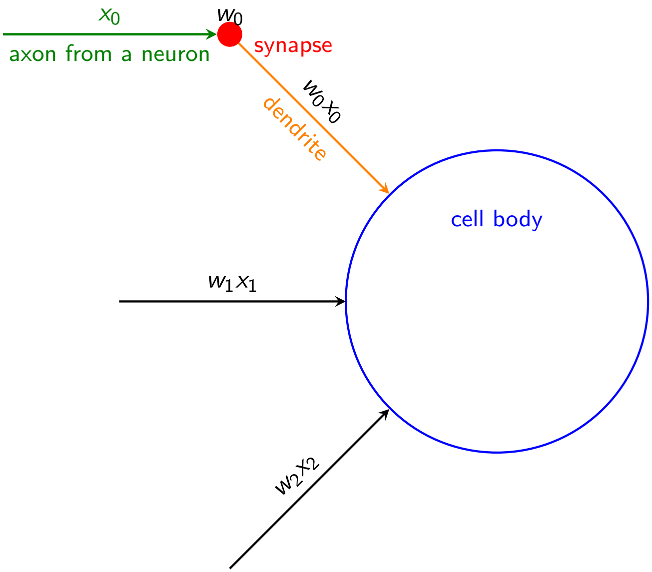

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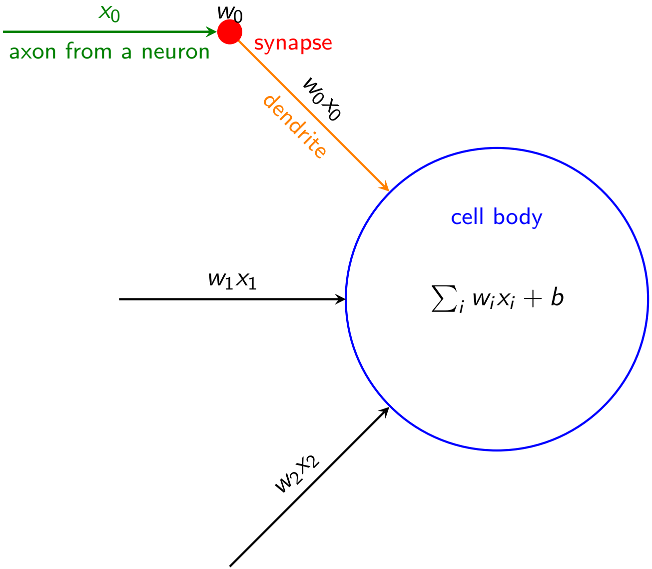

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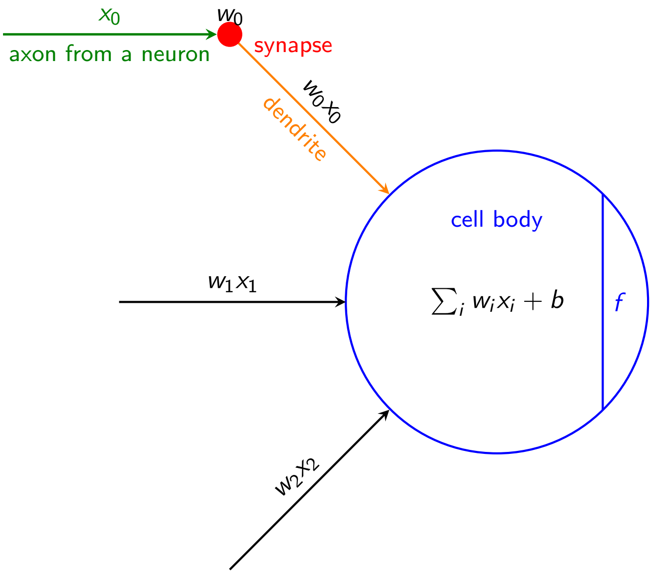

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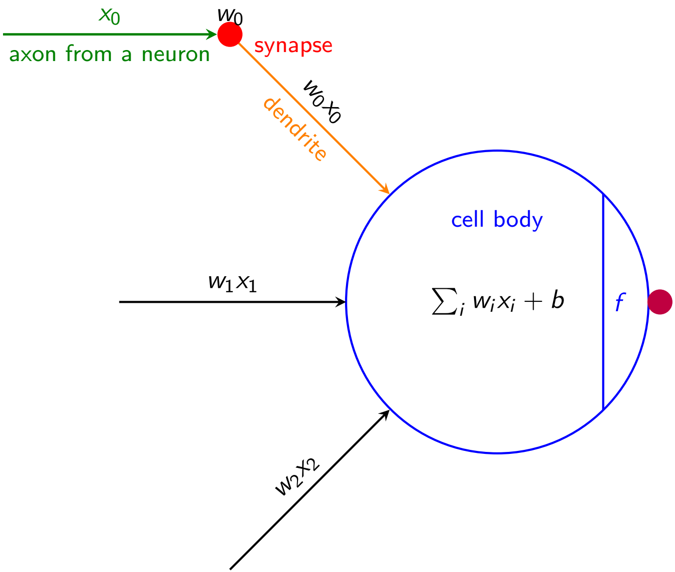

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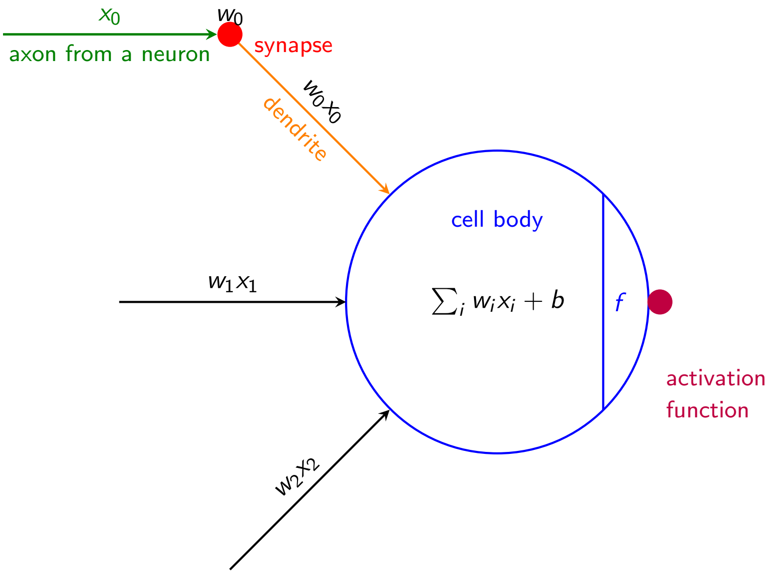

