COMP5212: Machine Learning

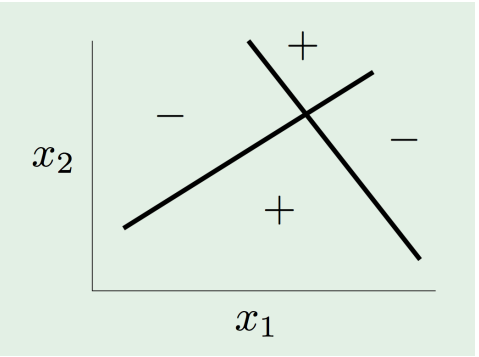
Lecture 12

Minhao Cheng

Neural networks

Another way to introduce nonlinearity

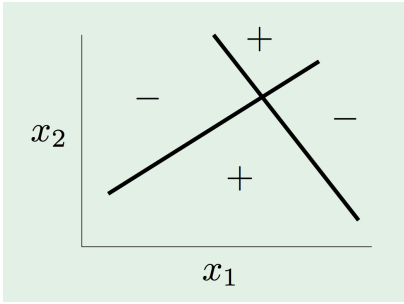
- How to generate this nonlinear hypothesis?



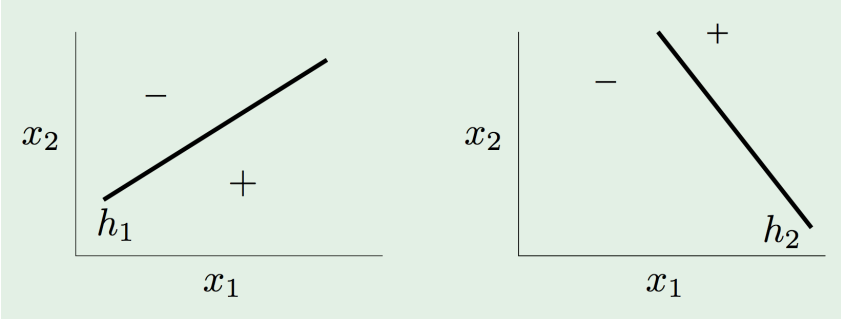
Neural network

Another way to introduce nonlinearity

- How to generate this nonlinear hypothesis?



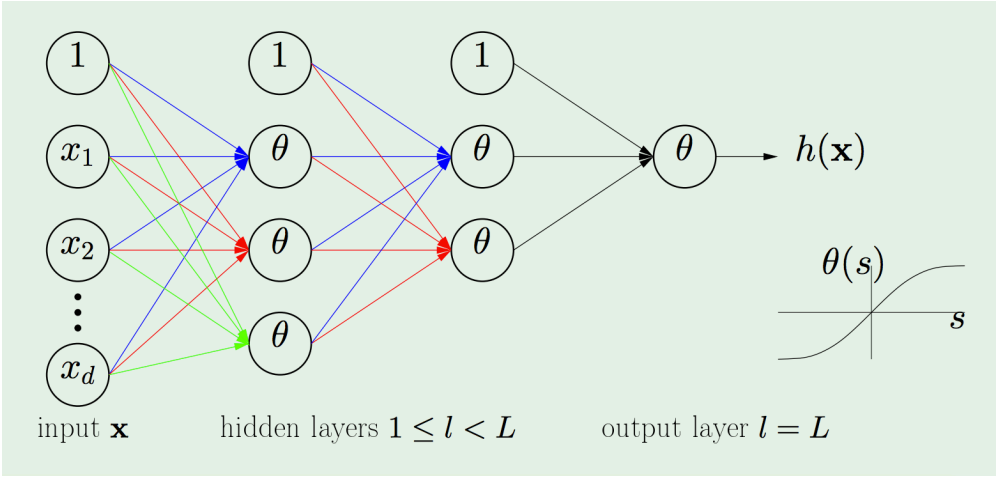
- Combining multiple linear hyperplanes to construct nonlinear hypothesis



Neural Network

Definition

- Input layer: d neurons (input features)
- Neurons from layer 1 to L: Linear combination of previous layers + activation function
  - $\theta(w^T x)$, θ : activation function
- Final layer: one neuron $\Rightarrow$ prediction by sign$(h(x))$

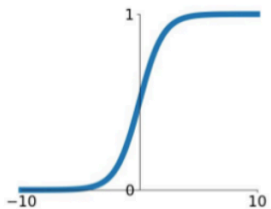


Neural network

Activation Function

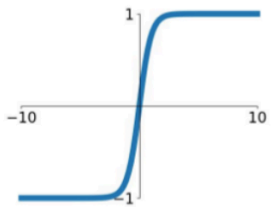
Sigmoid

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



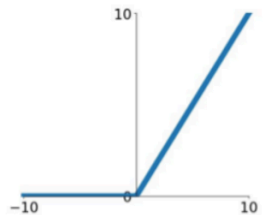
tanh

$$\tanh(x)$$



ReLU

$$\max(0, x)$$



Neural Network

Activation: Formal Definitions

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

- bias: $b_j^{(l)}$: added to the j-th neuron in the l-th layer

Neural Network

Formal Definitions

- Weight: $w_{ij}^{(l)}$ $\begin{cases} 1 \le l \le L & : \text{layers} \\ 0 \le i \le d^{(l-1)} & : \text{inputs} \\ 1 \le j \le d^{(l)} & : \text{outputs} \end{cases}$
- bias: $b_j^{(l)}$: added to the j-th neuron in the l-th layer
- j-th neuron in the l-the layer:
  - $x_j^{(l)} = \theta(s_j^{(l)}) = \theta(\sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)} x_i^{(l-1)} + b_j^{(l)})$

