Neural networks

CE-477: Machine Learning - CS-828: Theory of Machine Learning
Sharif University of Technology
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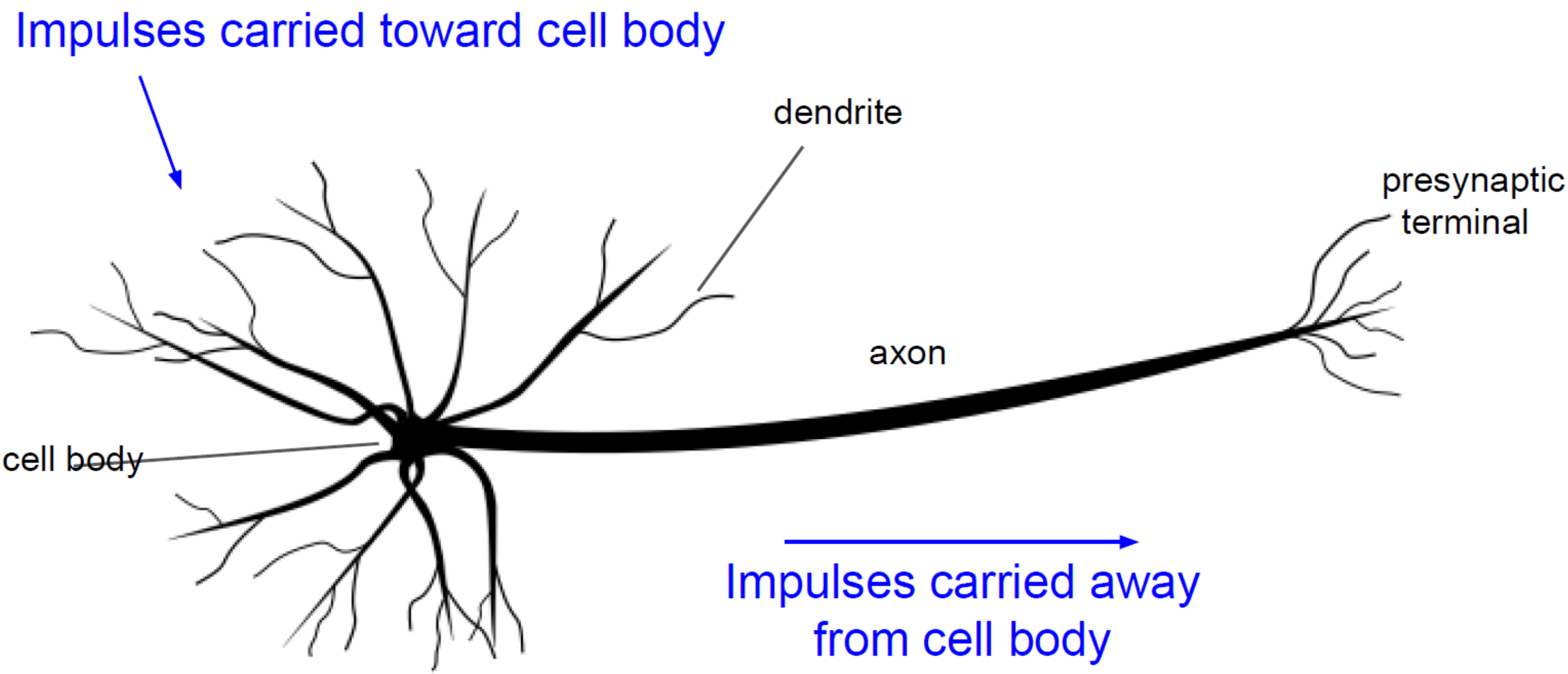
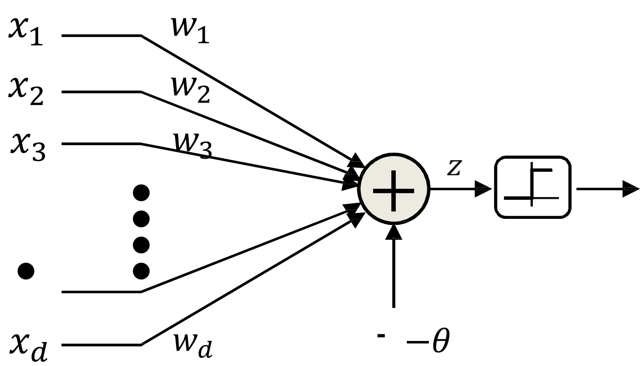
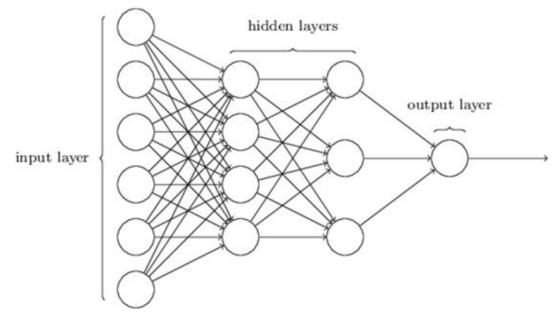
Neural cell

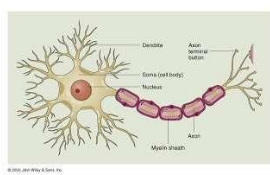


Impulses carried toward cell body
dendrite
presynaptic terminal
axon
cell body
Impulses carried away from cell body

Neural nets and the brain



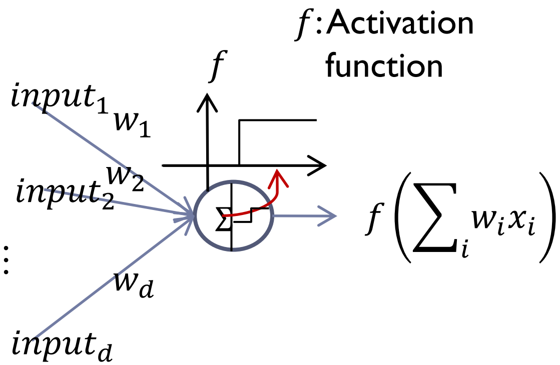


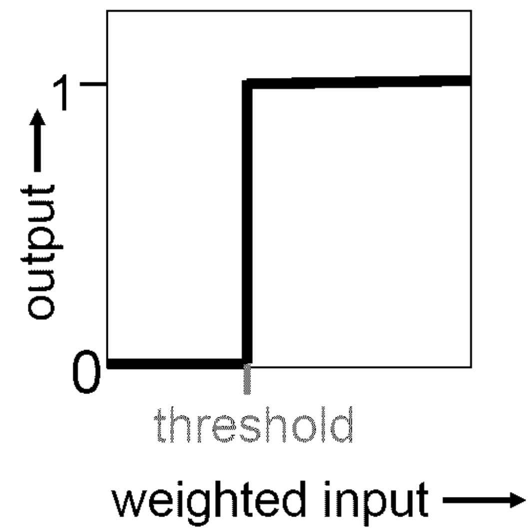


- Neural nets are composed of networks of computational models of neurons called perceptrons

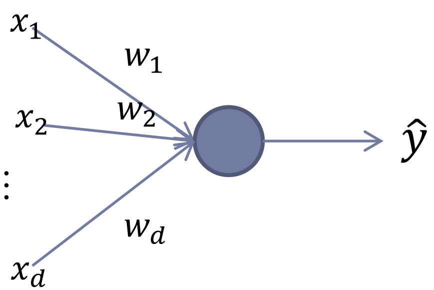
Binary threshold neurons

- McCulloch-Pitts (1943): influenced Von Neumann.
  - First compute a weighted sum of the inputs.
  - Send out a spike of activity if the weighted sum exceeds a threshold.