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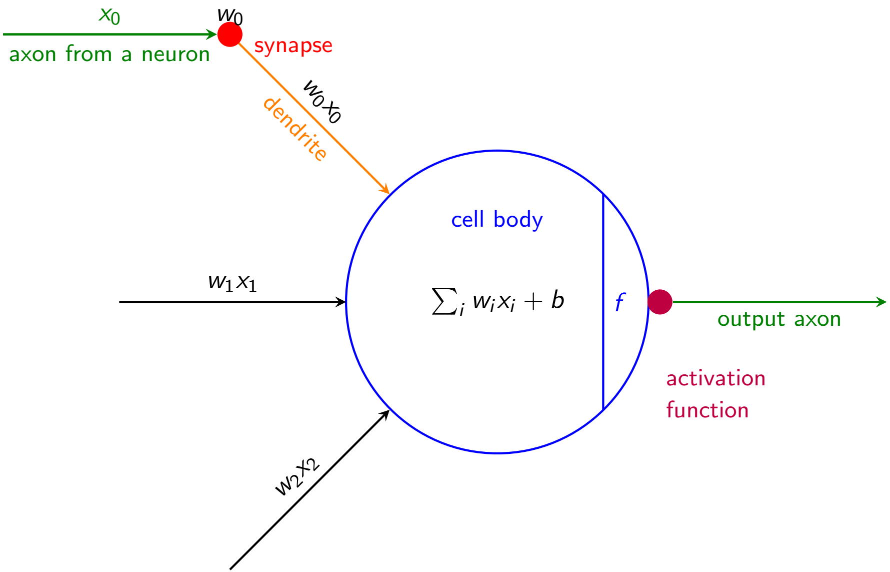

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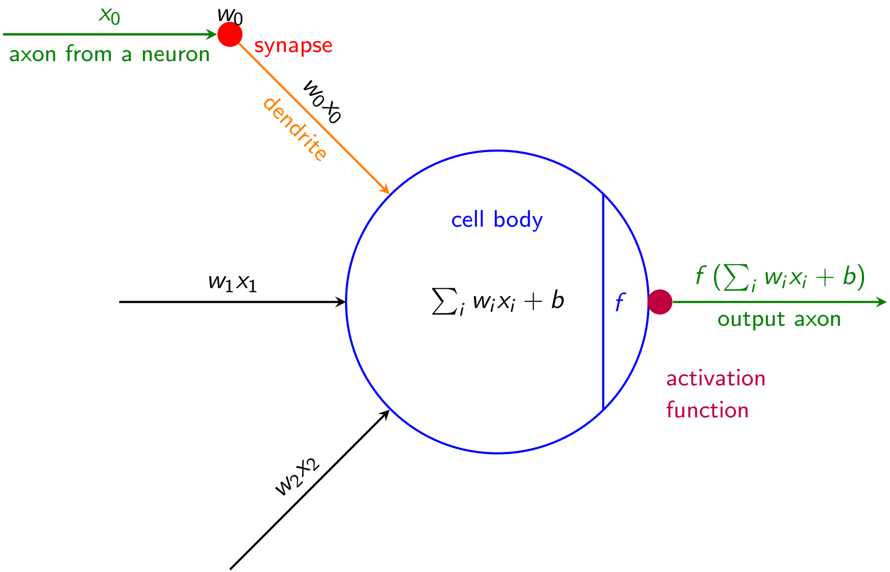

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- The output of a neuron is also called the *activation*

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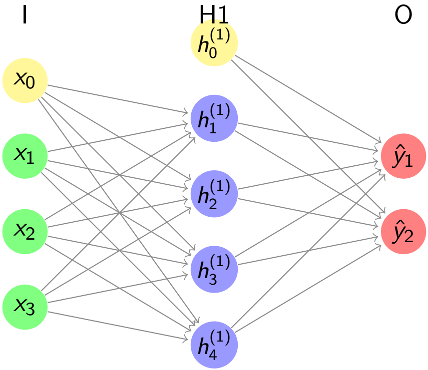
Two-layer neural network (with bias neurons)



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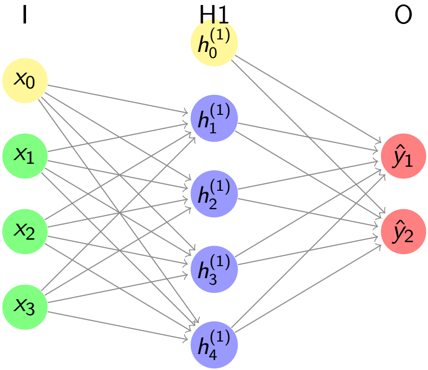

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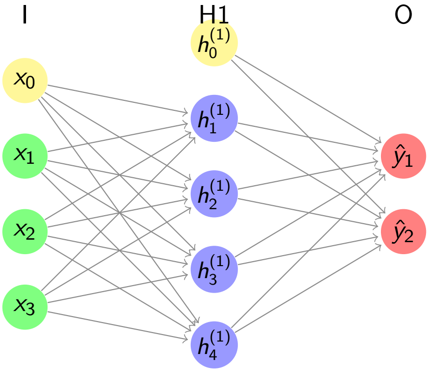

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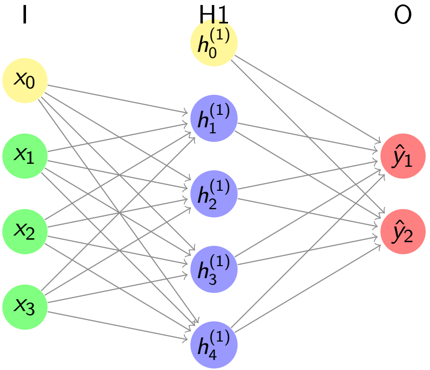