Neural Network

Formal Definitions

- Weight: $w_{ij}^{(l)}$ $\begin{cases} 1 \le l \le L & : \text{layers} \\ 0 \le i \le d^{(l-1)} & : \text{inputs} \\ 1 \le j \le d^{(l)} & : \text{outputs} \end{cases}$
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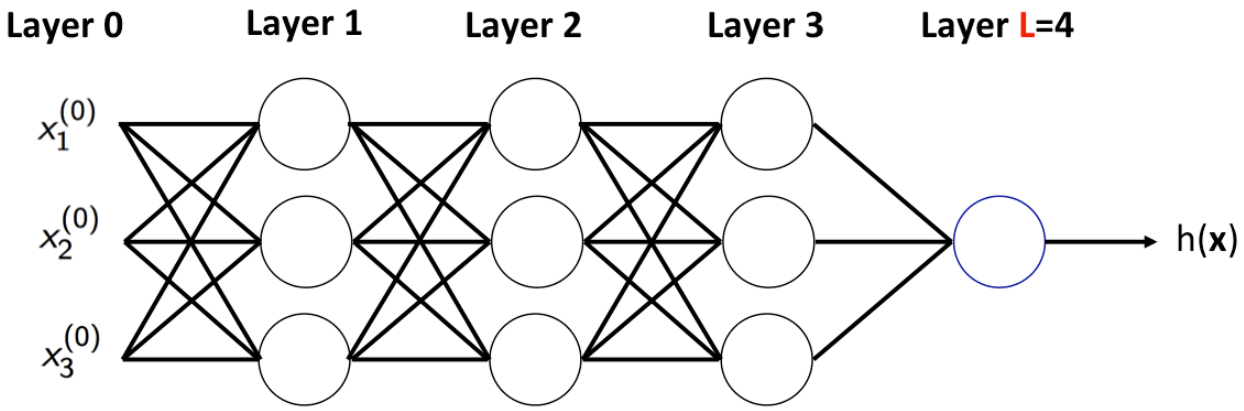
  - $x_j^{(l)} = \theta(s_j^{(l)}) = \theta(\sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)} x_i^{(l-1)} + b_j^{(l)})$
- Output:
  - $h(x) = x_1^{(L)}$

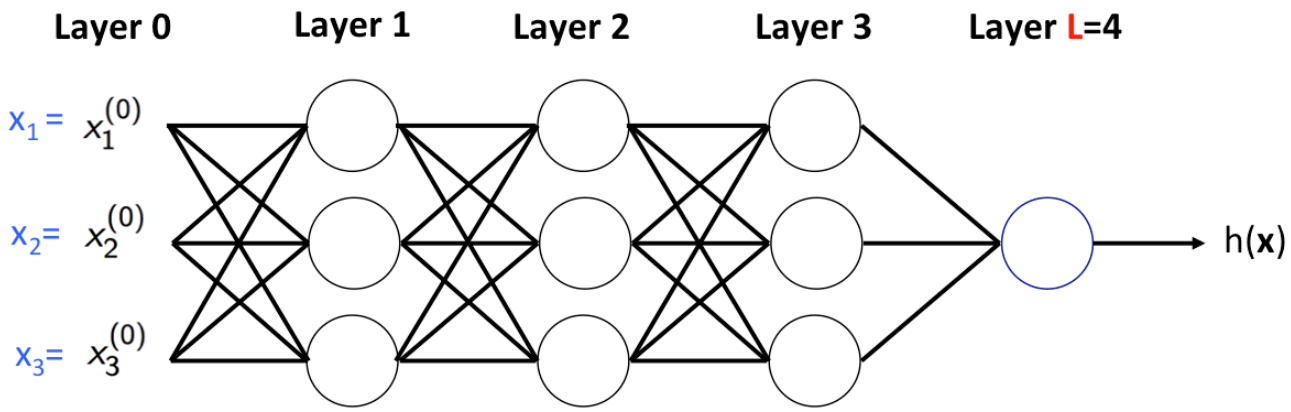
Neural Network

Forward propagation



Neural Network

Forward propagation

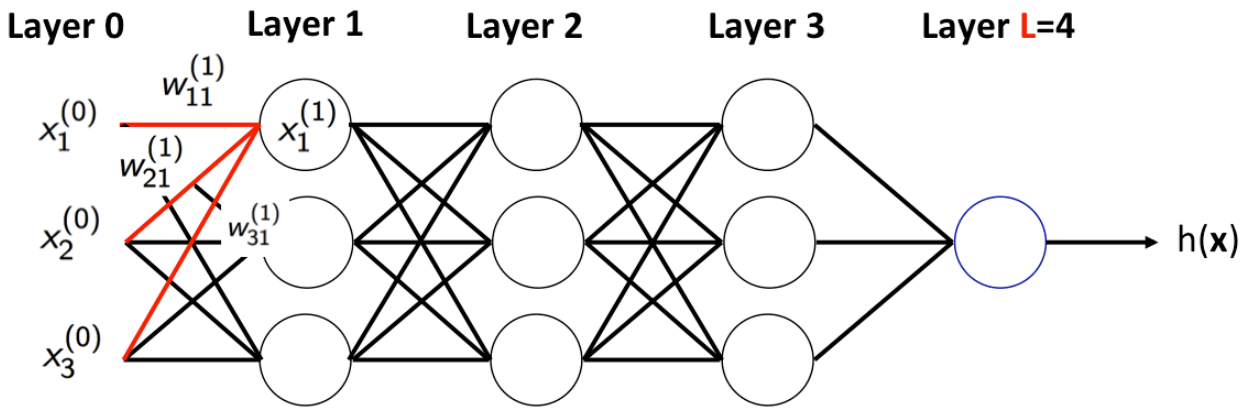


features for one data point

x = [x_1, x_2, x_3]