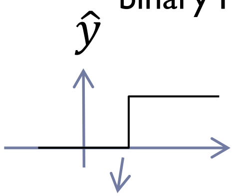




McCulloch-Pitts neuron: binary threshold



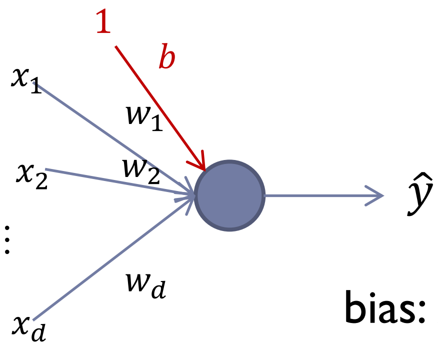
binary McCulloch-Pitts neuron

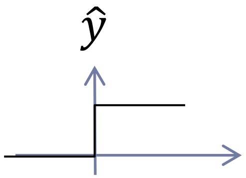


θ: activation threshold

$$\hat{y} = \begin{cases} 1, & z \geq \theta \\ 0, & z < \theta \end{cases}$$

Equivalent to



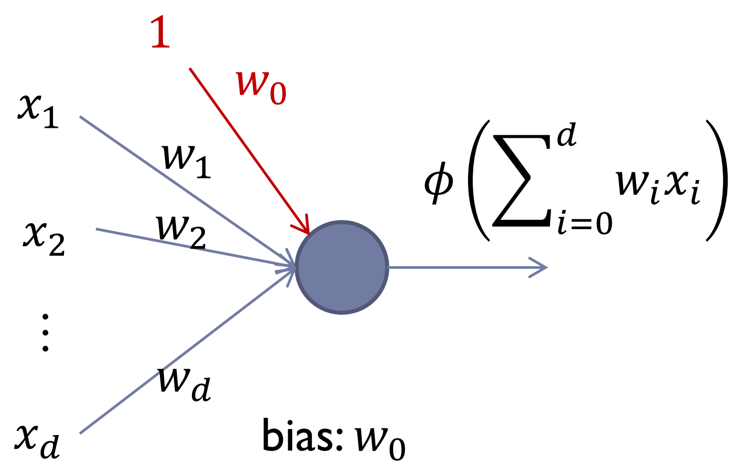


bias: $b = -\theta$

Single neuron

- Single neuron can be used as a linear decision boundary:
  - $\phi(\boldsymbol{w}^T\boldsymbol{x})$ shows the class of $\boldsymbol{x}$

- Training methods of a single neuron:
  - Perceptron (Rosenblatt, 1962)
    - We have seen it before!
  - ADALINE (Widrow and Hoff, 1960)
    - We have seen it before too !!!
  - …



Reminder: Perceptron Learning Algorithm

- Given N training instances $(\boldsymbol{x}^{(1)}, y^{(1)}), (\boldsymbol{x}^{(2)}, y^{(2)}), \ldots, (\boldsymbol{x}^{(N)}, y^{(N)})$
  - $y^{(n)} = +1$ or -1

- Initialize $\boldsymbol{w}$
- Cycle through the training instance
- While more classification errors
  - For $i = 1 \ldots N_{train}$

    $$\hat{y}^{(i)} = sign(\boldsymbol{w}^T \boldsymbol{x}^{(i)})$$

    - If $\hat{y}^{(i)} \neq y^{(i)}$

      $$\boldsymbol{w} = \boldsymbol{w} + y^{(i)} \boldsymbol{x}^{(i)}$$

- If instance misclassified:
  - If instance is positive class

    $$\boldsymbol{w} = \boldsymbol{w} + \boldsymbol{x}$$

  - If instance is negative class

    $$\boldsymbol{w} = \boldsymbol{w} - \boldsymbol{x}$$

Training of a single neuron

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta \nabla J_n(\boldsymbol{w}^{t})$$

- Weight update for a training pair $(\boldsymbol{x}^{(n)}, y^{(n)})$:
  - Perceptron: If $\text{sign}(\boldsymbol{w}^T \boldsymbol{x}^{(n)}) \neq y^{(n)}$ then

$$\nabla J_n(\boldsymbol{w}^{t}) = -\eta \boldsymbol{x}^{(n)} y^{(n)}$$

$J_n(\boldsymbol{w}) = -\boldsymbol{w}^T \boldsymbol{x}^{(n)} y^{(n)}$
if misclassified

  - ADALINE: $\nabla J_n(\boldsymbol{w}^{t}) = -\eta (y^{(n)} - \boldsymbol{w}^T \boldsymbol{x}^{(n)}) \boldsymbol{x}^{(n)}$
    - Widrow-Hoff, LMS, or delta rule

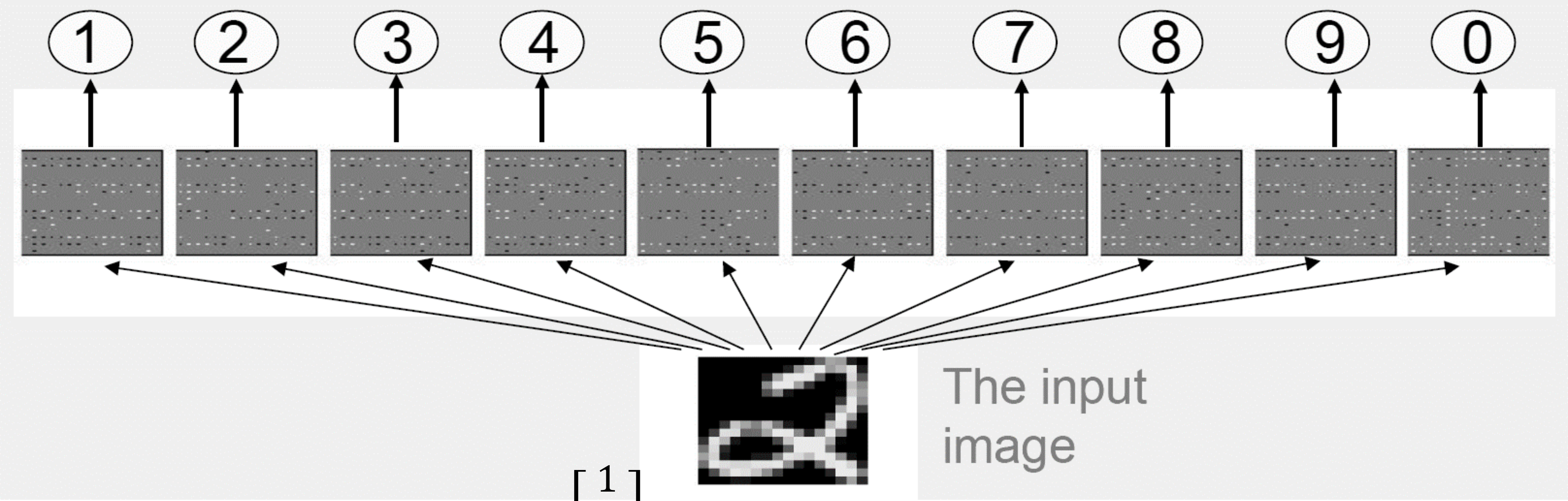
$J_n(\boldsymbol{w}) = \left(y^{(n)} - \boldsymbol{w}^T \boldsymbol{x}^{(n)}\right)^2$

Perceptron vs. Delta Rule

- Perceptron learning rule:
  - Guaranteed to succeed if training examples are linearly separable
- Delta rule:
  - Guaranteed to converge to the hypothesis with the minimum squared error
  - Succeed if sufficiently small learning rate
    - Even when training data contain noise or are not separable by a hyperplane
  - Can also be used for regression problems

How to learn the weights: multi class example

- 10 neuron next to each other to compose a single layer neural network

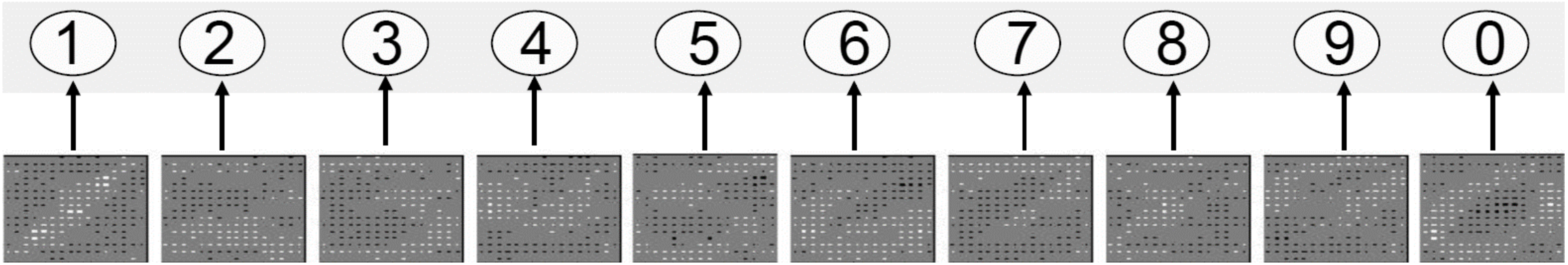


$$W = \begin{bmatrix} b_1 & w_{11} & \cdots & w_{1d} \\ \vdots & \ddots & \cdots & \vdots \\ b_k & w_{k1} & \cdots & w_{kd} \end{bmatrix} \quad \boldsymbol{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

 This slide has been adopted from Hinton's lectures, "NN for Machine Learning" course, 2015.

