MONASH University

ETC3555

Statistical Machine Learning

Neural networks

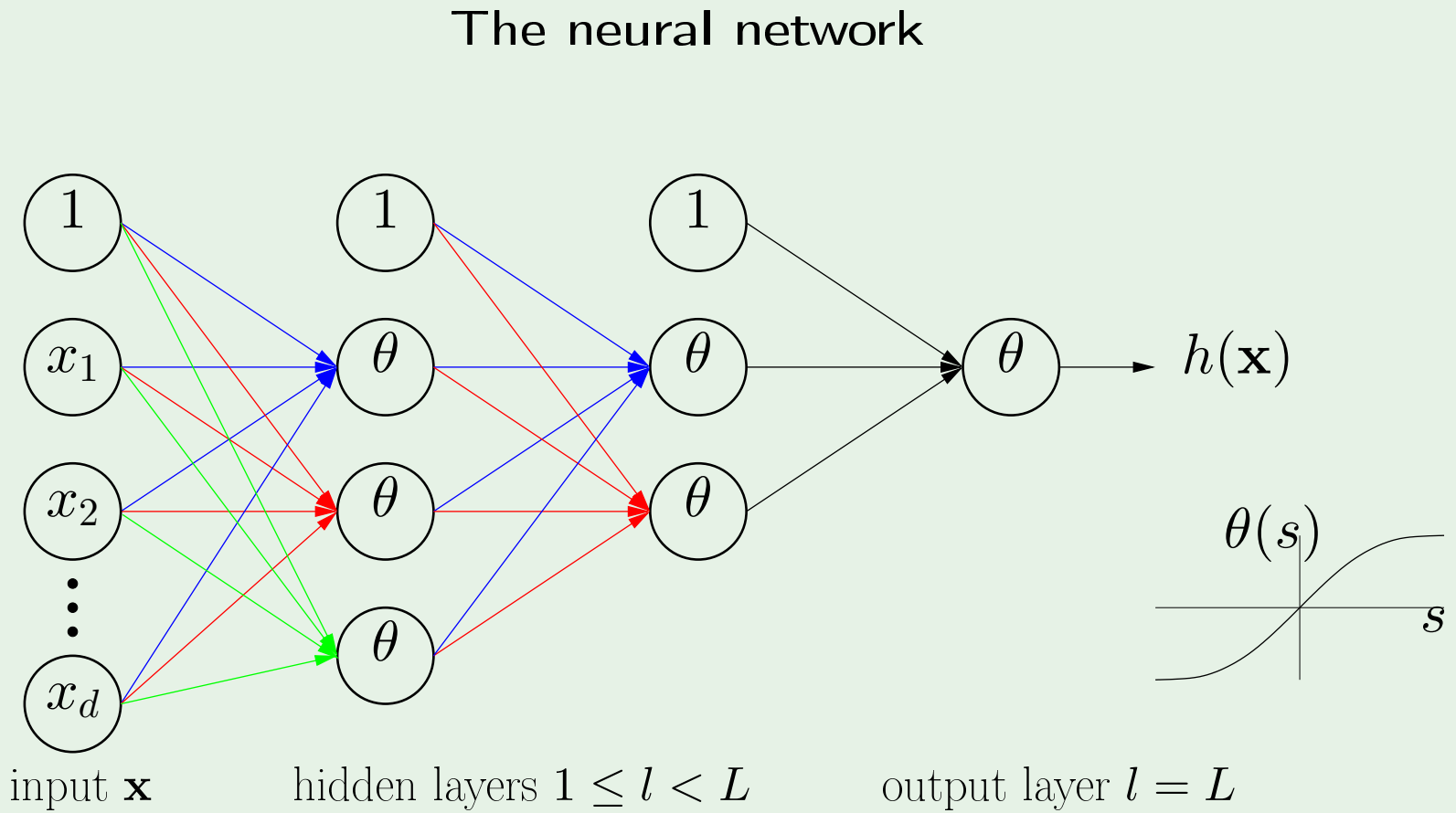
22 August 2018

Outline (subject to change)

Week	Topic
1	Introduction/The learning problem
2	The learning problem
3	Linear models
4	Gradient descent
5	Neural Networks
6	Neural Networks and Backpropagation
7	Deep Neural Networks
8	Support vector machines
9	Recommender systems and matrix completion
	Semester break
10	Text mining
11	Social networks
12	Project presentation