Neural Network

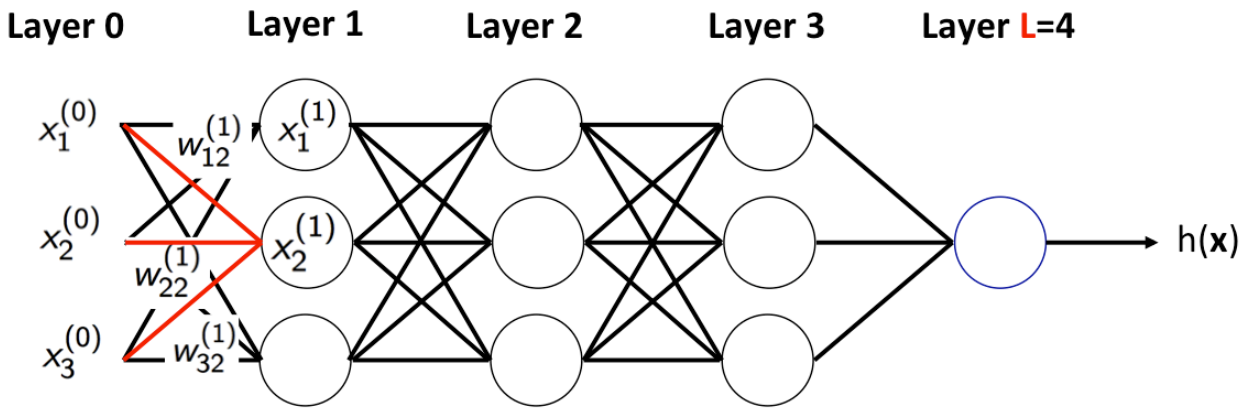
Forward propagation



$$x_1^{(1)} = \theta\left(\sum_{i=1}^{3} w_{i1}^{(1)} x_i^{(0)}\right)$$

Neural Network

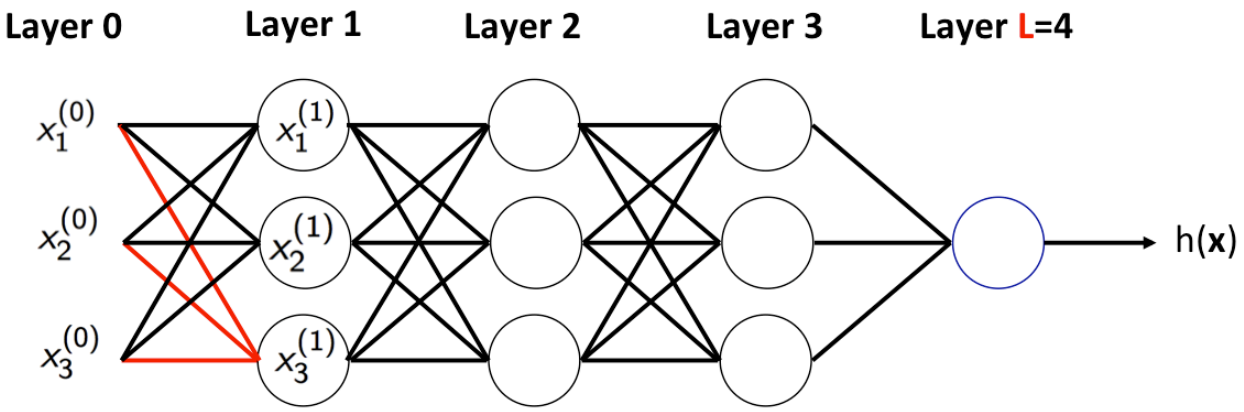
Forward propagation



$$x_2^{(1)} = \theta\left(\sum_{i=1}^{3} w_{i2}^{(1)} x_i^{(0)}\right)$$

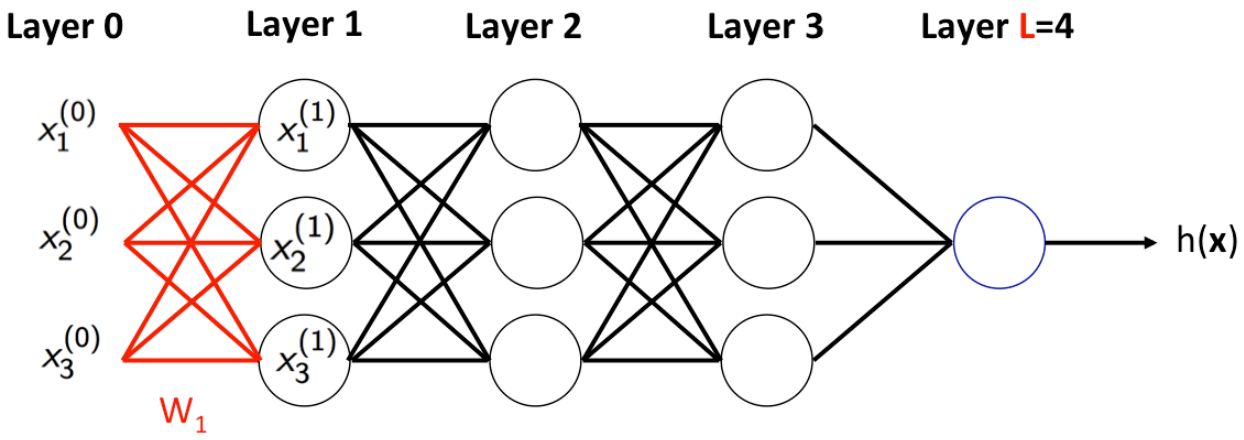
Neural Network

Forward propagation



Neural Network

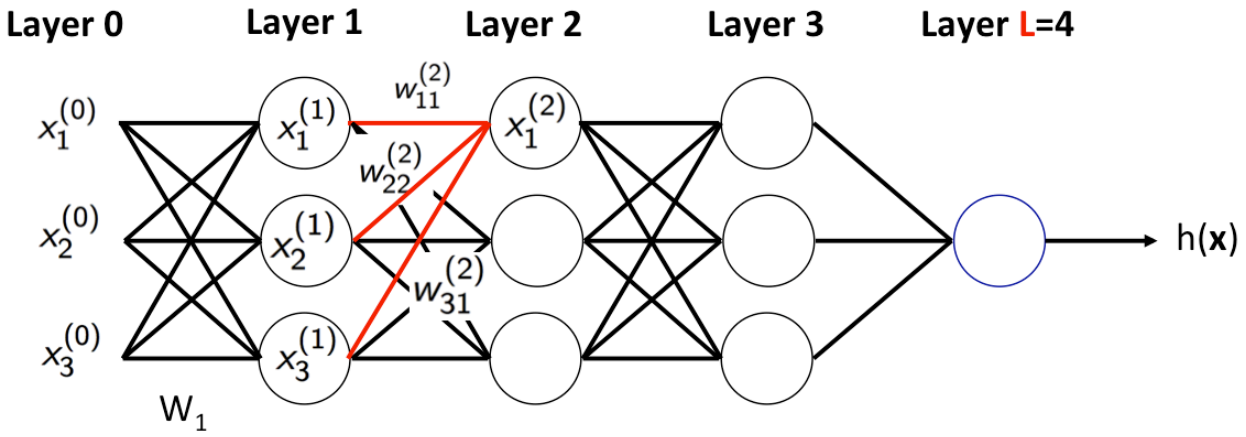
Forward propagation



$$\boldsymbol{x}^{(1)} = \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \end{bmatrix} = \theta \left(\begin{bmatrix} w_{11}^{(1)} & w_{21}^{(1)} & w_{31}^{(1)} \\ w_{12}^{(1)} & w_{22}^{(1)} & w_{32}^{(1)} \\ w_{13}^{(1)} & w_{23}^{(1)} & w_{33}^{(1)} \end{bmatrix} \times \begin{bmatrix} x_1^{(0)} \\ x_2^{(0)} \\ x_3^{(0)} \end{bmatrix} \right) = \theta(W_1 \boldsymbol{x}^{(0)})$$