How to learn the weights: multi class example

- Change of weights during training



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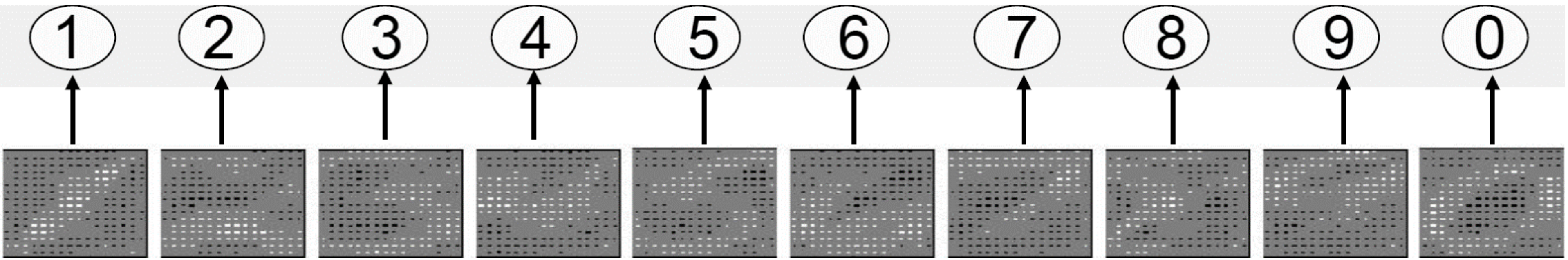

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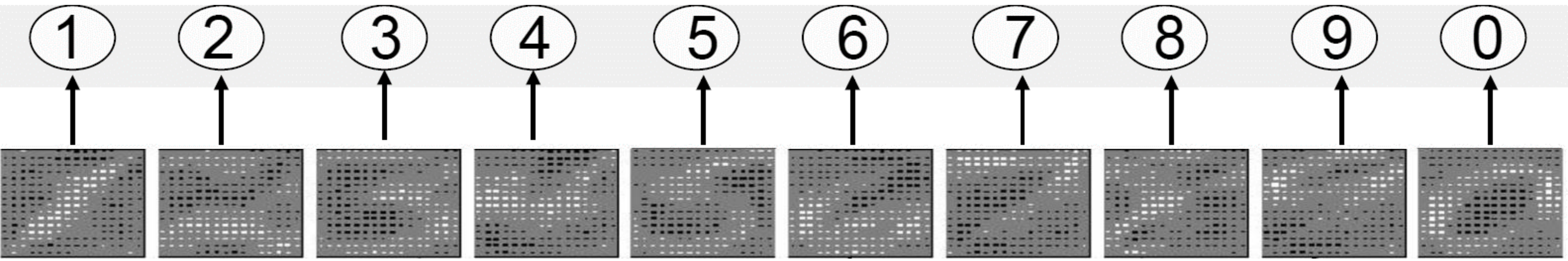

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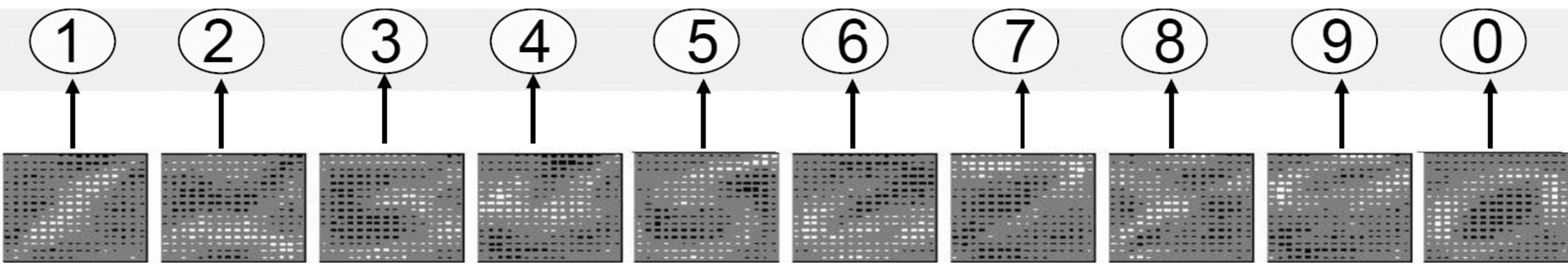

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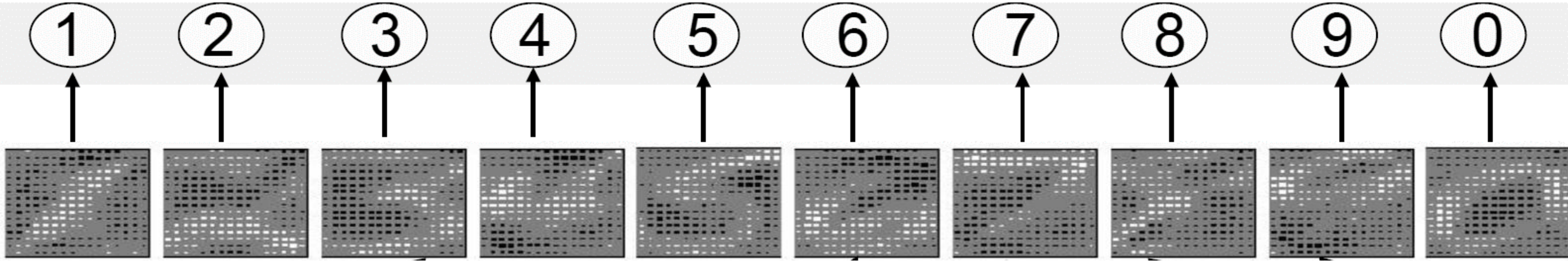

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How to learn the weights: multi class example

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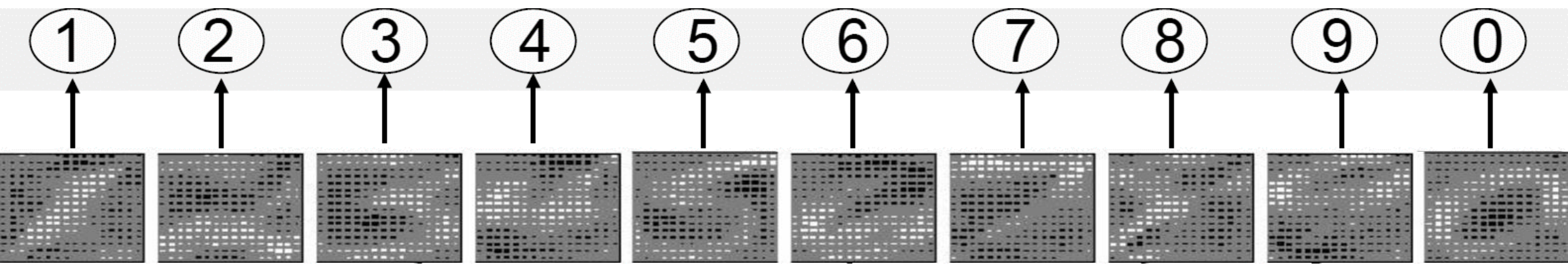

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Limitation of single layer network

- Single layer networks is equivalent to template matching
  - Weights for each class as a template for that class.

- The ways in which a digit can be written are much too complicated to be captured by simple template

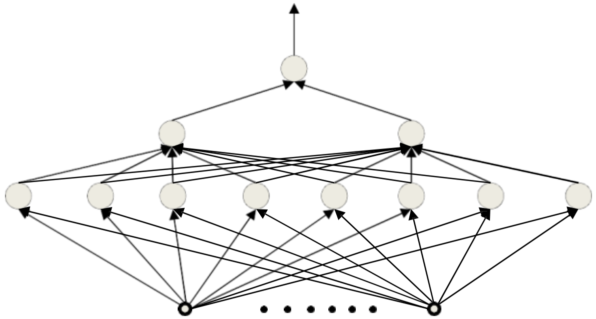
- Thus, networks without hidden units are very limited in the mappings that they can learn

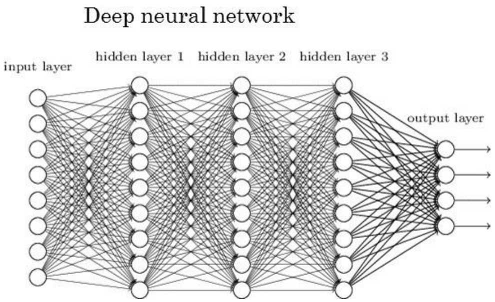
Networks with hidden units

- Networks without hidden units are very limited in the input-output mappings they can learn to model.
  - More layers of linear units do not help. Its still linear.
  - Fixed output non-linearities are not enough.