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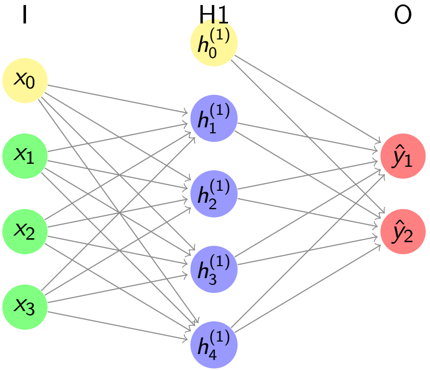

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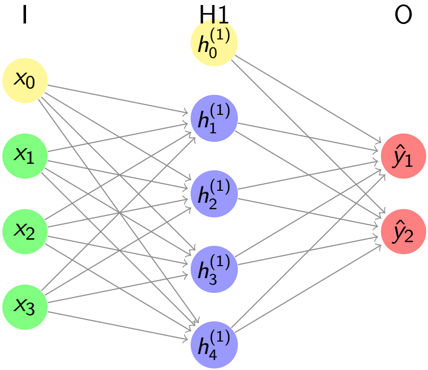

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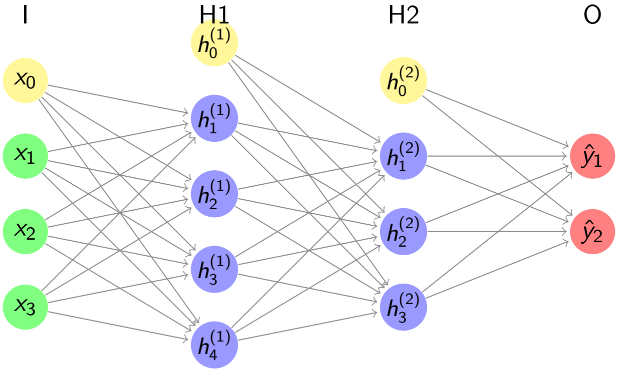

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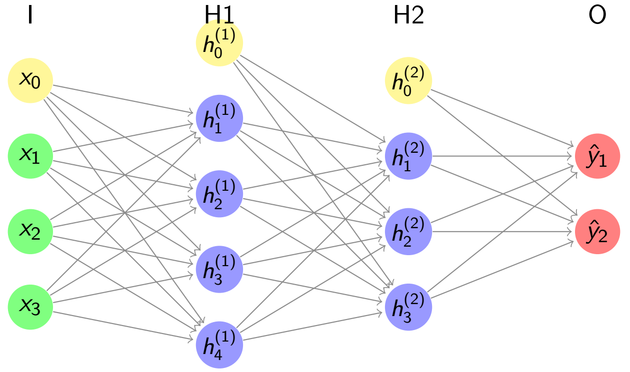

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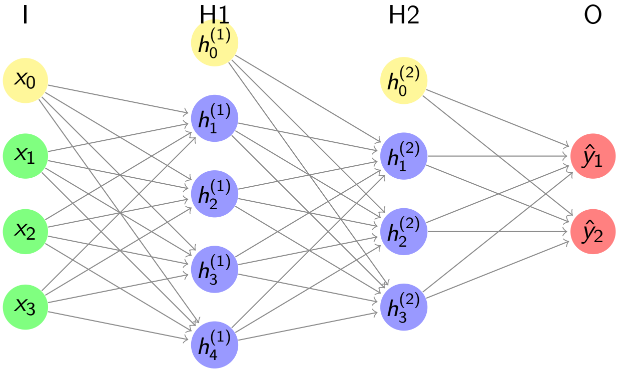

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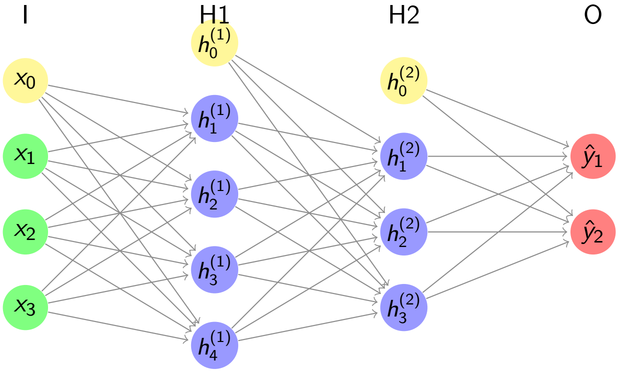

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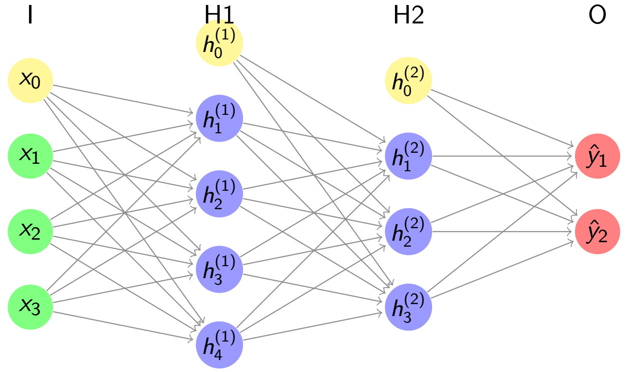

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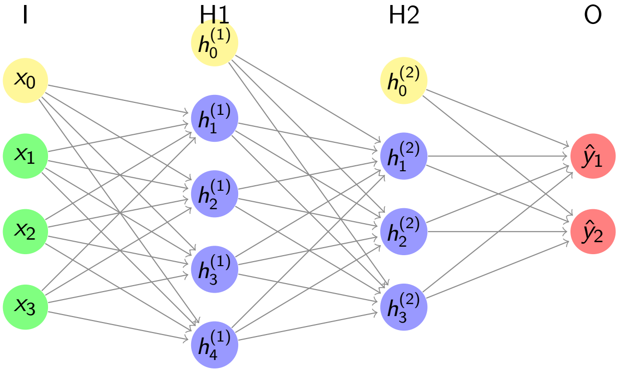

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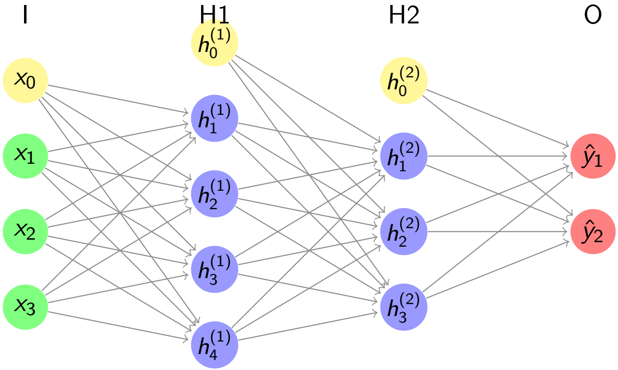