Neural Network

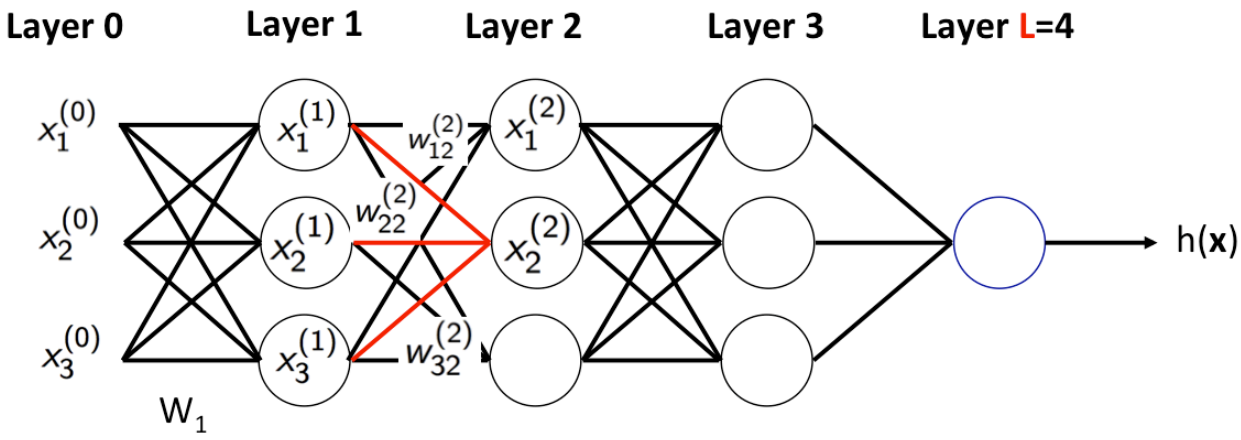
Forward propagation



$$x_1^{(2)} = \theta\left(\sum_{i=1}^{3} w_{i1}^{(2)} x_i^{(1)}\right)$$

Neural Network

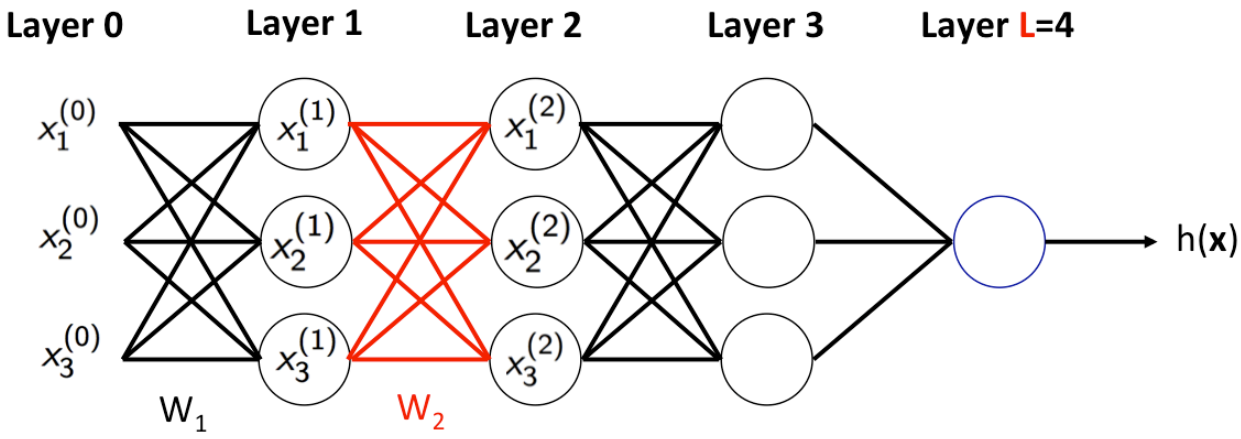
Forward propagation



$$x_2^{(2)} = \theta\left(\sum_{i=1}^{3} w_{i2}^{(2)} x_i^{(1)}\right)$$

Neural Network

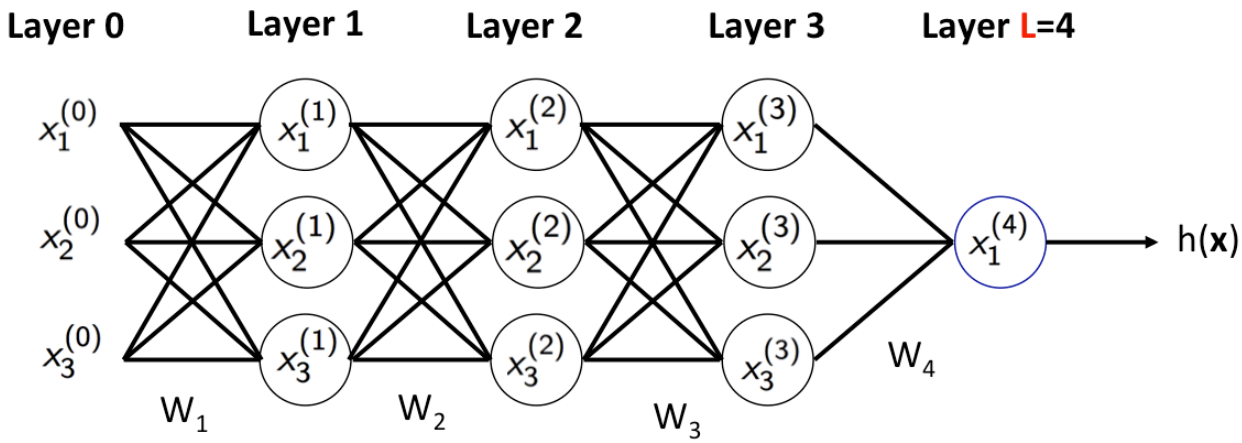
Forward propagation



$$\boldsymbol{x}^{(2)} = \begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \\ x_3^{(2)} \end{bmatrix} = \theta \left(\begin{bmatrix} w_{11}^{(2)} & w_{21}^{(2)} & w_{31}^{(2)} \\ w_{12}^{(2)} & w_{22}^{(2)} & w_{32}^{(2)} \\ w_{13}^{(2)} & w_{23}^{(2)} & w_{33}^{(2)} \end{bmatrix} \times \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \end{bmatrix} \right) = \theta(W_2 \boldsymbol{x}^{(1)})$$

