Deep Learning

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Big Idea

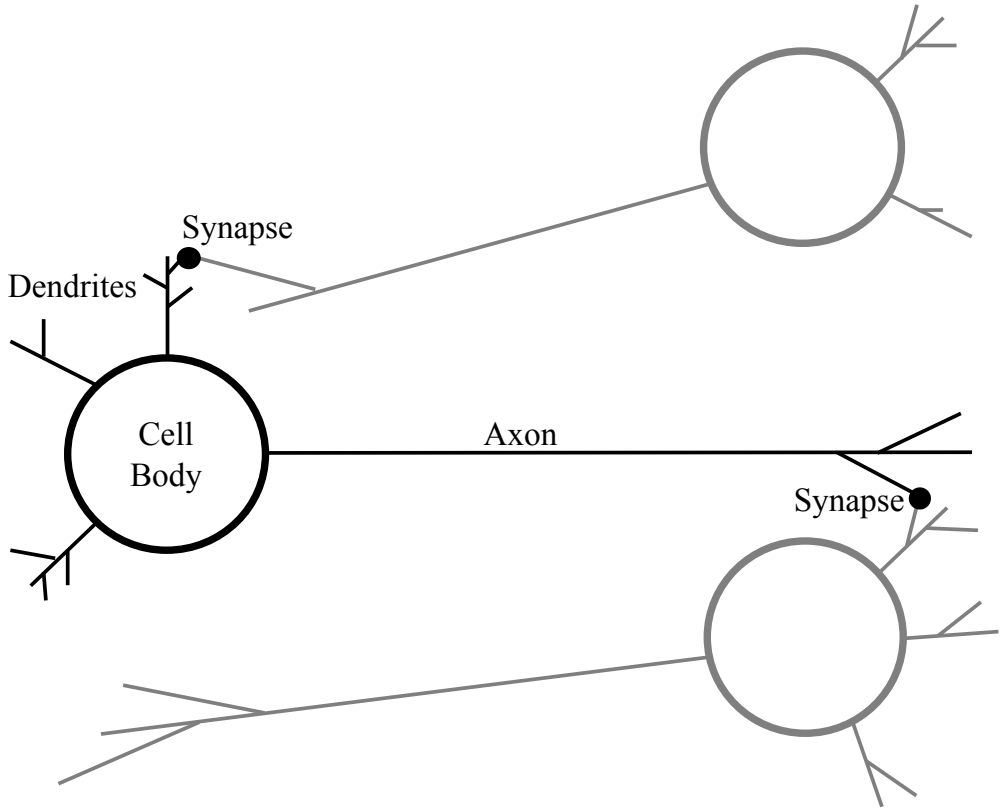


Figure 1: A high-level schematic of the structure of a neuron. This figure illustrates three interconnected neurons; the middle neuron is highlighted in black, and the major structural components of this neuron are labeled cell body, dendrites, and axon. Also marked are the synapses connecting the axon of one neuron and the dendrite of another, which allow signals to pass between the neurons.

Fundamentals

$$z = \underbrace{\mathbf{w}[0] \times \mathbf{d}[0] + \mathbf{w}[1] \times \mathbf{d}[1] + \cdots + \mathbf{w}[m] \times \mathbf{d}[m]}_{weighted\ sum} \tag{1}$$

$$= \sum_{j=0}^{m} \mathbf{w}[j] \times \mathbf{d}[j]$$

$$= \underbrace{\mathbf{w} \cdot \mathbf{d}}_{dot\ product} = \underbrace{\mathbf{w}^T \mathbf{d}}_{matrix\ product} = [w_0, w_1, \ldots, w_m] \begin{bmatrix} d_0 \\ d_2 \\ \vdots \\ d_m \end{bmatrix} \tag{2}$$

$$\mathbb{M}_{\mathbf{w}}(\mathbf{d}) = \begin{cases} 1 & \text{if } z \geq \theta \\ 0 & otherwise \end{cases} \tag{3}$$

$$rectifier(z) = max(0, z) \tag{4}$$

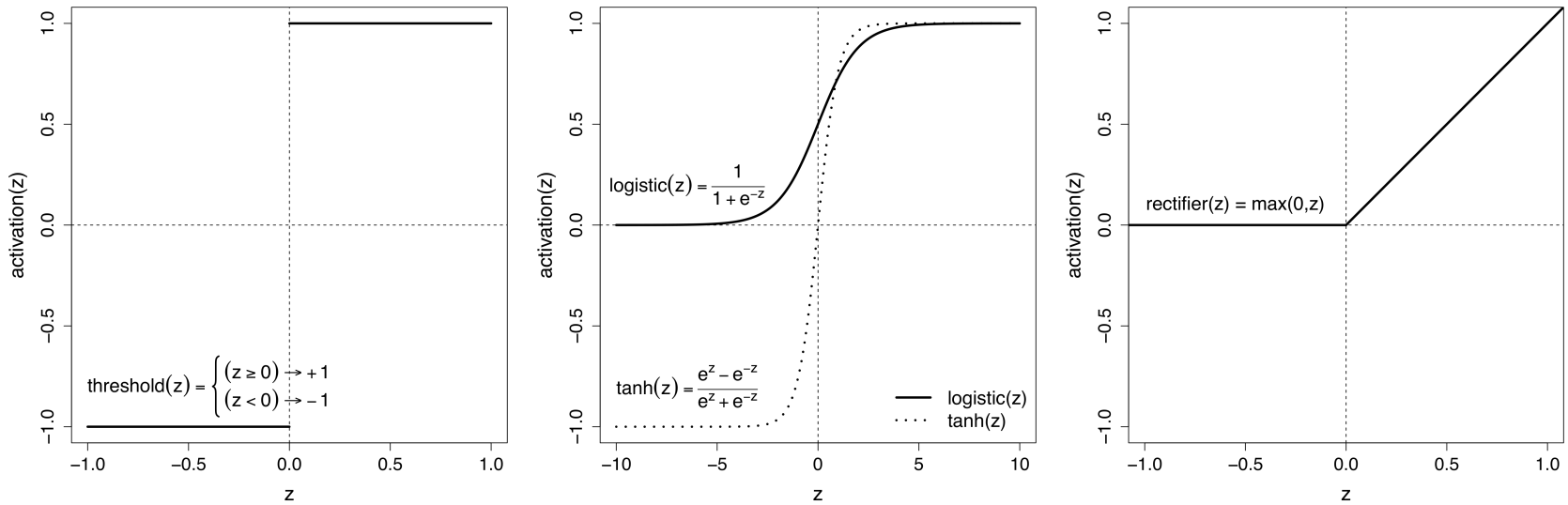


Figure 2: Plots for activation functions that have been popular in the history of neural networks.

$$\begin{aligned}
\mathbb{M}_{\mathbf{w}}(\mathbf{d}) &= \varphi\left(\mathbf{w}\left[0\right] \times \mathbf{d}\left[0\right] + \mathbf{w}\left[1\right] \times \mathbf{d}\left[1\right] + \cdots + \mathbf{w}\left[m\right] \times \mathbf{d}\left[m\right]\right) \\
&= \varphi\left(\sum_{i=0}^{m} w_i \times d_i\right) = \varphi\left(\underbrace{\mathbf{w} \cdot \mathbf{d}}_{dot\ product}\right) \\
&= \varphi\left(\underbrace{\mathbf{w}^T \mathbf{d}}_{matrix\ product}\right) = \varphi\left([w_0, w_1, \ldots, w_m] \begin{bmatrix} d_0 \\ d_2 \\ \vdots \\ d_m \end{bmatrix}\right)
\end{aligned} \tag{5}$$

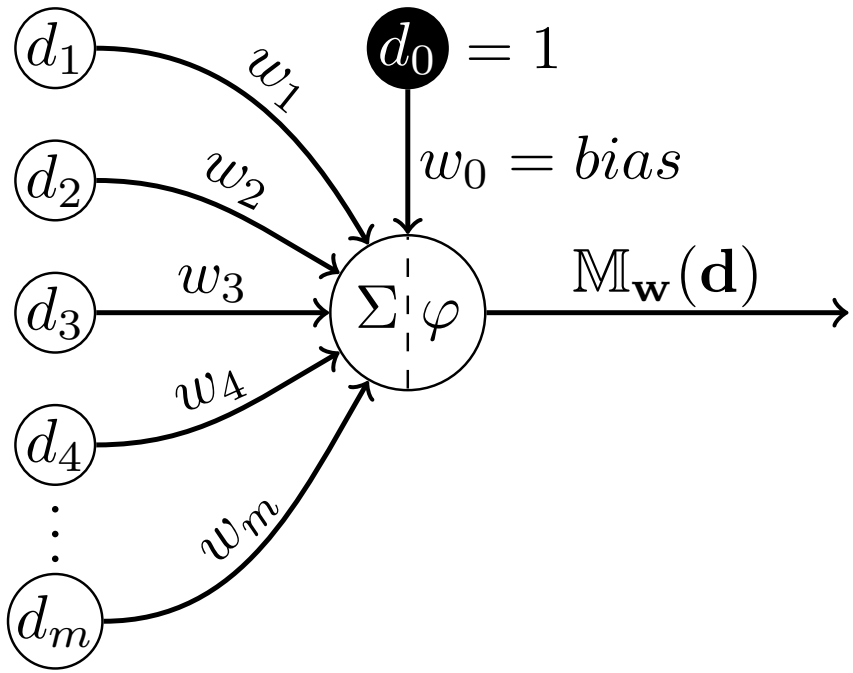


Figure 3: A schematic of an artificial neuron.

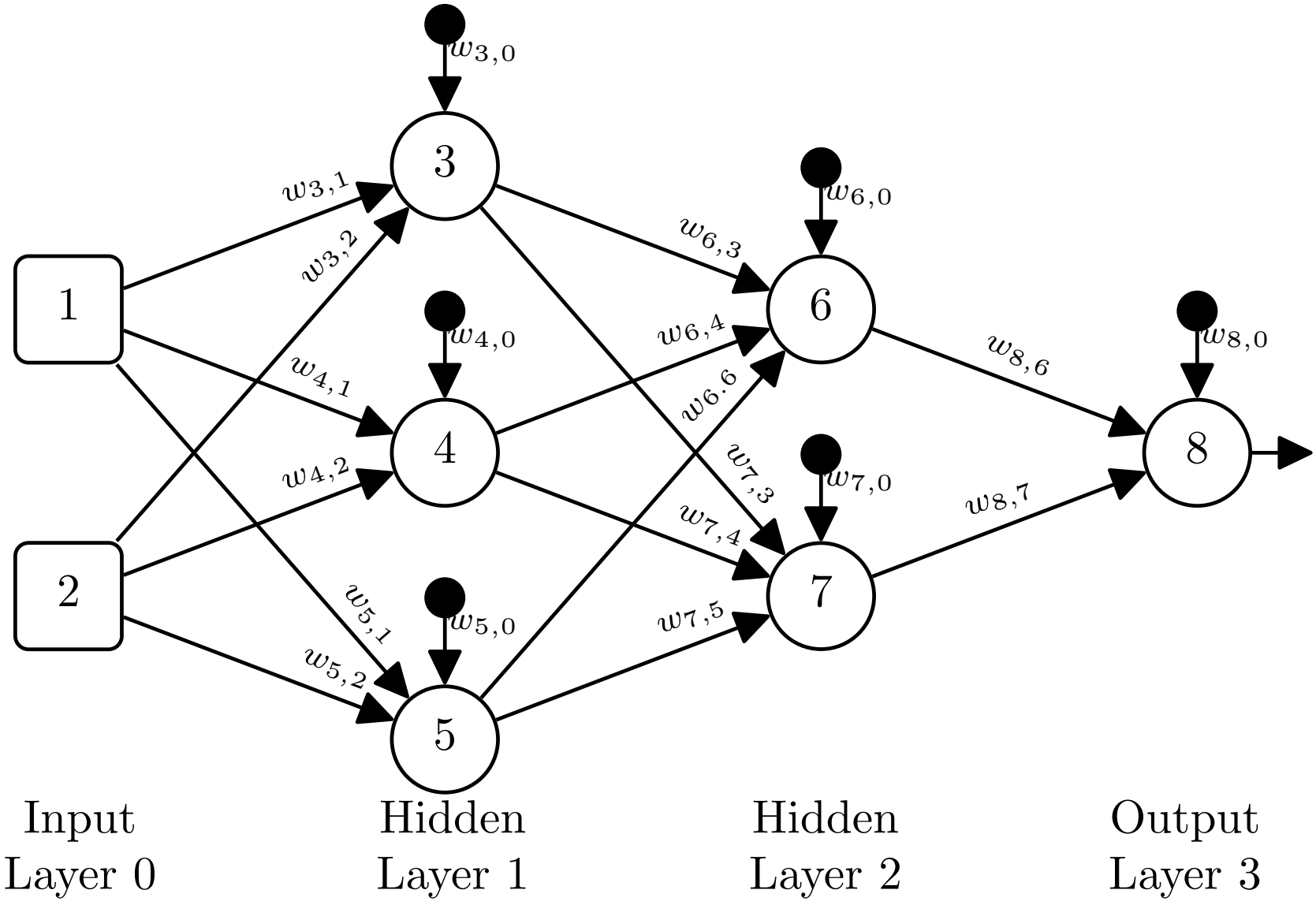


Figure 4: A schematic of a feedforward artificial neural network.

$$\mathbf{z}^{(\mathbf{2})} = \mathbf{W}^{(\mathbf{2})}\mathbf{a}^{(\mathbf{1})} \tag{6}$$

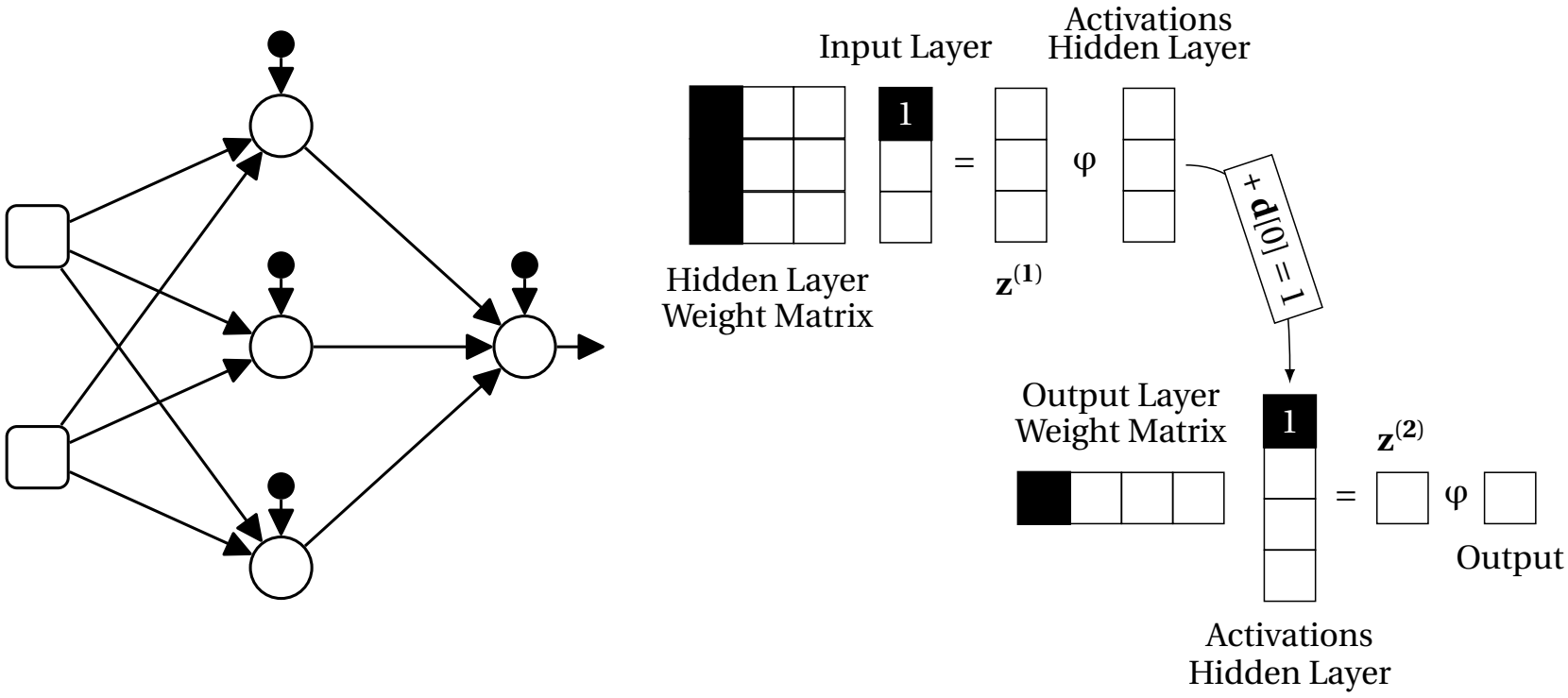


Figure 5: An illustration of the correspondence between graphical and matrix representations of a neural network. This figure is inspired by Figure 3.9 of (Kelleher, 2019).

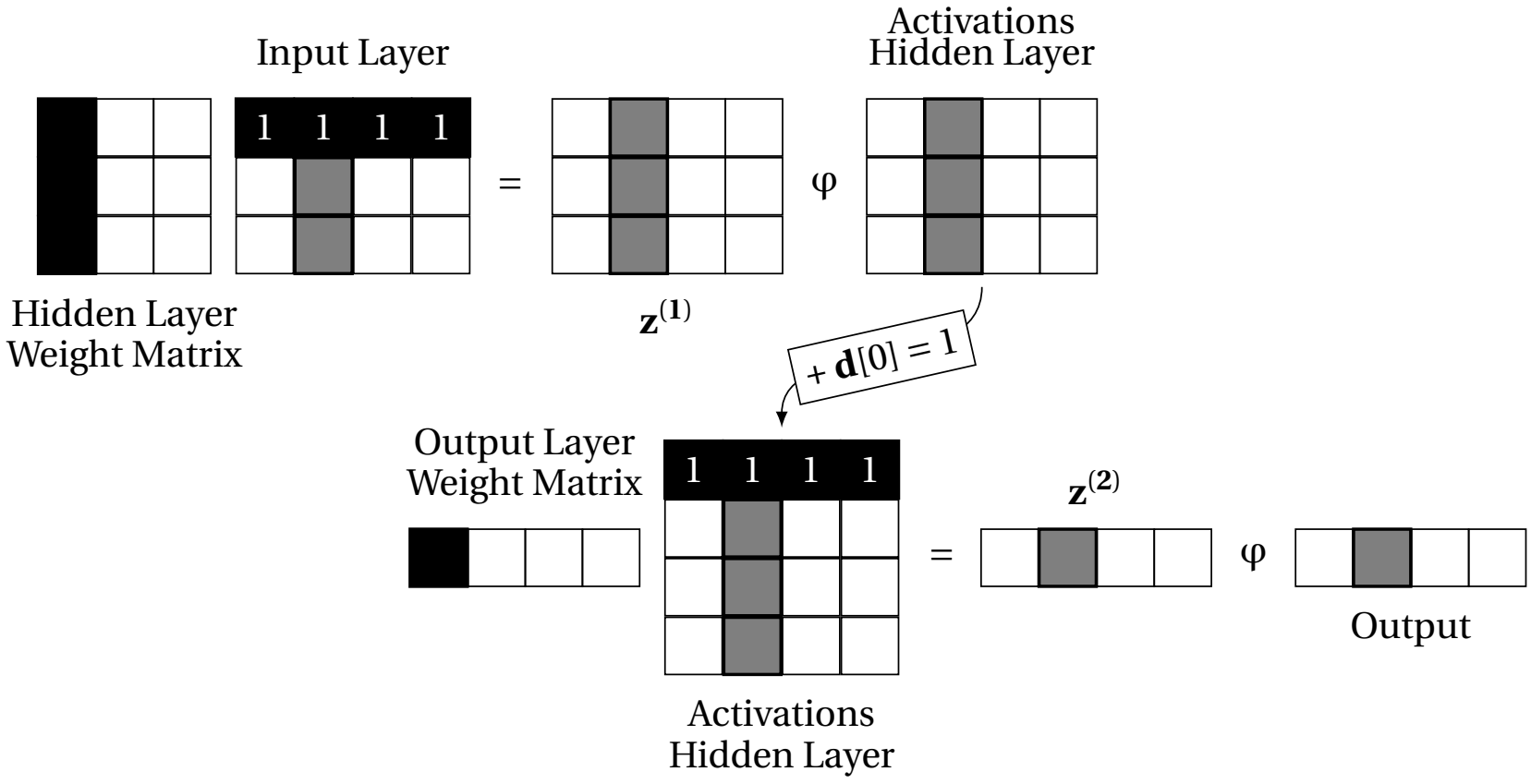


Figure 6: An illustration of how a batch of examples can be processed in parallel using matrix operations.

$$\mathbf{A}^{(1)} = \mathbf{W}^{(1)}\mathbf{A}^{(0)} \tag{7}$$

$$\mathbf{A}^{(2)} = \mathbf{W}^{(2)}\mathbf{A}^{(1)} \tag{8}$$

$$\mathbf{A}^{(2)} = \mathbf{W}^{(2)}\left(\mathbf{W}^{(1)}\mathbf{A}^{(0)}\right) \tag{9}$$

$$\mathbf{A}^{(2)} = \left(\mathbf{W}^{(2)}\mathbf{W}^{(1)}\right)\mathbf{A}^{(0)} \tag{10}$$

$$\mathbf{A}^{(2)} = \mathbf{W}'\mathbf{A}^{(0)} \tag{11}$$

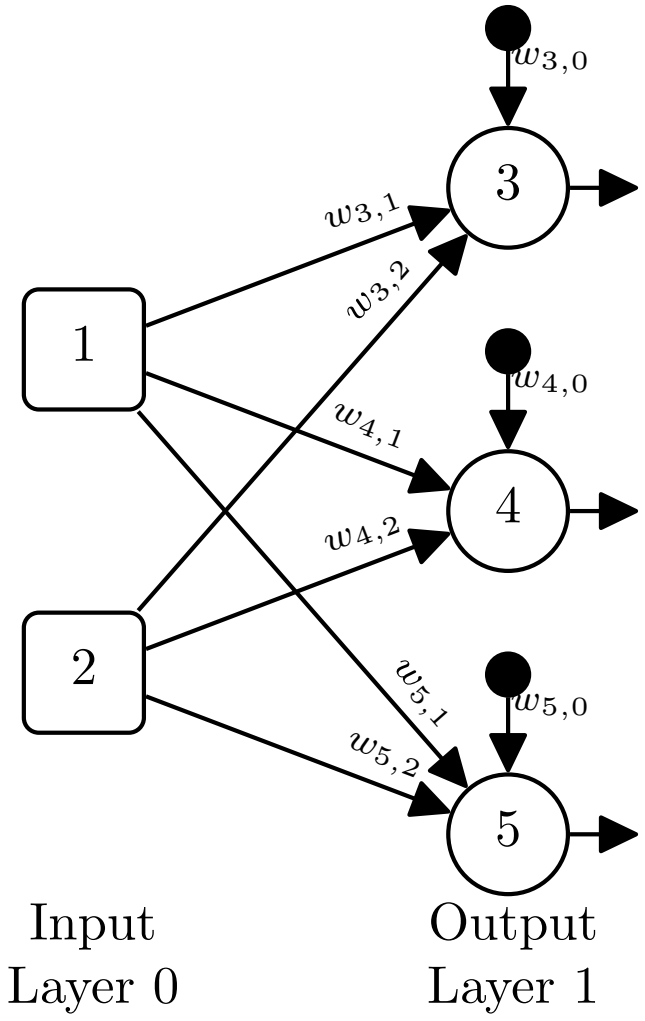


Figure 7: A single-layer network.

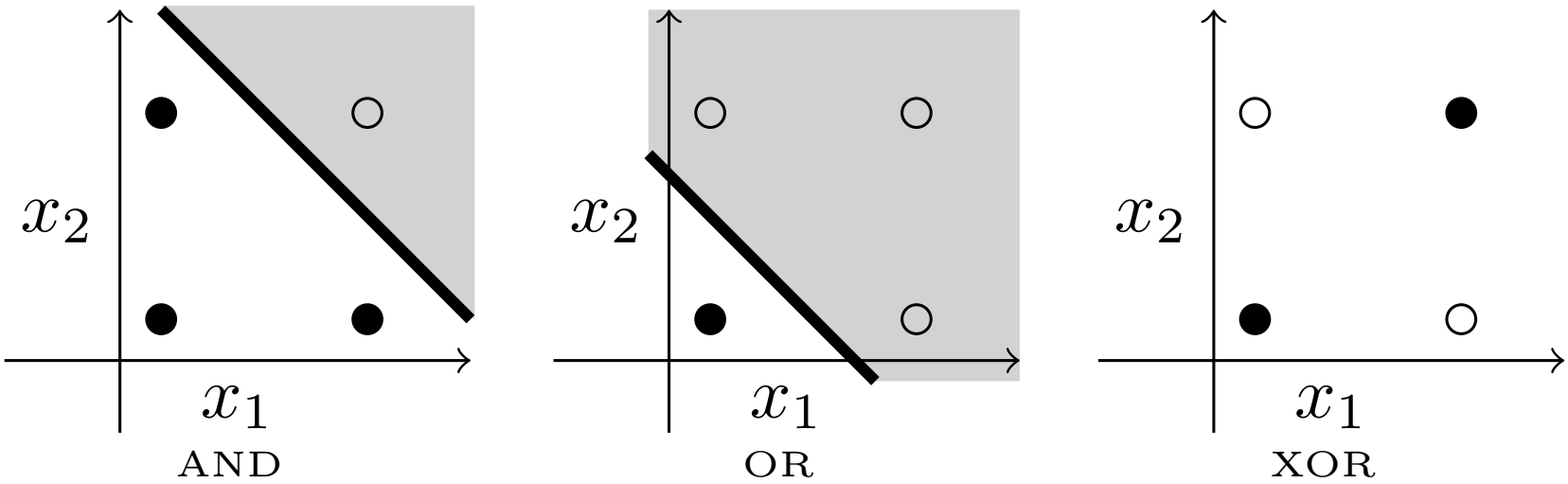


Figure 8: The logical AND and OR functions are linearly separable, but the XOR is not. This figure is Figure 4.2 of (Kelleher, 2019) and is used here with permission.

$$\mathbb{M}_{\mathbf{w}}(\mathbf{d}) = \begin{cases} 1 & \text{if } z \geq 1 \\ 0 & otherwise \end{cases} \tag{12}$$

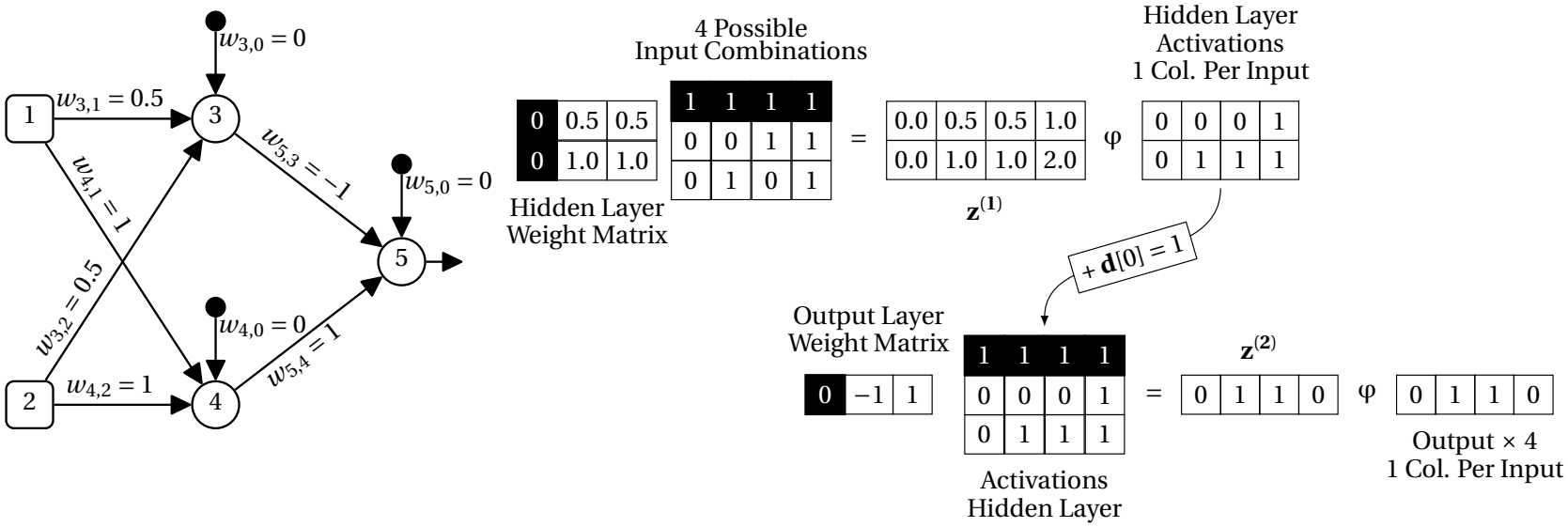


Figure 9: (left) The XOR function implemented as a two-layer neural network. (right) The network processing the four possible input combinations, one combination plus bias input per column: [*bias*, *FALSE*,*FALSE*] $\rightarrow$ [1,0,0]; [*bias*, *FALSE*,*TRUE*] $\rightarrow$ [1,0,1]; [*bias*, *TRUE*,*FALSE*] $\rightarrow$ [1,1,0]; [*bias*, *TRUE*,*TRUE*] $\rightarrow$ [1,1,1].