Outline

The neural network



How the network operates

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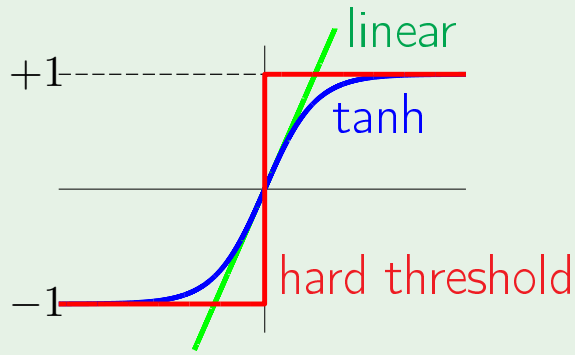
$$w_{ij}^{(l)} \quad \begin{cases} 1 \leq l \leq L & \text{layers} \\ 0 \leq i \leq d^{(l-1)} & \text{inputs} \\ 1 \leq j \leq d^{(l)} & \text{outputs} \end{cases}$$

$$x_j^{(l)} = \theta(s_j^{(l)}) = \theta\left(\sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)}\, x_i^{(l-1)}\right)$$



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

Apply $\mathbf{x}$ to $x_1^{(0)} \cdots x_{d^{(0)}}^{(0)} \rightarrow\rightarrow x_1^{(L)} = h(\mathbf{x})$

The activation function

- Every node with an input has a *transformation* or *activation* function, θ. In the previous example: $\theta(s) = \text{sign}(s)$.
- $\text{sign}(s)$ function can be approximated with $\tanh(s)$, the hyperbolic tangent function, a soft threshold. A smooth function $\rightarrow$ easier to optimize, e.g. gradient descent.
- For the nodes in the hidden layers, arbitrary activation functions can be used. They are often chosen to allow fast computation and efficient optimization.
- For the output node, a different sigmoid will be used depending on the learning problem
  - Classification: $\hat{y} = \theta(s) = \tanh(s)$ or $\text{logistic}(s)$
  - Regression: $\hat{y} = \theta(s) = s$

Tanh vs logistic

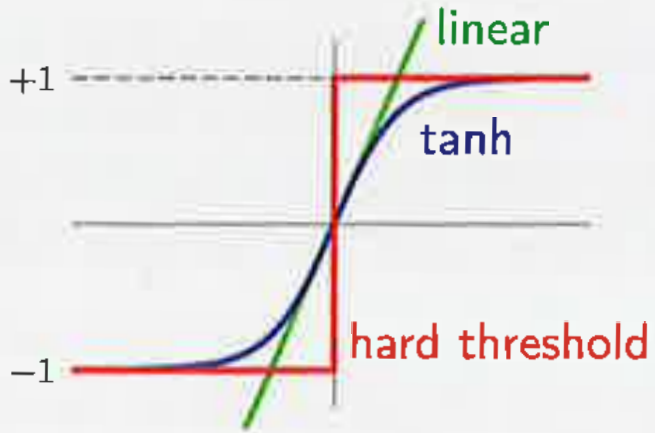
Exercise 3.5

Another popular soft threshold is the hyperbolic tangent

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

(a) How is $\tanh$ related to the logistic function θ? *[Hint: shift and scale]*

(b) Show that $\tanh(s)$ converges to a hard threshold for large $|s|$, and converges to no threshold for small $|s|$. *[Hint: Formalize the figure below.]*



Tanh vs logistic

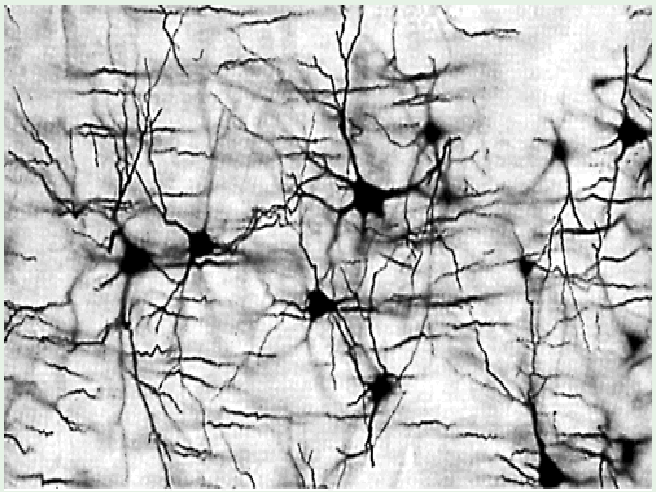
(a) $\tanh(s) = 2 \times \text{logistic}(2s) - 1$