Neural Network

Forward propagation



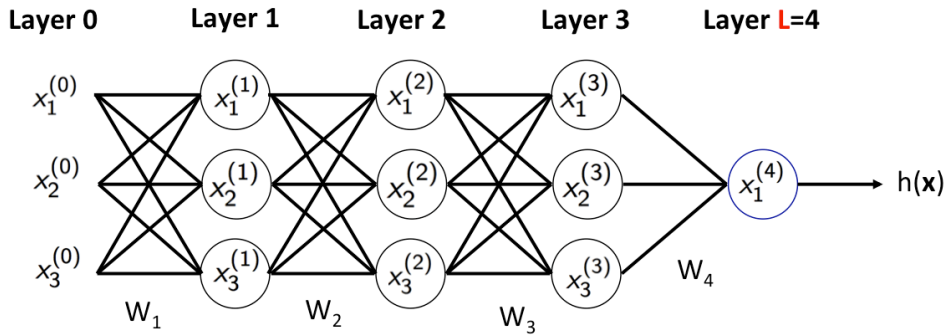
$$h(\boldsymbol{x}) = x_1^{(4)} = \theta(W_4 \boldsymbol{x}^{(3)}) = \theta(W_4 \theta(W_3 \boldsymbol{x}^{(2)}))$$
$$= \cdots = \theta(W_4 \theta(W_3 \theta(W_2 \theta(W_1 \boldsymbol{x}))))$$

Neural Network

Forward propagation

- With the bias term:

$$h(x) = \theta(W_4\theta(W_3\theta(W_2\theta(W_1x + b_1) + b_2) + b_3) + b_4)$$



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Neural Network

Capacity of neural networks

- Universal approximation theorem (Horink, 1991):
  - “A neural network with single hidden layer can approximate any continuous function arbitrarily well, given enough hidden units”
- True for commonly used activations (ReLU, sigmoid, …)

Neural Network

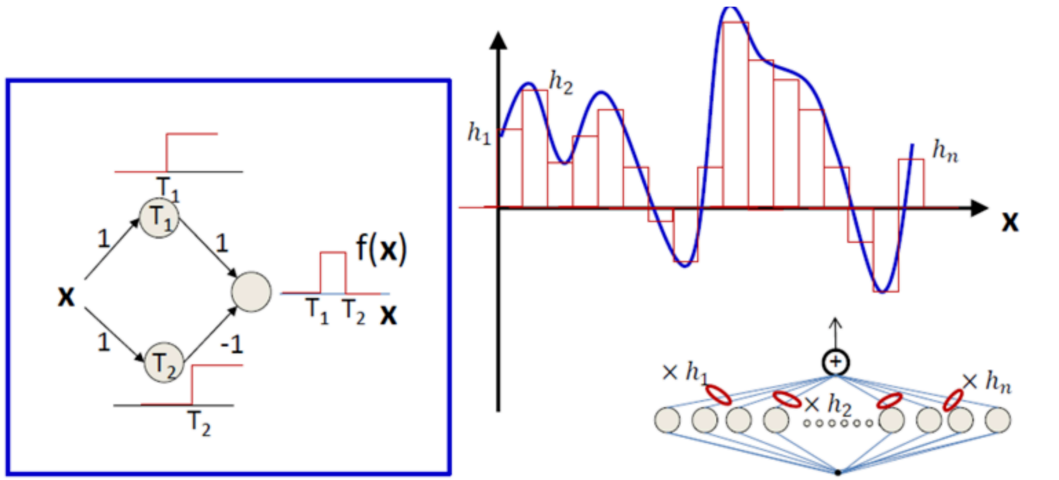
Capacity of neural networks

- Universal approximation theorem (Horink, 1991):
  - “A neural network with single hidden layer can approximate any continuous function arbitrarily well, given enough hidden units”
- True for commonly used activations (ReLU, sigmoid, …)
- However,
  - Can’t have infinitely number of hidden units in practice
  - Only shows the ideal model exists, but we may not be able to find it

Neural Network

Universal approximation for step activation

- How to approximate an arbitrary function by single-layer NN with step function as activation:



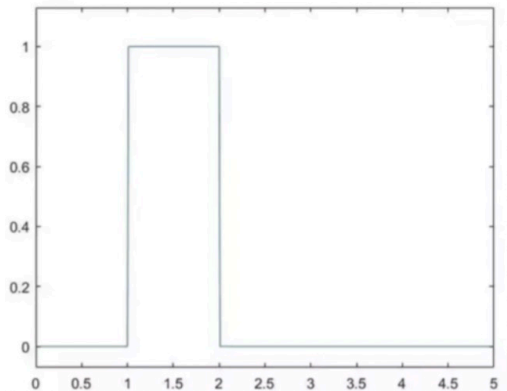
2 hidden units to form a "rectangle" **any function can be approximated by rectangles**

(figure from https://medium.com/analytics-vidhya)

Neural Network

Universal approximation for ReLU

- Use ReLU to approximate a rectangle:
  - $\frac{1}{\epsilon}(\max(0,x-a)-\max(0,x-a-\epsilon)-\max(0,x-b)+\max(0,x-b-\epsilon))$



- Use (approximate) rectangles to approximate arbitrary function

Neural Network

Training

- Weights $W = \{W_1, \ldots, W_L\}$ and bias $\{b_1, \cdots, b_L\}$ determine $h(x)$
- Learning the weights: solve ERM with SGD