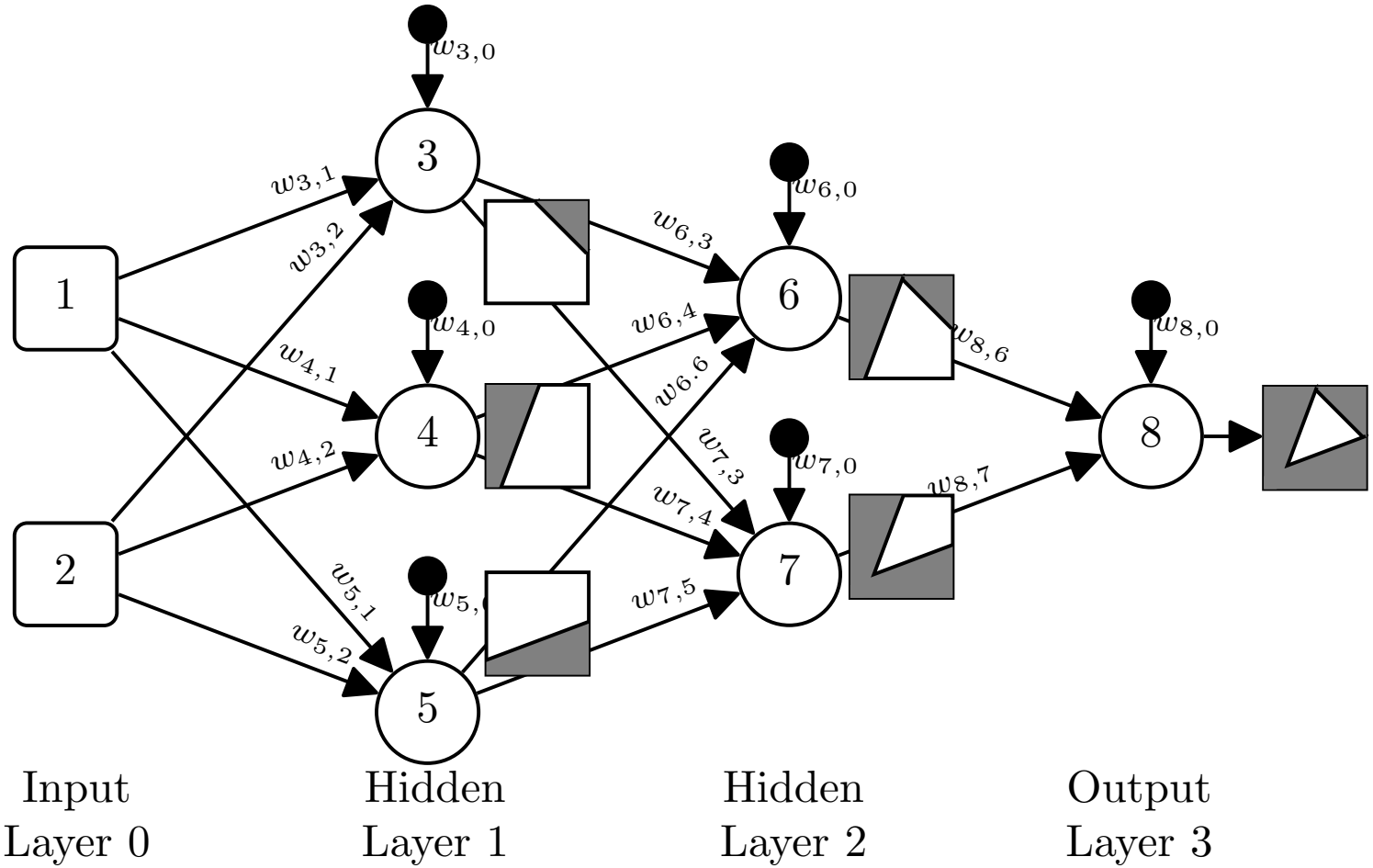


Figure 10: An illustration of how the representational capacity of a network increases as more layers are added to the network. This figure was inspired by Figure 4.2 in (Reed and Marks, 1999) and Figure 3.10 in (Marsland, 2011).

Standard Approach: Backpropagation and Gradient Descent

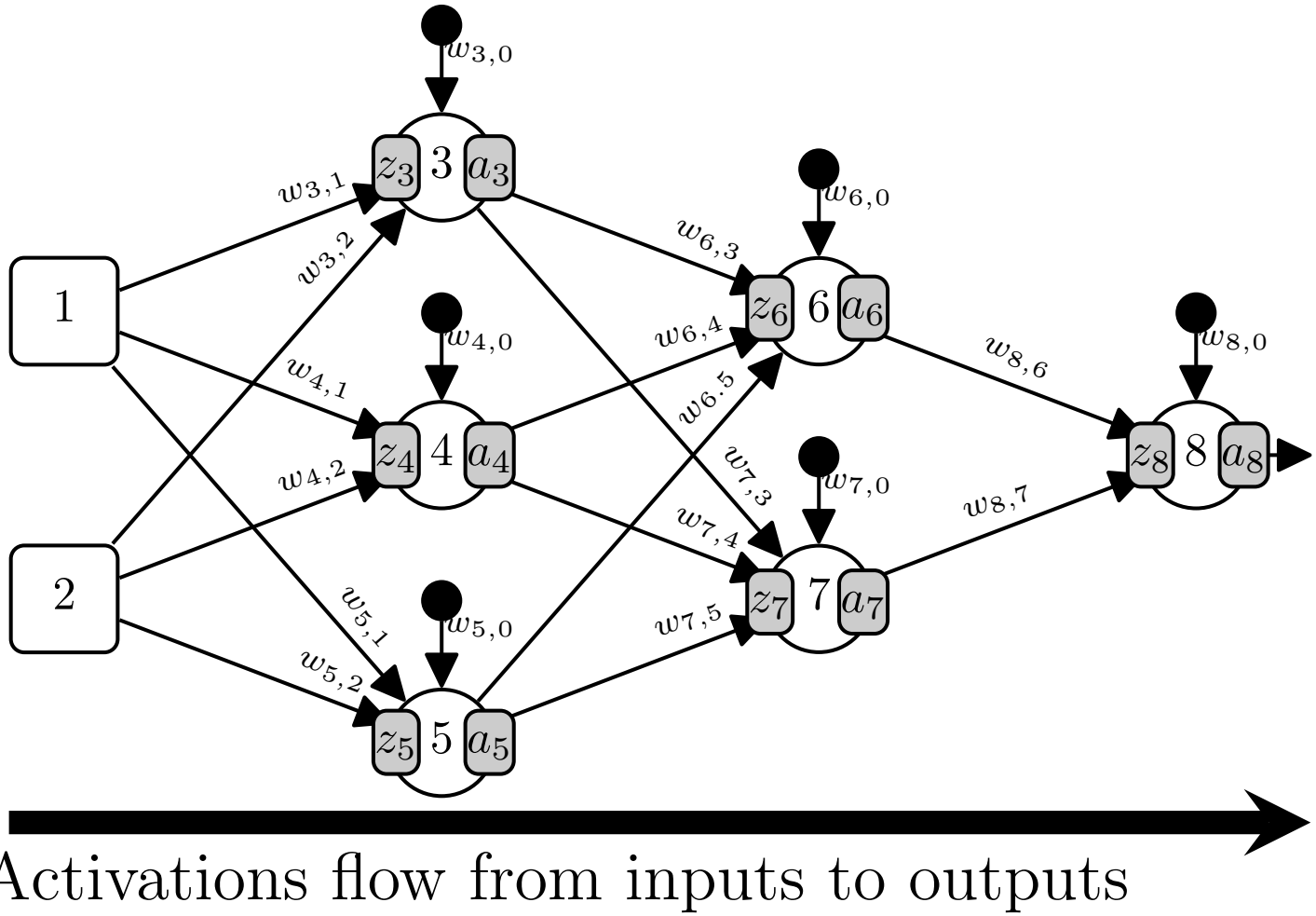


Figure 11: The calculation of the z values and activations of each neuron during the forward pass of the backpropagation algorithm. This figure is based on Figure 6.5 of (Kelleher, 2019).

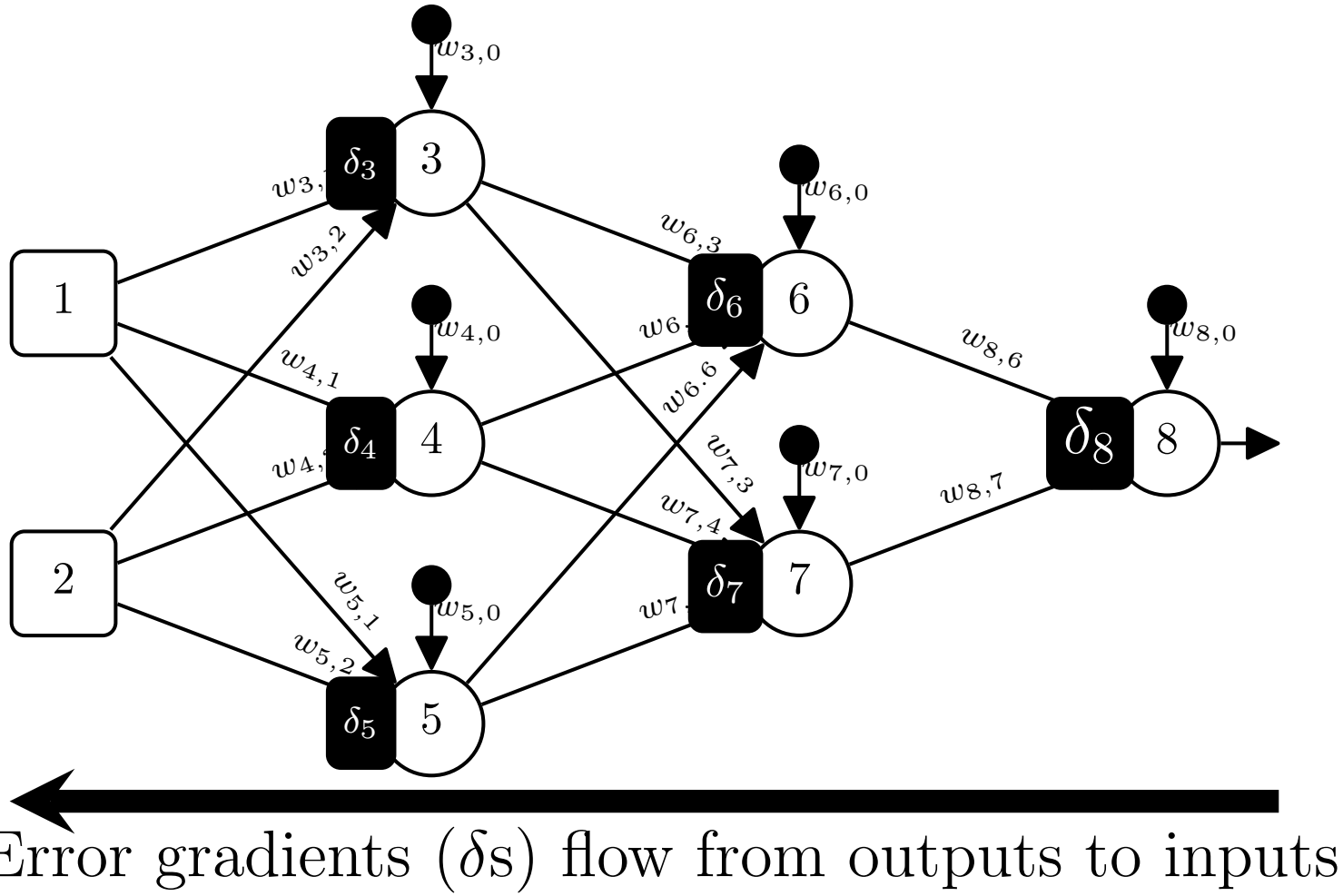


Figure 12: The backpropagation of the δ values during the backward pass of the backpropagation algorithm. This figure is based on Figure 6.6 of (Kelleher, 2019).

rate of change of error w.r.t. neuron k:
1. rate of change of E w.r.t. activation
2. rate of change of activation w.r.t. weighted sum

$$\boldsymbol{\delta}_k = \frac{\partial \mathcal{E}}{\partial z_k} \tag{13}$$

$$\boldsymbol{\delta}_k = \frac{\partial a_k}{\partial z_k} \times \frac{\partial \mathcal{E}}{\partial a_k} \tag{14}$$

2.) calculate rate of change of activation w.r.t. weighted sum

$$\frac{d}{dz} logistic(z) = logistic(z) \times (1 - logistic(z)) \tag{15}$$

$$\begin{aligned} \frac{d}{dz} logistic(z = 0) &= logistic(0) \times (1 - logistic(0)) \\ &= 0.5 \times (1 - 0.5) \\ &= 0.25 \end{aligned} \tag{16}$$

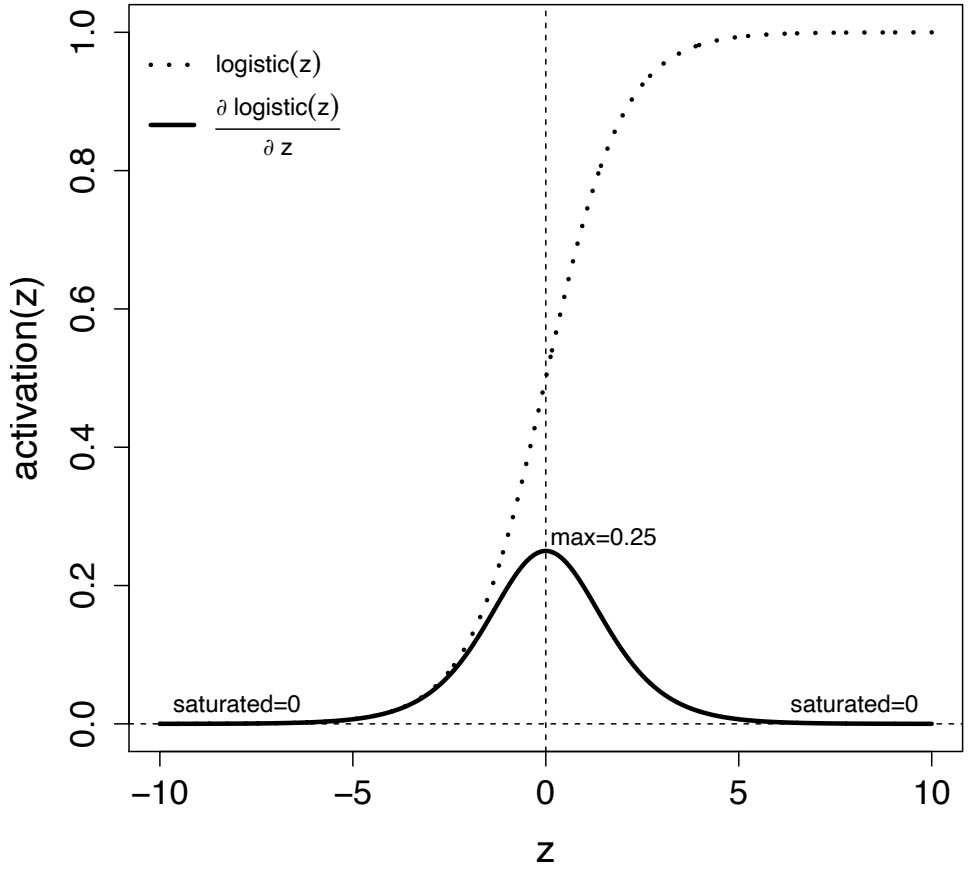


Figure 13: Plots of the logistic function and its derivative. This figure is Figure 4.6 of (Kelleher, 2019) and is used here with permission.

1.) rate of change of error w.r.t. activation for output neuron
(error calc'd via Loss function)

$$L_2(\mathbb{M}_{\mathbf{w}}, \mathcal{D}) = \frac{1}{2}\sum_{i=1}^{n}\left(t_i - \mathbb{M}_{\mathbf{w}}\left(\mathbf{d}_i\right)\right)^2 \tag{17}$$

$$\frac{\partial}{\partial \mathbf{w}\left[j\right]} L_2\left(\mathbb{M}_{\mathbf{w}}, \mathbf{d}\right) = \left(t - \mathbb{M}_{\mathbf{w}}(\mathbf{d})\right) \times -\mathbf{d}\left[j\right] \tag{18}$$

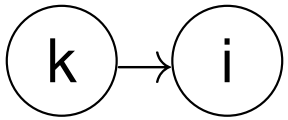
$$\frac{\partial \mathcal{E}}{\partial a_k} = \frac{\partial L_2\left(\mathbb{M}_{\mathbf{w}}, \mathbf{d}\right)}{\partial \mathbb{M}_{\mathbf{w}}(\mathbf{d}))} = t - \mathbb{M}_{\mathbf{w}}(\mathbf{d}) = t_k - a_k \tag{19}$$

$$\frac{\partial \mathcal{E}}{\partial a_k} = -\left(t_k - a_k\right) \tag{20}$$

putting 1 & 2 together for output neuron

$$\begin{aligned}
\boldsymbol{\delta}_k &= \frac{\partial a_k}{\partial z_k} \times \frac{\partial \mathcal{E}}{\partial a_k} \\
&= \frac{\partial a_k}{\partial z_k} \times -(t_k - a_k) \\
&= \underbrace{\frac{d}{dz} logistic(z)}_{\text{Assuming a logistic activation function}} \times -(t_k - a_k) \\
&= \underbrace{(logistic(z) \times (1 - logistic(z)))}_{\text{Assuming a logistic activation function}} \times -(t_k - a_k) \qquad (21)
\end{aligned}$$

putting 1 & 2 together for processing neuron



$$\frac{\partial \mathcal{E}}{\partial a_k} = \sum_{i=1}^{n} w_{i,k} \times \boldsymbol{\delta}_i \tag{22}$$

$$\begin{aligned}
\boldsymbol{\delta}_k &= \frac{\partial a_k}{\partial z_k} \times \frac{\partial \mathcal{E}}{\partial a_k} \\
&= \frac{\partial a_k}{\partial z_k} \times \left(\sum_{i=1}^{n} w_{i,k} \times \boldsymbol{\delta}_i \right) \\
&= \underbrace{\frac{d}{dz} logistic(z)}_{\text{Assuming a logistic activation function}} \times \left(\sum_{i=1}^{n} w_{i,k} \times \boldsymbol{\delta}_i \right) \\
&= \underbrace{(logistic(z) \times (1 - logistic(z)))}_{\text{Assuming a logistic activation function}} \times \left(\sum_{i=1}^{n} w_{i,k} \times \boldsymbol{\delta}_i \right) \qquad (23)
\end{aligned}$$

calculate delta for weight
zi = wik * ak
derivative of zi w.r.t. wik -> ak

$$\frac{\partial \mathcal{E}}{\partial w_{i,k}} = \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial z_i} \times \frac{\partial z_i}{\partial w_{i,k}} \tag{24}$$

$$\begin{aligned} \frac{\partial \mathcal{E}}{\partial w_{i,k}} &= \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial z_i} \times \frac{\partial z_i}{\partial w_{i,k}} \\ &= \boldsymbol{\delta}_i \times \frac{\partial z_i}{\partial w_{i,k}} \end{aligned} \tag{25}$$

$$\frac{\partial z_i}{\partial w_{i,k}} = a_k \tag{26}$$

calculate delta for weight
zi = wik * ak
derivative of zi w.r.t. wik -> ak

$$\begin{aligned}\frac{\partial \mathcal{E}}{\partial w_{i,k}} &= \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial z_i} \times \frac{\partial z_i}{\partial w_{i,k}} \\ &= \boldsymbol{\delta}_i \times \frac{\partial z_i}{\partial w_{i,k}} \\ &= \boldsymbol{\delta}_i \times a_k \end{aligned} \tag{27}$$

adjust weight by -learning_rate * (dE/dwik … weight blame)

$$w_{i,k} \leftarrow w_{i,k} - \alpha \times \boldsymbol{\delta}_i \times a_k \tag{28}$$

batch gradient descent (sum deltas for all m instances in batch)
di,j is delta value of neuron i for instance j
ak,j is activation of neuron i for instance j

$$\Delta w_{i,k} = \sum_{j=1}^{m} \boldsymbol{\delta}_{i,j} \times a_{k,j} \tag{29}$$

$$w_{i,k} \leftarrow w_{i,k} - \alpha \times \Delta w_{i,k} \tag{30}$$

Require: set of training instances $\mathcal{D}$
Require: a learning rate α that controls how quickly the algorithm converges
Require: a batch size B specifying the number of examples in each batch
Require: a convergence criterion

Shuffle $\mathcal{D}$ and create the mini-batches: $[(\mathbf{X}^{(1)}, \mathbf{Y}^{(1)}), \ldots, (\mathbf{X}^{k}, \mathbf{Y}^{k})]$
Initialize the weight matrices for each layer: $\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)}$
repeat ▷ Each repeat loop is one epoch
  for t=1 to number of mini-batches **do** ▷ Each for loop is one iteration
    $\mathbf{A}^{(0)} \leftarrow \mathbf{X}^{(t)}$
    for l=1 to L **do**
      $\mathbf{v} \leftarrow [1_0, \ldots 1_m]$ ▷ Create $\mathbf{v}$ the vector of bias terms
      $\mathbf{A}^{(l-1)} \leftarrow [\mathbf{v}; \mathbf{A}^{(l-1)}]$ ▷ Insert $\mathbf{v}$ into the activation matrix
      $\mathbf{Z}^{(l)} \leftarrow \mathbf{W}^{l}\mathbf{A}^{(l-1)}$
      $\mathbf{A}^{(l)} \leftarrow \varphi(\mathbf{Z}^{(l)})$ ▷ Elementwise application of φ to $\mathbf{Z}^{(l)}$
    end for
    for each weight $w_{i,k}$ in the network **do**
      $\Delta w_{i,k} = 0$
    end for
    for each example in the mini-batch **do** ▷ Backpropagate the δs
      for each neuron i in the output layer **do**
        $\delta_i = \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial z_i}$ ▷ See Equation (21)[28]
      end for
      for l = L-1 to 1 **do**
        for each neuron i in the layer l **do**
          $\delta_i = \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial z_i}$ ▷ See Equation (23)[29]
        end for
      end for
      for each weight $w_{i,k}$ in the network **do**
        $\Delta w_{i,k} = \Delta w_{i,k} + (\delta_i \times a_k)$ ▷ Equation (29)[33]
      end for
    end for
    for each weight $w_{i,k}$ in the network **do**
      $w_{i,k} \leftarrow w_{i,k} - \alpha \times \Delta w_{i,k}$ ▷ Equation (30)[33]
    end for
  end for
  shuffle($[(\mathbf{X}^{(1)}, \mathbf{Y}^{(1)}), \ldots, (\mathbf{X}^{k}, \mathbf{Y}^{k})]$)
until convergence occurs

Table 1: Hourly samples of ambient factors and full load electrical power output of a combined cycle power plant.

ID	Ambient Temperature °C	Relative Humidity %	Electrical Output MW
1	03.21	86.34	491.35
2	31.41	68.50	430.37
3	19.31	30.59	463.00
4	20.64	99.97	447.14

Table 2: The minimum and maximum values for the AMBIENT TEMPERATURE, RELATIVE HUMIDITY, and ELECTRICAL OUTPUT features in the power plant dataset.

	AMBIENT TEMPERATURE	RELATIVE HUMIDITY	ELECTRICAL OUTPUT
Min	$1.81°$C	25.56%	420.26MW
Max	$37.11°$C	100.16%	495.76MW

Table 3: The *range-normalized* hourly samples of ambient factors and full load electrical power output of a combined cycle power plant, rounded to two decimal places.