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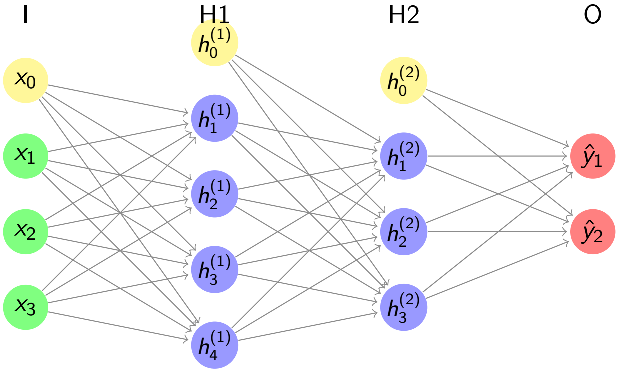

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  Thus

$$\boldsymbol{z}_\ell = \varphi_\ell(\boldsymbol{a}_\ell) \tag{7}$$

- In the historic MLP, the activation function was the non-differentiable Heaviside function (difficult to train)
- Later on, the sigmoid was introduced (smooth, trainable/differentiable)

Examples of activation functions

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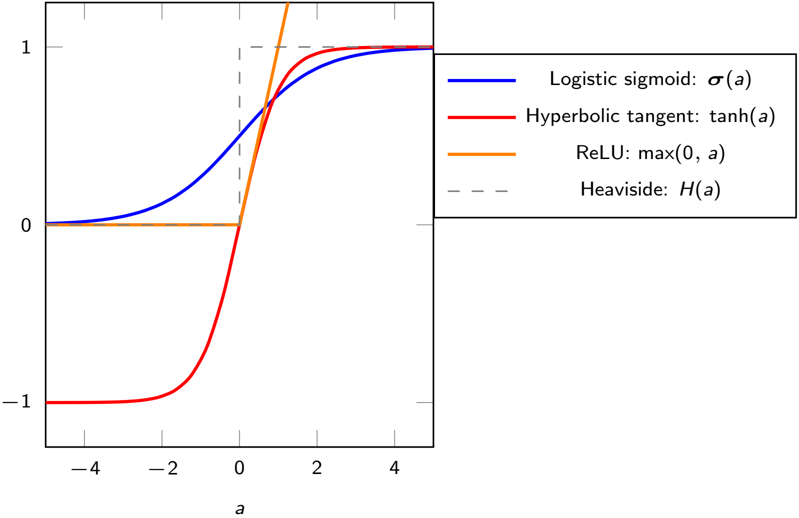

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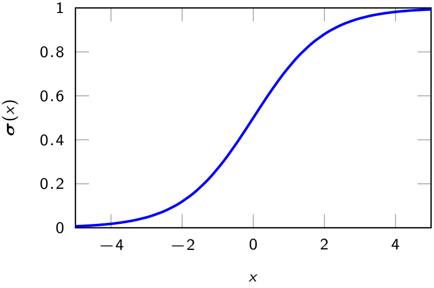

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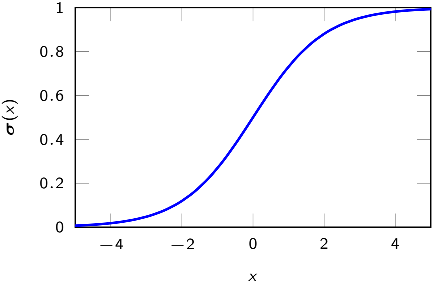

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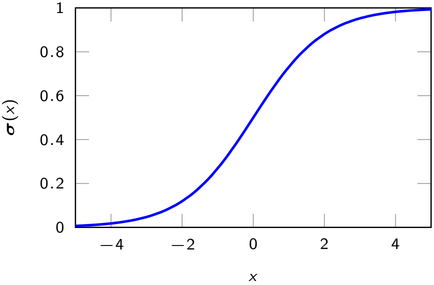

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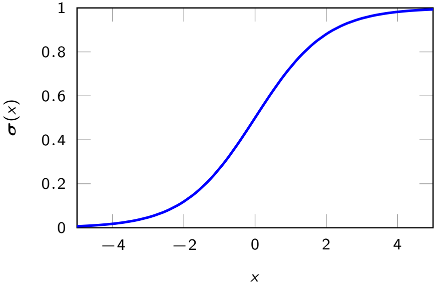

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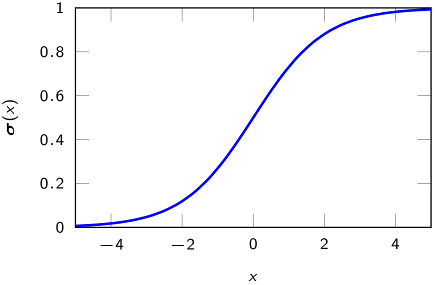

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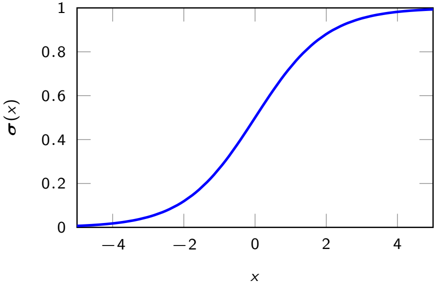

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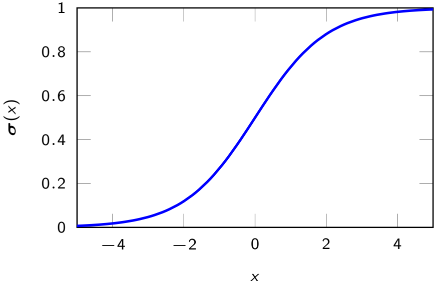

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- Recently, it has been superseded by the hyperbolic tangent due to its (a) gradient saturation and (b) non-zero-centeredness.