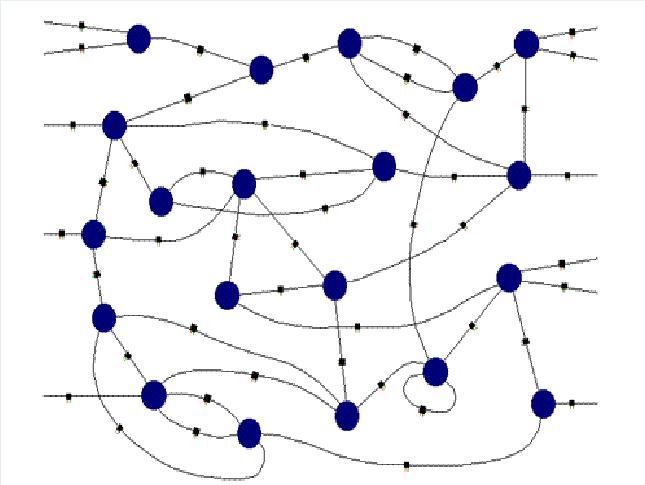
(b) Use a taylor expansion around zero.

Biological inspiration

Biological inspiration

biological function $\longrightarrow$ biological structure





Outline

Applying SGD

Applying SGD

All the weights $\mathbf{w} = \{w_{ij}^{(l)}\}$ determine $h(\mathbf{x})$

Error on example $(\mathbf{x}_n, y_n)$ is

$$\mathbf{e}\left(h(\mathbf{x}_n), y_n\right) = \mathbf{e}(\mathbf{w})$$

To implement SGD, we need the gradient

$$\nabla \mathbf{e}(\mathbf{w}): \quad \frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, w_{ij}^{(l)}} \quad \text{for all } i, j, l$$

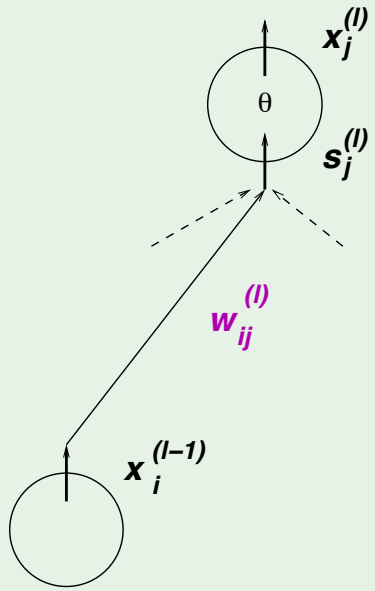
Computing partial derivatives efficiently

Computing $\frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, w_{ij}^{(l)}}$

We can evaluate $\frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, w_{ij}^{(l)}}$ one by one: analytically or numerically

A trick for efficient computation:

$$\frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, w_{ij}^{(l)}} = \frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, s_j^{(l)}} \times \frac{\partial\, s_j^{(l)}}{\partial\, w_{ij}^{(l)}}$$



We have $\frac{\partial\, s_j^{(l)}}{\partial\, w_{ij}^{(l)}} = x_i^{(l-1)}$ We only need: $\frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, s_j^{(l)}} = \delta_j^{(l)}$

A $\delta_j^{(l)}$ will be associated to each $\frac{\partial\, e(w)}{\partial\, s_j^{(l)}}$.

Computing partial derivatives efficiently

δ for the final layer

$$\delta_j^{(l)} = \frac{\partial\, \mathrm{e}(\mathbf{w})}{\partial\, s_j^{(l)}}$$

For the final layer $l = L$ and $j = 1$:

$$\delta_1^{(L)} = \frac{\partial\, \mathrm{e}(\mathbf{w})}{\partial\, s_1^{(L)}}$$

$$\mathrm{e}(\mathbf{w}) = (\, x_1^{(L)} - y_n)^2$$

$$x_1^{(L)} = \theta(s_1^{(L)})$$

$$\theta'(s) = 1 - \theta^2(s) \qquad \text{for the tanh}$$

$$e(\boldsymbol{w}) = e(h(\boldsymbol{x}_n), y_n) = e(x_1^{(L)}, y_n) = (x_1^{(L)} - y_n)^2$$