ID	Ambient Temperature °C	Relative Humidity %	Electrical Output MW
1	0.04	0.81	0.94
2	0.84	0.58	0.13
3	0.50	0.07	0.57
4	0.53	1.00	0.36

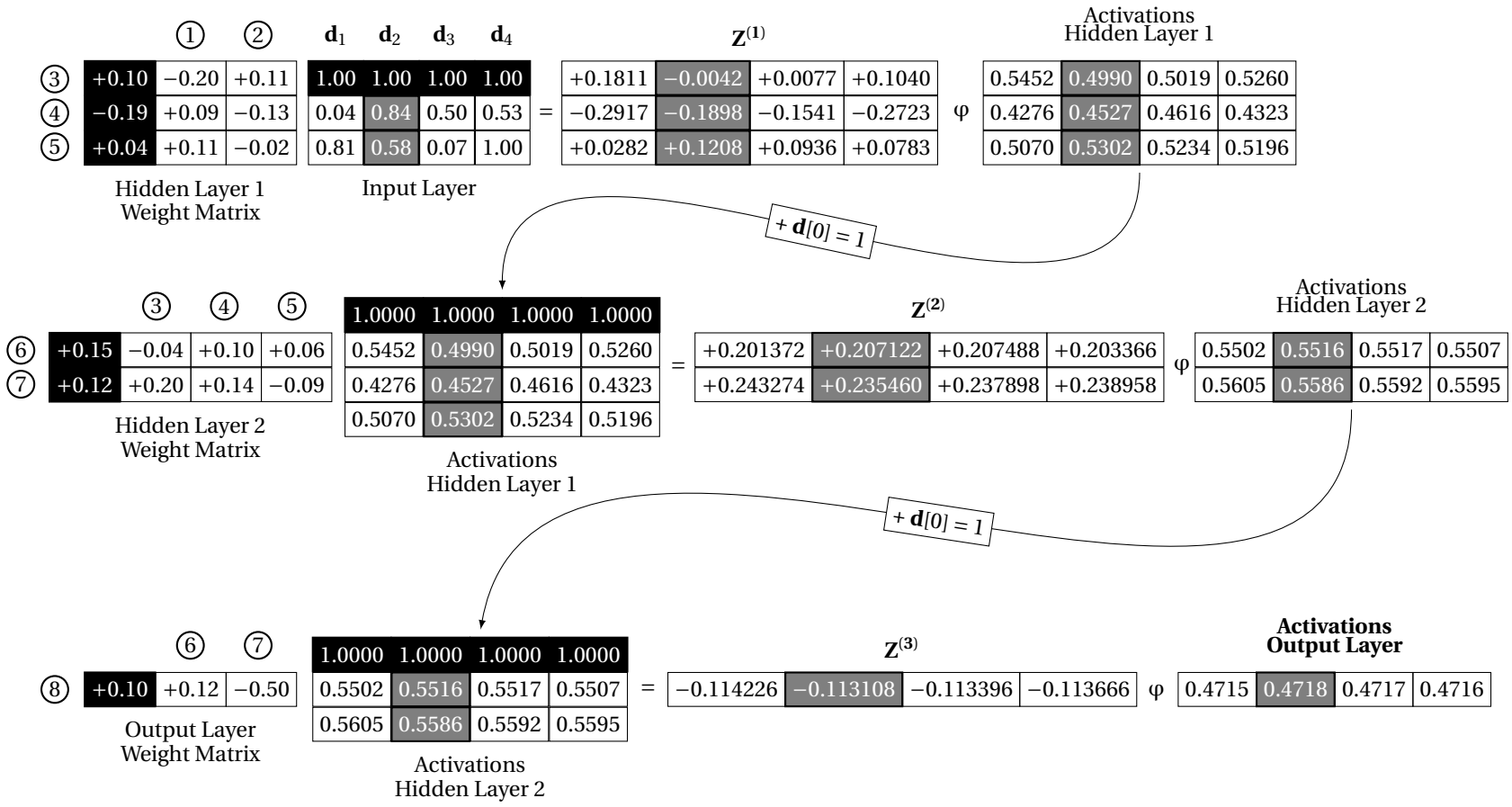


Figure 14: The forward pass of the examples listed in Table 3[38] through the network in Figure 4[11].

Table 4: The per example error after the forward pass illustrated in Figure 14[39], the per example $\partial \mathcal{E} / \partial a_8$, and the **sum of squared errors** for the model over the dataset of four examples.

	$\mathbf{d}_1$	$\mathbf{d}_2$	$\mathbf{d}_3$	$\mathbf{d}_4$
Target	0.9400	0.1300	0.5700	0.3600
Prediction	0.4715	0.4718	0.4717	0.4716
Error	0.4685	-0.3418	0.0983	-0.1116
$\partial \mathcal{E} / \partial a_8$: Error $\times -1$	-0.4685	0.3418	-0.0983	0.1116
Error^2	0.21949225	0.11682724	0.00966289	0.01245456
SSE:				0.17921847

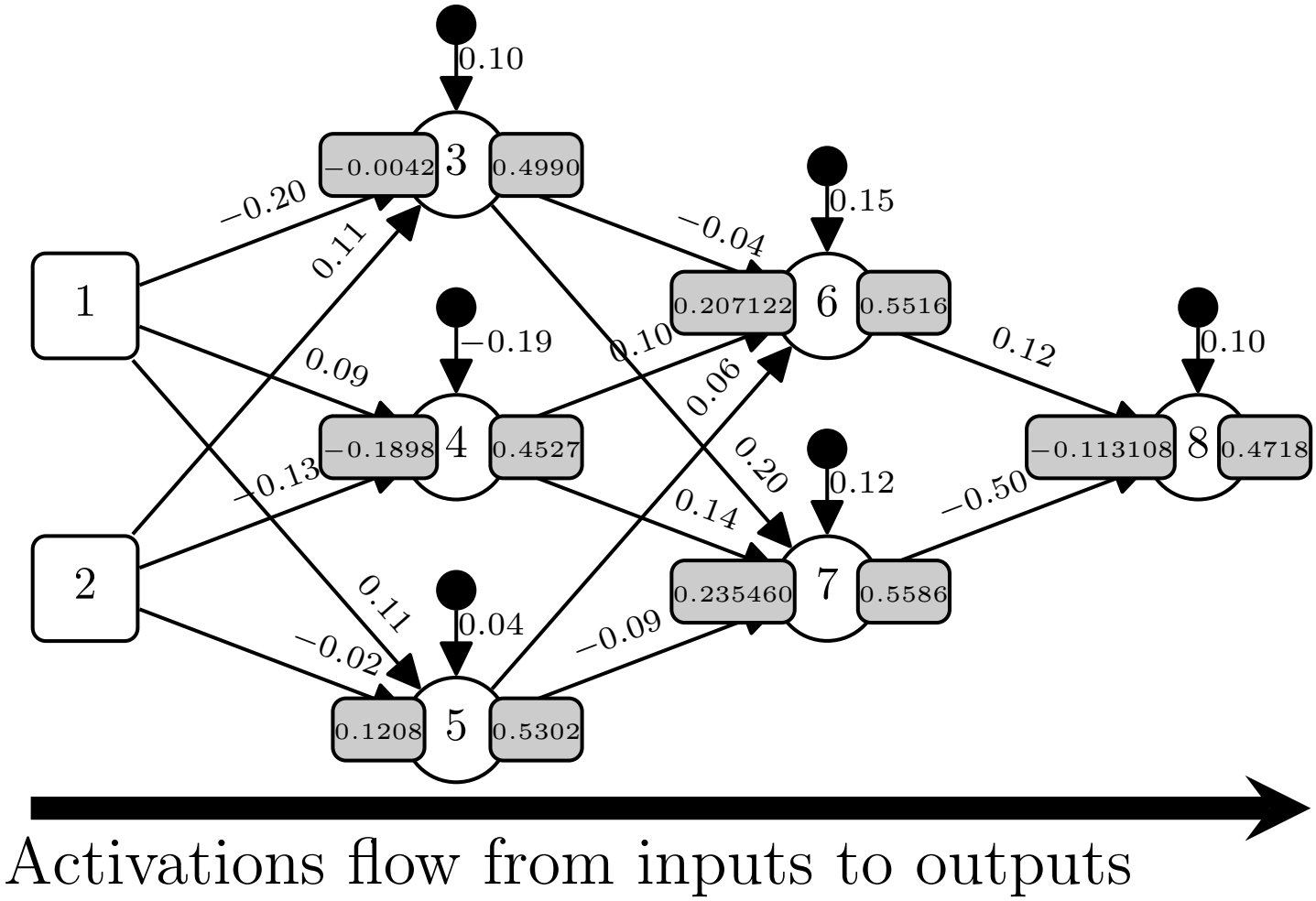


Figure 15: An illustration of the forward propagation of $\mathbf{d}_2$ through the network showing the weights on each connection, and the weighted sum z and activation a value for each neuron in the network.

$$\frac{\partial \mathcal{E}}{\partial a} = 0.3418 \tag{31}$$

$$\begin{aligned} \delta_8 = & \frac{\partial \mathcal{E}}{\partial a_8} \times \frac{\partial a_8}{\partial z_8} \\ =& 0.3418 \times 0.2492 \\ =& 0.0852 \end{aligned} \tag{32}$$

Table 5: The $\partial a/\partial z$ for each neuron for Example 2 rounded to four decimal places.

NEURON	z	$\partial a/\partial z$
3	-0.004200	0.2500
4	-0.189800	0.2478
5	0.120800	0.2491
6	0.207122	0.2473
7	0.235460	0.2466
8	-0.113108	0.2492

$$
\begin{aligned}
\delta_6 = & \frac{\partial \mathcal{E}}{\partial a_6} \times \frac{\partial a_6}{\partial z_6} \\
= & \left(\sum \delta_i \times w_{i,6} \right) \times \frac{\partial a_6}{\partial z_6} \\
= & \left(\delta_8 \times w_{8,6} \right) \times \frac{\partial a_6}{\partial z_6} \\
= & (0.0852 \times 0.12) \times 0.2473 \\
= & \quad 0.0025
\end{aligned} \tag{33}
$$

$$
\begin{aligned}
\delta_7 = & \frac{\partial \mathcal{E}}{\partial a_7} \times \frac{\partial a_7}{\partial z_7} \\
= & \left(\sum \delta_i \times w_{i,7} \right) \times \frac{\partial a_7}{\partial z_7} \\
= & \left(\delta_8 \times w_{8,7} \right) \times \frac{\partial a_6}{\partial z_6} \\
= & (0.0852 \times -0.50) \times 0.2466 \\
= & -0.0105
\end{aligned} \tag{34}
$$

$$
\begin{aligned}
\delta_3 = & \frac{\partial \mathcal{E}}{\partial a_3} \times \frac{\partial a_3}{\partial z_3} \\
= & \left(\sum \delta_i \times w_{i,3} \right) \times \frac{\partial a_3}{\partial z_3} \\
= & \left((\delta_6 \times w_{6,3}) + (\delta_7 \times w_{7,3}) \right) \times \frac{\partial a_3}{\partial z_3} \\
= & ((0.0025 \times -0.04) + (-0.0105 \times 0.20)) \times 0.2500 \\
= & -0.0006
\end{aligned} \tag{35}
$$

$$
\begin{aligned}
\delta_4 = & \frac{\partial \mathcal{E}}{\partial a_4} \times \frac{\partial a_4}{\partial z_4} \\
= & \left(\sum \delta_i \times w_{i,4} \right) \times \frac{\partial a_4}{\partial z_4} \\
= & \left((\delta_6 \times w_{6,4}) + (\delta_7 \times w_{7,4}) \right) \times \frac{\partial a_4}{\partial z_4} \\
= & ((0.0025 \times 0.10) + (-0.0105 \times 0.14)) \times 0.2478 \\
= & -0.0003
\end{aligned} \tag{36}
$$

$$
\begin{aligned}
\delta_5 = & \frac{\partial \mathcal{E}}{\partial a_5} \times \frac{\partial a_5}{\partial z_5} \\
= & \left(\sum \delta_i \times w_{i,5} \right) \times \frac{\partial a_5}{\partial z_5} \\
= & \left((\delta_6 \times w_{6,5}) + (\delta_7 \times w_{7,5}) \right) \times \frac{\partial a_5}{\partial z_5} \\
= & ((0.0025 \times 0.06) + (-0.0105 \times -0.09)) \times 0.2491 \\
= & 0.0003
\end{aligned} \tag{37}
$$

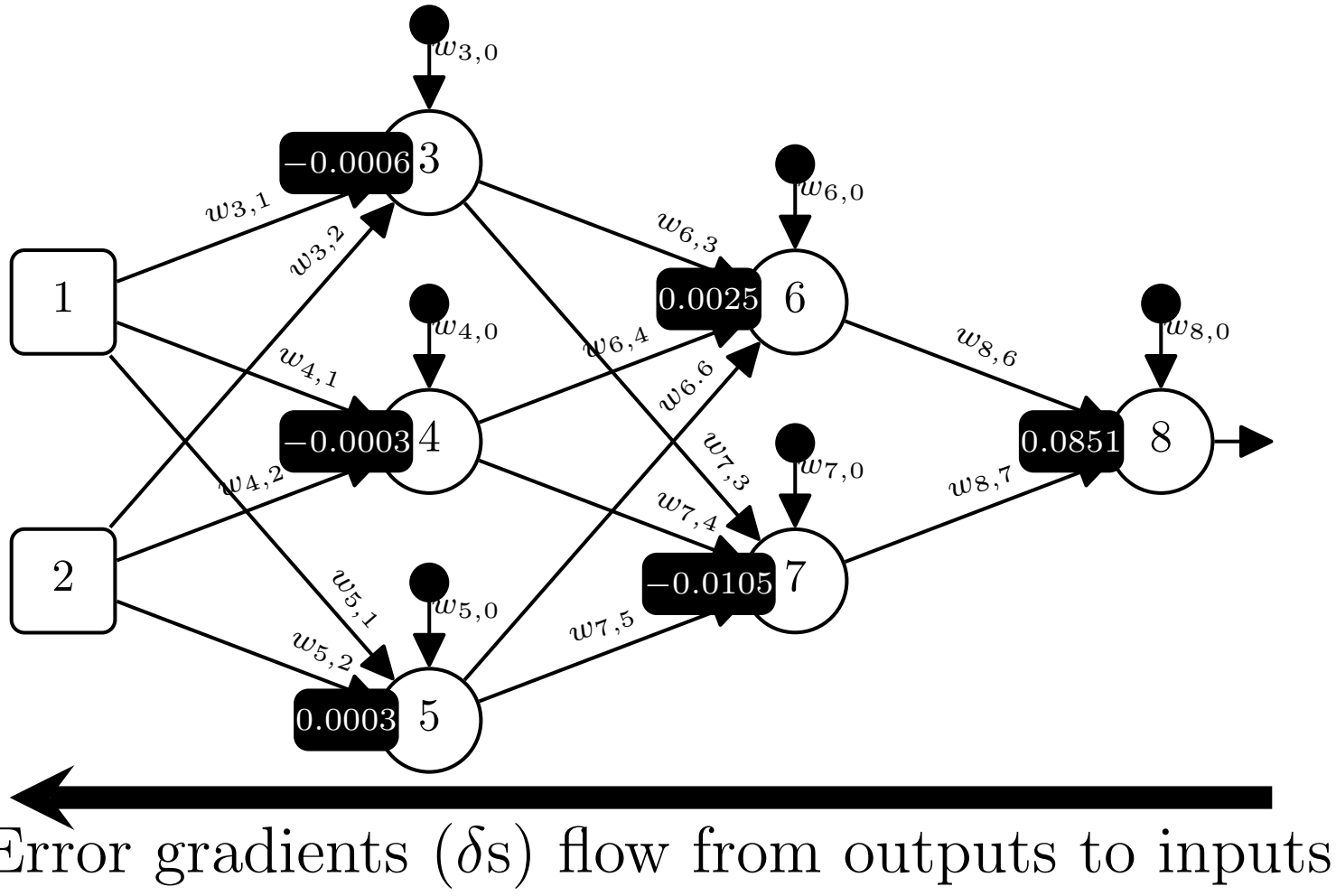


Figure 16: The δs for each of the neurons in the network for Ex. 2.

Table 6: The $\partial \mathcal{E}/\partial w_{i,k}$ calculations for $\mathbf{d}_2$ for every weight in the network. The neuron index 0 denotes the bias input for each neuron.

NEURON$_i$	NEURON$_k$	$w_{i,k}$	δ_i	a_k	$\partial \mathcal{E}/\partial w_{i,k}$
8	0	$w_{8,0}$	0.0852	1	$0.0852 \times 1 = 0.0852$
8	6	$w_{8,6}$	0.0852	0.5516	$0.0852 \times 0.5516 = 0.04699632$
8	7	$w_{8,7}$	0.0852	0.5586	$0.0852 \times 0.5586 = 0.04759272$
7	0	$w_{7,0}$	-0.0105	1	$-0.0105 \times 1 = -0.0105$
7	3	$w_{7,3}$	-0.0105	0.4990	$-0.0105 \times 0.4527 = -0.0052395$
7	4	$w_{7,4}$	-0.0105	0.4527	$-0.0105 \times 0.4527 = -0.00475335$
7	5	$w_{7,5}$	-0.0105	0.5302	$-0.0105 \times 0.5302 = -0.0055671$
6	0	$w_{6,0}$	0.0025	1	$0.0025 \times 1 = 0.0025$
6	3	$w_{6,3}$	0.0025	0.4990	$0.0025 \times 0.4527 = 0.0012475$
6	4	$w_{6,4}$	0.0025	0.4527	$0.0025 \times 0.4527 = 0.00113175$
6	5	$w_{6,5}$	0.0025	0.5302	$0.0025 \times 0.5302 = 0.0013255$
5	0	$w_{5,0}$	0.0003	1	$0.0003 \times 1 = 0.0003$
5	1	$w_{5,1}$	0.0003	0.84	$0.0003 \times 0.84 = 0.000252$
5	2	$w_{5,2}$	0.0003	0.58	$0.0003 \times 0.58 = 0.000174$
4	0	$w_{4,0}$	-0.0003	1	$-0.0003 \times 1 = -0.0003$
4	1	$w_{4,1}$	-0.0003	0.84	$-0.0003 \times 0.84 = -0.000252$
4	2	$w_{4,2}$	-0.0003	0.58	$-0.0003 \times 0.58 = -0.000174$
3	0	$w_{3,0}$	-0.0006	1	$-0.0006 \times 1 = -0.0006$
3	1	$w_{3,1}$	-0.0006	0.84	$-0.0006 \times 0.84 = -0.000504$
3	2	$w_{3,2}$	-0.0006	0.58	$-0.0006 \times 0.58 = -0.000348$

stochastic: update weights for each instance
(process each instance, 1 by 1)

$$
\begin{aligned}
w_{7,5} &= w_{7,5} - \alpha \times \boldsymbol{\delta}_7 \times a_5 \\
&= w_{7,5} - \alpha \times \frac{\partial \mathcal{E}}{\partial w_{i,k}} \\
&= -0.09 - 0.2 \times -0.0055671 \\
&= -0.08888658
\end{aligned} \tag{38}
$$

if batch, weight delta based on batch of data (sum deltas)

Table 7: The calculation of $\Delta w_{7,5}$ across our four examples.

MINI-BATCH EXAMPLE	$\frac{\partial \mathcal{E}}{\partial w_{7,5}}$
$\mathbf{d}_1$	0.00730080
$\mathbf{d}_2$	-0.00556710
$\mathbf{d}_3$	0.00157020
$\mathbf{d}_4$	-0.00176664
$\Delta w_{7,5}=$	0.00153726

batch: update weights for batch of instance
(process batch update, with multiple data instances)

$$\begin{aligned} w_{7,5} &= w_{7,5} - \alpha \times \Delta w_{i,k} \\ &= -0.09 - 0.2 \times 0.00153726 \\ &= -0.0903074520 \end{aligned} \tag{39}$$

after weight updates and running second epoch of training -> error reduction

Table 8: The per example error after each weight has been updated once, the per example $\partial \mathcal{E}/\partial a_8$, and the **sum of squared errors** for the model.

	$\mathbf{d}_1$	$\mathbf{d}_2$	$\mathbf{d}_3$	$\mathbf{d}_4$
Target	0.9400	0.1300	0.5700	0.3600
Prediction	0.4738	0.4741	0.4740	0.4739
Error	0.4662	-0.3441	0.0960	-0.1139
$\partial \mathcal{E}/\partial a_8$: Error $\times -1$	-0.4662	0.3441	-0.0960	0.1139
Error^2	0.21734244	0.11840481	0.009216	0.01297321
SSE:				0.17896823

Table 9: The per example prediction, error, and the sum of squared errors after training has converged to an $SSE < 0.0001$.

	$\mathbf{d}_1$	$\mathbf{d}_2$	$\mathbf{d}_2$	$\mathbf{d}_2$
Target	0.9400	0.1300	0.5700	0.3600
Prediction	0.9266	0.1342	0.5700	0.3608
Error	0.0134	-0.0042	0.0000	-0.0008
Error^2	0.00017956	0.00001764	0.00000000	0.00000064
SSE:				0.00009892

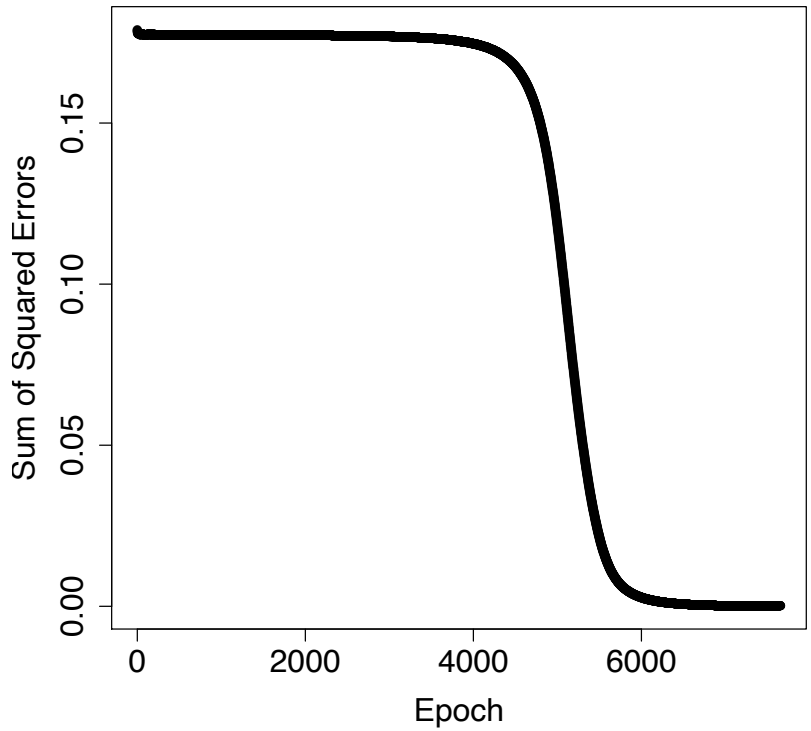


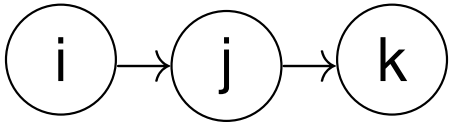
Figure 17: A plot showing how the sum of squared errors of the network changed during training.

Extensions and Variations

gradients vanish due to multiplying smaller and smaller gradients back through the network

$$\begin{aligned}\frac{\partial \mathcal{E}}{\partial w_{i,k}} &= \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial z_i} \times \frac{\partial z_i}{\partial w_{i,k}} \\ &= \boldsymbol{\delta}_i \times \frac{\partial z_i}{\partial w_{i,k}}\end{aligned} \tag{40}$$

gradient vanishes due to repeatedly multiplying by small deltas
and due to logistic function derivation (max value .25, large or small Z -> derivative of 0



$$
\begin{aligned}
\delta_i &= \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial z_i} \\
&= \overbrace{w_{j,i} \times \delta_j}^{} \times \frac{\partial a_i}{\partial z_i} \\
&= w_{j,i} \times \overbrace{w_{k,j} \times \delta_k \times \frac{\partial a_j}{\partial z_j}}^{} \times \frac{\partial a_i}{\partial z_i} \\
&= w_{j,i} \times w_{k,j} \times \overbrace{\frac{\partial \mathcal{E}}{\partial a_k} \times \frac{\partial a_k}{\partial z_k}} \times \frac{\partial a_j}{\partial z_j} \times \frac{\partial a_i}{\partial z_i}
\end{aligned}
\tag{41}
$$

address vanishing gradient by changing activation function

$$rectifier(z) = max(0, z) = \begin{cases} z & \text{if } z > 0 \\ 0 & otherwise \end{cases} \tag{42}$$

$$\frac{d}{dz} rectifier(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & otherwise \end{cases} \tag{43}$$

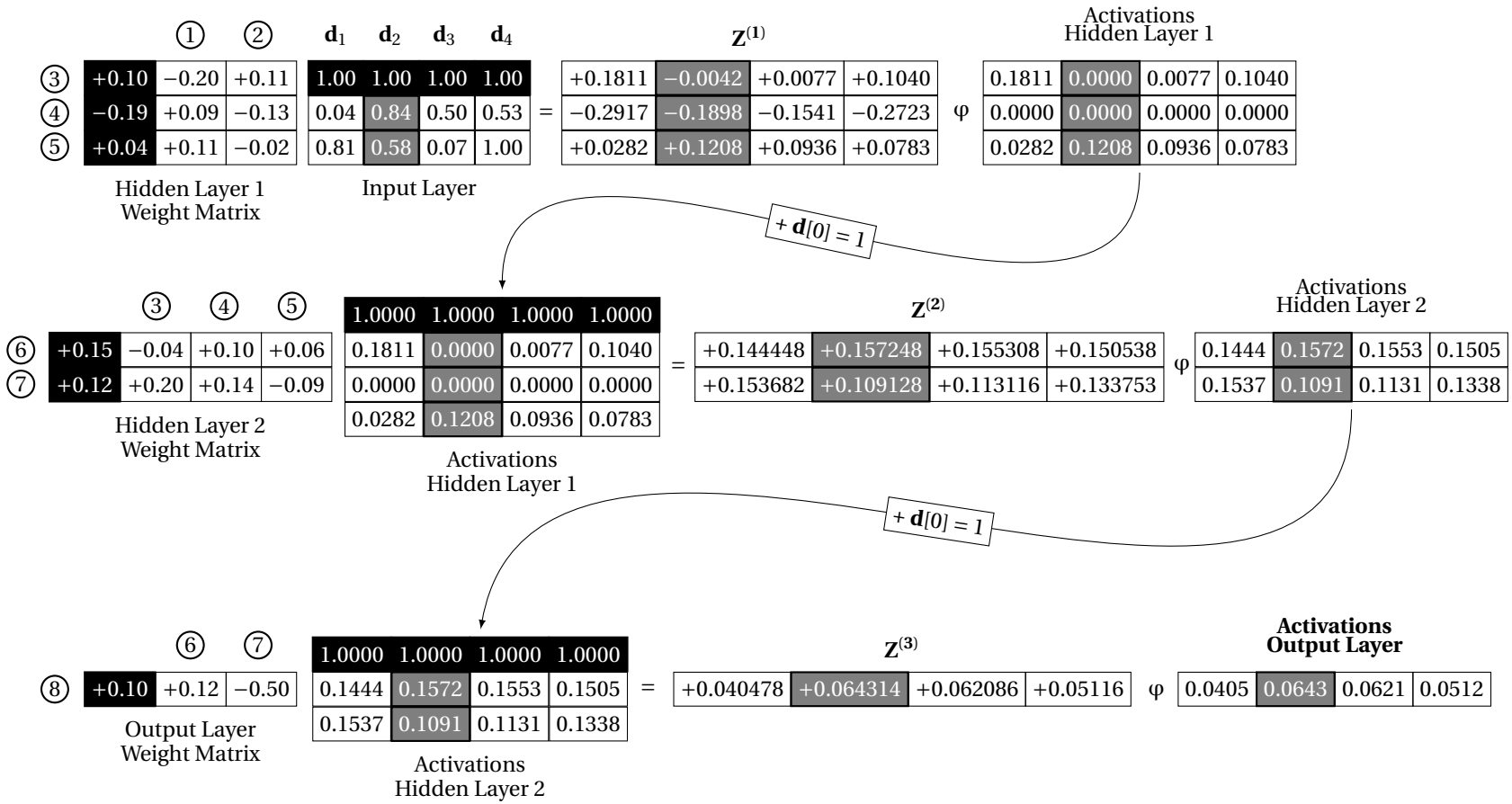


Figure 18: The forward pass of the examples listed in Table 3[38] through the network in Figure 4[11] when all the neurons are ReLUs.