- We need multiple layers of adaptive, non-linear hidden units. But how can we train such nets?

The multi-layer neural network

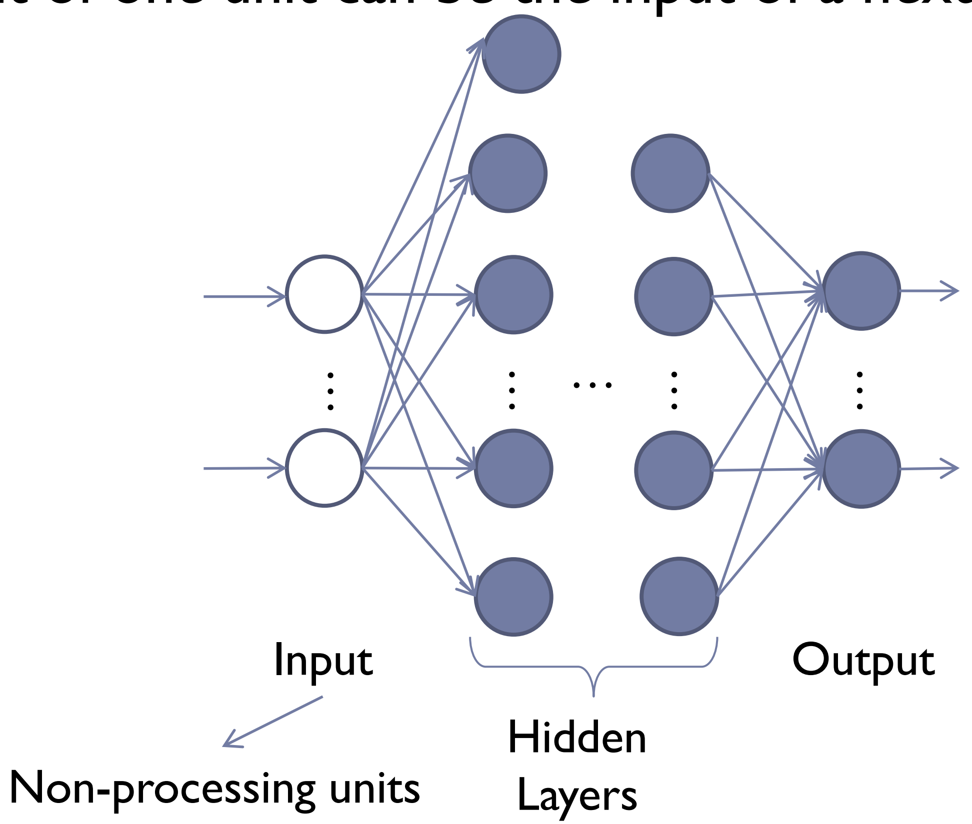




- A network of perceptrons
  - Generally “layered”
  - Also called multi layer perceptron

Feed-forward neural networks

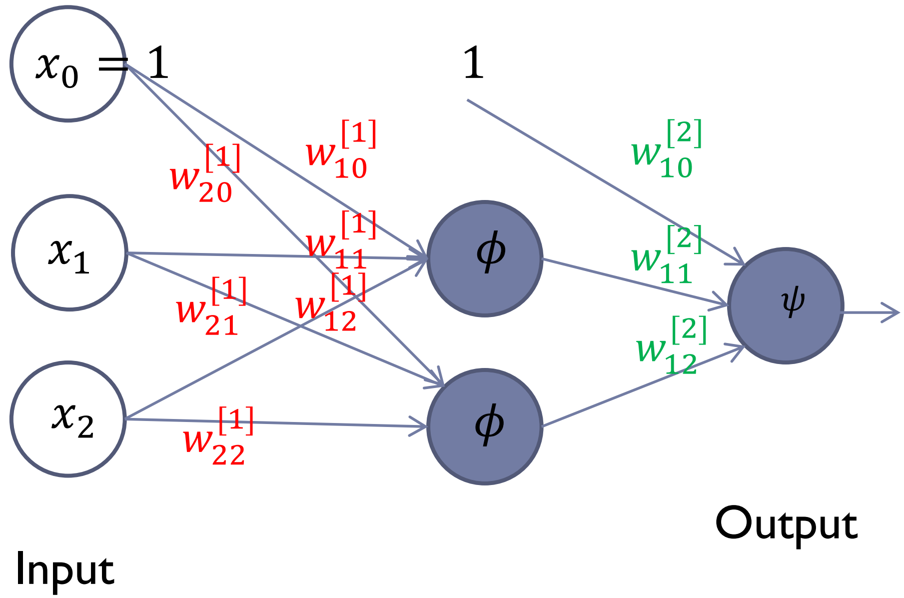
- We need multiple layers of adaptive, non-linear hidden units.
  - Also called **Multi-Layer Perceptron (MLP)**
- Each *unit* takes some inputs and produces one output.
  - Output of one unit can be the input of a next layer(s) unit.



Weights on links can be adapted using training data and a learning algorithm

Multi-layer Neural Network

- Φ: activation function
  - A nonlinear function



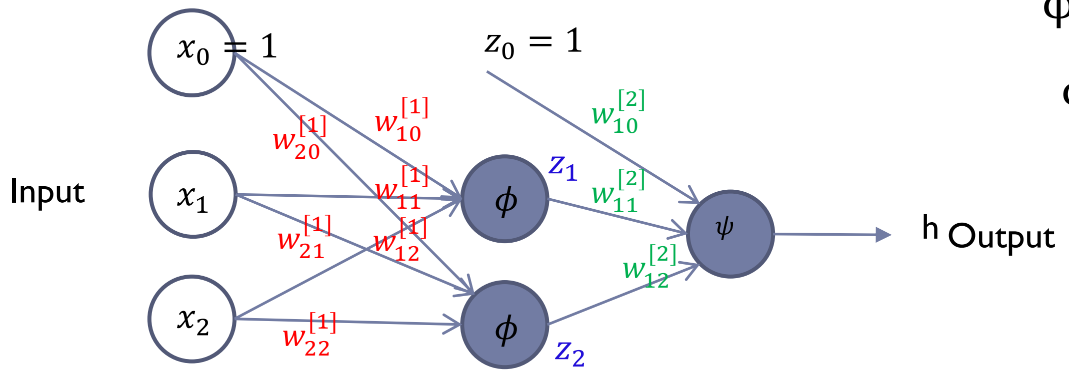
Multi-layer Neural Network

ϕ: fixed activation function

Examples:

$$\phi(z) = \max(0, z)$$

$$\phi(z) = \frac{1}{1 + e^{-z}}$$

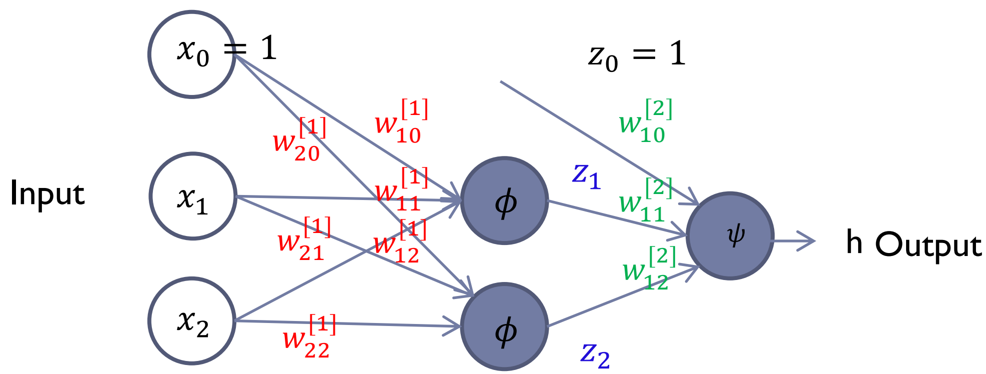


$$z_j = \phi\left(\sum_{i=0}^{d} w_{ji}^{[1]} x_i\right)$$

$$h = \psi\left(\sum_{j=0}^{2} w_{kj}^{[2]} z_j\right) = \left(\sum_{j=0}^{2} w_{kj}^{[2]} \phi\left(\sum_{i=0}^{d} w_{ji}^{[1]} x_i\right)\right)$$