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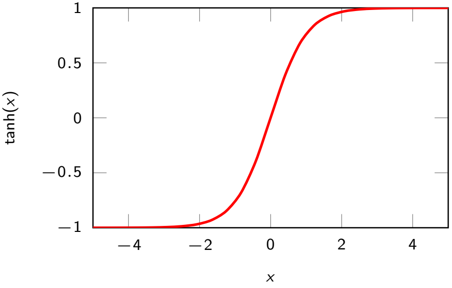

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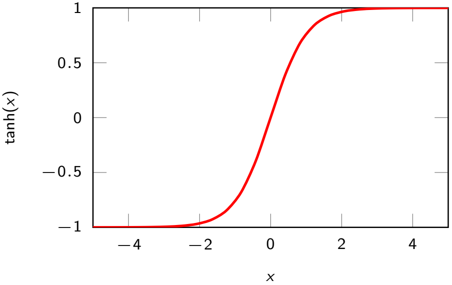

- Preferred to sigmoid activation function due to its zero-centeredness.

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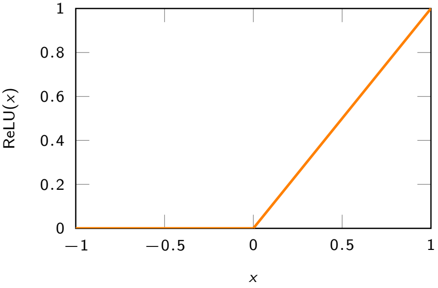

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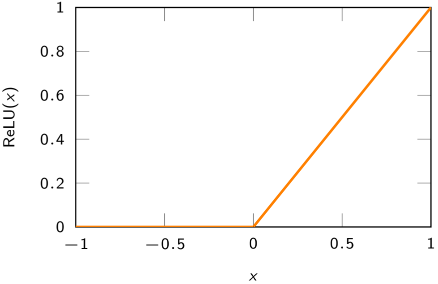

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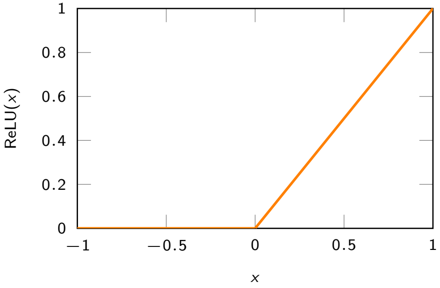

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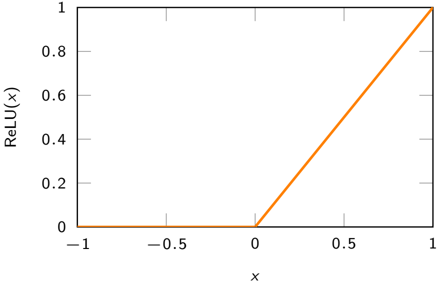

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- Popular for deep convolutional networks (several hidden layers)
- Neurons can be fragile, however, requiring care in selection of learning rate

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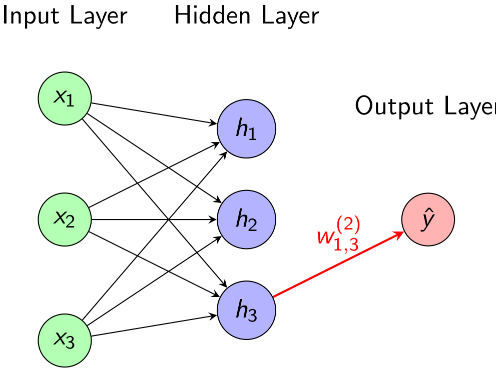

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Given the activation vector (D neurons) in the zeroth (input) layer:

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Example: If Layer 1 had only two neurons, then the weight matrix $\boldsymbol{W}$ would have only 2 rows.

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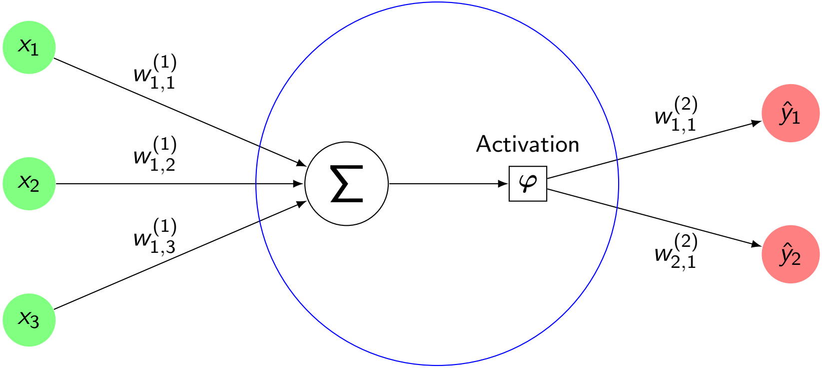
This simple MLP has 2 layers (1 hidden, one outer), and



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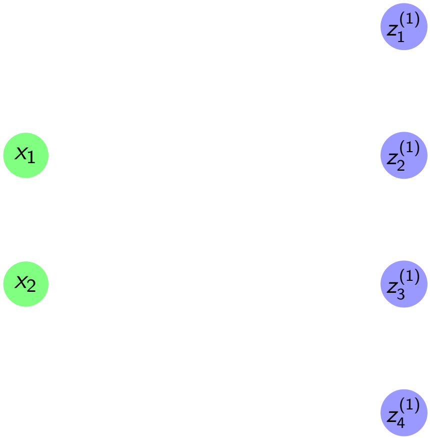

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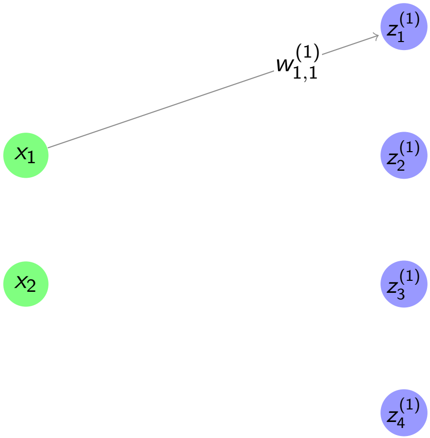