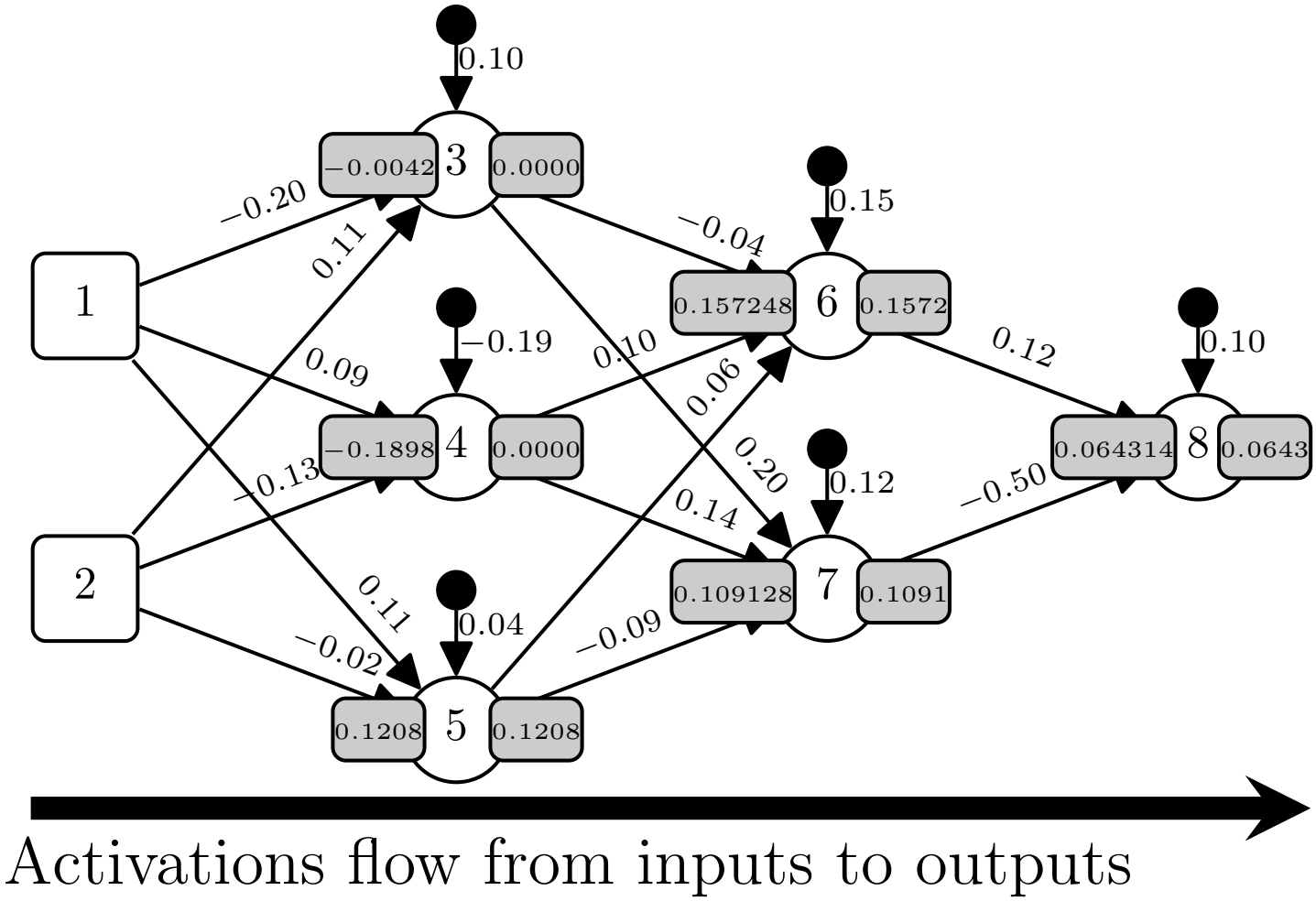


Figure 19: An illustration of the forward propagation of $\mathbf{d}_2$ through the ReLU network showing the weights on each connection, and the weighted sum z and activation a value for each neuron in the network.

Table 10: The per example error of the ReLU network after the forward pass illustrated in Figure 18[61], the per example $\partial \mathcal{E}/\partial a_8$, and the **sum of squared errors** for the ReLU model.

	$\mathbf{d}_1$	$\mathbf{d}_2$	$\mathbf{d}_3$	$\mathbf{d}_4$
Target	0.9400	0.1300	0.5700	0.3600
Prediction	0.0405	0.0643	0.0621	0.0512
Error	0.8995	0.0657	0.5079	0.3088
$\partial \mathcal{E}/\partial a_8$: Error $\times -1$	-0.8995	-0.0657	-0.5079	-0.3088
Error^2	0.80910025	0.00431649	0.25796241	0.09535744
SSE:				0.58336829

Table 11: The $\partial a/\partial z$ for each neuron for $\mathbf{d}_2$ rounded to four decimal places.

NEURON	z	$\partial a/\partial z$
3	-0.004200	0
4	-0.189800	0
5	0.120800	1
6	0.157248	1
7	0.109128	1
8	0.064314	1

$$
\begin{aligned}
\delta_k &= \frac{\partial \mathcal{E}}{\partial a_k} \times \frac{\partial a_k}{\partial z_i} \\
\delta_8 &= -0.0657 \times 1.0 \\
&= -0.0657 \\
\delta_7 &= \left(\delta_8 \times w_{8,7}\right) \times \frac{\partial a_7}{\partial z_7} \\
&= (-0.0657 \times -0.50) \times 1 \\
&= 0.0329 \\
\delta_6 &= \left(\delta_8 \times w_{8,6}\right) \times \frac{\partial a_6}{\partial z_6} \\
&= (-0.0657 \times 0.12) \times 1 \\
&= -0.0079 \\
\delta_5 &= \left(\left(\delta_6 \times w_{6,5}\right) + \left(\delta_7 \times w_{7,5}\right)\right) \times \frac{\partial a_5}{\partial z_5} \\
&= ((-0.0079 \times 0.06) + (0.0329 \times -0.09)) \times 1 \\
&= -0.0034 \\
\delta_4 &= \left(\left(\delta_6 \times w_{6,4}\right) + \left(\delta_7 \times w_{7,4}\right)\right) \times \frac{\partial a_4}{\partial z_4} \\
&= ((-0.0079 \times 0.10) + (0.0329 \times 0.14)) \times 0 \\
&= 0 \\
\delta_3 &= \left(\left(\delta_6 \times w_{6,3}\right) + \left(\delta_7 \times w_{7,3}\right)\right) \times \frac{\partial a_3}{\partial z_3} \\
&= ((-0.0079 \times -0.04) + (0.0329 \times 0.20)) \times 0 \\
&= 0
\end{aligned}
$$

(44)

Table 12: The ReLU network's per example prediction, error, and the sum of squared errors after training has converged to an $SSE < 0.0001$.

	$\mathbf{d}_1$	$\mathbf{d}_2$	$\mathbf{d}_3$	$\mathbf{d}_4$
Target	0.9400	0.1300	0.5700	0.3600
Prediction	0.9487	0.1328	0.5772	0.3679
Error	-0.0087	-0.0028	-0.0072	-0.0079
Error^2	0.00007569	0.00000784	0.00005184	0.00006241
SSE:				0.00009889

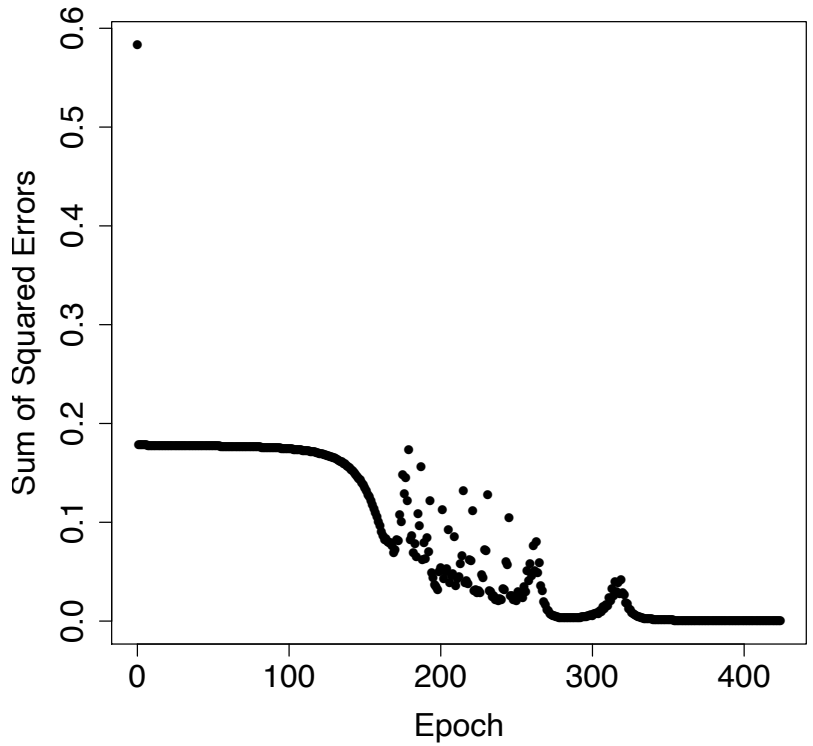


Figure 20: A plot showing how the sum of squared errors of the ReLU network changed during training when $\alpha = 0.2$.

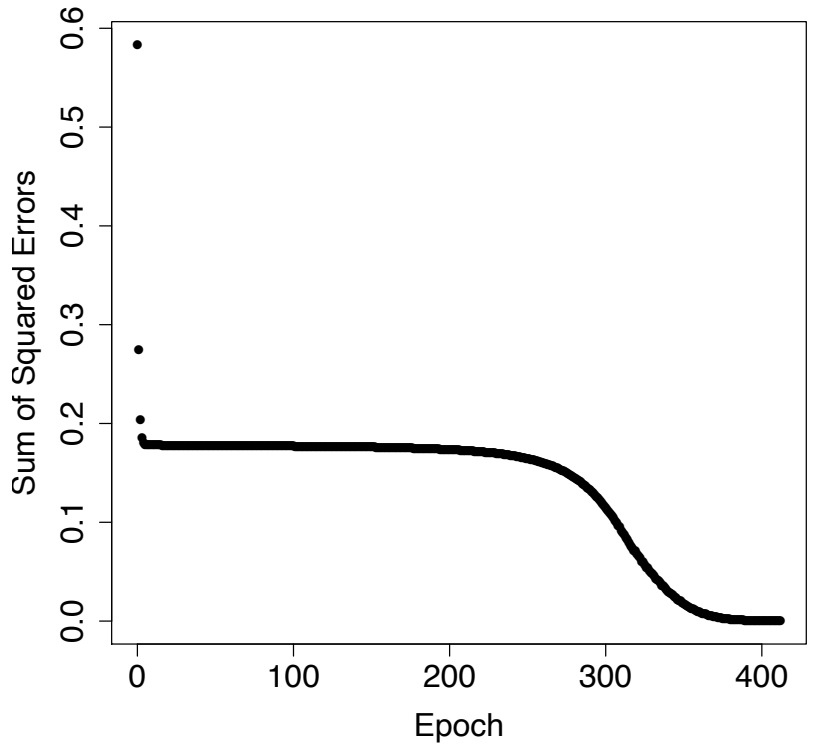


Figure 21: A plot showing how the sum of squared errors of the ReLU network changed during training when $\alpha = 0.1$.

$$rectifier_{leaky}(z) = \begin{cases} z & \text{if } z > 0 \\ 0.01 \times z & otherwise \end{cases} \tag{45}$$

$$\frac{d}{dz} rectifier_{leaky}(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0.01 & otherwise \end{cases} \tag{46}$$

$$rectifier_{parametric}(z_i) = \begin{cases} z_i & \text{if } z_i > 0 \\ \lambda_i \times z_i & otherwise \end{cases} \tag{47}$$

$$\frac{d}{dz} rectifier_{parametric}(z_i) = \begin{cases} 1 & \text{if } z_i > 0 \\ \lambda_i & otherwise \end{cases} \tag{48}$$

lambda becomes a learnable parameter for parametric ReLU

$$\frac{\partial \mathcal{E}}{\partial \lambda_i} = \frac{\partial \mathcal{E}}{\partial a_i} \times \frac{\partial a_i}{\partial \lambda_i} \tag{49}$$

$$\frac{\partial a_i}{\partial \lambda_i} = \begin{cases} 0 & \text{if } z_i > 0 \\ z_i & otherwise \end{cases} \tag{50}$$

$$\lambda_i \leftarrow \lambda_i - \alpha \times \frac{\partial \mathcal{E}}{\partial \lambda_i} \tag{51}$$

1. activation function is critical (large pos / neg can push activation towards saturation (0) if logistic, large negatives can lead to dying ReLUs)
2. learning rate is critical (large learning rates can push weights to extremes)
3. initialization of weights is critical (extremely large weights -> exploding gradient, extremely small weights -> vanishing gradient)

$$\delta_i = \underbrace{w_{j,i} \times w_{k,j} \times}_{\substack{\text{extreme weights} \\ \rightarrow \\ \text{unstable gradients}}} \frac{\partial \mathcal{E}}{\partial a_k} \underbrace{\times \frac{\partial a_k}{\partial z_k} \times \frac{\partial a_j}{\partial z_j} \times \frac{\partial a_i}{\partial z_i}}_{\substack{\text{extreme weights} \\ \rightarrow \\ \text{saturated activations} \\ \rightarrow \\ \text{vanishing gradients}}} \tag{52}$$

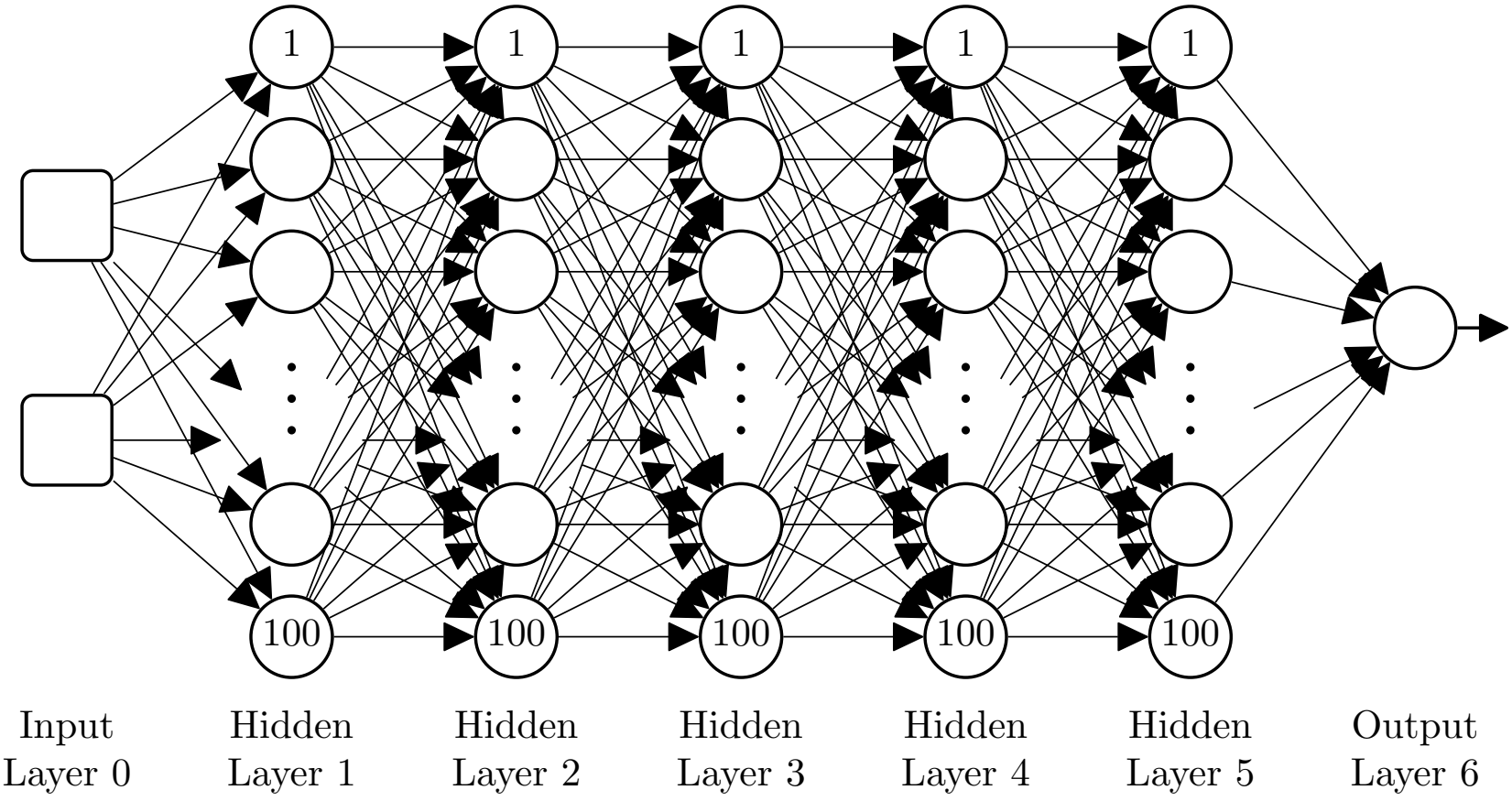
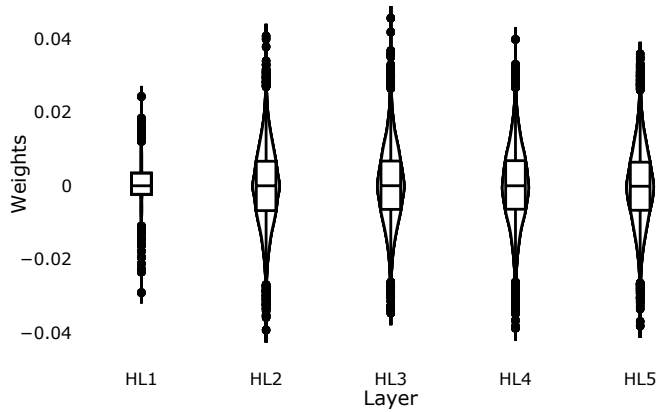
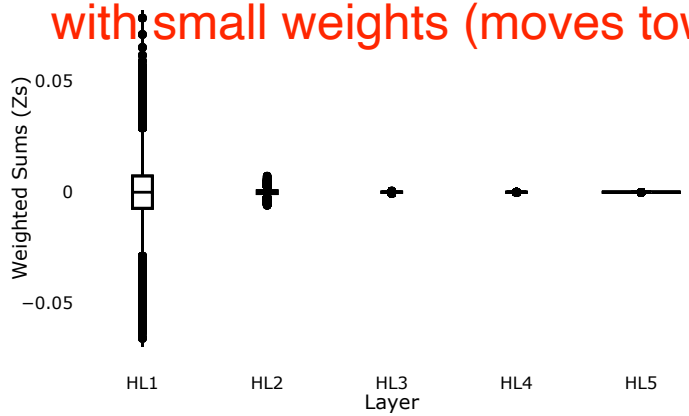


Figure 22: The architecture of the neural network used in the weight initialization experiments. Note that the neurons in this network use a linear activation function: $a_i = z_i$.

variance of z decreases bc weighted sum with small weights (moves towards 0)

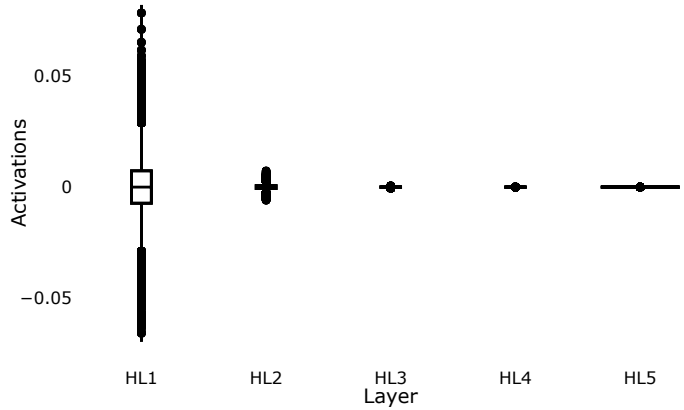


(a) Weights by Layer

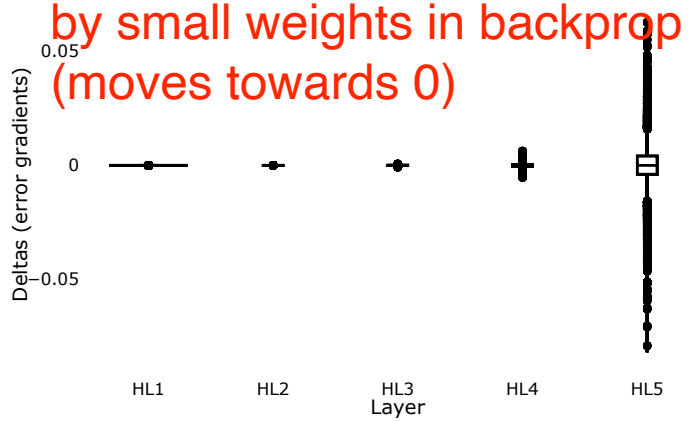


(b) Weighted Sum (z) by Layer

variance of delta decreases bc multiplying by small weights in backprop (moves towards 0)



(c) Activations by Layer

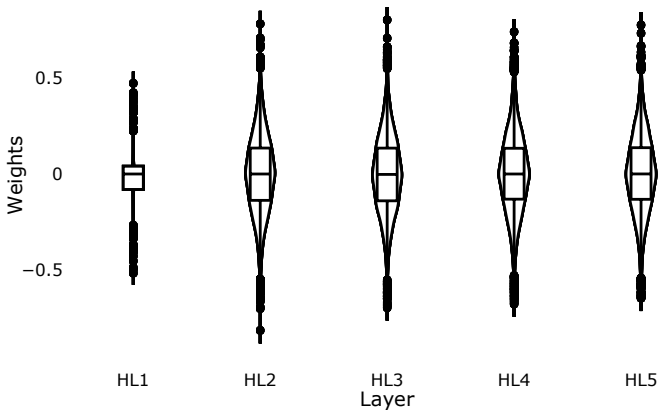


(d) δs by Layer

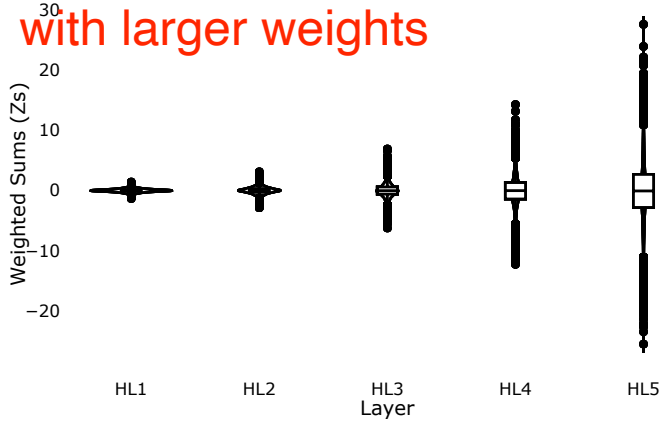
Figure 23: The internal dynamics of the network in Figure 22[73] during the first training iteration when the weights were initialized using a normal distribution with $\mu=0.0, \sigma=0.01$.

Weight Initialization and Unstable Gradients

variance of z increases bc weighted sum with larger weights

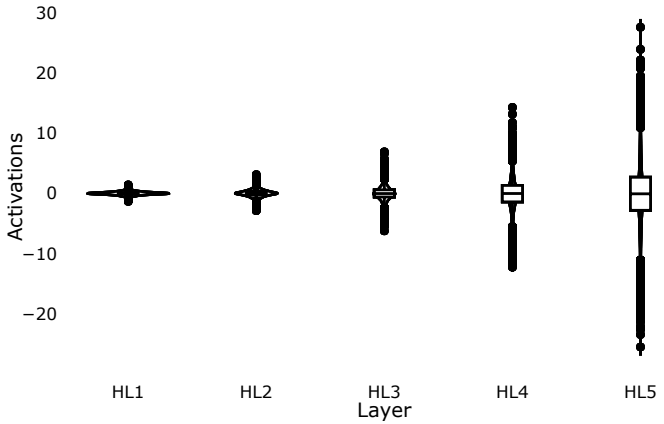


(a) Weights by Layer

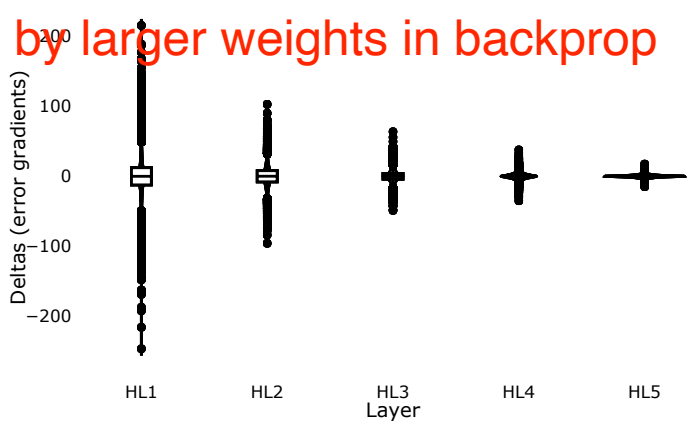


(b) Weighted Sum (z) by Layer

variance of delta increases bc multiplying by larger weights in backprop



(c) Activations by Layer



(d) δs by Layer

Figure 24: The internal dynamics of the network in Figure 22[73] during the first training iteration when the weights were initialized using a normal distribution with $\mu = 0.0$ and $\sigma = 0.2$.

$$z = (w_1 \times d_1) + (w_2 \times d_2) + \cdots + (w_{n_{in}} \times d_{n_{in}}) \tag{53}$$

$$var\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} var\left(X_i\right) \tag{54}$$

$$
\begin{aligned}
var(z) &= var\left((w_1 \times d_1) + (w_2 \times d_2) + \ldots (w_{n_{in}} \times d_{n_{in}})\right) \\
&= \sum_{i=1}^{n_{in}} var(w_i \times d_i) \qquad (55)
\end{aligned}
$$

$$var(w \times d) = [E(\mathbf{W})]^2\, var(\mathbf{d}) + [E(\mathbf{d})]^2\, var(\mathbf{W}) + var(\mathbf{W})\, var(\mathbf{d}) \quad (56$$

$$var(w \times d) = var(\mathbf{W}) var(\mathbf{d}) \qquad (57)$$

there is a relationship between variance of weighted sum (z) and # of inputs * variance of weights * variance of input data

increase any of these factors -> increase in variance of z

What if we initialized W with var = 1/n_in? -> n_in * 1/n_in

and if d is standardized, var = 1

$$var(z) = \sum_{i=1}^{n_{in}} var(w_i \times d_i) = n_{in}\, var(\mathbf{W})\, var(\mathbf{d}) \tag{58}$$

Why Vanishing Gradient, in terms of variance?