Emperical Risk Minimization

- Loss on example (x_n, y_n) is
  - $e(h(x_n), y_n) = e(W)$

Neural Network

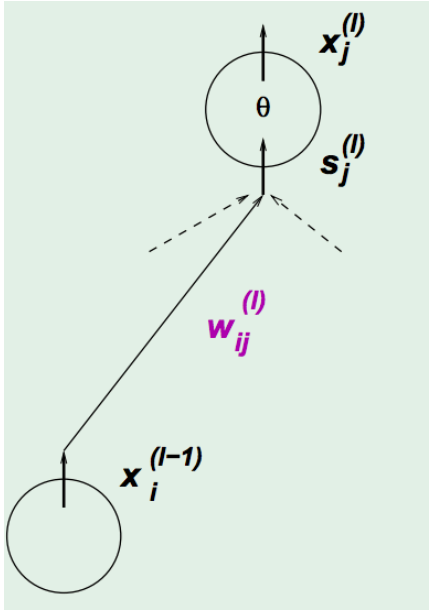
Training

- Weights $W = \{W_1, \ldots, W_L\}$ and bias $\{b_1, \cdots, b_L\}$ determine $h(x)$
- Learning the weights: solve ERM with SGD
- Loss on example (x_n, y_n) is
  - $e(h(x_n), y_n) = e(W)$
- To implement SGD, we need the gradient
  - $\nabla e(W) : \{\frac{\partial e(W)}{\partial w_{ij}^{(l)}}\}$ for all i, j, l (for simplicity we ignore bias in the derivations)

Neural Network

Computing Gradient $\frac{\partial e(W)}{\partial w_{ij}^{(l)}}$

- Use chain rule:
  - $$\frac{\partial e(W)}{\partial w_{ij}^{(l)}} = \frac{\partial e(W)}{\partial s_j^{(l)}} \times \frac{\partial s_j^{(l)}}{\partial w_{ij}^{(l)}}$$
  - $$s_j^{(l)} = \sum_{i=1}^{d} x_i^{(l-1)} w_{ij}^{(l)}$$
- We have $$\frac{\partial s_j^{(l)}}{\partial w_{ij}^{(l)}} = x_i^{(l-1)}$$



Neural Network

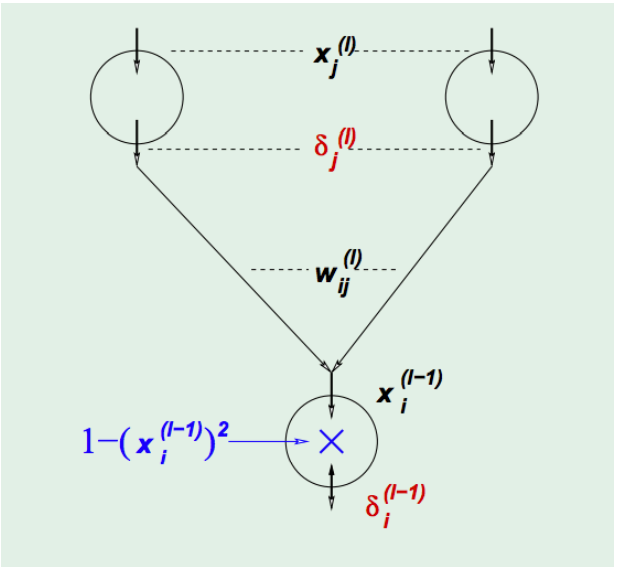
Computing Gradient $\frac{\partial e(W)}{\partial w_{ij}^{(l)}}$

- Define $\delta_j^{(l)} := \frac{\partial e(W)}{\partial s_j^{(l)}}$
- Compute by layer-by-layer:

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

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

- $$= \sum_{j=1}^{d} \delta_j^{(l)} \times w_{ij}^{(l)} \times \theta'(s_i^{(l-1)}),$$
  - where $\theta'(s) = 1 - \theta^2(s)$ for tanh $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
- $\delta_i^{(l-1)} = (1 - (x_i^{(l-1)})^2) \sum_{j=1}^{d} w_{ij}^{(l)} \delta_j^{(l)}$



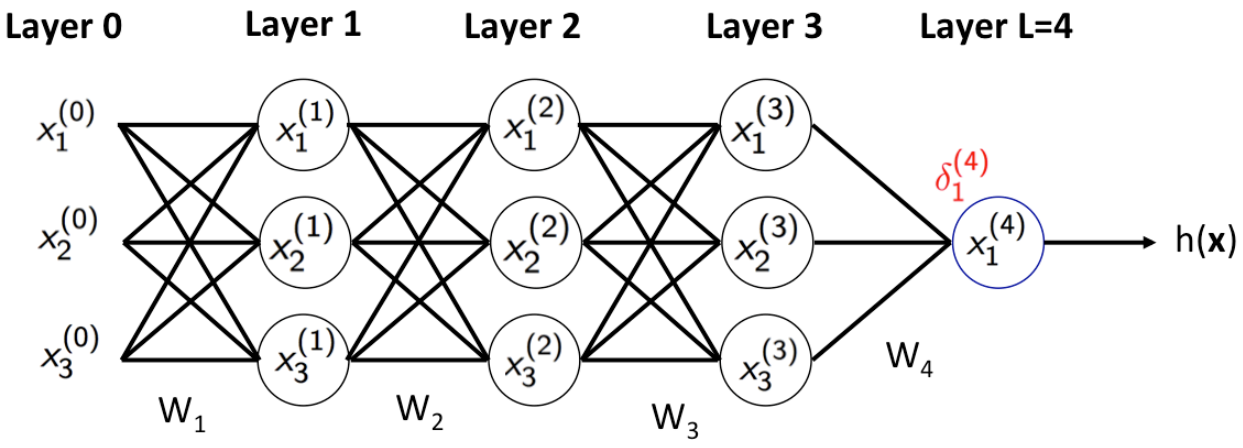
Neural Network

Final layer

- (Assume square loss)
  - $e(W) = (x_1^{(L)} - y_n)^2$
  - $x_1^{(L)} = \theta(s_1^{(L)})$
- So,
  - $$\delta_1^{(L)} = \frac{\partial e(W)}{\partial s_1^{(L)}}$$
  - $$= \frac{\partial e(W)}{\partial x_1^{(L)}} \times \frac{\partial x_1^{(L)}}{\partial s_1^{(L)}}$$
  - $$= 2(x_1^{(L)} - y_n) \times \theta'(s_1^{(L)})$$