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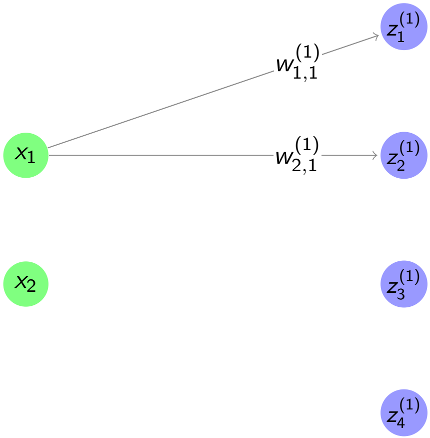

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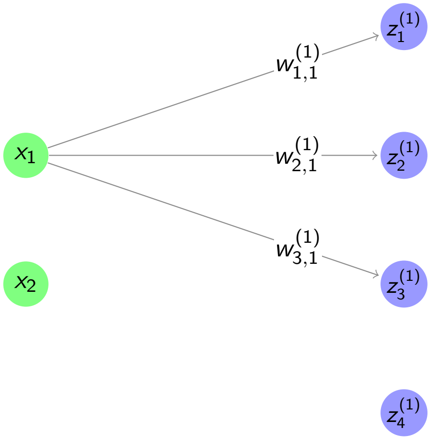

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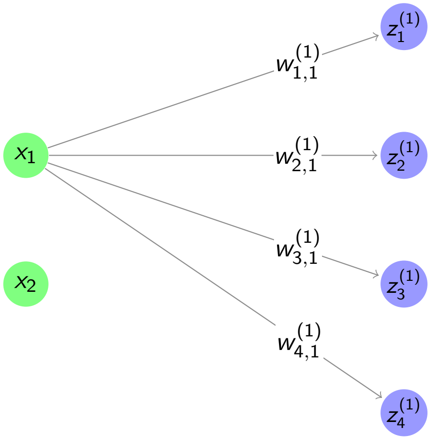

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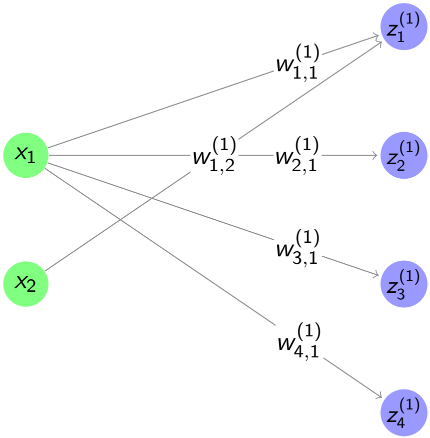

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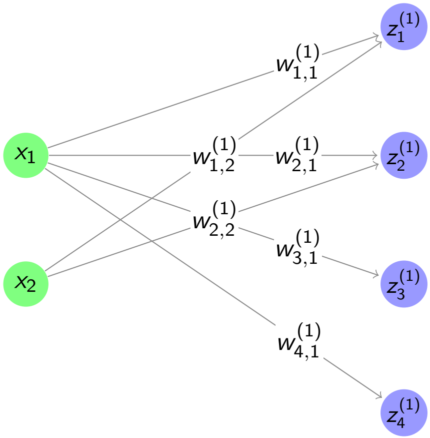

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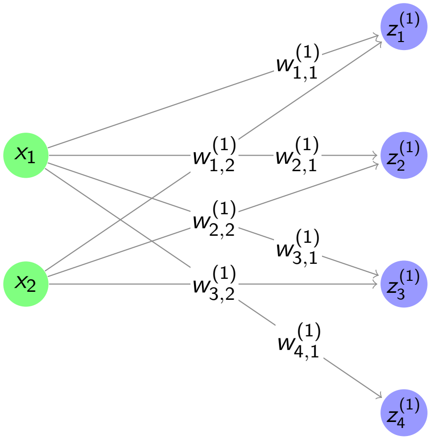

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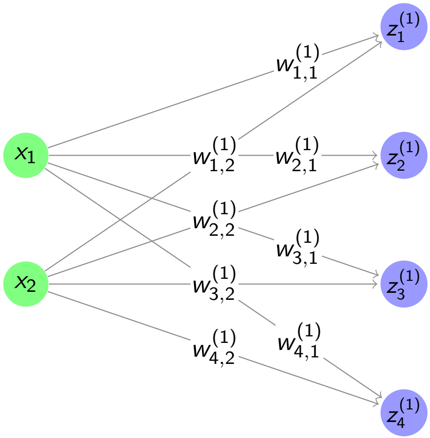

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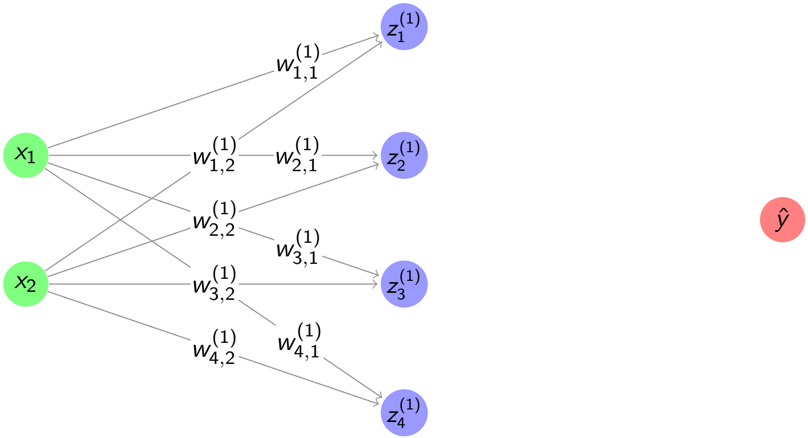

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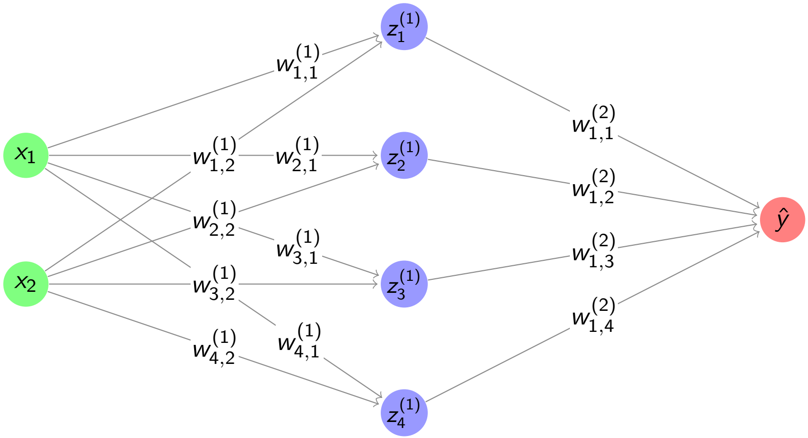