First Layer

$$
\begin{aligned}
var(Z^{(HL1)}) &= n_{in}^{(HL1)} \times var(\mathbf{W}^{(HL1)}) \times var(\mathbf{d}^{(HL1)}) \\
&= 2 \times 0.0001 \times 1 \\
&= 0.0002
\end{aligned}
\tag{59}
$$

second layer, more inputs, weight variance same..
but input data variance inherited from prior layer:
layer 1 output -> layer 2 input

$$
\begin{aligned}
var(Z^{(HL2)}) &= n_{in}^{(HL2)} \times var(\mathbf{W}^{(HL2)}) \times var(\mathbf{d}^{(HL2)}) \\
&= 100 \times 0.0001 \times 0.0002 \\
&= 0.000002
\end{aligned}
\tag{60}
$$

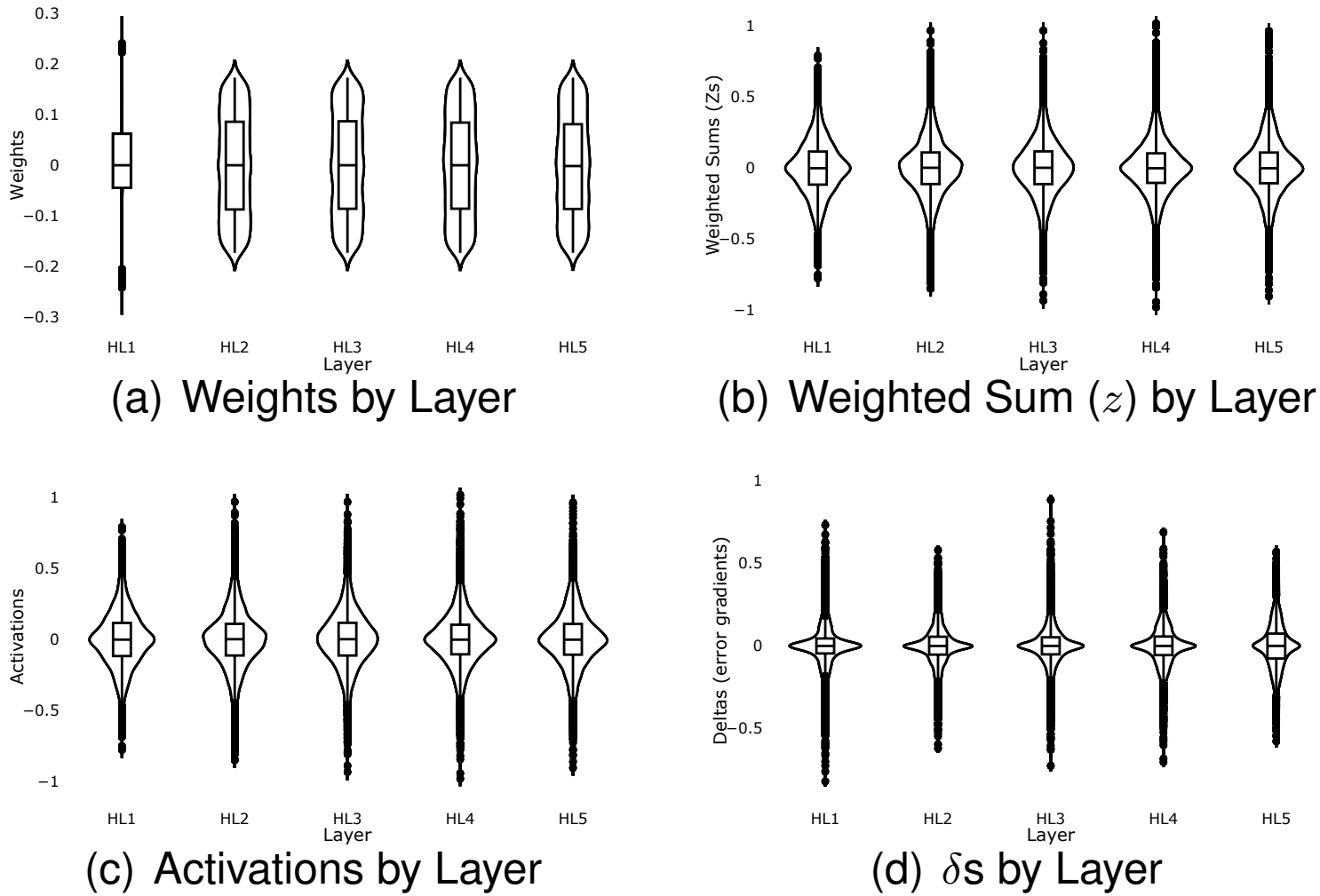
Therefore, variance will shrink towards 0
bc of var(d) … layer by layer

Xavier initialization:
carefully select variance of initialized weights vs random initialization

typically used with Logistic / TanH activation functions

$$var(\mathbf{W}^{(k)}) = \frac{2}{n_{in}^{(k)} + n_{out}^{(k)}} \tag{61}$$

$$var(\mathbf{W}^{(k)}) = \frac{1}{n_{in}^{(k)}} \tag{62}$$



(a) Weights by Layer

(b) Weighted Sum (z) by Layer

(c) Activations by Layer

(d) δs by Layer

Figure 25: The internal dynamics of the network in Figure 22[73] during the first training iteration when the weights were initialized using Xavier initialization.

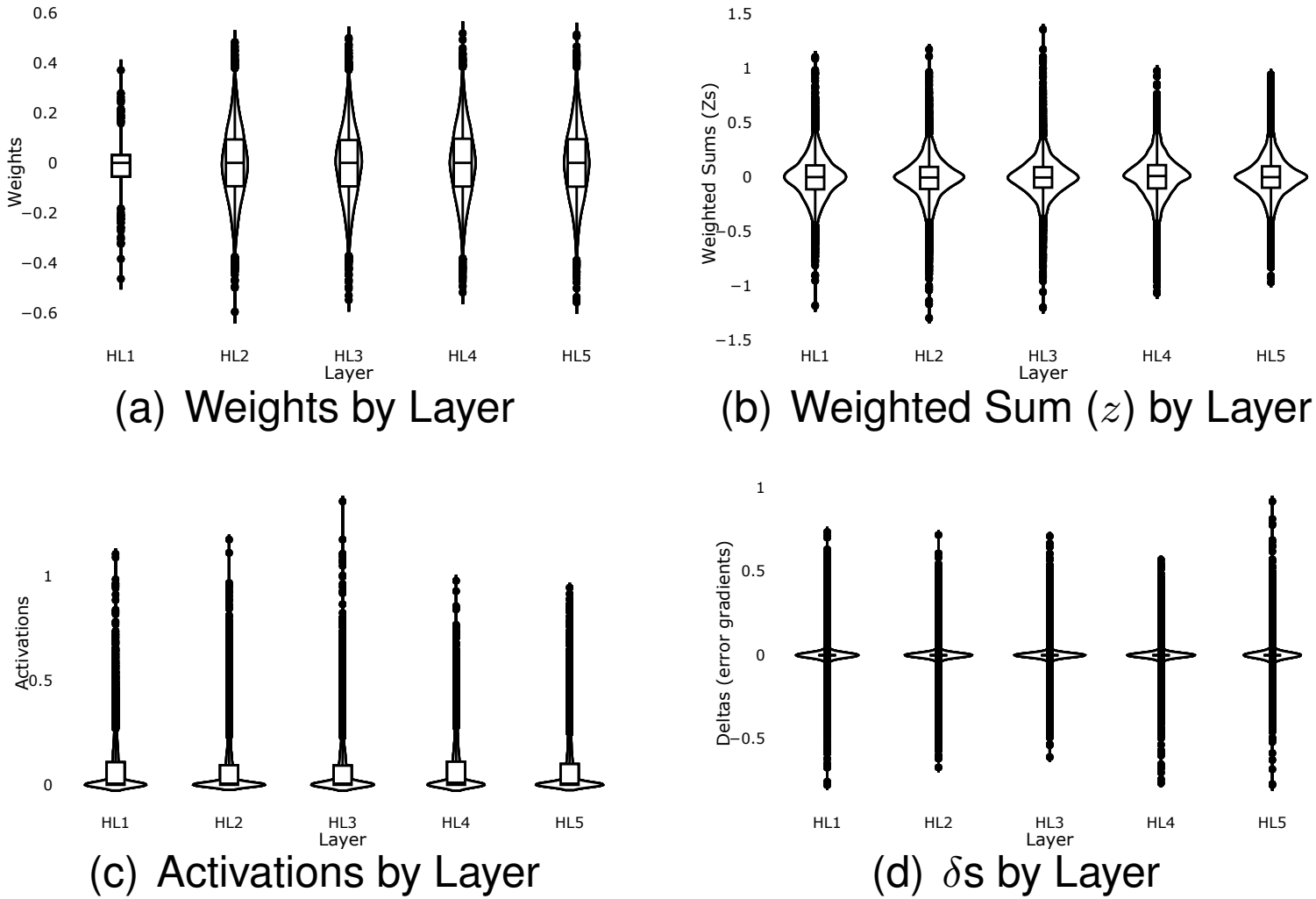
He / Kaiming initialization:
carefully select variance of initialized weights vs random initialization

typically used with ReLU activation functions

$$var(\mathbf{W}^{(k)}) = \frac{2}{n_{in}^{(k)}} \tag{63}$$

For ex: 3 layer network
First layer's (100 inputs) weight (mean, std) -> Xavier
Layers 2 (80 inputs) and 3 (50 inputs) weight (mean, std) -> He / Kaiming

$$
\begin{aligned}
W^{(1)} &\sim \mathcal{N}\left(0, \sqrt{\frac{1}{100}}\right) \\
W^{(2)} &\sim \mathcal{N}\left(0, \sqrt{\frac{2}{80}}\right) \\
W^{(3)} &\sim \mathcal{N}\left(0, \sqrt{\frac{2}{50}}\right)
\end{aligned} \tag{64}
$$



(a) Weights by Layer

(b) Weighted Sum (z) by Layer

(c) Activations by Layer

(d) δs by Layer

Figure 26: The internal dynamics of the network in Figure 22[73], using ReLUs, during the first training iteration when the weights were initialized using He initialization.

1. represent the target feature using **one-hot encoding**;
2. change the output layer of the network to be a **softmax layer**; and
3. change the error (or loss) function we use for training to be the **cross-entropy** function.

Table 13: The *range-normalized* hourly samples of ambient factors and full load electrical power output of a combined cycle power plant, rounded to two decimal places, and with the (binned) target feature represented using one-hot encoding.

ID	Ambient Temperature	Relative Humidity	Electrical Output		
	°C	%	*low*	*medium*	*high*
1	0.04	0.81	0	0	1
2	0.84	0.58	1	0	0
3	0.50	0.07	0	1	0
4	0.53	1.00	0	1	0

softmax produces probability outputs (weighted outputs for each neuron because dividing by sum of all output neurons)

non-normalized values are called logits

for ex: 2 outputs could be <.25, .75>

$$\varphi_{sm}\left(z_i\right) = \frac{e^{z_i}}{\sum_{j=1}^{m} e^{z_m}} \tag{65}$$

Table 14: The calculation of the softmax activation function φ_{sm} over a vector of three logits $\mathbf{l}$.

	$\mathbf{l}_0$	$\mathbf{l}_1$	$\mathbf{l}_2$
$\mathbf{l}$	1.5	-0.9	0.6
$e^{\mathbf{l}_i}$	4.48168907	0.40656966	1.8221188
$\sum_i e^{\mathbf{l}_i}$			6.71037753
$\varphi_{sm}(\mathbf{l}_i)$	0.667874356	0.060588195	0.27153745

normalized outputs can be interpreted as probabilities
(for each predicted class)

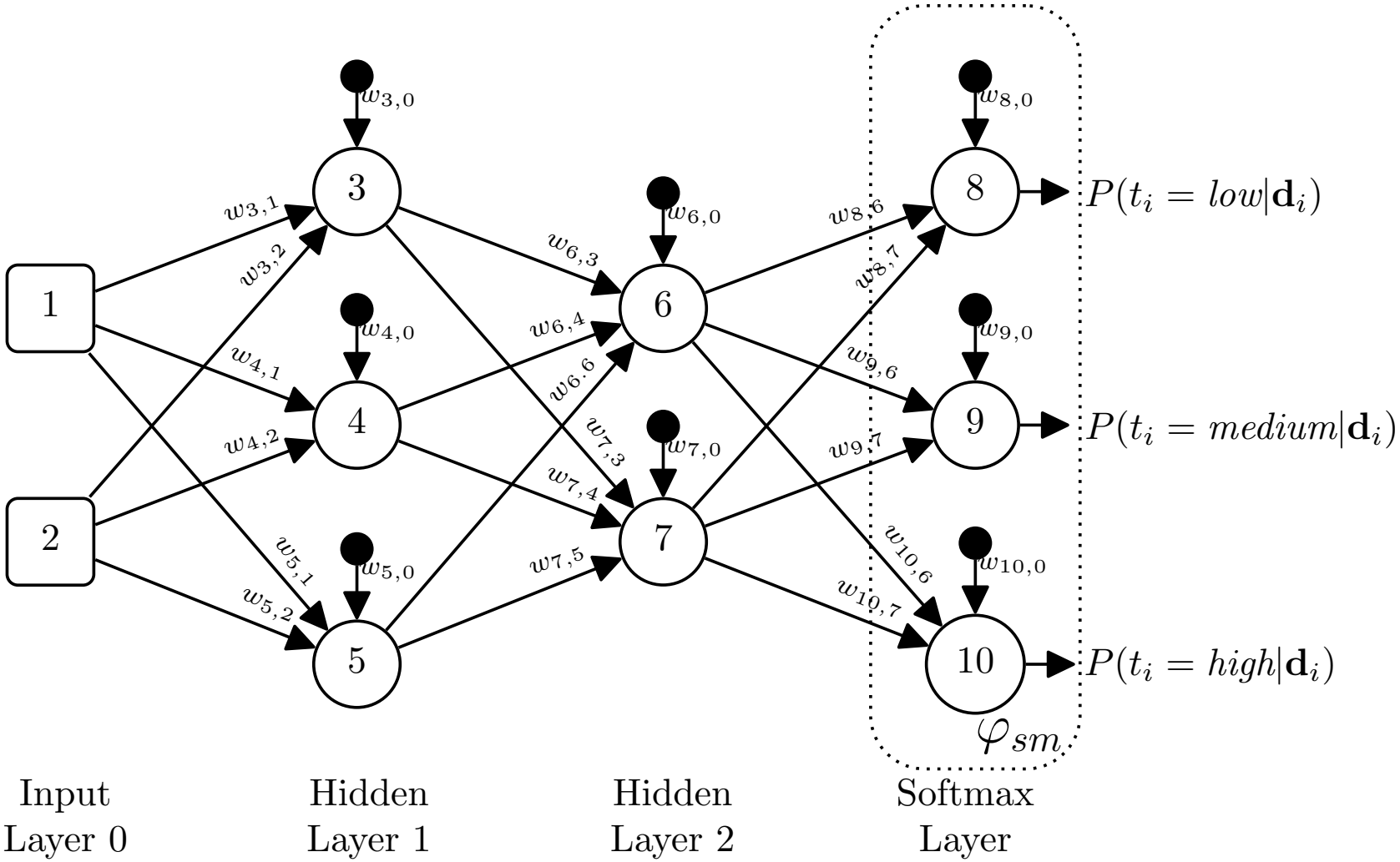


Figure 27: A schematic of a feedforward artificial neural network with a three-neuron softmax output layer.

- each output neuron predicts P for 1 level (class in classification)

Scenario 1: Wrong
target: <1, 0, 0>
predicted: <0, 0, 1>
Loss: -(1*-Inf + 0*-Inf + 0*-0) = Big #

Scenario 3: Correct
target: <1, 0, 0>
predicted: <1, 0, 0>
Loss: -(1*0 + 0*-Inf + 0*-Inf) = 0

$$L_{CE}\left(\mathbf{t}, \hat{\mathbf{P}}\right) = -\sum_j \mathbf{t}_j \ln\left(\hat{\mathbf{P}}_j\right) \tag{66}$$

$$L_{CE}\left(\mathbf{t}, \hat{\mathbf{P}}\right) = -\ln\left(\hat{\mathbf{P}}_\star\right) \text{ Simpler representation of LCE} \tag{67}$$

Scenario 3: Wrong
target: <1, 0, 0>
predicted: <0.01, 0.01, 0.98>
Loss: -(1*-4.6 + 0*-4.6 + 0*-.02) = 4.6

Scenario 4: Correct
target: <0, 0, 1>
predicted: <0.01, 0.01, 0.98>
Loss: -(0*-4.6 + 0*-4.6 + 1*-.02) = .02

Derivation of simpler representation of LCE

$$
\begin{aligned}
L_{CE}\left(\mathbf{t}, \hat{\mathbf{P}}\right) &= -\sum_{j} \mathbf{t}_j \ln\left(\hat{\mathbf{P}}_j\right) \\
&= -\left(\left(\mathbf{t}_0 \ln\left(\hat{\mathbf{P}}_0\right)\right) + \left(\mathbf{t}_1 \ln\left(\hat{\mathbf{P}}_1\right)\right) + \left(\mathbf{t}_2 \ln\left(\hat{\mathbf{P}}_2\right)\right)\right) \\
&= -\left(\left(0 \ln\left(\hat{\mathbf{P}}_0\right)\right) + \left(1 \ln\left(\hat{\mathbf{P}}_1\right)\right) + \left(0 \ln\left(\hat{\mathbf{P}}_2\right)\right)\right) \\
&= -1 \ln\left(\hat{\mathbf{P}}_1\right) \qquad (68)
\end{aligned}
$$

$$\boldsymbol{\delta}_k = \frac{\partial \mathcal{E}}{\partial z_k} \tag{69}$$

$$= \frac{\partial L_{CE}\left(\mathbf{t}, \hat{\mathbf{P}}\right)}{\partial \mathbf{l}_k} \tag{70}$$

$$= \frac{\partial - \ln\left(\hat{\mathbf{P}}_\star\right)}{\partial \mathbf{l}_k} \tag{71}$$

$$= \frac{\partial - \ln\left(\hat{\mathbf{P}}_\star\right)}{\partial\left(\hat{\mathbf{P}}_\star\right)} \times \frac{\partial\left(\hat{\mathbf{P}}_\star\right)}{\partial \mathbf{l}_k} \tag{72}$$

$$\frac{d \ln x}{dx} = \frac{1}{x} \tag{73}$$

$$\frac{\partial - \ln\left(\hat{\mathbf{P}}_{\star}\right)}{\partial\left(\hat{\mathbf{P}}_{\star}\right)} = -\frac{1}{\hat{\mathbf{P}}_{\star}} \tag{74}$$

$$\frac{\partial\left(\hat{\mathbf{P}}_{\star}\right)}{\partial \mathbf{l}_k} = \begin{cases} \hat{\mathbf{P}}_{\star}\left(1 - \hat{\mathbf{P}}_k\right) & \text{if } k = \star \\ -\hat{\mathbf{P}}_{\star}\hat{\mathbf{P}}_k & otherwise \end{cases} \tag{75}$$

$$\boldsymbol{\delta}_k = \frac{\partial - \ln\left(\hat{\mathbf{P}}_\star\right)}{\partial\left(\hat{\mathbf{P}}_\star\right)} \times \frac{\partial\left(\hat{\mathbf{P}}_\star\right)}{\partial \mathbf{l}_k} \tag{76}$$

$$= -\frac{1}{\hat{\mathbf{P}}_\star} \times \frac{\partial\left(\hat{\mathbf{P}}_\star\right)}{\partial \mathbf{l}_k} \tag{77}$$

$$= -\frac{1}{\hat{\mathbf{P}}_\star} \times \begin{cases} \hat{\mathbf{P}}_\star\left(1 - \hat{\mathbf{P}}_k\right) & \text{if } k = \star \\ -\hat{\mathbf{P}}_\star \hat{\mathbf{P}}_k & otherwise \end{cases} \tag{78}$$

$$= \begin{cases} -\left(1 - \hat{\mathbf{P}}_k\right) & \text{if } k = \star \\ \hat{\mathbf{P}}_k & otherwise \end{cases} \tag{79}$$

$$\boldsymbol{\delta}_{k=\star} = -\left(1 - \hat{\mathbf{P}}_k\right) \tag{80}$$

$$\boldsymbol{\delta}_{k\neq\star} = \hat{\mathbf{P}}_k \tag{81}$$

Handling Categorical Target Features: Softmax Output Layers and Cross-Entropy Loss Functions

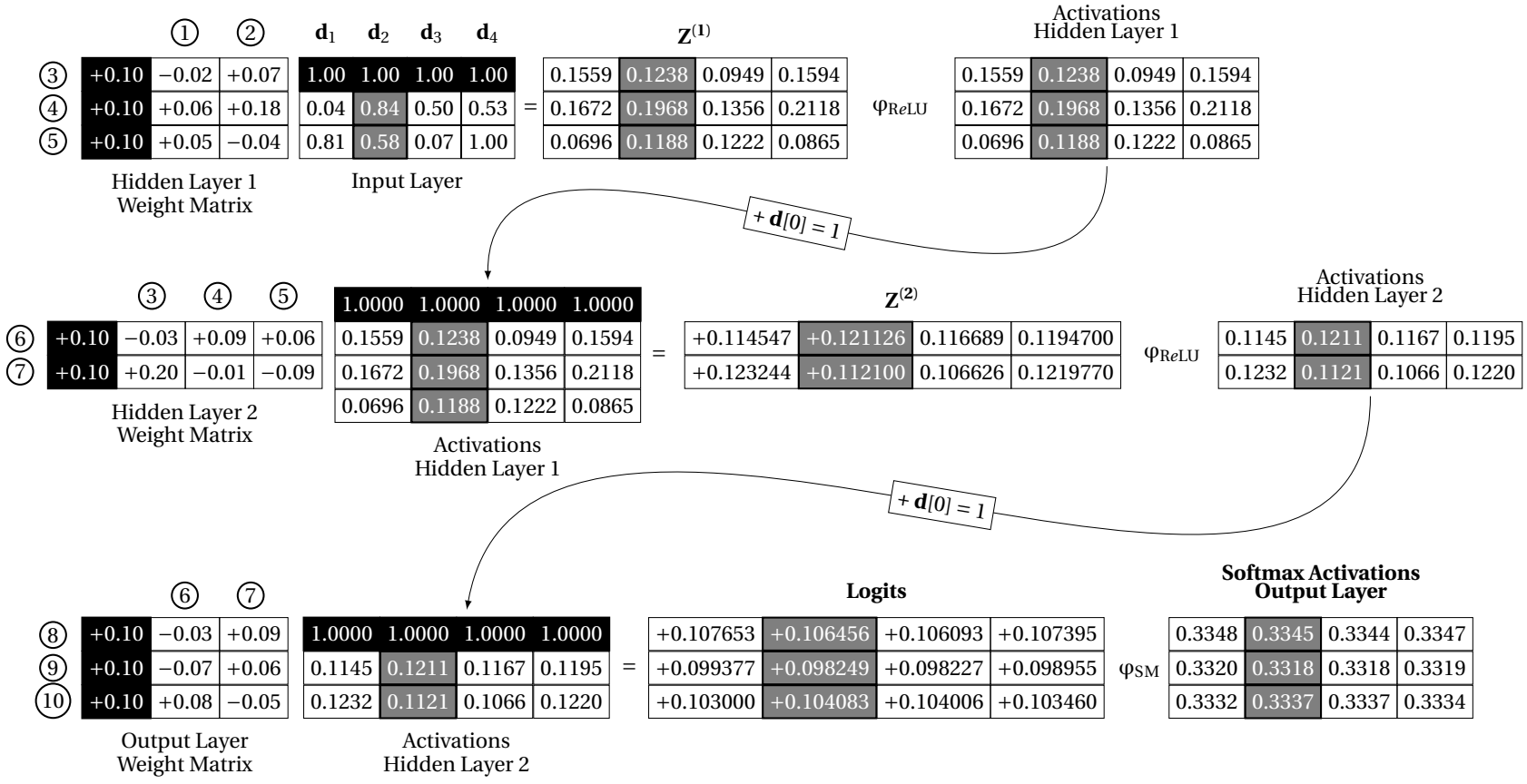


Figure 28: The forward pass of the mini-batch of examples listed in Table 13[88] through the network in Figure 27[91].

Table 15: The calculation of the softmax activations for each of the neurons in the output layer for each example in the mini-batch, and the calculation of the δ for each neuron in the output layer for each example in the mini-batch.