Multi-layer Neural Network

$$W^{[1]} = \begin{bmatrix} w_{10}^{[1]} & w_{11}^{[1]} & w_{12}^{[1]} \\ w_{20}^{[1]} & w_{21}^{[1]} & w_{22}^{[1]} \end{bmatrix}$$



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Examples:

$$\phi(z) = \max(0, z)$$

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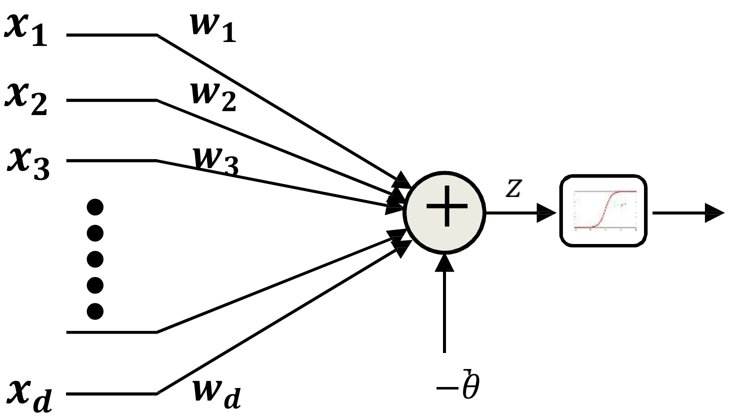
$$z_j = \phi\left(\sum_{i=0}^{d} w_{ji}^{[1]} x_i\right)$$

$$\text{h} = \psi\left(\Sigma_{j=0}^{2} w_{kj}^{[2]} z_j\right) = \left(\Sigma_{j=0}^{2} w_{kj}^{[2]} \phi\left(\Sigma_{i=0}^{d} w_{ji}^{[1]} x_i\right)\right)$$

Matrix form: $\boldsymbol{z} = \phi\left(W^{[1]}\boldsymbol{x}\right)$

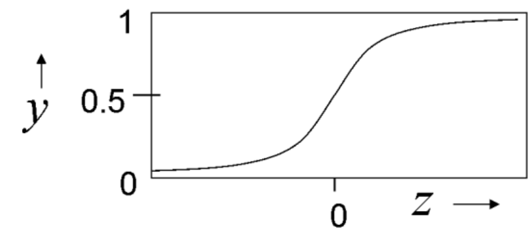
$$\text{h}(\boldsymbol{x}) = \psi(\boldsymbol{W}^{[2]}\boldsymbol{z}) = \psi\left(\boldsymbol{W}^{[2]}\phi(\boldsymbol{W}^{[1]}\boldsymbol{x})\right)$$

Sigmoid



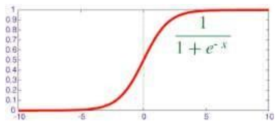
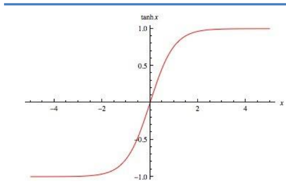
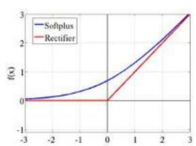
$$z = \sum_i w_i x_i - \theta$$

$$\hat{y} = \frac{1}{1 + \exp(-z)}$$



- A “squashing” function instead of a threshold
  - The sigmoid “activation” replaces the threshold
    - These give a real-valued output that is a smooth and bounded function of their input.
    - They have nice derivatives.

Activations and their derivatives

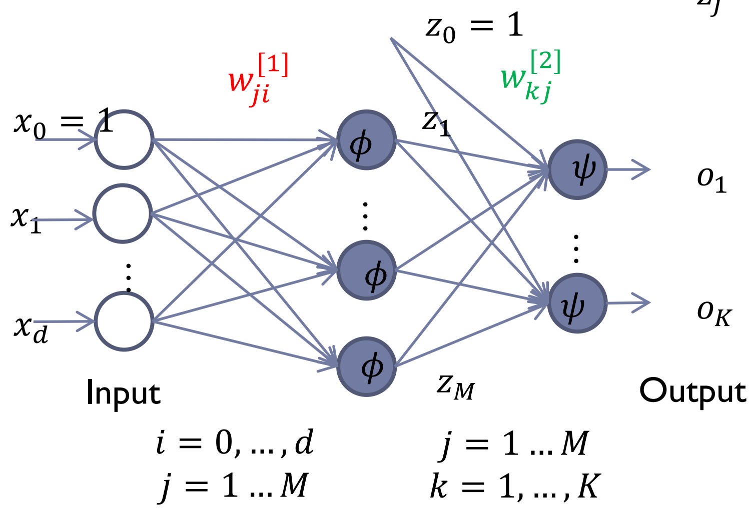
 $f(z) = \dfrac{1}{1+\exp(-z)}$	$f'(z) = f(z)(1 - f(z))$
 $f(z) = \tanh(z)$	f $f'(z) = 1 - f^2(z)$
 $f(z) = \begin{cases} 0, & z < 0 \\ z, & z \geq 0 \end{cases}$	$f'(z) = \begin{cases} 1, z \geq 0 \\ 0, z < 0 \end{cases}$
$f(z) = \log(1 + \exp(z))$	$f'(z) = \dfrac{1}{1+\exp(-z)}$

- Some popular activation functions and their derivatives

MLP with single hidden layer

- Two-layer MLP (Number of layers of adaptive weights is counted)

$$o_k(\boldsymbol{x}) = \psi\left(\sum_{j=0}^{M} w_{kj}^{[2]} z_j\right) \Rightarrow o_k(\boldsymbol{x}) = \psi\left(\sum_{j=0}^{M} w_{kj}^{[2]} \underbrace{\phi\left(\sum_{i=0}^{d} w_{ji}^{[1]} x_i\right)}_{z_j}\right)$$



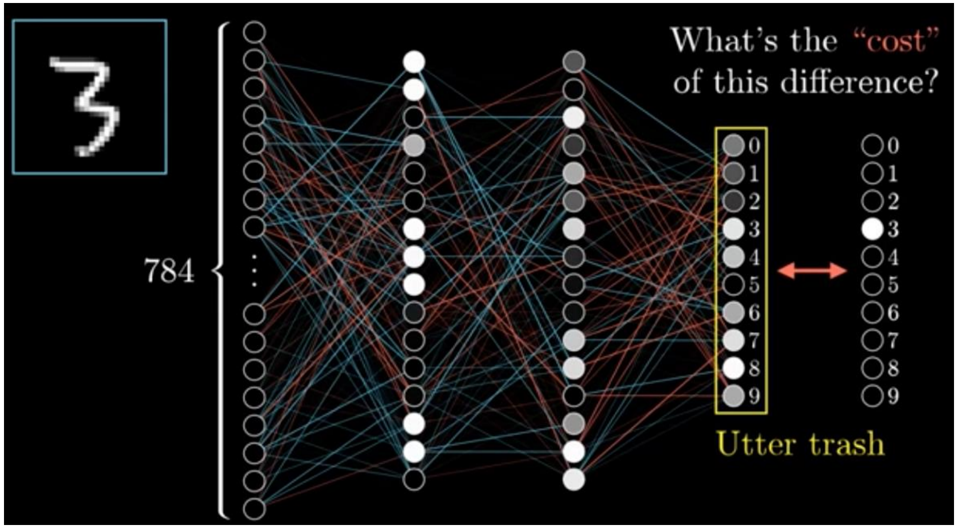
- Thus, we don't need expert knowledge or time consuming tuning of hand-crafted features
  - Compared to kernel method in which we need to perform a feature engineering phase

Training multi-layer networks

- Back-propagation
  - Training algorithm that is used to adjust weights in multi-layer networks
    - The backpropagation algorithm is based on gradient descent
      - The direction of the most rapid decrease in the cost function
  - Use chain rule to efficiently compute gradients