Computing partial derivatives efficiently

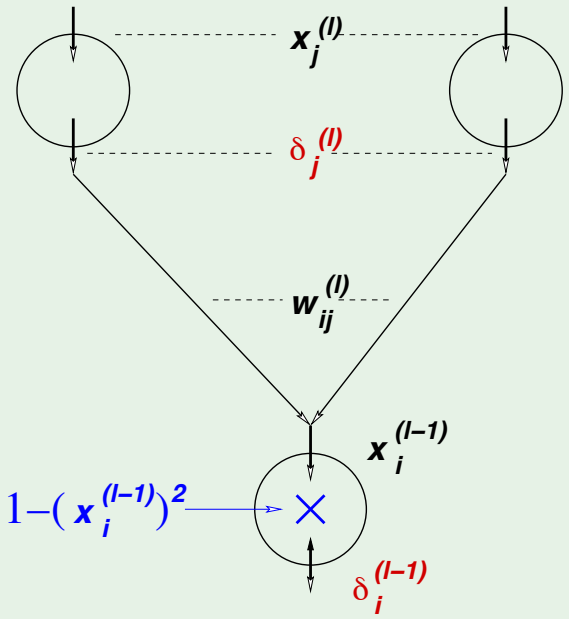
Back propagation of δ

$$\delta_i^{(l-1)} = \frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, s_i^{(l-1)}}$$

$$= \sum_{j=1}^{d^{(l)}} \frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, s_j^{(l)}} \times \frac{\partial\, s_j^{(l)}}{\partial\, x_i^{(l-1)}} \times \frac{\partial\, x_i^{(l-1)}}{\partial\, s_i^{(l-1)}}$$

$$= \sum_{j=1}^{d^{(l)}} \delta_j^{(l)} \times w_{ij}^{(l)} \times \theta'(s_i^{(l-1)})$$

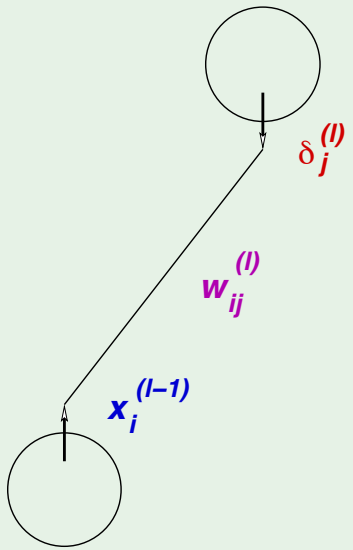
$$\delta_i^{(l-1)} = (1 - (x_i^{(l-1)})^2) \sum_{j=1}^{d^{(l)}} w_{ij}^{(l)}\, \delta_j^{(l)}$$



Backpropagation algorithm

Backpropagation algorithm

1: Initialize all weights $w_{ij}^{(l)}$ at random
2: **for** $t = 0, 1, 2, \ldots$ **do**
3: Pick $n \in \{1, 2, \cdots, N\}$
4: *Forward:* Compute all $x_j^{(l)}$
5: *Backward:* Compute all $\delta_j^{(l)}$
6: Update the weights: $w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \eta\, x_i^{(l-1)} \delta_j^{(l)}$
7: Iterate to the next step until it is time to stop
8: Return the final weights $w_{ij}^{(l)}$

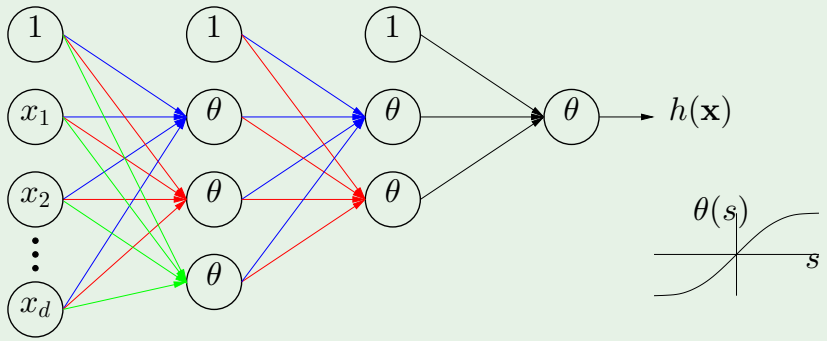


Automatic feature extraction

Final remark: hidden layers

learned nonlinear transform

interpretation?