	$\mathbf{d}_1$	$\mathbf{d}_2$	$\mathbf{d}_3$	$\mathbf{d}_4$
Per Neuron Per Example logits				
Neuron 8	0.107653	0.106456	0.106093	0.107395
Neuron 9	0.099377	0.098249	0.098227	0.098955
Neuron 10	0.103000	0.104083	0.1040060	0.103460
Per Neuron Per Example $e^{\mathbf{l}_i}$				
Neuron 8	1.113661238	1.112328983	1.111925281	1.11337395
Neuron 9	1.104482611	1.103237457	1.103213186	1.104016618
Neuron 10	1.108491409	1.109692556	1.109607113	1.109001432
$\sum_i e^{\mathbf{l}_i}$	3.326635258	3.325258996	3.324745579	3.326392
Per Neuron Per Example Softmax Activations				
Neuron 8	0.3348	0.3345	0.3344	0.3347
Neuron 9	0.3320	0.3318	0.3318	0.3319
Neuron 10	0.3332	0.3337	0.3337	0.3334
Per Neuron Target One-Hot Encodings				
Neuron 8	0	1	0	0
Neuron 9	0	0	1	1
Neuron 10	1	0	0	0
Per Neuron Per Example δs				
Neuron 8	0.3348	-0.6655	0.3344	0.3347
Neuron 9	0.3320	0.3318	-0.6682	-0.6681
Neuron 10	-0.6668	0.3337	0.3337	0.3334

$$
\begin{aligned}
\Delta w_{9,6} &= \sum_{j=1}^{4} \boldsymbol{\delta}_{9,j} \times a_{6,j} \\
&= (0.3320 \times 0.1145) + (0.3318 \times 0.1211) \\
&\quad + (-0.6682 \times 0.1167) + (-0.6681 \times 0.1195) \\
&= 0.038014 + 0.04018098 + -0.07797894 + -0.07983795 \\
&= -0.07962191 \qquad (82)
\end{aligned}
$$

$$
\begin{aligned}
w_{9,6} &= w_{9,6} - \alpha \times \Delta w_{9,6} \\
&= -0.07 - 0.01 \times -0.07962191 \\
&= -0.07 - (-0.000796219) \\
&= -0.069203781
\end{aligned} \tag{83}
$$

Like other ML models, we seek to build generalizable NNs

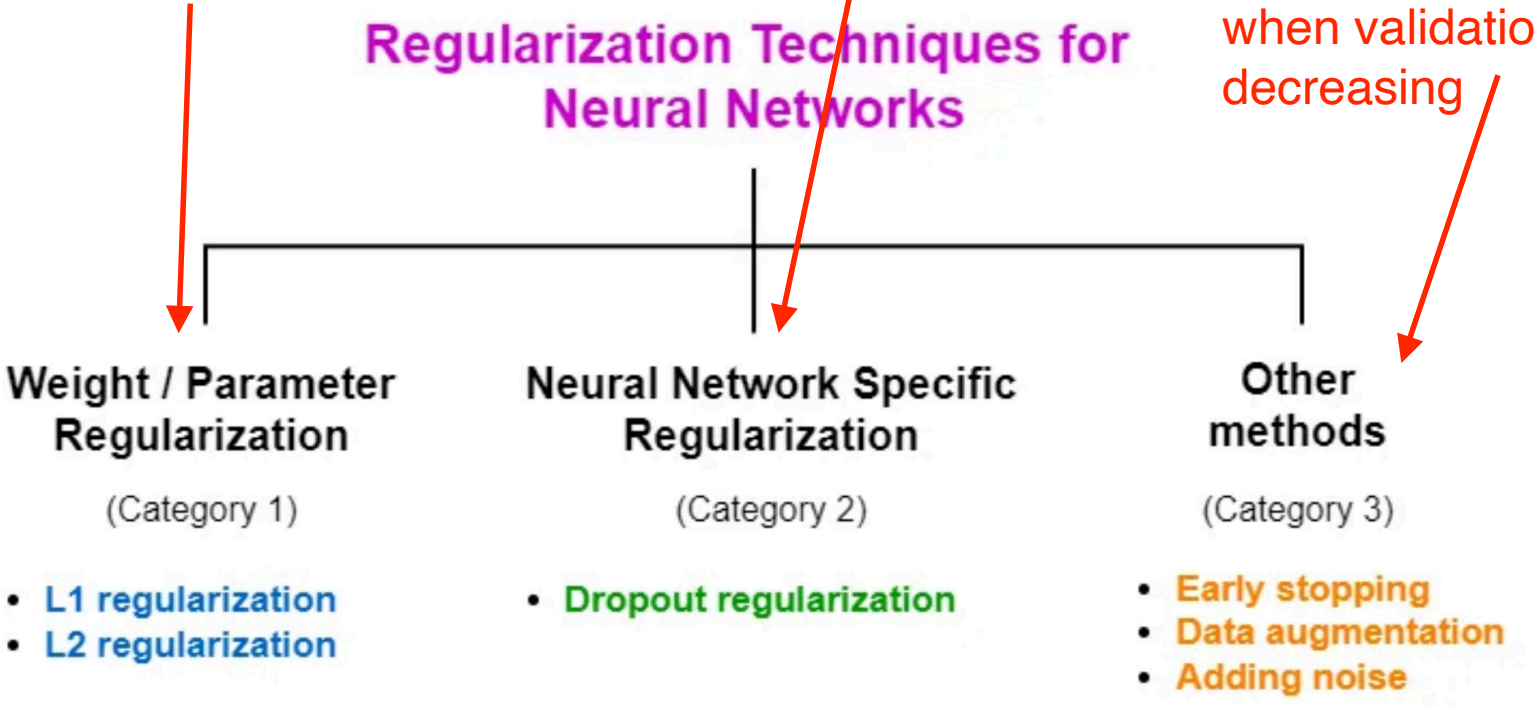
NNs can have billions of parameters, need to push them away from a tendency to overfit

3 core techniques:

weight decay (using optimizer or custom Loss function)

dropout: randomly turn off neurons during training

- Noise: can add random noise to data, weights, activations
- Data Aug: can synthesize new (similar data) from existing data
- Early Stopping: stop training when validation loss stops decreasing



Algorithm 1 The early stopping algorithm

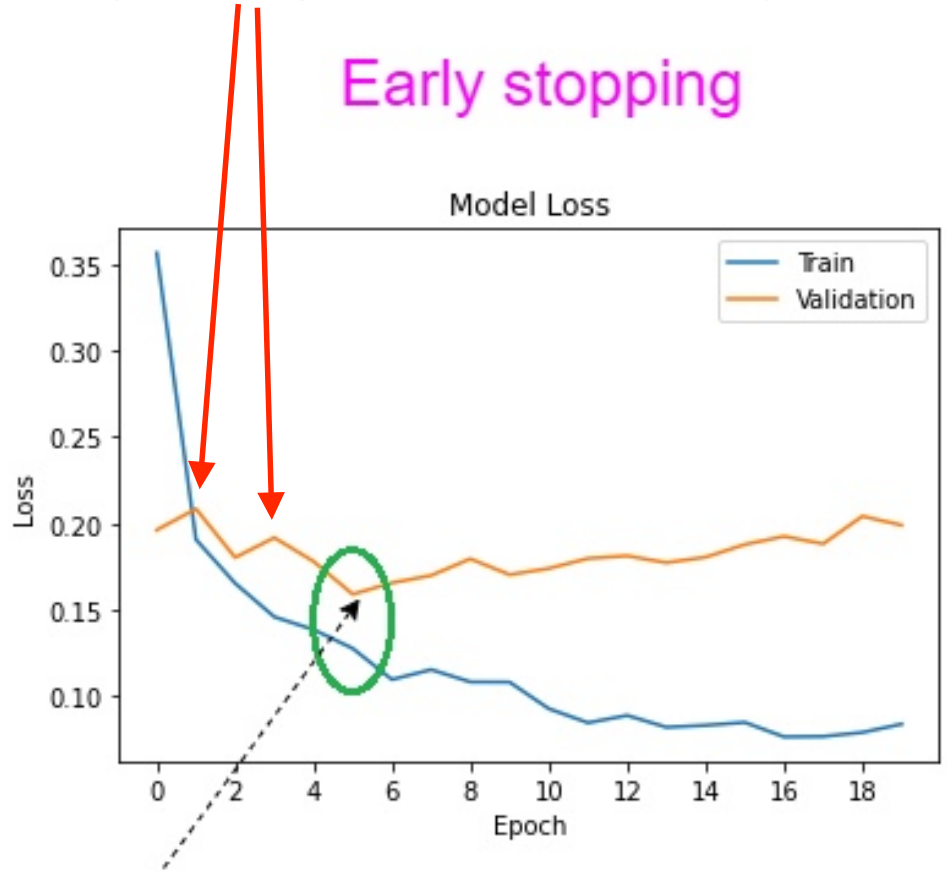
Require: p the patience parameter
Require: $\mathcal{D}_\nu$ a validation set
1: bestValidationError $= \infty$
2: tmpValidationError $= 0$
3: $\theta =$ initial model parameters
4: $\theta^{best} = 0$
5: patienceCount = 0
6: **while** patienceCount $< p$ **do**
7: $\theta =$ new model parameters after most recent weight update
8: tmpValidationError = calculateValidationError(θ, $\mathcal{D}_\nu$)
9: **if** bestValidationError $\geq$ tmpValidationError **then**
10: bestValidationError = tmpValidationError
11: $\theta^{best} = \theta$
12: patienceCount = 0
13: **else**
14: patienceCount = patienceCount + 1
15: **end if**
16: **end while**
17: **return** Best Model Parameters θ^{best}

- if current val error <= best val error, reset patience to 0 and capture model params
- if current val error > best error, increment patience

- training stops when patience > p limit param

Example of Early Stopping with Patience = 3

- patience is used to prevent training from terminating prematurely (due to spike in validation loss)



Right Fit Region

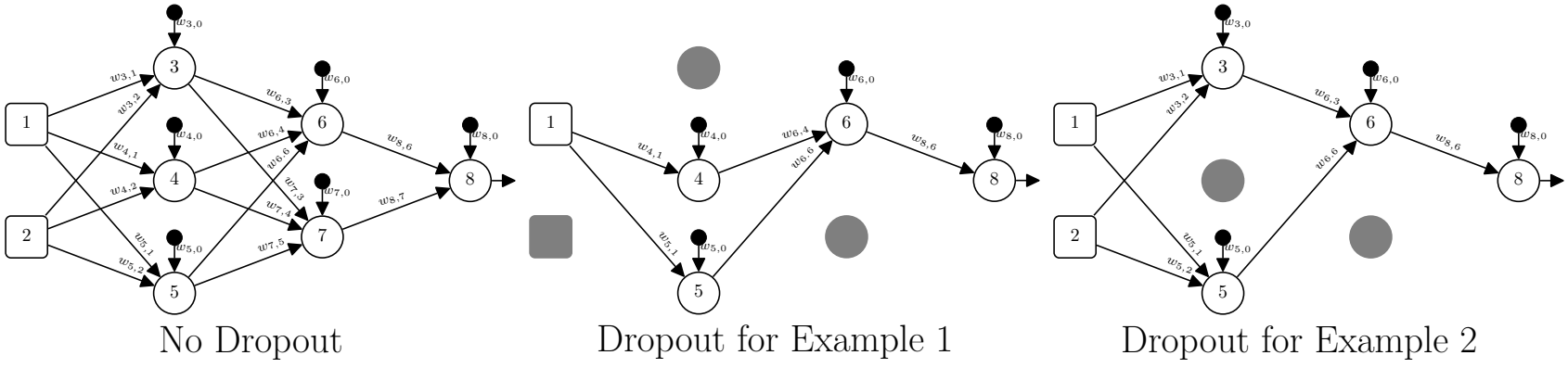


Figure 29: An illustration of how different small networks are generated for different training examples by applying dropout to the original large network. The gray nodes mark the neurons that have been dropped from the network for the training example.

- for each training iteration, turn off a random set of neurons (activation = 0), therefore not involved in forward pass and do not receive weight updates in backprop
- reduces overfitting by reducing reliance on a small set of inputs and neurons
- spread weight updates across more weights -> keeps weights small and improves model stability w.r.t. small changes in inputs

Algorithm 2 Extensions to Backpropagation to Use Inverted Dropout

Require: ρ probability that a neuron in a layer will not be dropped

▷ Forward Pass

1: **for** each input or hidden layer l **do**
2: $\quad \mathbf{DropMask}^{(l)} = (m_1, \ldots, m_{size(l)}) \sim Bernoulli(\rho)$
3: $\quad \mathbf{a}^{(l)'} = \mathbf{a}^{(l)} \odot \mathbf{DropMax}^{(l)}$
4: $\quad \mathbf{a}^{(l)''} = \frac{1}{\rho}\mathbf{a}^{(l)'}$
5: **end for**

▷ Backward Pass

6: **for** each layer l in backward pass **do**
7: $\quad \delta^{(l)} = \delta^{(l)} \odot \mathbf{DropMax}^{(l)}$
8: **end for**

Figure 30: Samples of the handwritten digit images from the MNIST dataset. Image attribution: Josef Steppan, used here under the Creative Commons Attribution-Share Alike 4.0 International license https://creativecommons.org/licenses/by-sa/4.0) and was sourced via Wikimedia Commons

RGB images are 3 channels
MNIST is grayscale -> 1 channel of pixel intensities (encoding a 4)
255 -> white, 0 -> black

$$\begin{bmatrix} 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & \mathbf{255} & 000 & 000 & 000 & 000 \\ 000 & \mathbf{255} & 000 & \mathbf{255} & 000 & 000 \\ 000 & \mathbf{255} & \mathbf{255} & \mathbf{255} & \mathbf{255} & 000 \\ 000 & 000 & 000 & \mathbf{255} & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 \end{bmatrix} \tag{84}$$

ex: a neuron processing inputs (pixel intensities) from top left corner of image (neuron's receptive field)

each neuron is responsible for a specific receptive field in the image

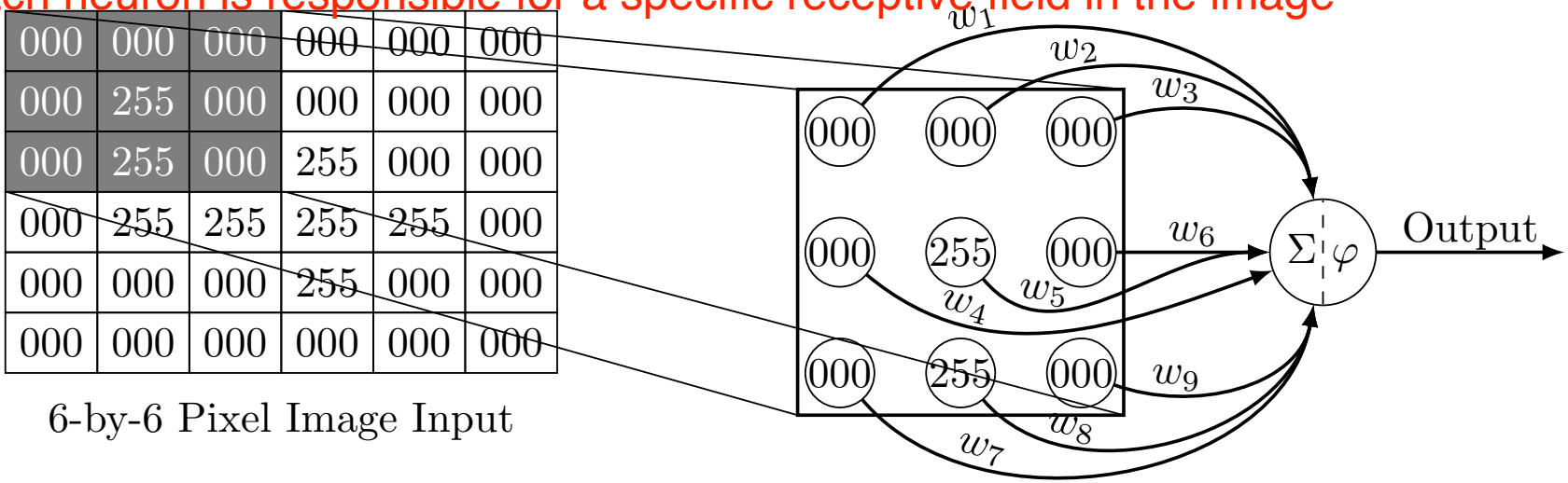


Figure 31: A 6-by-6 matrix representation of a grayscale image of a 4, and a neuron with a receptive field that covers the top-left corner of the image. This figure was inspired by Figure 2 of (Kelleher and Dobnik, 2017).

given a set of example weights, neuron performs 1.) weighted sum 2.) activation (based on inputs from prior image)

$$\begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix} \tag{85}$$

$$\begin{aligned} a_i &= rectifier((w_1 \times 000) + (w_2 \times 000) + (w_3 \times 000) \\ &\quad + (w_4 \times 000) + (w_5 \times 255) + (w_6 \times 000) \\ &\quad + (w_7 \times 000) + (w_8 \times 255) + (w_9 \times 000)) \\ &= rectifier((0 \times 000) + (0 \times 000) + (0 \times 000) \\ &\quad + (1 \times 000) + (1 \times 255) + (1 \times 000) \\ &\quad + (0 \times 000) + (0 \times 255) + (0 \times 000)) \\ &= 255 \end{aligned} \tag{86}$$

ex: different neuron with different receptive field

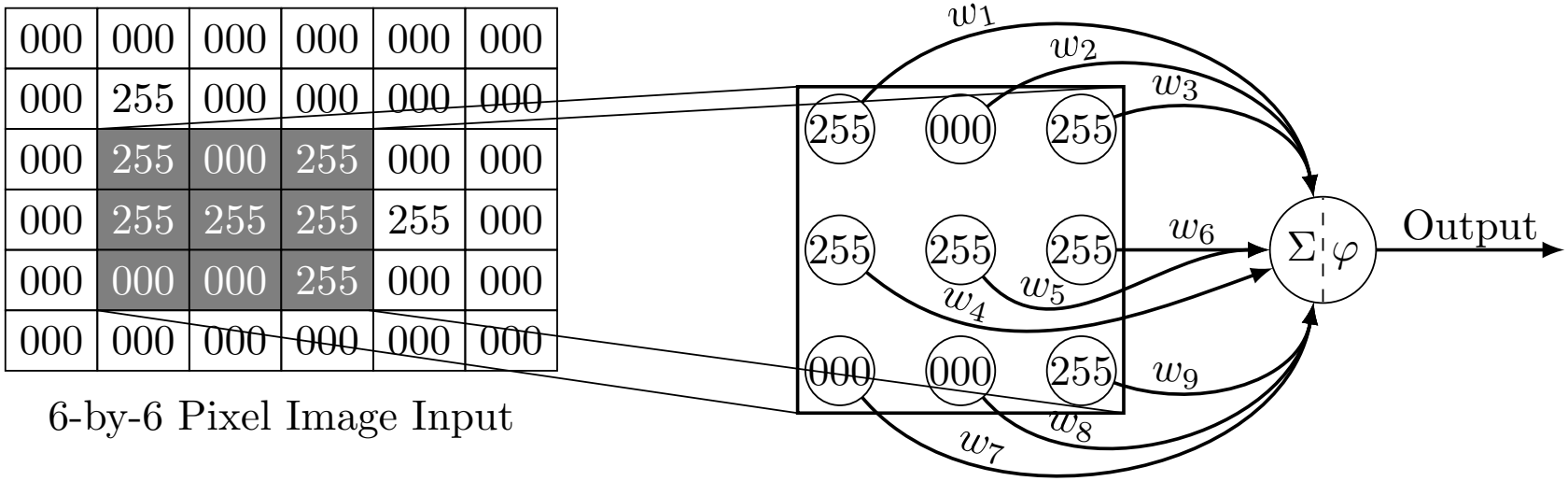


Figure 32: A 6-by-6 matrix representation of a grayscale image of a 4, and a neuron with a different receptive field from the neuron in Figure 31[107]. This figure was inspired by Figure 2 of (Kelleher and Dobnik, 2017).

maximum value (based on weights, neuron is rudimentary detector of horizontal lines)

$$\begin{aligned} a_i &= rectifier((w_1 \times 255) + (w_2 \times 000) + (w_3 \times 255) \\ &\quad + (w_4 \times 255) + (w_5 \times 255) + (w_6 \times 255) \\ &\quad + (w_7 \times 000) + (w_8 \times 000) + (w_9 \times 255)) \\ &= rectifier((0 \times 255) + (0 \times 000) + (0 \times 255) \\ &\quad + (1 \times 255) + (1 \times 255) + (1 \times 255) \\ &\quad + (0 \times 000) + (0 \times 000) + (0 \times 255)) \\ &= 765 \end{aligned} \tag{87}$$

weight matrices are called filters (i.e., filter inputs by returning high activations for certain patterns and low activations for others

weight matrices are learned via training (network learns which visual patterns are useful to extract from visual input to perform task)

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & +1 & -1 \\ -1 & +1 & -1 \\ -1 & +1 & -1 \end{bmatrix} \quad \begin{bmatrix} -1 & -1 & -1 \\ +1 & +1 & +1 \\ -1 & -1 & -1 \end{bmatrix} \tag{88}$$

multiple neurons, sharing same weight matrix (filter), scan the image

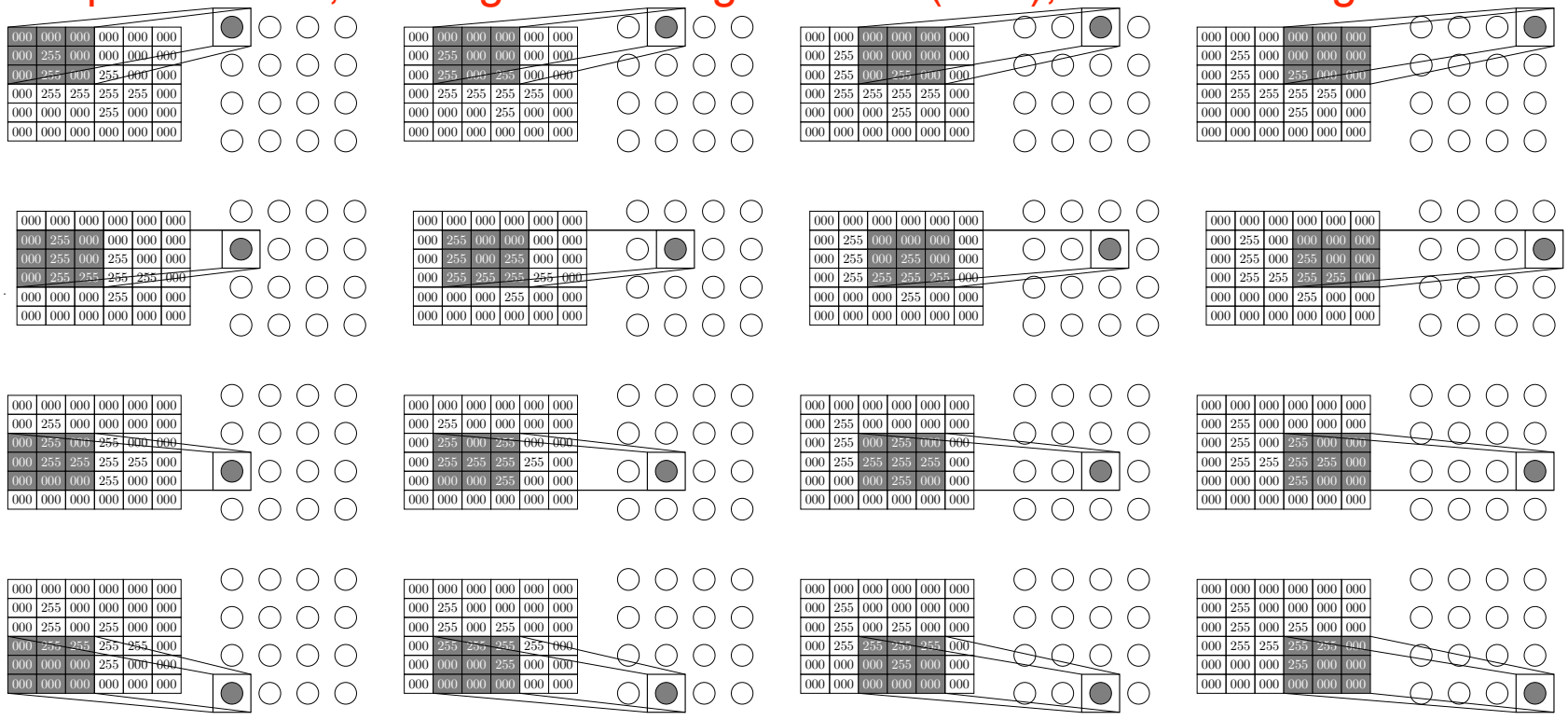


Figure 33: Illustration of the organization of a set of neurons that share weights (use the same filter) and their local receptive fields such that together the receptive fields cover the entirety of the input image.

m neurons share the same weight filter, so calculate weight updates for each neuron and sum it all together. apply sum to update the weights

$$\Delta w_{i,*} = \sum_{i=1}^{m} \boldsymbol{\delta}_i \times a_*$$
$$w_{i,*} \leftarrow w_{i,*} - \alpha \times \Delta w_{i,*} \tag{89}$$

$$\underbrace{\begin{bmatrix} 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & \mathbf{255} & 000 & 000 & 000 & 000 \\ 000 & \mathbf{255} & 000 & \mathbf{255} & 000 & 000 \\ 000 & \mathbf{255} & \mathbf{255} & \mathbf{255} & \mathbf{255} & 000 \\ 000 & 000 & 000 & \mathbf{255} & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 \end{bmatrix}}_{\text{Input Image}} \rightarrow \underbrace{\begin{bmatrix} -1 & +1 & -1 \\ -1 & +1 & -1 \\ -1 & +1 & -1 \end{bmatrix}}_{\text{Convolved Filter}} \rightarrow \underbrace{\begin{bmatrix} 510 & 0 & 255 & 0 \\ 510 & 0 & 0 & 0 \\ 255 & 0 & 255 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{\text{Feature Map}}$$

+ pass through ReLU

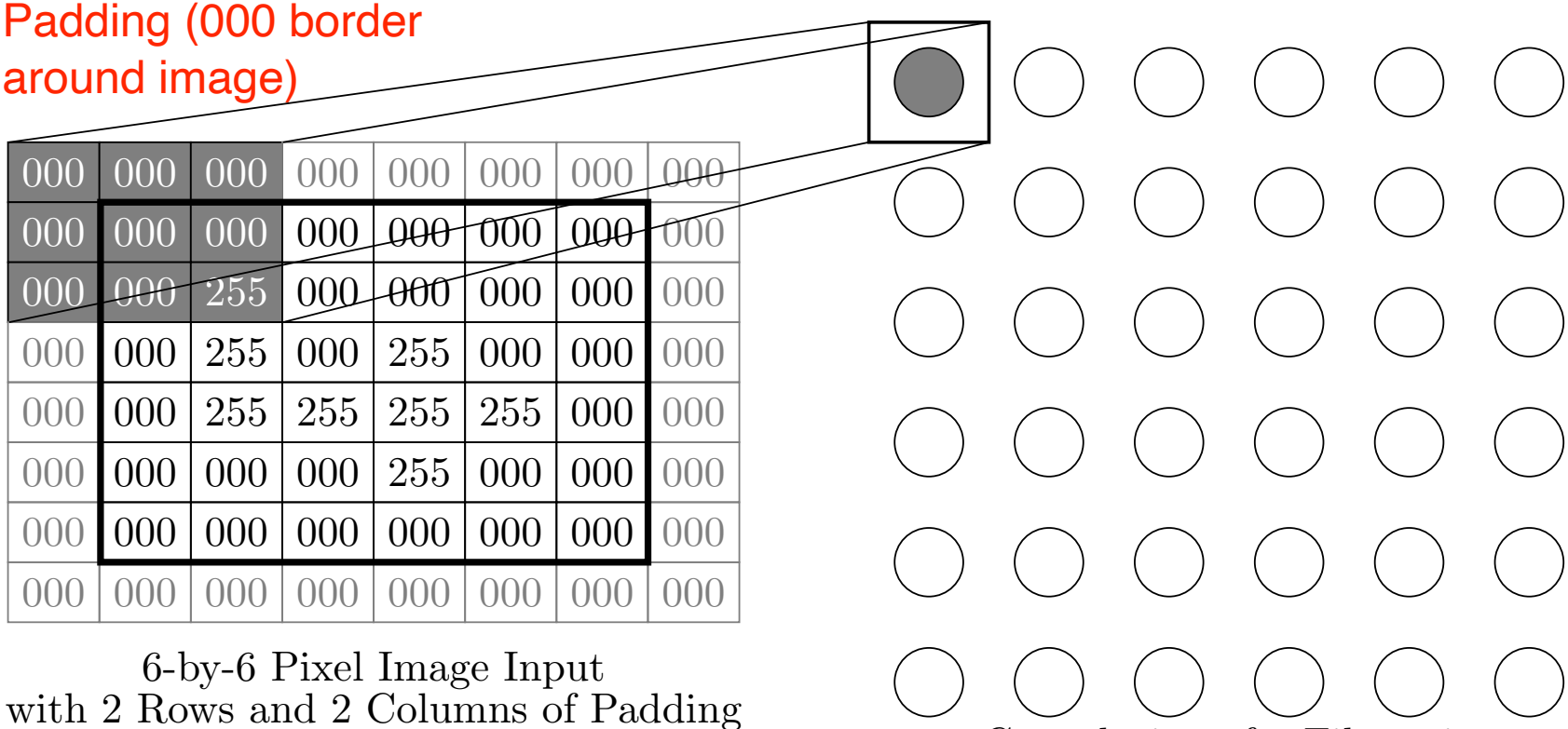
(90)

$$\underbrace{\begin{bmatrix} 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & \mathbf{255} & 000 & 000 & 000 & 000 \\ 000 & \mathbf{255} & 000 & \mathbf{255} & 000 & 000 \\ 000 & \mathbf{255} & \mathbf{255} & \mathbf{255} & \mathbf{255} & 000 \\ 000 & 000 & 000 & \mathbf{255} & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 \end{bmatrix}}_{\text{Input Image}} \rightarrow \underbrace{\begin{bmatrix} -1 & -1 & -1 \\ +1 & +1 & +1 \\ -1 & -1 & -1 \end{bmatrix}}_{\text{Convolved Filter}} \rightarrow \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 255 & 0 & 255 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{\text{Feature Map}}$$

+ pass through ReLU

(91)

Padding (000 border around image)



6-by-6 Pixel Image Input with 2 Rows and 2 Columns of Padding

Convolution of a Filter via Set of Neurons Sharing Weights

Figure 34: A grayscale image of a 4 after padding has been applied to the original 6-by-6 matrix representation, and the local receptive field of a neuron that includes both valid and padded pixels.