Find the weights by optimizing the cost

- Start from random weights and then adjust them iteratively to get lower cost.
- Update the weights according to the gradient of the cost function



Source: http://3b1b.co

Training Neural Nets through Gradient Descent

- The cost function to train the neural network,
  - $\boldsymbol{h}_{\boldsymbol{W}}^{(n)}$ as the output of a network with $\boldsymbol{n}$ layers

$$\text{J} = \sum_{n=1}^{N} loss\left(\boldsymbol{h}_{\boldsymbol{W}}^{(n)}, \boldsymbol{y}^{(n)}\right)$$

- Gradient descent algorithm
- Initialize all weights and biases $\left\{w_{ji}^{[k]}\right\}$
  - Using the extended notation : the bias is also weight
- Do :
  - For every layer k for all i, j update:
    - $w_{ji}^{[k]} = w_{ji}^{[k]} - \eta \frac{dJ}{dw_{ji}^{[k]}}$
- Until J has converged

Training multi-layer networks

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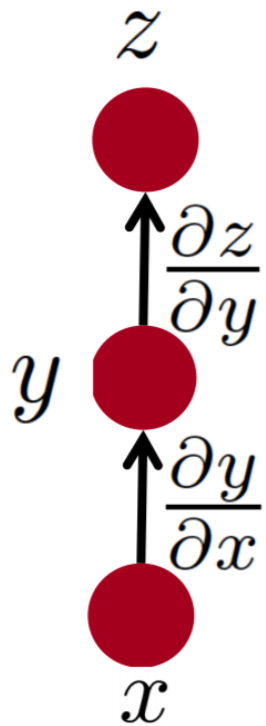
Simple chain rule

- $z = f\big(g(x)\big)$
- $y = g(x)$



$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$

Calculus Refresher: Basic rules of calculus

$$y = f(x)$$

with derivative

$$\frac{dy}{dx}$$

the following must hold for sufficiently small Δx $\Rightarrow$ $\Delta y \approx \frac{dy}{dx}\Delta x$

$$\frac{dy}{dx} \approx \frac{\Delta y}{\Delta x}$$

For any differentiable function

$$y = f(x_1, x_2, \ldots, x_M)$$

with partial derivatives

$$\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \ldots, \frac{\partial y}{\partial x_M}$$

the following must hold for sufficiently small $\Delta x_1, \Delta x_2, \ldots, \Delta x_M$

$$\Delta y \approx \frac{\partial y}{\partial x_1}\Delta x_1 + \frac{\partial y}{\partial x_2}\Delta x_2 + \cdots + \frac{\partial y}{\partial x_M}\Delta x_M$$

Calculus Refresher: Chain rule

For any nested function $y = f(g(x))$

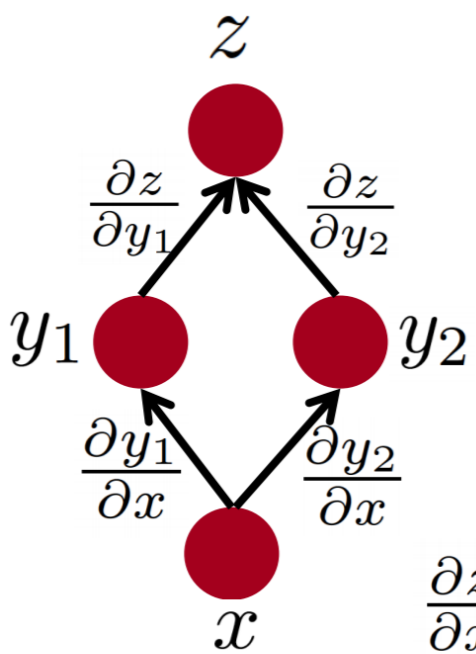
$$\boxed{\frac{dy}{dx} = \frac{\partial f}{\partial g(x)} \frac{dg(x)}{dx}}$$

Check – we can confirm that : $\Delta y = \frac{dy}{dx} \Delta x$

$z = g(x) \Rightarrow \Delta z = \frac{dg(x)}{dx} \Delta x$

$y = f(z) \Rightarrow \Delta y = \frac{df}{dz} \Delta z = \frac{df}{dz} \frac{dg(x)}{dx} \Delta x$ ✓

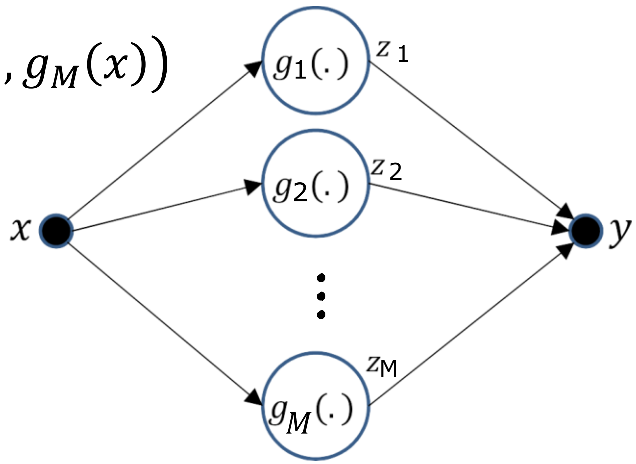
Multiple paths chain rule



$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

Distributed Chain Rule: Influence Diagram

$$y = f\big(g_1(x), g_2(x), \dots, g_M(x)\big)$$



- x affects y through each $g_1, \dots, g_M$

Calculus Refresher: Distributed Chain rule

$$y = f\left(g_1(x), g_1(x), \dots, g_M(x)\right)$$

$$\boxed{\frac{dy}{dx} = \frac{\partial f}{\partial g_1(x)}\frac{dg_1(x)}{dx} + \frac{\partial f}{\partial g_2(x)}\frac{dg_2(x)}{dx} + \cdots + \frac{\partial f}{\partial g_M(x)}\frac{dg_M(x)}{dx}}$$

Check:

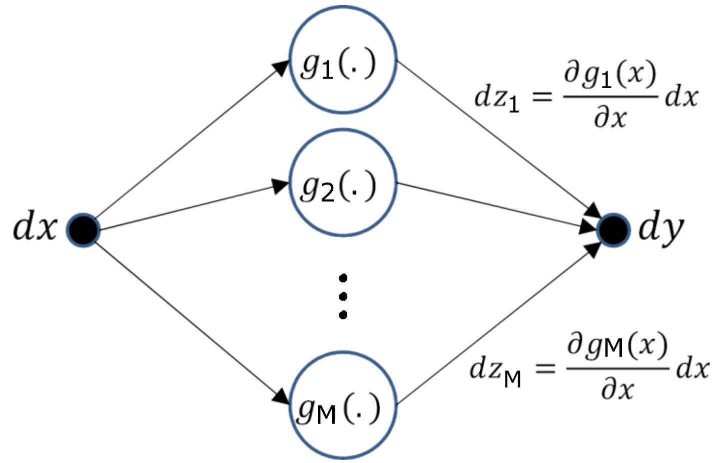
$$\Delta y = \frac{dy}{dx}\Delta x$$

$$\Delta y = \frac{\partial f}{\partial g_1(x)}\Delta g_1(x) + \frac{\partial f}{\partial g_2(x)}\Delta g_2(x) + \cdots + \frac{\partial f}{\partial g_M(x)}\Delta g_M(x)$$

$$\boxed{\Delta y = \frac{\partial f}{\partial g_1(x)}\frac{dg_1(x)}{dx}\Delta x + \frac{\partial f}{\partial g_2(x)}\frac{dg_2(x)}{dx}\Delta x + \cdots + \frac{\partial f}{\partial g_M(x)}\frac{dg_M(x)}{dx}\Delta x}$$

$$\boxed{\Delta y = \left(\frac{\partial f}{\partial g_1(x)}\frac{dg_1(x)}{dx} + \frac{\partial f}{\partial g_2(x)}\frac{dg_2(x)}{dx} + \cdots + \frac{\partial f}{\partial g_M(x)}\frac{dg_M(x)}{dx}\right)\Delta x} \checkmark$$