Matrix notations

layer ℓ parameters

signals in	$\mathbf{s}^{(\ell)}$	$d^{(\ell)}$ dimensional input vector
outputs	$\mathbf{x}^{(\ell)}$	$d^{(\ell)}+1$ dimensional output vector
weights in	$\mathrm{W}^{(\ell)}$	$(d^{(\ell-1)}+1)\times d^{(\ell)}$ dimensional matrix
weights out	$\mathrm{W}^{(\ell+1)}$	$(d^{(\ell)}+1)\times d^{(\ell+1)}$ dimensional matrix

Forward propagation

Forward propagation to compute $h(\mathbf{x})$:

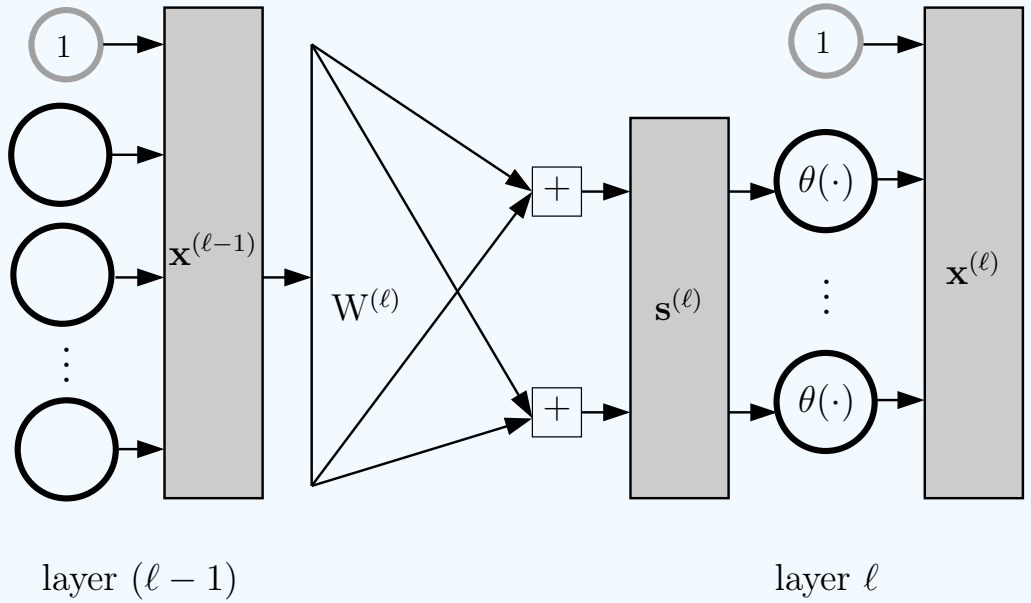
1: $\mathbf{x}^{(0)} \leftarrow \mathbf{x}$ **[Initialization]**