Neural Network

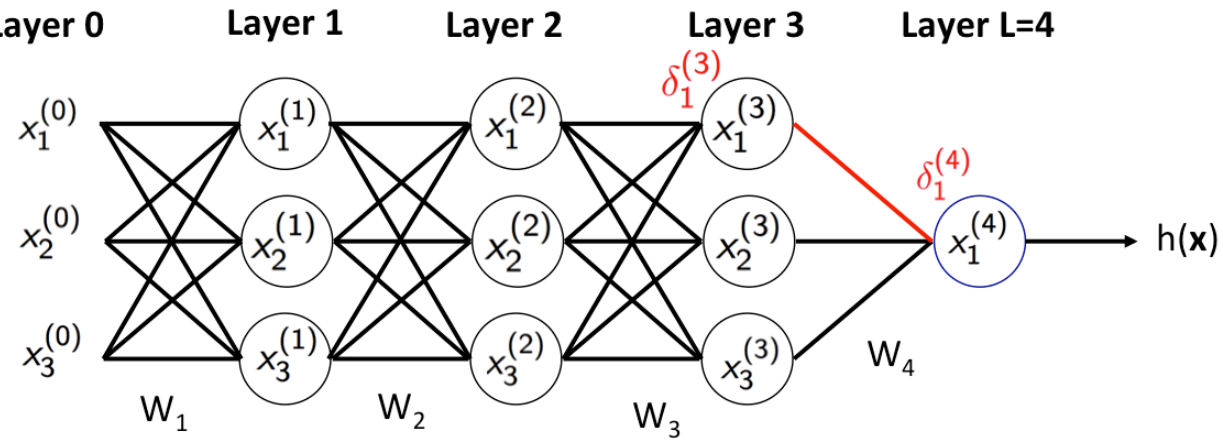
Backward propagation



$$\delta_1^{(4)} = 2(x_1^{(4)} - y_n) \times (1 - (x_1^{(4)})^2)$$

Neural Network

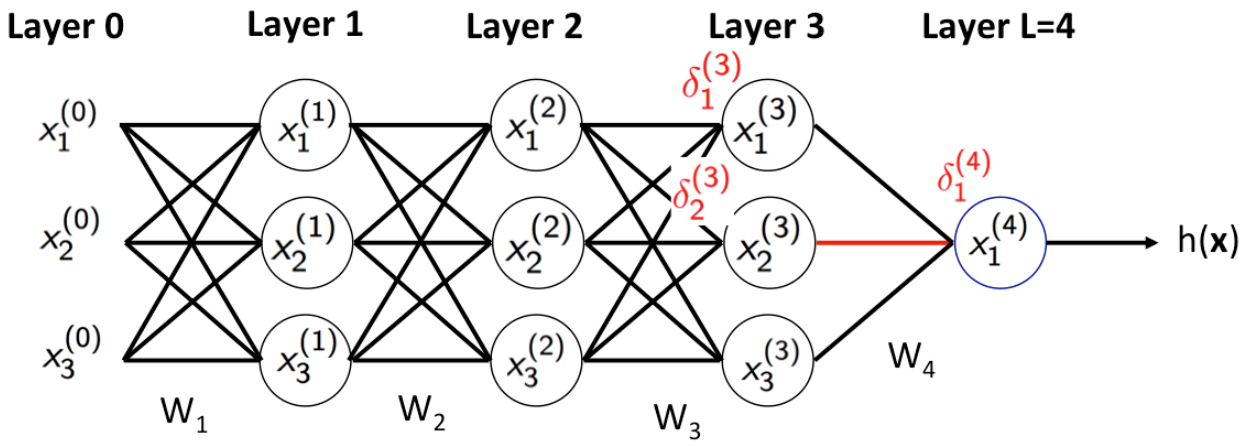
Backward propagation



$$\delta_1^{(3)} = (1 - (x_1^{(3)})^2) \times \delta_1^{(4)} \times w_{11}^{(4)}$$

Neural Network

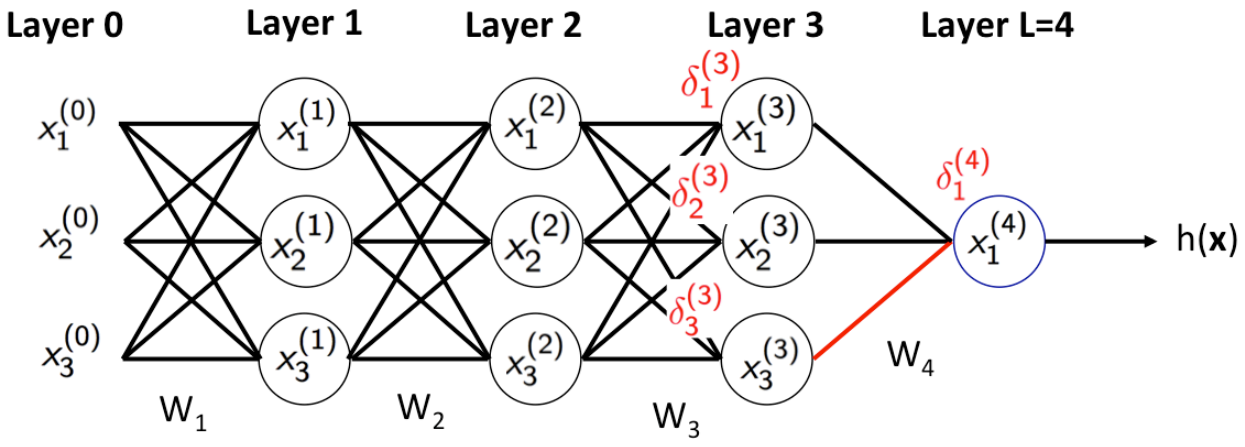
Backward propagation



$$\delta_2^{(3)} = (1 - (x_2^{(3)})^2) \times \delta_1^{(4)} \times w_{21}^{(4)}$$