Distributed Chain Rule: Influence Diagram



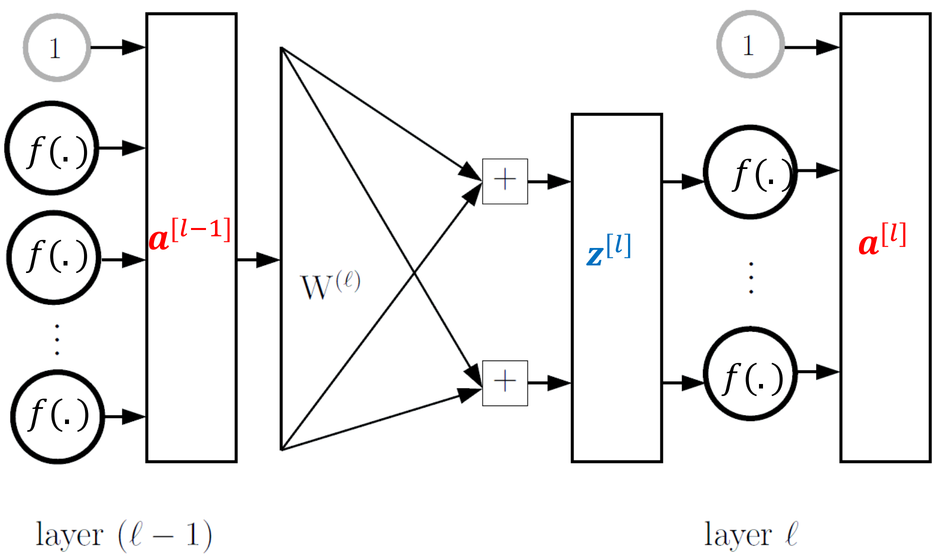
- Small perturbations in x cause small perturbations in each of $g_1 \cdots g_M$, which individually additively perturbs y

Returning to our problem

- How to compute $$\frac{d\,\boldsymbol{J}}{dw_{ji}^{[k]}}$$

Backpropagation: Notation

- $\boldsymbol{a}^{[0]} \leftarrow Input$
- $output \leftarrow \boldsymbol{a}^{[L]}$
- f as the activation function



Backpropagation: Last layer gradient

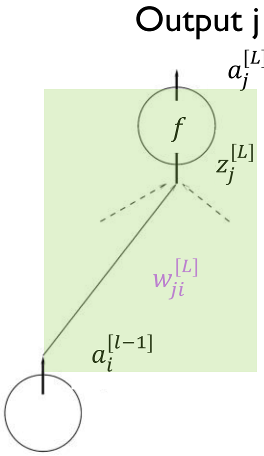
$$a_j^{[L]} = f\left(z_j^{[L]}\right)$$

$$z_j^{[L]} = \sum_{i=0}^{M} w_{ji}^{[L]} a_i^{[L-1]}$$

$$\frac{\partial loss}{\partial w_{ji}^{[L]}} = \frac{\partial loss}{\partial a_j^{[L]}} \frac{\partial a_j^{[L]}}{\partial w_{ji}^{[L]}}$$

$$\frac{\partial a^{[L]}}{\partial w_{ji}^{[L]}} = f'\left(z_j^{[L]}\right) \frac{\partial z_j^{[L]}}{\partial w_{ji}^{[L]}} = f'\left(z_j^{[L]}\right) a_i^{[L-1]}$$

$$\frac{\partial loss}{\partial w_{ji}^{[L]}} = \frac{\partial loss}{\partial a_j^{[L]}} f'\left(z_j^{[L]}\right) a_i^{[L-1]}$$



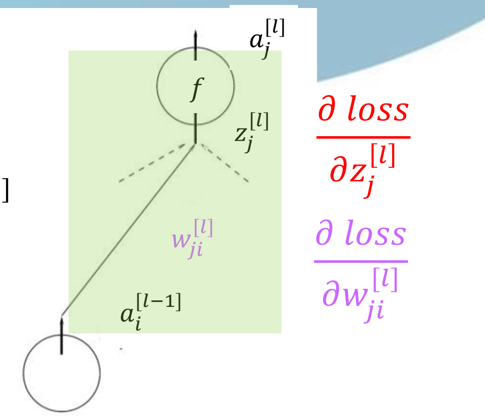
$$\frac{\partial loss}{\partial a_j^{[L]}}$$

$$\frac{\partial loss}{\partial w_{ji}^{[L]}}$$

Previous layers gradients

$$a_j^{[l]} = f\left(z_j^{[l]}\right)$$

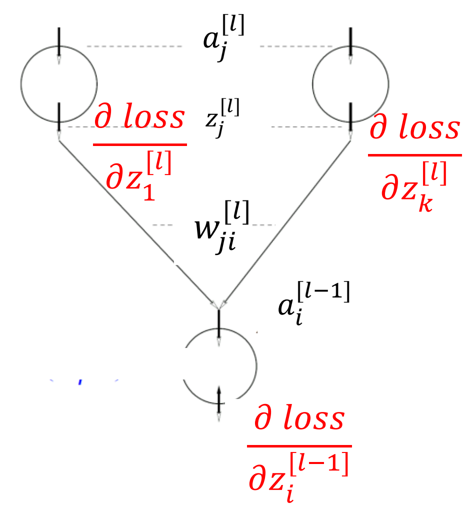
$$z_j^{[l]} = \sum_{i=0}^{M} w_{ji}^{[l]} a_i^{[l-1]}$$



$$\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \frac{\partial\, loss}{\partial z_j^{[l]}} \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}}$$

$$\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \frac{\partial\, loss}{\partial z_j^{[l]}} a_i^{[l-1]}$$

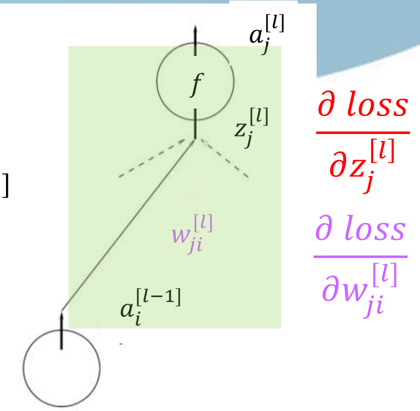
$$\frac{\partial\, loss}{\partial z_j^{[l]}} =?$$



Previous layers gradients

$$a_j^{[l]} = f\left(z_j^{[l]}\right)$$

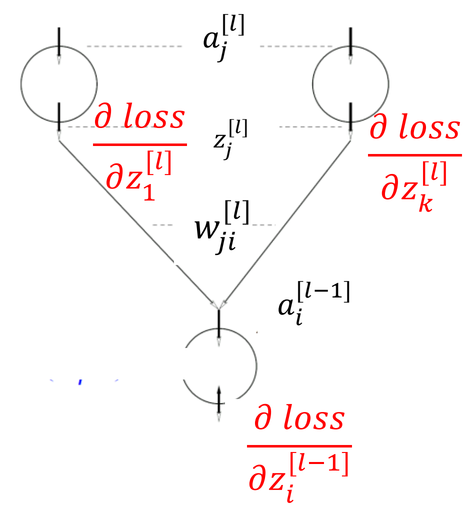
$$z_j^{[l]} = \sum_{i=0}^{M} w_{ji}^{[l]} a_i^{[l-1]}$$



$$\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \frac{\partial\, loss}{\partial z_j^{[l]}} \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}} = \frac{\partial\, loss}{\partial z_j^{[l]}} a_i^{[l-1]}$$

$$\frac{\partial\, loss}{\partial z_i^{[l-1]}} = \frac{\partial a_i^{[l-1]}}{\partial z_i^{[l-1]}} \sum_{j=1}^{d^{[l]}} \frac{\partial\, loss}{\partial z_j^{[l]}} \times \frac{\partial z_j^{[l]}}{\partial a_i^{[l-1]}}$$

$$= f'\left(z_i^{[l-1]}\right) \sum_{j=1}^{d^{[l]}} \frac{\partial\, loss}{\partial z_j^{[l]}} \times w_{ji}^{[l]}$$