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Given an observation x_{nd} with $d = 1, \ldots, D$ features, these equations describe the output from a 2-layer network:

$$
\begin{aligned}
z_m^{(1)} &= \varphi\left(\sum_{d=1}^{D} w_{1,d}^{(1)} x_{nd} + b_d^{(1)}\right) \\
y_i(x_i) &= \sum_{m=1}^{M} w_{1,m}^{(2)} z_m^{(1)} + b^{(2)}
\end{aligned}
$$

- D is number of input neurons
- M is number of hidden neurons
- Total number of learnable parameters: $M(D+1)$ weights and $(D+1)$ biases
- Linear/identity activation is used in output

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- In neural networks, the gradients are computed via **backpropagation**

Backpropagation overview

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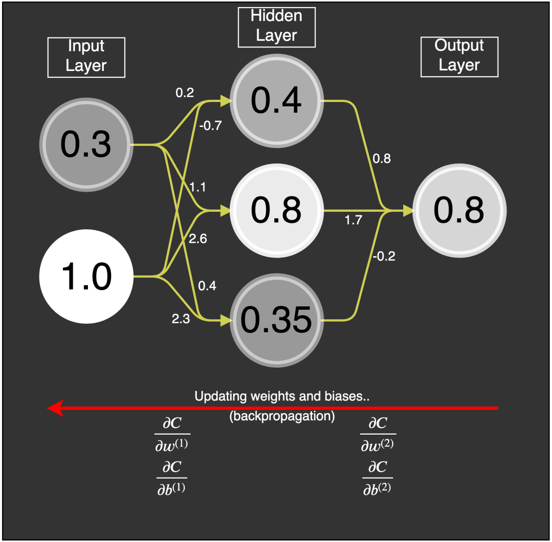

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  where L is the last layer and $\boldsymbol{a} = \boldsymbol{W}\boldsymbol{z}^{\ell-1} + \boldsymbol{b}$
- Repeat the forward and backward passes until cost is sufficiently minimized

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$$\frac{\partial \mathcal{L}}{\partial w^{(L-1)}} = \frac{\partial \mathcal{L}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial w^{(L-1)}} \tag{33}$$

$$= \frac{\partial \mathcal{L}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L)}} \frac{\partial z^{(L)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial w^{(L-1)}} \tag{34}$$

$$\frac{\partial \mathcal{L}}{\partial b^{(L-1)}} = \frac{\partial \mathcal{L}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial b^{(L-1)}} \tag{35}$$

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Backward pass (cont.)

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Backward pass (cont.)

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$$w^{(L-1),r+1} = w^{(L-1),r} - \eta \frac{\partial \mathcal{L}}{\partial w^{(L-1)}} \tag{37}$$

Backward pass (cont.)

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Once these gradients are computed, we update the weights for the $(r+1)$th iteration using:

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$$b^{(L-1),r+1} = b^{(L-1),r} - \eta \frac{\partial \mathcal{L}}{\partial b^{(L-1)}} \tag{38}$$

Summary: forward pass

1. ($r = 0$): Initialize weights and biases: $w^{(l),0}$, $b^{(l),0}$

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At output layer:

$$a^{(L),0} = w^{(L),0} \times z^{(L-1),0} + b^{(L),0} \quad (41)$$

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At output layer:

$$a^{(L),0} = w^{(L),0} \times z^{(L-1),0} + b^{(L),0} \quad (41)$$
$$o = \varphi(a^{(L),0}) \quad (42)$$
$$C = (o - y)^2 \quad (43)$$

Summary: backward pass—outer layer

3. Backward pass, outer layer (L):

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Summary: backward pass—outer layer

3. Backward pass, outer layer (L):
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$$\frac{\partial \mathcal{L}}{\partial w^{(L)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial w^{(L)}} \qquad (44)$$

Summary: backward pass—outer layer

3. Backward pass, outer layer (L):
    1. Compute gradients:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w^{(L)}} &= \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial w^{(L)}} \\
\frac{\partial \mathcal{L}}{\partial b^{(L)}} &=
\end{aligned}
\tag{44}
$$

Summary: backward pass—outer layer

3. Backward pass, outer layer (L):
   1. Compute gradients:

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Summary: backward pass—outer layer

3. Backward pass, outer layer (L):
   1. Compute gradients:

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$$\frac{\partial \mathcal{L}}{\partial b^{(L)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial b^{(L)}} \tag{45}$$

   2. Update weights:

Summary: backward pass—outer layer

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   1. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial w^{(L)}} \quad (44)$$

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Summary: backward pass—outer layer

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$$\frac{\partial \mathcal{L}}{\partial b^{(L)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial b^{(L)}} \tag{45}$$

   2. Update weights:

$$w^{(L),1} = w^{(L),0} - \eta \frac{\partial C^0}{\partial w^{(L)}} \tag{46}$$

Summary: backward pass—outer layer

3. Backward pass, outer layer (L):
   1. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial w^{(L)}} \tag{44}$$

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$$b^{(L),1} = b^{(L),0} - \eta \frac{\partial C^0}{\partial b^{(L)}} \tag{47}$$

Summary: backward pass—last hidden layer

3. Backward pass, layer $(L-1)$:

Summary: backward pass—last hidden layer

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3. Backward pass, layer $(L-1)$:
    3. Compute gradients:

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Summary: backward pass—last hidden layer

3. Backward pass, layer $(L-1)$:
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$$\frac{\partial \mathcal{L}}{\partial w^{(L-1)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial w^{(L-1)}} \tag{48}$$

Summary: backward pass—last hidden layer

3. Backward pass, layer $(L-1)$:
   3. Compute gradients:

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$$\frac{\partial \mathcal{L}}{\partial b^{(L-1)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial b^{(L-1)}} \quad (49)$$