Output Size of Feature Map: (Input Size - Filter Size + 2*Padding)/Stride +1
Rounded down if decimal

Convolution with padding (feature map output size remains 6x6)

$$\underbrace{\begin{bmatrix} 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & 000 & \mathbf{255} & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & \mathbf{255} & \mathbf{255} & \mathbf{255} & 000 & 000 \\ 000 & 000 & 000 & 000 & \mathbf{255} & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \end{bmatrix}}_{\text{Input Image}} \rightarrow \underbrace{\begin{bmatrix} -1 & +1 & -1 \\ -1 & +1 & -1 \\ -1 & +1 & -1 \end{bmatrix}}_{\text{Convolved Filter}} \rightarrow \underbrace{\begin{bmatrix} 0 & 255 & 0 & 0 & 0 & 0 \\ 0 & 510 & 0 & 255 & 0 & 0 \\ 0 & 510 & 0 & 0 & 0 & 0 \\ 0 & 255 & 0 & 255 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 255 & 0 & 0 \end{bmatrix}}_{\text{Feature Map}}$$

(92)

Convolution with padding (feature map output size remains 6x6)

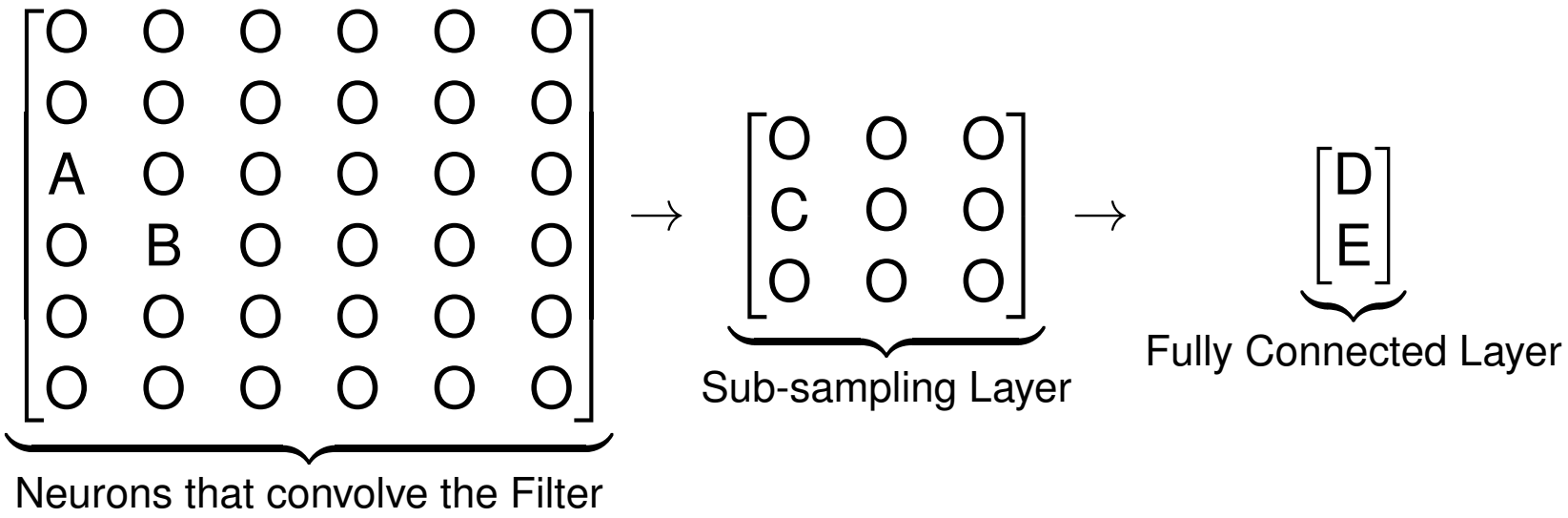
$$\underbrace{\begin{bmatrix} 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & 000 & \mathbf{255} & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & \mathbf{255} & \mathbf{255} & \mathbf{255} & 000 & 000 \\ 000 & 000 & 000 & 000 & \mathbf{255} & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \end{bmatrix}}_{\text{Input Image}} \rightarrow \underbrace{\begin{bmatrix} -1 & -1 & -1 \\ +1 & +1 & +1 \\ -1 & -1 & -1 \end{bmatrix}}_{\text{Convolved Filter}} \rightarrow \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 255 & 0 & 255 & 0 & 255 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\text{Feature Map}}$$

(93)

2x2 max pooling as a subsampling technique
local receptive fields do not overlap

$$\underbrace{\begin{bmatrix} 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & 000 & \mathbf{255} & 000 & 000 & 000 \\ 000 & 000 & \mathbf{255} & \mathbf{255} & \mathbf{255} & \mathbf{255} & 000 & 000 \\ 000 & 000 & 000 & 000 & \mathbf{255} & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \\ 000 & 000 & 000 & 000 & 000 & 000 & 000 & 000 \end{bmatrix}}_{\text{Input Image}} \rightarrow \underbrace{\begin{bmatrix} -1 & -1 & -1 \\ +1 & +1 & +1 \\ -1 & -1 & -1 \end{bmatrix}}_{\text{Convolved Filter}} \rightarrow$$

$$\rightarrow \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 255 & 0 & 255 & 0 & 255 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\text{Feature Map}} \rightarrow \text{max pooling} \rightarrow \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 255 & 255 & 255 \\ 0 & 0 & 0 \end{bmatrix}}_{\text{Output from Sub-sampling}}$$


O O O O O O
O O O O O O
A O O O O O
O B O O O O
O O O O O O
O O O O O O
Neurons that convolve the Filter
O O O
C O O
O O O
Sub-sampling Layer
D
E
Fully Connected Layer

(95)

$$\begin{aligned}\delta_C &= \frac{\partial \mathcal{E}}{\partial a_C} \times \frac{\partial a_C}{\partial z_C} \\ &= ((\delta_D \times w_{D,C}) + (\delta_E \times w_{E,C})) \times 1\end{aligned} \tag{96}$$

$$\begin{aligned}\delta_B &= \frac{\partial \mathcal{E}}{\partial a_B} \times \frac{\partial a_B}{\partial z_B} \\ &= (\delta_D \times w_{C,B}) \times \frac{\partial a_B}{\partial z_B} \\ &= (\delta_D \times 1) \times 1\end{aligned} \tag{97}$$

3 dimensional filter for RGB image (1 weight matrix for each channel)

$$\left[\underbrace{w_0}_{\text{bias}} \begin{bmatrix} w_1 & w_2 \\ w_3 & w_4 \end{bmatrix} \begin{bmatrix} w_5 & w_6 \\ w_7 & w_8 \end{bmatrix} \begin{bmatrix} w_9 & w_{10} \\ w_{11} & w_{12} \end{bmatrix} \right] \tag{98}$$

3 dimensional filter for RGB image (1 weight matrix for each channel)

$$\left[\underbrace{w_0 = 0.5}_{\text{bias}} \underbrace{\begin{bmatrix} w_1 = 1 & w_2 = 1 \\ w_3 = 0 & w_4 = 0 \end{bmatrix}}_{\text{Red Channel}} \underbrace{\begin{bmatrix} w_5 = 0 & w_6 = 1 \\ w_7 = 0 & w_8 = 1 \end{bmatrix}}_{\text{Green Channel}} \underbrace{\begin{bmatrix} w_9 = 1 & w_{10} = 0 \\ w_{11} = 0 & w_{12} = 1 \end{bmatrix}}_{\text{Blue Channel}} \right] \tag{99}$$

3 pixels x 3 pixels RGB Image (with 3 channels)

$$\left[\underbrace{\begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\text{Red Channel}} \underbrace{\begin{bmatrix} 0 & 0 & 2 \\ 0 & 0 & 2 \\ 0 & 0 & 2 \end{bmatrix}}_{\text{Green Channel}} \underbrace{\begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{bmatrix}}_{\text{Blue Channel}} \right] \tag{100}$$

for ex: start at top left of image as inputs for first convolution

$$\left[\underbrace{\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}}_{\text{Red Channel}} \underbrace{\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}}_{\text{Green Channel}} \underbrace{\begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}}_{\text{Blue Channel}}\right] \tag{101}$$

output activation for neuron (top left receptive field)

$$
\begin{aligned}
z &= ((w_0 \times 1) \\
&\quad + (w_1 \times 1) + (w_2 \times 1) + (w_3 \times 0) + (w_4 \times 0) \\
&\quad + (w_5 \times 0) + (w_6 \times 0) + (w_7 \times 0) + (w_8 \times 0) \\
&\quad + (w_9 \times 3) + (w_{10} \times 0) + (w_{11} \times 0) + (w_{12} \times 3)) \\
&= 0.5 + 1 + 1 + 0 + 0 + 0 + 0 + 0 + 0 + 3 + 0 + 0 + 3 \\
&= 8.5 \\
a &= rectifier(z) \\
&= rectifier(8.5) \\
&= 8.5
\end{aligned}
\tag{102}
$$

if all convolutions performed, feature map output of 3 channel RB image -> 2x2

$$\begin{bmatrix} 8.5 & 6.5 \\ 0.5 & 10.5 \end{bmatrix} \tag{103}$$

can apply multiple filters
(create stacked outputs)

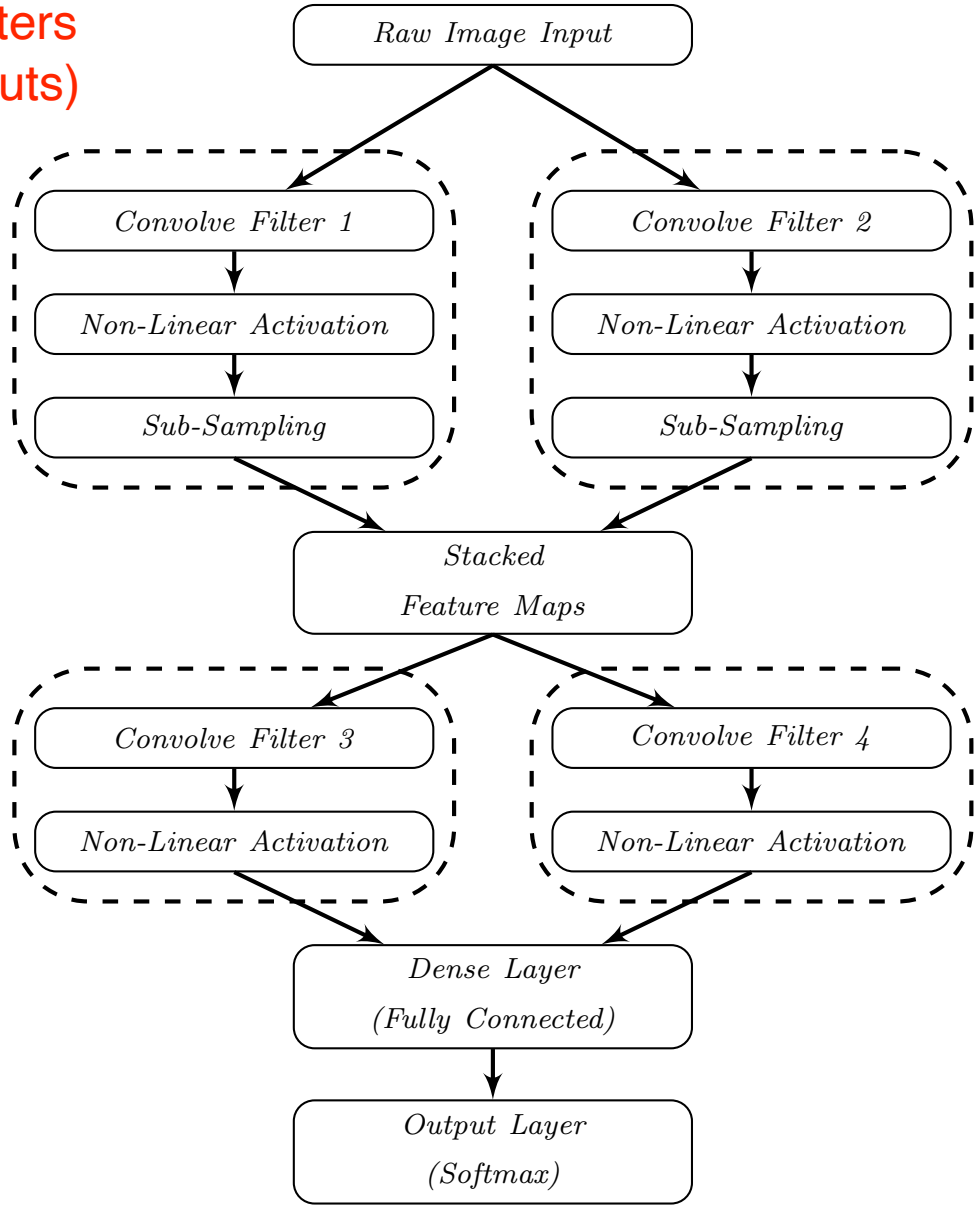


Figure 35: Schematic of the typical sequences of layers found in a convolutional neural network.

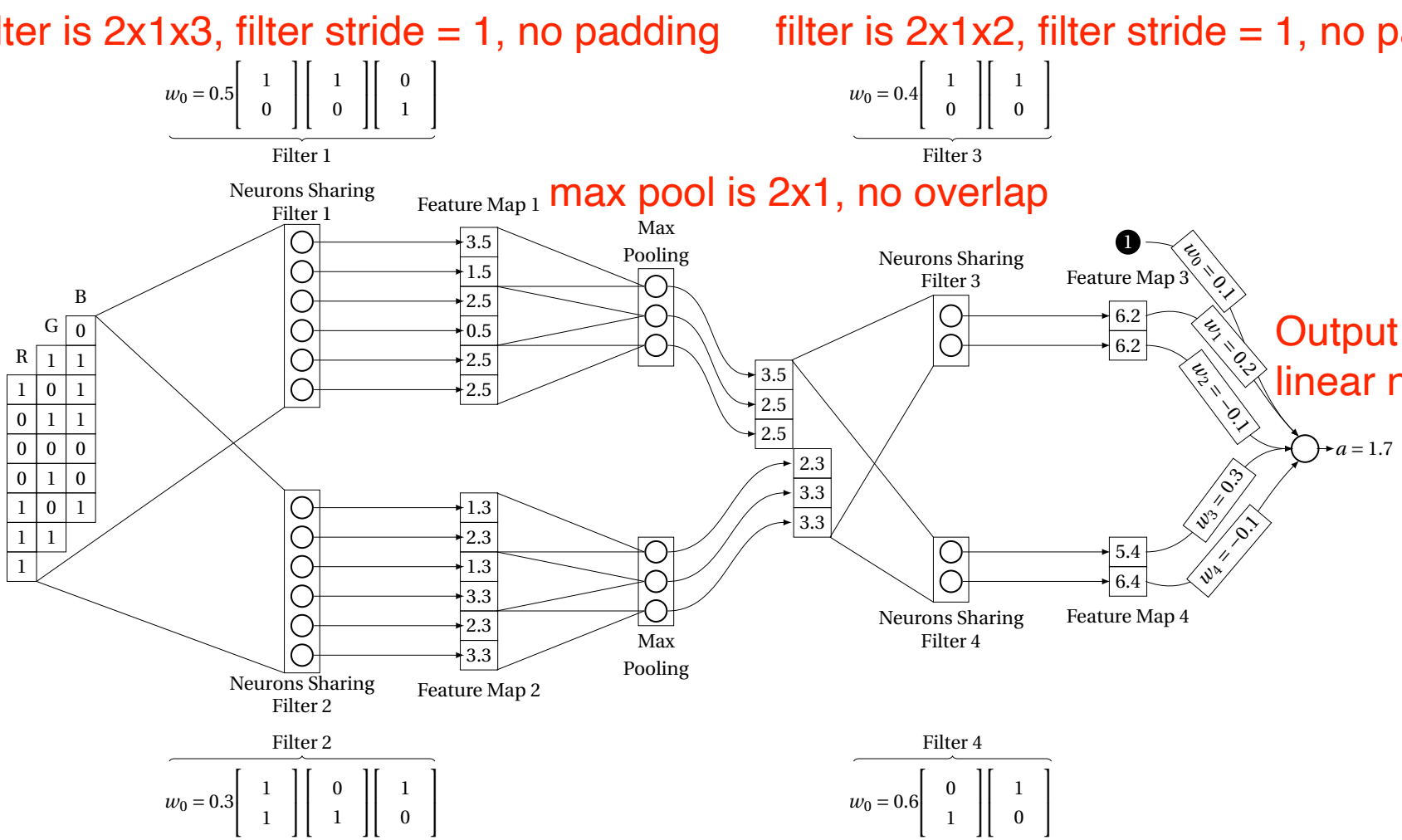


Figure 36: Worked example illustrating the dataflow through a multilayer, multifilter CNN.

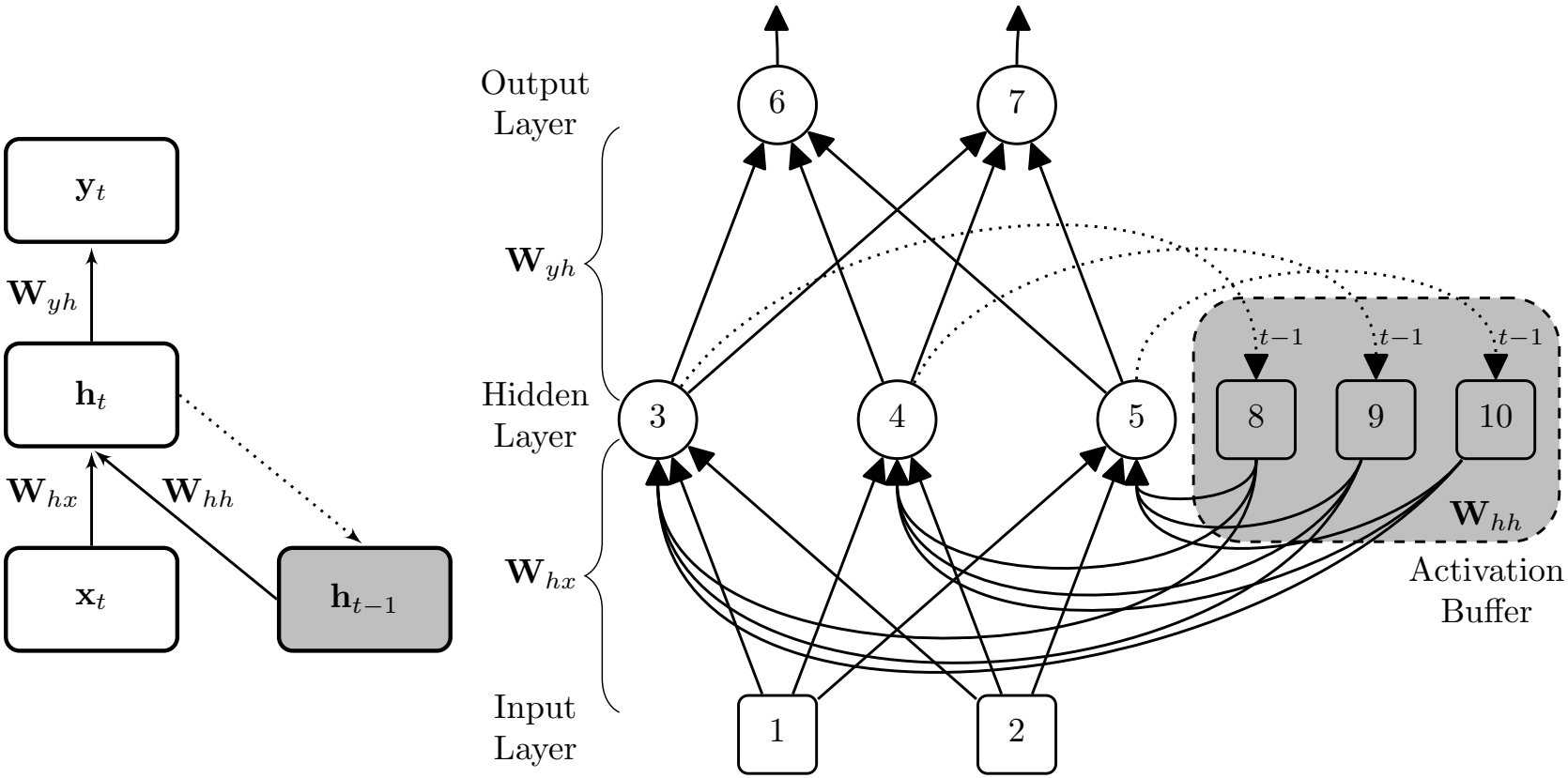


Figure 37: Schematic of the simple recurrent neural architecture.

$$\mathbf{h}_t = \varphi\left((\mathbf{W}_{hh} \cdot \mathbf{h}_{t-1}) + (\mathbf{W}_{hx} \cdot \mathbf{x}_t) + \mathbf{w}_0\right) \tag{104}$$

$$\mathbf{y}_t = \varphi\left(\mathbf{W}_{yh} \cdot \mathbf{h}_t\right) \tag{105}$$

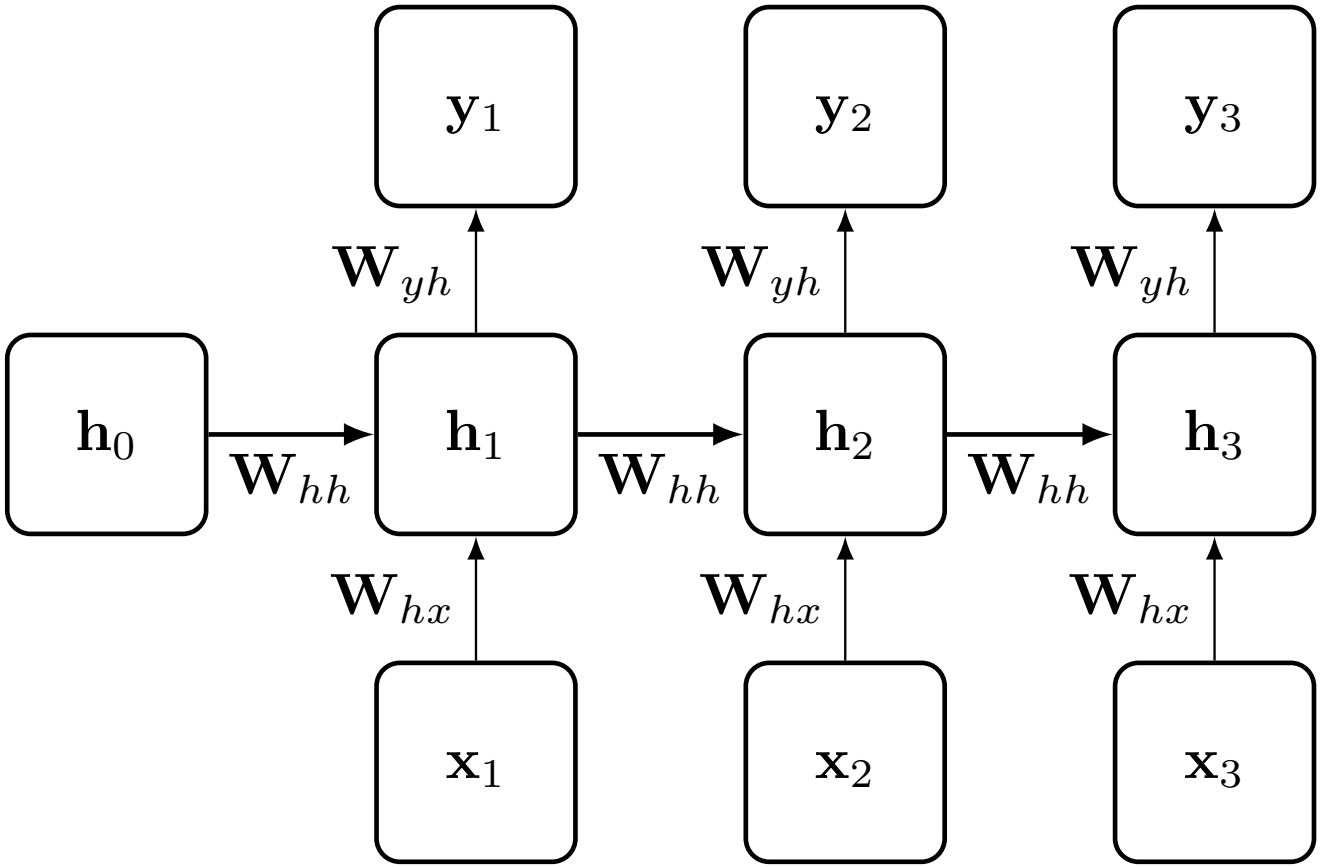


Figure 38: A simple RNN model unrolled through time (in this instance, three time-steps).

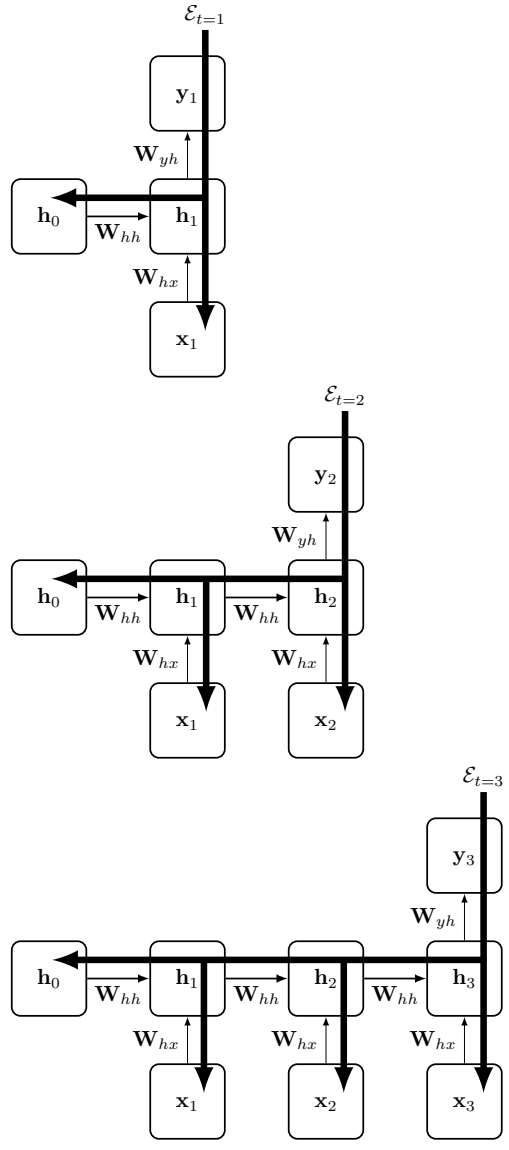


Figure 39: An illustration of the different iterations of backpropagation during backpropagation through time.