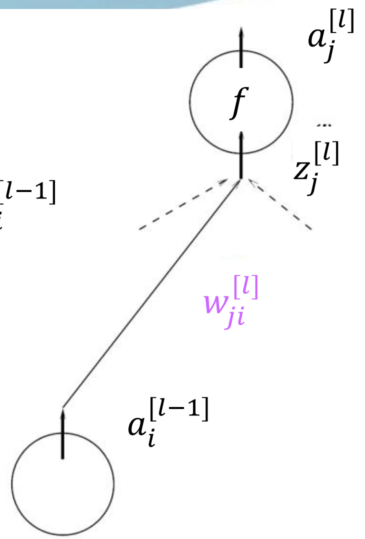
Backpropagation:

$$\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \boxed{\frac{\partial\, loss}{\partial z_j^{[l]}}} \times \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}}$$

$$= \boxed{\delta_j^{[l]}} \times a_i^{[l-1]}$$

$$a_j^{[l]} = f\left(z_j^{[l]}\right)$$

$$z_j^{[l]} = \sum_{i=0}^{M} w_{ji}^{[l]} a_i^{[l-1]}$$



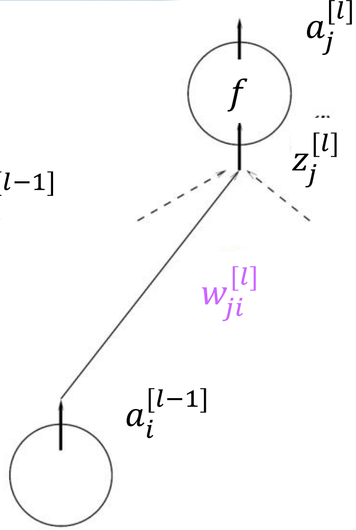
Backpropagation:

$$\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \boxed{\frac{\partial\, loss}{\partial z_j^{[l]}}} \times \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}}$$

$$= \boxed{\delta_j^{[l]}} \times a_i^{[l-1]}$$

$$a_j^{[l]} = f\left(z_j^{[l]}\right)$$

$$z_j^{[l]} = \sum_{i=0}^{M} w_{ji}^{[l]} a_i^{[l-1]}$$



- $\delta_j^{[l]} = \frac{\partial\, loss}{\partial z_j^{[l]}}$ is the sensitivity of the loss to $z_j^{[l]}$
- Sensitivity vectors can be obtained by running a backward process in the network architecture (hence the name backpropagation.)

We will compute $\boldsymbol{\delta}^{[l-1]}$ from $\boldsymbol{\delta}^{[l]}$:

$$\delta_i^{[l-1]} = f'\left(z_i^{[l-1]}\right) \sum_{j=1}^{d^{[l]}} \delta_j^{[l]} \times w_{ji}^{[l]}$$

Backward process on sensitivity vectors

- For the final layer $l = L$:

$$\delta_j^{[L]} = \frac{\partial\, loss}{\partial z_j^{[L]}}$$

- Compute $\boldsymbol{\delta}^{[l-1]}$ from $\boldsymbol{\delta}^{[l]}$: by running a backward process in the network architecture:

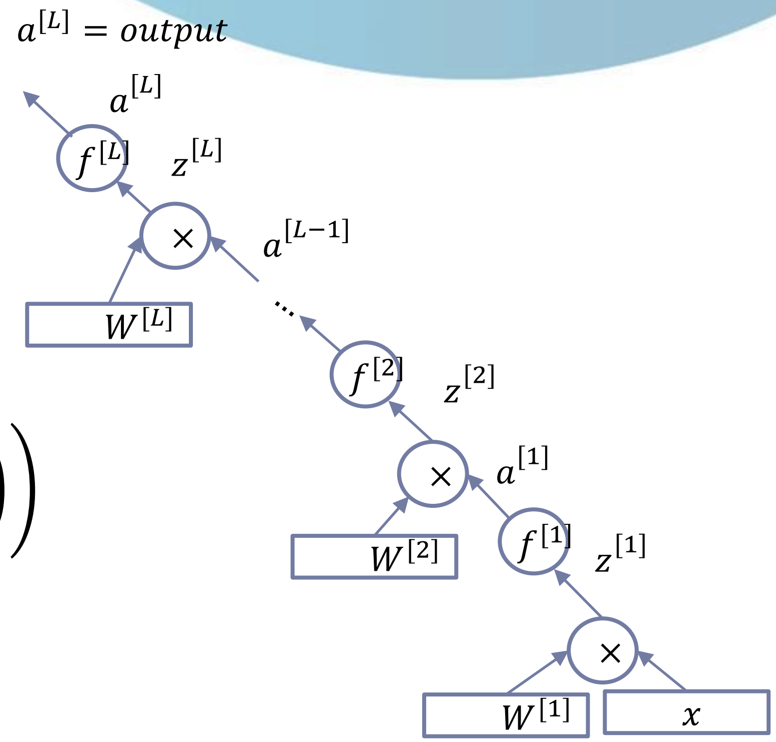
$$\delta_i^{[l-1]} = f'\left(z_i^{[l-1]}\right) \sum_{j=1}^{d^{[l]}} \delta_j^{[l]} \times w_{ji}^{[l]}$$

Backpropagation Algorithm

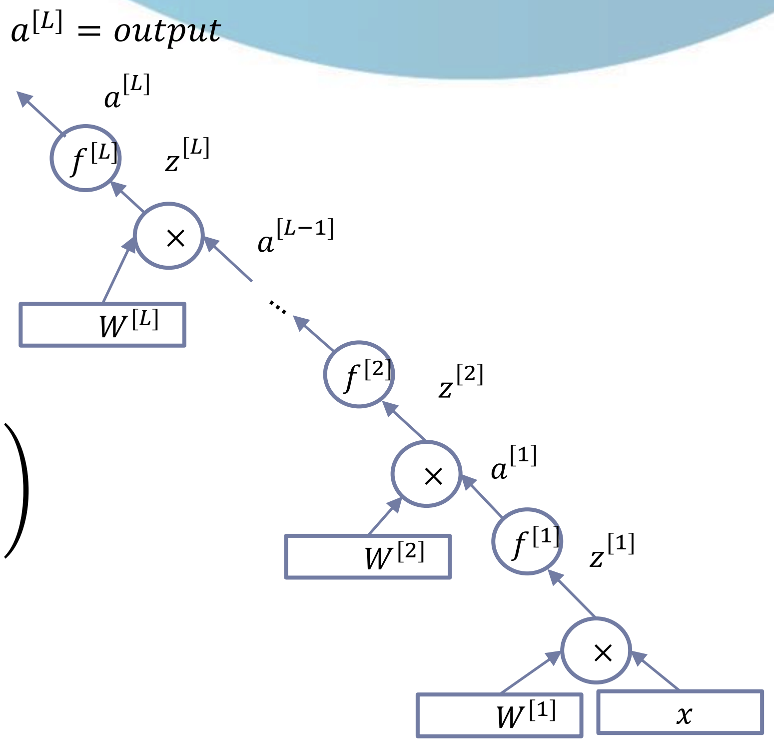
- Initialize all weights to small random numbers.
- **While not satisfied**
- **For** each training example **do**:
  1. Feed forward the training example to the network and compute the outputs of all units in forward step (z and a) and the loss
  2. For each unit find its δ in the backward step
  3. Update each network weight $w_{ji}^{[l]}$ as $w_{ji}^{[l]} \leftarrow w_{ji}^{[l]} - \eta \frac{\partial\, loss}{\partial w_{ji}^{[l]}}$ where $\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \delta_j^{[l]} \times a_i^{[l-1]}$

Multi-layer network: Matrix notation

$$Output = a^{[L]}$$
$$= f\left(z^{[L]}\right)$$
$$= f\left(W^{[L]}a^{[L-1]}\right)$$
$$= f\left(W^{[L]}f(W^{[L-1]}a^{[L-2]}\right)$$
$$= f\left(W^{[L]}f\left(W^{[L-1]} \dots f\left(W^{[2]}f(W^{[1]}x)\right)\right)\right)$$



Multi-layer network: Matrix notation



$$Output = a^{[L]}$$
$$= f\left(z^{[L]}\right)$$
$$= f\left(W^{[L]}a^{[L-1]}\right)$$
$$= f\left(W^{[L]}f(W^{[L-1]}a^{[L-2]}\right)$$
$$= f\left(W^{[L]}f\left(W^{[L-1]}\dots f\left(W^{[2]}f(W^{[1]}x)\right)\right)\right)$$

$$\frac{\partial\, loss}{\partial W^{[l]}} = \frac{\partial\, loss}{\partial z^{[l]}} a^{[l-1]^T}$$

$$\frac{\partial\, loss}{\partial z^{[l]}} = f'(z^{[l]}) W^{[l+1]^T} \frac{\partial\, loss}{\partial z^{[l+1]}}$$

References

- Mahdieh Soleymani, Machine learning, Sharif university