Summary: backward pass—last hidden layer

3. Backward pass, layer $(L-1)$:
   3. Compute gradients:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w^{(L-1)}} &= \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial w^{(L-1)}} \qquad (48) \\
\frac{\partial \mathcal{L}}{\partial b^{(L-1)}} &= \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial b^{(L-1)}} \qquad (49)
\end{aligned}
$$

   4. Update weights:

Summary: backward pass—last hidden layer

3. Backward pass, layer $(L-1)$:
   3. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L-1)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial w^{(L-1)}} \quad (48)$$

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3. Backward pass, layer $(L-1)$:
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   4. Update weights:

$$w^{(L-1),1} =$$

Summary: backward pass—last hidden layer

3. Backward pass, layer $(L-1)$:
   3. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L-1)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial w^{(L-1)}} \quad (48)$$

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   4. Update weights:

$$w^{(L-1),1} = w^{(L-1),0} -$$

Summary: backward pass—last hidden layer

3. Backward pass, layer $(L-1)$:
   3. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L-1)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial w^{(L-1)}} \quad (48)$$

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Summary: backward pass—last hidden layer

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$$b^{(L-1),1} =$$

Summary: backward pass—last hidden layer

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Summary: backward pass—last hidden layer

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   4. Update weights:

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$$b^{(L-1),1} = b^{(L-1),0} - \eta \frac{\partial \mathcal{L}}{\partial b^{(L-1)}} \tag{51}$$

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:
    5. Compute gradients:

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:
   5. Compute gradients:

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:
    5. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L-2)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}}$$

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:
   5. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L-2)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial z^{(L-2)}}$$

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:
   5. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L-2)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial z^{(L-2)}} \frac{\partial z^{(L-2)}}{\partial a^{(L-2)}} \frac{\partial a^{(L-2)}}{\partial w^{(L-2)}} \tag{52}$$

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:
   5. Compute gradients:

$$\frac{\partial \mathcal{L}}{\partial w^{(L-2)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \frac{\partial a^{(L-1)}}{\partial z^{(L-2)}} \frac{\partial z^{(L-2)}}{\partial a^{(L-2)}} \frac{\partial a^{(L-2)}}{\partial w^{(L-2)}} \quad (52)$$

$$\frac{\partial \mathcal{L}}{\partial b^{(L-2)}} = \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}}$$

Summary: backward pass—second-to-last hidden layer

3. Backward pass, layer $(L-2)$:
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Summary: backward pass—first hidden layer

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$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial w^{(1)}} &= \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \cdots \frac{\partial a^{(2)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial w^{(1)}} \qquad (56) \\ \frac{\partial \mathcal{L}}{\partial b^{(1)}} &= \frac{\partial \mathcal{L}}{\partial o^{(L)}} \frac{\partial o^{(L)}}{\partial a^{(L)}} \frac{\partial a^{(L)}}{\partial z^{(L-1)}} \frac{\partial z^{(L-1)}}{\partial a^{(L-1)}} \end{aligned}$$

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1. Fix initial weights $w^{(l),0}$, $b^{(l),0}$ and perform a forward sweep/pass through the network computing the activations a (outputs) of each layer l as:

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3. Then, we *backpropagate* the errors through each layer in order to compute the gradients $\frac{\partial \mathcal{L}}{\partial w^{(l)}}$, $\frac{\partial \mathcal{L}}{\partial b^{(l)}}$ and weight updates $w^{(l),r+1}$ and $b^{(l),r+1}$
4. Repeat the forward and backward passes until cost is sufficiently minimized

Example: backpropagation for 3-layer network

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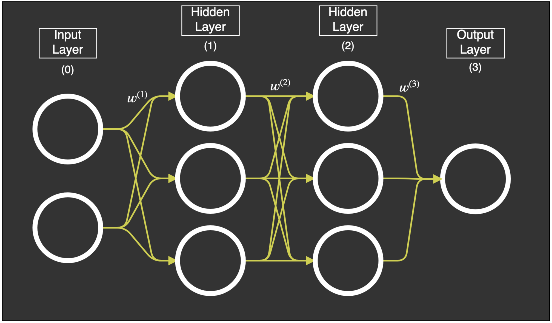

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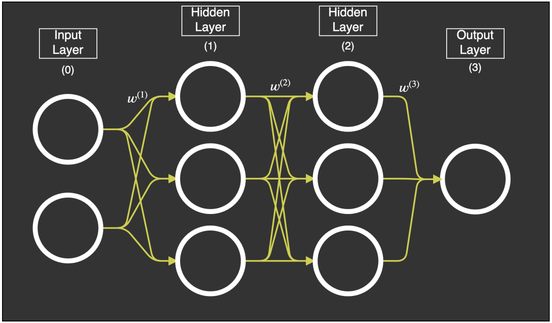

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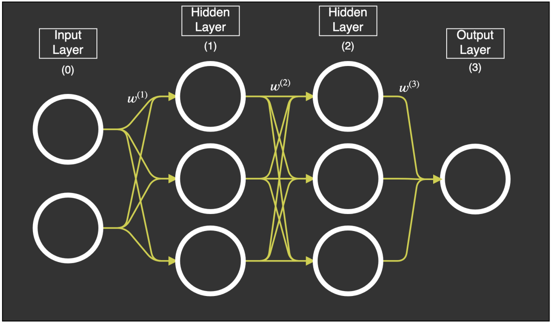

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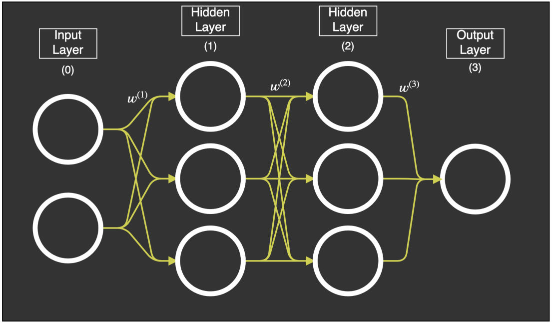

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$$\frac{\partial \mathcal{L}}{\partial w^{(1)}} = \frac{\partial \mathcal{L}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial w^{(1)}} \tag{63}$$

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loss function	MSE or MAE/Huber

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Other types of neural networks

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- Long short-term memory networks (LSTMs): time-series, pattern identification, etc.

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- Experiment in this **playground**