Algorithm 3 The Backpropagation Through Time Algorithm

Require: h_0 initialized hidden state
Require: $\mathbf{x}$ a sequence of inputs
Require: $\mathbf{y}$ a sequence of target outputs
Require: n length of the input sequence
Require: Initialized weight matrices (with associated biases)
Require: $\Delta\mathbf{w}$ a data structure to accumulate the summed weight updates for each weight across time-steps

for $t = 1$ to n **do**
    $Inputs = [x_0, \ldots, x_t]$
    $h_{tmp} = h_0$
    for $i = 0$ to t **do** ▷ Unroll the network through t steps
        $h_{tmp} = ForwardPropagate(Inputs[i], h_{tmp})$
    end for
    $\hat{y}_t = OutputLayer(h_{tmp})$ ▷ Generate the output for time-step t
    $\mathcal{E}_t = \mathbf{y}[t] - \hat{y}_t$ ▷ Calculate the error at time-step t
    $Backpropagate(\mathcal{E}_t)$ ▷ Backpropagate $\mathcal{E}_t$ through t steps
    For each weight, sum the weight updates across the unrolled network and update $\Delta\mathbf{w}$
end for
Update the network weights using $\Delta\mathbf{w}$

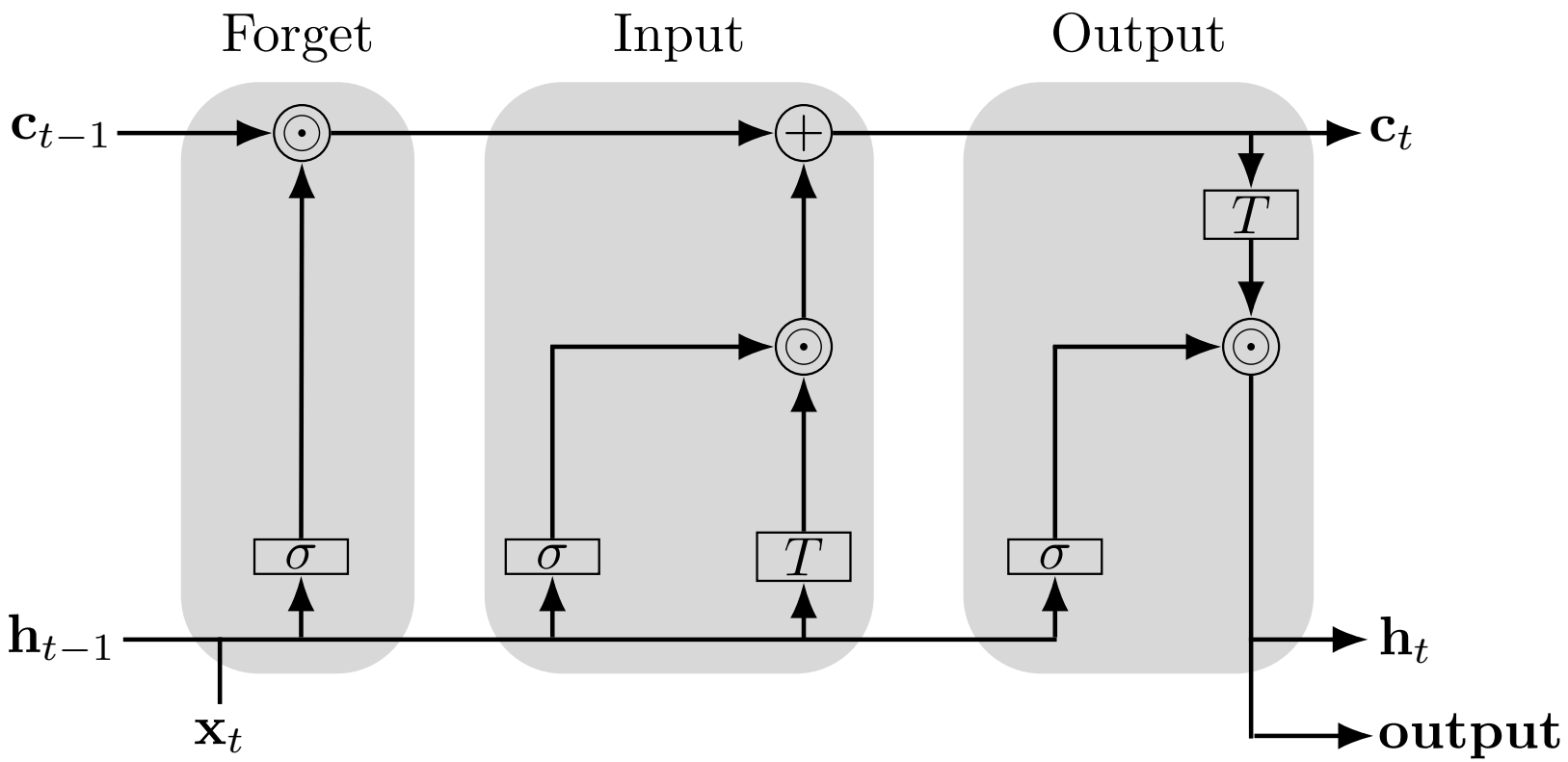


Figure 40: A schematic of the internal structure of a long short-term memory unit. This figure is based on Figure 5.4 of (Kelleher, 2019), which in turn was inspired by an image by Christopher Olah (available at: http://colah.github.io/posts/2015-08-Understanding-LSTMs/).

$$\mathbf{f}_t = \varphi_{sigmoid}(\mathbf{W}^{(f)} \cdot \mathbf{hx}_t) \tag{106}$$

$$\mathbf{c}_t^{\ddagger} = \mathbf{c}_{t-1} \odot \mathbf{f}_t \tag{107}$$

$$\mathbf{c}_{t-1} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \mathbf{h}_{t-1} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \mathbf{x}_t = \begin{bmatrix} 4 \end{bmatrix}$$

$$\mathbf{W}^{(f)} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 0 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{108}$$

$$\underbrace{\begin{bmatrix} 0 & 1 & 1 & 1 \\ 0 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{\mathbf{W}^{(f)}} \times \underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \\ 4 \end{bmatrix}}_{\mathbf{hx}_t} = \underbrace{\begin{bmatrix} 6 \\ -6 \\ 0 \end{bmatrix}}_{\mathbf{z}_t^{(f)}} \rightarrow \varphi_{sigmoid} \rightarrow \underbrace{\begin{bmatrix} 0.997527377 \\ 0.002472623 \\ 0.500000000 \end{bmatrix}}_{\mathbf{f}_t}$$

$$\underbrace{\begin{bmatrix} 0.997527377 \\ 0.002472623 \\ 0.500000000 \end{bmatrix}}_{\mathbf{f}_t} \odot \underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}}_{\mathbf{c}_{t-1}} = \underbrace{\begin{bmatrix} 0.997527377 \\ 0.002472623 \\ 0.500000000 \end{bmatrix}}_{\mathbf{c}\ddagger}$$

(109)

$$\mathbf{i}\dagger_t = \varphi_{sigmoid}(\mathbf{W}^{(i\dagger)} \cdot \mathbf{hx}_t) \tag{110}$$

$$\mathbf{i}\ddagger_t = \varphi_{tanh}(\mathbf{W}^{(i\ddagger)} \cdot \mathbf{hx}_t) \tag{111}$$

$$\mathbf{i}_t = \mathbf{i}\dagger_t \odot \mathbf{i}\ddagger_t \tag{112}$$

$$\mathbf{c}_t = \mathbf{c}\ddagger + \mathbf{i}_t \tag{113}$$

$$\mathbf{o}\dagger_t = \varphi_{sigmoid}(\mathbf{W}^{(o\dagger)} \cdot \mathbf{hx}_t) \tag{114}$$

$$\mathbf{o}\ddagger_t = \varphi_{tanh}(\mathbf{W}^{(o\ddagger)} \cdot \mathbf{c}_t) \tag{115}$$

$$\mathbf{o}_t = \mathbf{o}\dagger_t \odot \mathbf{o}\ddagger_t \tag{116}$$

$$\mathbf{h}_{t+1} = \mathbf{o}_t \tag{117}$$

$$
\begin{aligned}
\mathbf{f}_t &= \varphi_{sigmoid}(\mathbf{W}^{(f)} \cdot \mathbf{hx}_t) \\
\mathbf{c}\ddagger &= \mathbf{c}_{t-1} \odot \mathbf{f}_t \\
\mathbf{i}\dagger_t &= \varphi_{sigmoid}(\mathbf{W}^{(i\dagger)} \cdot \mathbf{hx}_t) \\
\mathbf{i}\ddagger_t &= \varphi_{tanh}(\mathbf{W}^{(i\ddagger)} \cdot \mathbf{hx}_t) \\
\mathbf{i}_t &= \mathbf{i}\dagger_t \odot \mathbf{i}\ddagger_t \\
\mathbf{c}_t &= \mathbf{c}\ddagger + \mathbf{i}_t \\
\mathbf{o}\dagger_t &= \varphi_{sigmoid}(\mathbf{W}^{(o\dagger)} \cdot \mathbf{hx}_t) \\
\mathbf{o}\ddagger_t &= \varphi_{tanh}(\mathbf{W}^{(o\ddagger)} \cdot \mathbf{c}_t) \\
\mathbf{o}_t &= \mathbf{o}\dagger_t \odot \mathbf{o}\ddagger_t \\
\mathbf{h}_{t+1} &= \mathbf{o}_t
\end{aligned}
$$

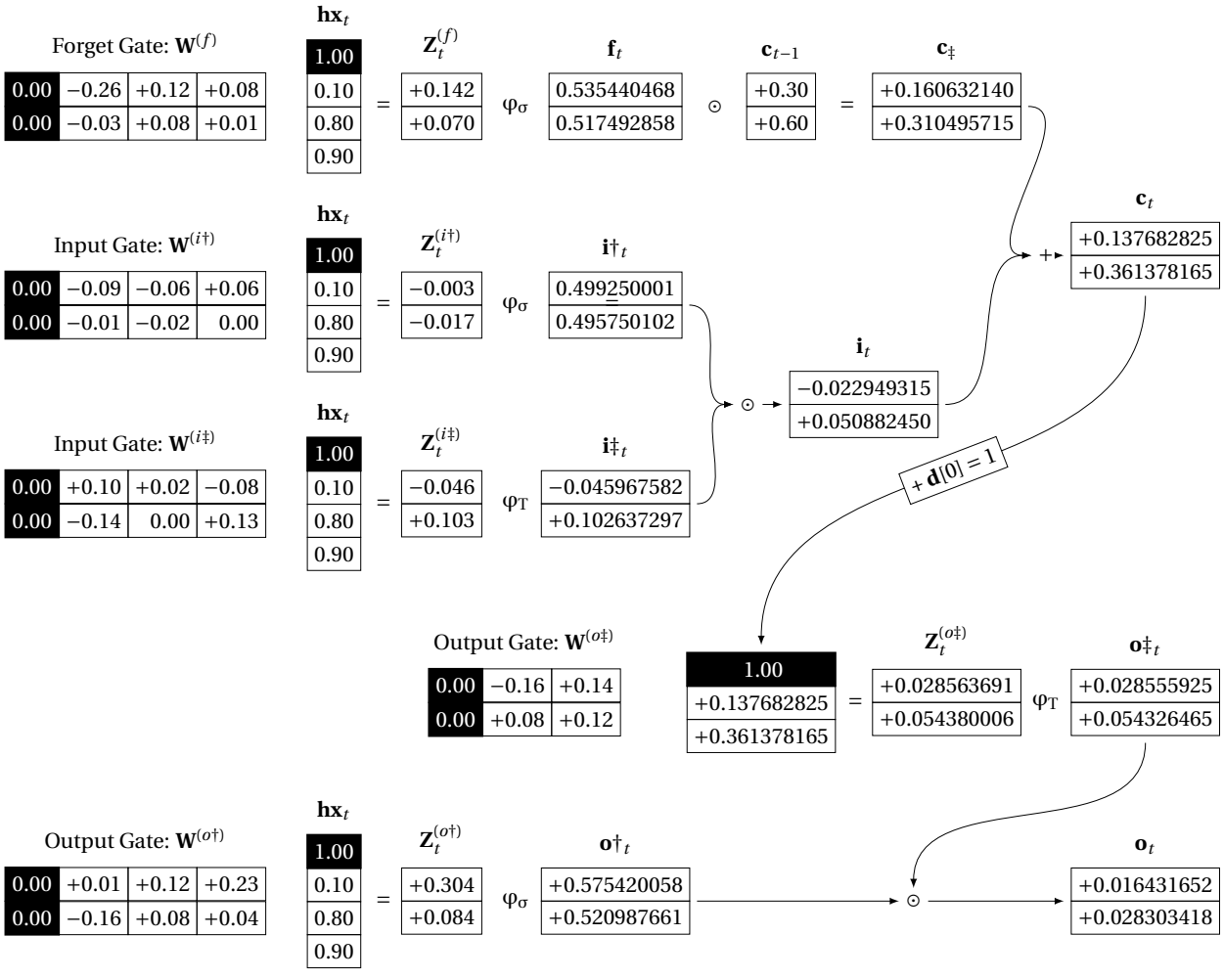


Figure 41: The flow of activations through a long short-term memory unit during forward propagation when $\mathbf{c}_{t-1} = [0.3, 0.6]$, $\mathbf{h}_t = [0.1, 0.8]$, and $\mathbf{x}_t = [0.9]$.

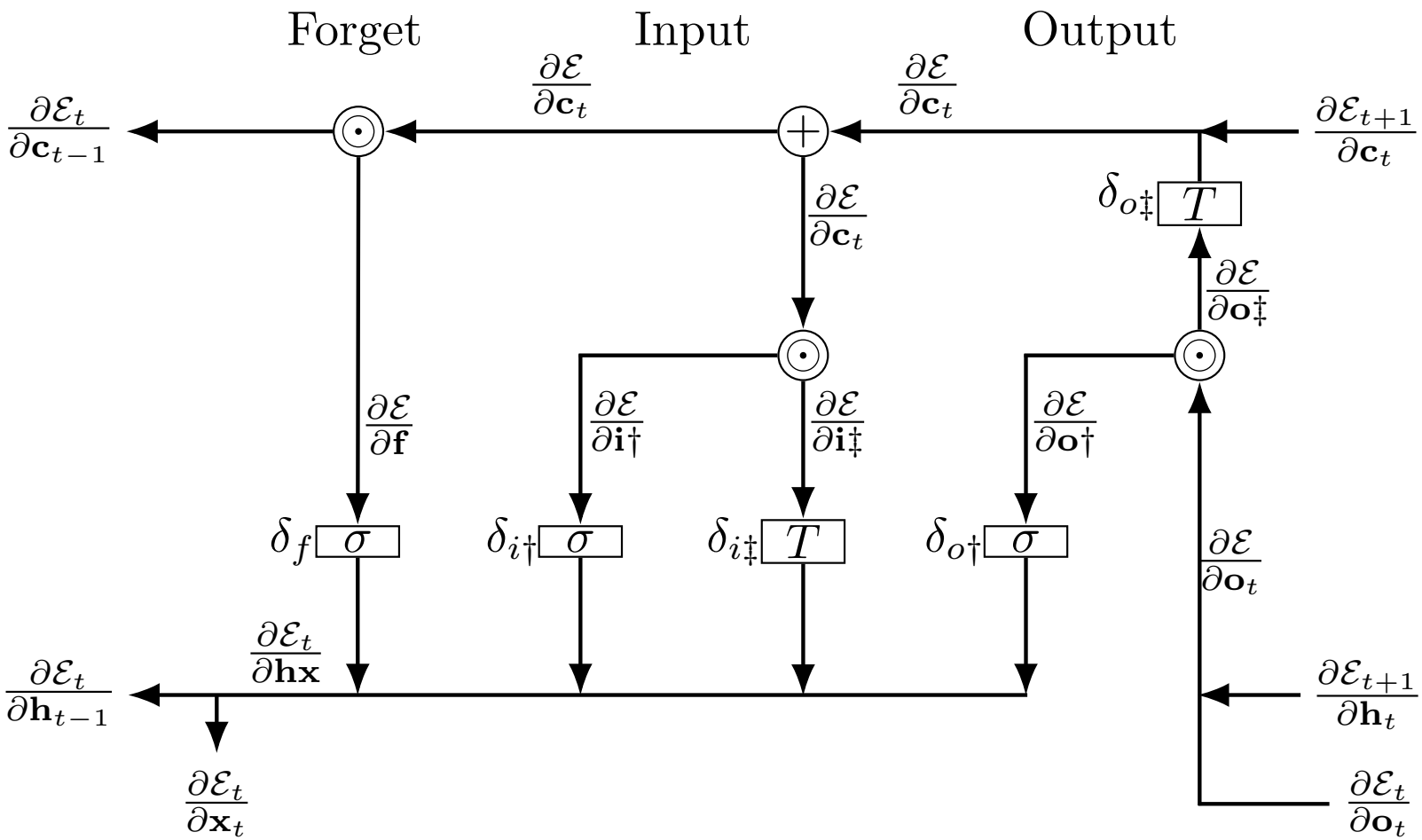


Figure 42: The flow of error gradients through a long short-term memory unit during backpropagation.

$$\frac{\partial \mathcal{E}}{\partial \mathbf{o}_t} = \frac{\partial \mathcal{E}_t}{\partial \mathbf{o}_t} + \frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{h}_t} \tag{118}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{o}\ddagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{o}_t} \odot \mathbf{o}\dagger \tag{119}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{o}\dagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{o}_t} \odot \mathbf{o}\ddagger \tag{120}$$

$$\delta_{o\ddagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{o}\ddagger} \odot \frac{\partial \mathbf{o}\ddagger_t}{\partial \mathbf{c}_{t\ddagger}} = \frac{\partial \mathcal{E}}{\partial \mathbf{o}\ddagger} \odot \underbrace{\left(\mathbf{1} - tanh^2(\mathbf{c}\ddagger_t)\right)}_{\text{Derivate of tanh, i.e.: } \frac{\partial a}{\partial z}} \tag{121}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{c}_t} = \delta_{o\ddagger} + \frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{c}_t} \tag{122}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{i}\ddagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{c}_t} \odot \mathbf{i}\dagger \tag{123}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{i}\dagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{c}_t} \odot \mathbf{i}\ddagger \tag{124}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{c}_{t-1}} = \frac{\partial \mathcal{E}}{\partial \mathbf{c}_t} \odot \mathbf{f}_t \tag{125}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{f}} = \frac{\partial \mathcal{E}}{\partial \mathbf{c}_t} \odot \mathbf{c}_{t-1} \tag{126}$$

$$\delta_f = \frac{\partial \mathcal{E}}{\partial \mathbf{f}} \odot \frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_f} = \frac{\partial \mathcal{E}}{\partial \mathbf{f}} \odot (\mathbf{f}_t \odot (\mathbf{1} - \mathbf{f}_t)) \tag{127}$$

$$\delta_{i\dagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{i}\dagger} \odot \frac{\partial \mathbf{i}\dagger_t}{\partial \mathbf{z}_{i\dagger}} = \frac{\partial \mathcal{E}}{\partial \mathbf{i}\dagger} \odot (\mathbf{i}\dagger_t \odot (\mathbf{1} - \mathbf{i}\dagger_t)) \tag{128}$$

$$\delta_{i\ddagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{i}\ddagger} \odot \frac{\partial \mathbf{i}\ddagger_t}{\partial \mathbf{z}_{i\ddagger}} = \frac{\partial \mathcal{E}}{\partial \mathbf{i}\ddagger} \odot \left(\mathbf{1} - tanh^2(\mathbf{i}\ddagger_t)\right) \tag{129}$$

$$\delta_{o\dagger} = \frac{\partial \mathcal{E}}{\partial \mathbf{o}\dagger} \odot \frac{\partial \mathbf{o}\dagger_t}{\partial \mathbf{z}_{o\dagger}} = \frac{\partial \mathcal{E}}{\partial \mathbf{o}\dagger} \odot (\mathbf{o}\dagger_t \odot (\mathbf{1} - \mathbf{o}\dagger_t)) \tag{130}$$

$$\Delta \mathbf{W}^{(f)} = \delta_f \cdot \mathbf{h}\mathbf{x}^\intercal \tag{131}$$

$$\frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{c}_t} = \begin{bmatrix} 0.35 \\ 0.50 \end{bmatrix} \quad \frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{h}_t} = \begin{bmatrix} 0.75 \\ 0.25 \end{bmatrix} \quad \frac{\partial \mathcal{E}_t}{\partial \mathbf{o}_t} = \begin{bmatrix} 0.15 \\ 0.60 \end{bmatrix}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{o}_t} = \underbrace{\begin{bmatrix} 0.75 \\ 0.25 \end{bmatrix}}_{\partial \mathcal{E}_{t+1}/\partial \mathbf{h}_t} + \underbrace{\begin{bmatrix} 0.15 \\ 0.60 \end{bmatrix}}_{\partial \mathcal{E}_t/\partial \mathbf{o}_t} = \begin{bmatrix} 0.9 \\ 0.85 \end{bmatrix} \tag{132}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{o}\ddagger} = \underbrace{\begin{bmatrix} 0.9 \\ 0.85 \end{bmatrix}}_{\partial \mathcal{E}/\partial \mathbf{o}_t} \odot \underbrace{\begin{bmatrix} 0.575420058 \\ 0.52098661 \end{bmatrix}}_{\mathbf{o}\dagger} = \begin{bmatrix} 0.517878052 \\ 0.442839512 \end{bmatrix} \tag{133}$$

$$\delta_{o\ddagger} = \underbrace{\begin{bmatrix} 0.517878052 \\ 0.442839512 \end{bmatrix}}_{\partial \mathcal{E}/\partial \mathbf{o}\ddagger} \odot \underbrace{\begin{bmatrix} 0.999184559 \\ 0.997048635 \end{bmatrix}}_{1-tanh(\mathbf{c}_t)} = \begin{bmatrix} 0.517455753 \\ 0.441532531 \end{bmatrix} \tag{134}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{c}_t} = \underbrace{\begin{bmatrix} 0.517455753 \\ 0.441532531 \end{bmatrix}}_{\delta_{o\ddagger}} + \underbrace{\begin{bmatrix} 0.35 \\ 0.50 \end{bmatrix}}_{\partial \mathcal{E}_{t+1}/\partial \mathbf{c}_t} = \begin{bmatrix} 0.867455753 \\ 0.941532531 \end{bmatrix} \tag{135}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{f}} = \underbrace{\begin{bmatrix} 0.867455753 \\ 0.941532531 \end{bmatrix}}_{\partial \mathcal{E}/\partial \mathbf{c}_t} \odot \underbrace{\begin{bmatrix} 0.3 \\ 0.6 \end{bmatrix}}_{\mathbf{c}_{t-1}} = \begin{bmatrix} 0.260236726 \\ 0.564919518 \end{bmatrix} \tag{136}$$

$$\delta_f = \underbrace{\begin{bmatrix} 0.260236726 \\ 0.564919518 \end{bmatrix}}_{\partial \mathcal{E}/\partial \mathbf{f}} \odot \underbrace{\begin{bmatrix} 0.248743973 \\ 0.249694 \end{bmatrix}}_{\mathbf{f}_t \odot (1 - \mathbf{f}_t)} = \begin{bmatrix} 0.064732317 \\ 0.141057014 \end{bmatrix} \tag{137}$$

$$\begin{aligned} \Delta \mathbf{W}^{(f)} &= \underbrace{\begin{bmatrix} 0.064732317 \\ 0.141057014 \end{bmatrix}}_{\delta_f} \cdot \underbrace{\begin{bmatrix} 1.00 & 0.10 & 0.80 & 0.90 \end{bmatrix}}_{\mathbf{h}\mathbf{x}^\intercal} \\ &= \begin{bmatrix} 0.064732317 & 0.006473232 & 0.051785854 & 0.058259085 \\ 0.141057014 & 0.014105701 & 0.112845611 & 0.126951313 \end{bmatrix} \end{aligned} \tag{138}$$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{hx}} = \left(\mathbf{W}^{(f)\intercal} \cdot \delta_f\right) + \left(\mathbf{W}^{(i\dagger)\intercal} \cdot \delta_{i\dagger}\right) + \left(\mathbf{W}^{(i\ddagger)\intercal} \cdot \delta_{i\ddagger}\right) + \left(\mathbf{W}^{(o\dagger)\intercal} \cdot \delta_{o\dagger}\right) \tag{139}$$

$$
\begin{aligned}
\frac{\partial \mathcal{E}}{\partial \mathbf{c}_{t-1}} &= \mathbf{f}_t \odot \frac{\partial \mathcal{E}}{\partial \mathbf{c}_t} \\
&= \mathbf{f}_t \odot \left(\frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{c}_t} + \delta_{o\ddagger} \right) \\
&= \mathbf{f}_t \odot \left(\frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{c}_t} + \left(\left(\mathbf{1} - tanh^2(\mathbf{c}\ddagger_t) \right) \odot \frac{\partial \mathcal{E}}{\partial \mathbf{o}\ddagger} \right) \right) \\
&= \mathbf{f}_t \odot \left(\frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{c}_t} + \left(\left(\mathbf{1} - tanh^2(\mathbf{c}\ddagger_t) \right) \odot \left(\mathbf{o}\dagger \odot \frac{\partial \mathcal{E}}{\partial \mathbf{o}_t} \right) \right) \right) \\
&= \mathbf{f}_t \odot \left(\frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{c}_t} + \left(\left(\mathbf{1} - tanh^2(\mathbf{c}\ddagger_t) \right) \odot \left(\mathbf{o}\dagger \odot \left(\frac{\partial \mathcal{E}_{t+1}}{\partial \mathbf{h}_t} + \frac{\partial \mathcal{E}_t}{\partial \mathbf{o}_t} \right) \right) \right) \right)
\end{aligned}
\tag{140}
$$

Summary

- Deep neural networks to learn and represent complex mappings from inputs to outputs
- The standard algorithm for training a deep neural network combines the backpropagation algorithm
- Unstable gradients (either vanishing or exploding gradients) can make training a deep network with backpropagation and gradient descent difficult
  - Activation Functions (ReLUs)
  - Weight Initialization
- Dropout is a very simple and effective method that helps to stop overfitting.
- We can tailor the structure of a network toward the characteristics of the data
  - Convolutional Neural Networks
  - Recurrent Neural Networks

Further Reading

- Other texts on neural networks and deep learning: (Bishop, 1996; Reed and Marks, 1999; Kelleher, 2019; Goodfellow et al., 2016)
- Programming focused introductions to deep learning: (Charniak, 2019; Trask, 2019)
- Introduction to neural networks for natural language processing: (Goldberg, 2017)
- Computer architecture perspective on deep learning: (Reagen et al., 2017)
- Recent developments in the field: **batch normalization** (Ioffe and Szegedy, 2015), adaptively learning algorithms such as **Adam** (Kingma and Ba, 2014), **Generative Adversarial Networks** (Goodfellow et al., 2014), and attention-based architectures such as the **Transformer** (Vaswani et al., 2017).

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