2: **for** $\ell = 1$ to L **do** **[Forward Propagation]**

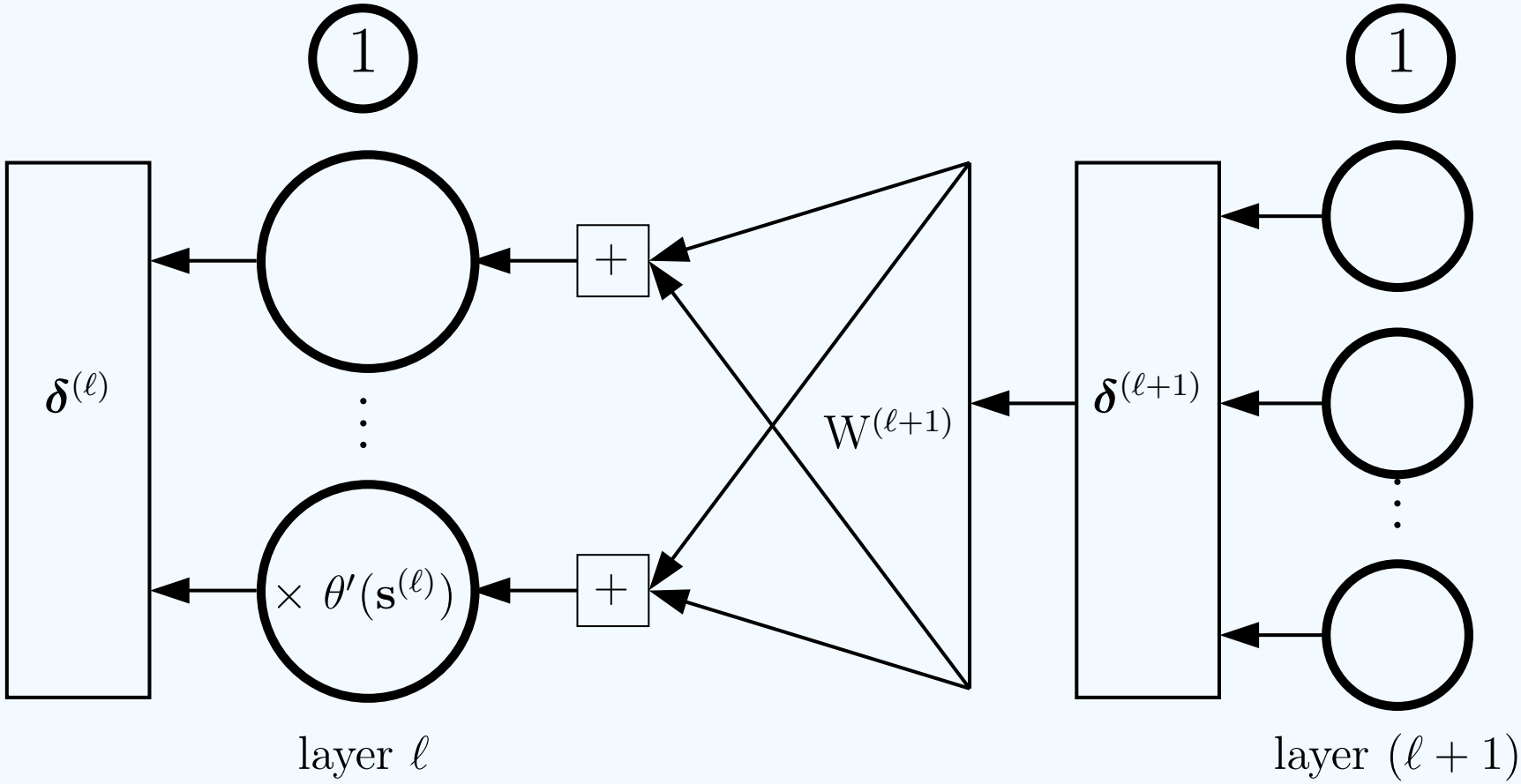
3: $\quad \mathbf{s}^{(\ell)} \leftarrow (\mathrm{W}^{(\ell)})^{\mathrm{T}} \mathbf{x}^{(\ell-1)}$

4: $\quad \mathbf{x}^{(\ell)} \leftarrow \begin{bmatrix} 1 \\ \theta(\mathbf{s}^{(\ell)}) \end{bmatrix}$

5: $h(\mathbf{x}) = \mathbf{x}^{(L)}$ **[Output]**



Backpropagation



Backpropagation

$$\frac{\partial \mathsf{e}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)} (\boldsymbol{\delta}^{(\ell)})^{\mathrm{T}}$$

Backpropagation to compute sensitivities $\boldsymbol{\delta}^{(\ell)}$.
Input: a data point $(\mathbf{x}, y)$.

0: Run forward propagation on $\mathbf{x}$ to compute and save:

$$\begin{array}{ll} \mathbf{s}^{(\ell)} & \text{for } \ell = 1, \ldots, L; \\ \mathbf{x}^{(\ell)} & \text{for } \ell = 0, \ldots, L. \end{array}$$

1: $\delta^{(L)} \leftarrow 2(x^{(L)} - y)\theta'(s^{(L)})$ **[Initialization]**

$$\theta'(s^{(L)}) = \begin{cases} 1 - (x^{(L)})^2 & \theta(s) = \tanh(s); \\ 1 & \theta(s) = s. \end{cases}$$

2: **for** $\ell = L - 1$ to 1 **do** **[Back-Propagation]**

3: Let $\theta'(\mathbf{s}^{(\ell)}) = \left[1 - \mathbf{x}^{(\ell)} \otimes \mathbf{x}^{(\ell)}\right]_1^{d^{(\ell)}}$.

4: Compute the sensitivity $\boldsymbol{\delta}^{(\ell)}$ from $\boldsymbol{\delta}^{(\ell+1)}$:

$$\boldsymbol{\delta}^{(\ell)} \leftarrow \theta'(\mathbf{s}^{(\ell)}) \otimes \left[\mathrm{W}^{(\ell+1)} \boldsymbol{\delta}^{(\ell+1)}\right]_1^{d^{(\ell)}}$$