Neural Network

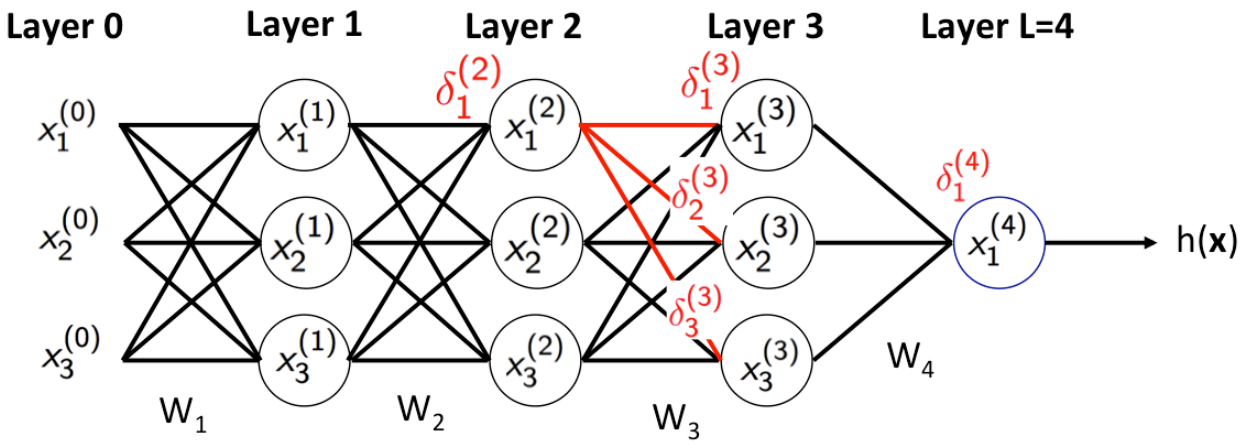
Backward propagation



$$\delta_3^{(3)} = (1 - (x_3^{(3)})^2) \times \delta_1^{(4)} \times w_{31}^{(4)}$$

Neural Network

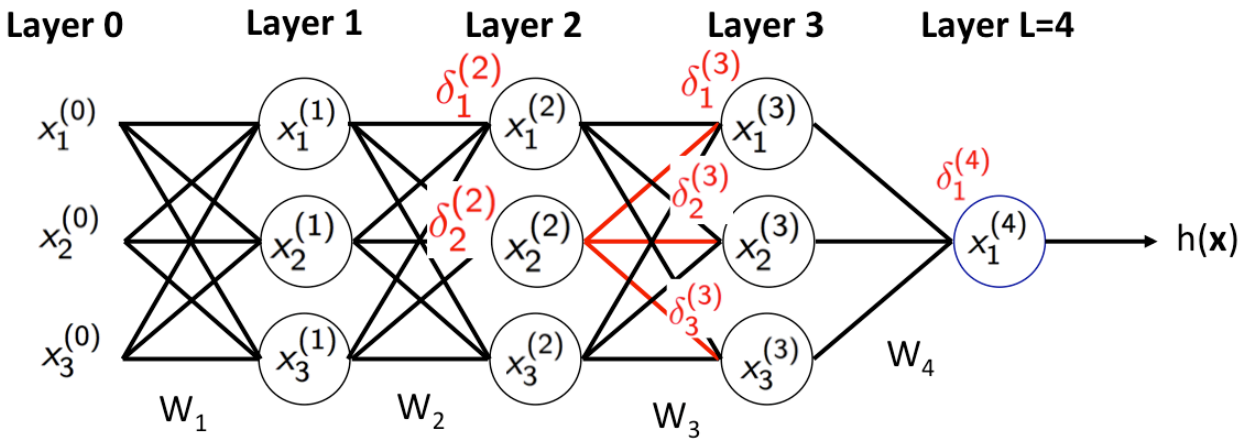
Backward propagation



$$\delta_1^{(2)} = (1 - (x_1^{(2)})^2) \sum_{j=1}^{3} \delta_j^{(3)} w_{1j}^{(3)}$$

Neural Network

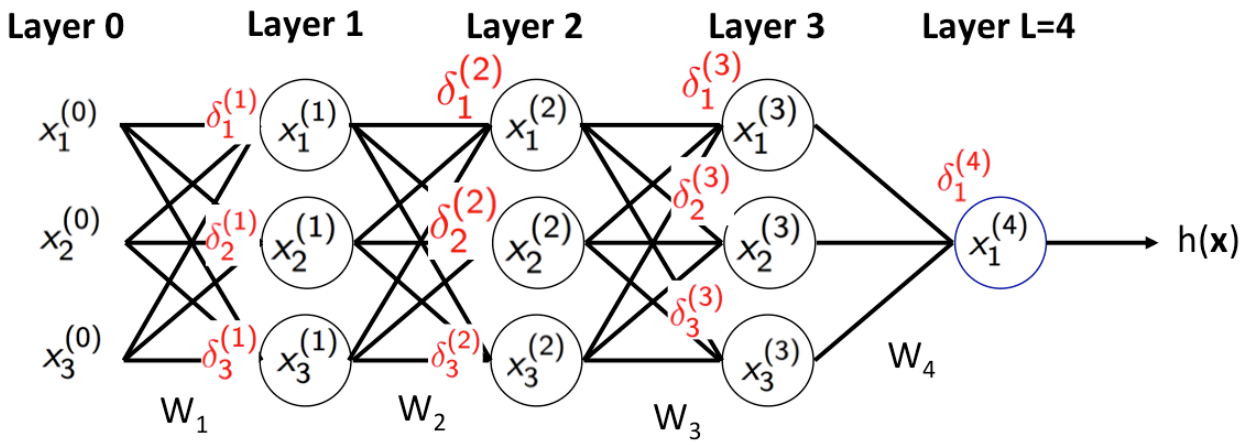
Backward propagation



$$\delta_2^{(2)} = (1 - (x_2^{(2)})^2) \sum_{j=1}^{3} \delta_j^{(3)} w_{2j}^{(3)}$$

Neural Network

Backward propagation

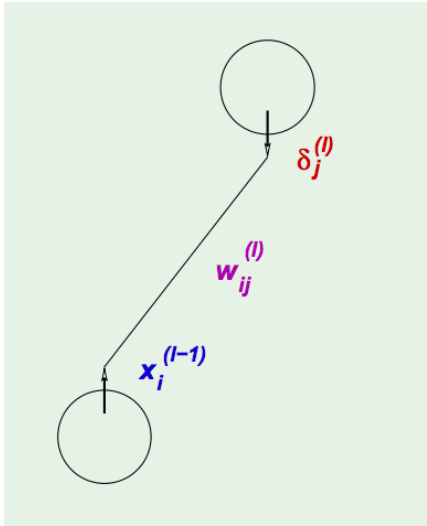


Neural Network

Backpropagation

SGD for neural networks

- Initialize all weights $w_{ij}^{(l)}$ **at random**
- For iter $= 0, 1, 2, \cdots$
  - Forward: Compute all $x_j^{(l)}$ from input to output
  - Backward: Compute all $\delta_j^{(l)}$ from output to input
  - Update all the weights $w_{ij}^l \leftarrow w_{ij}^{(l)} - \eta x_i^{(l-1)} \delta_j^{(l)}$



Neural Network

Backpropagation

- Just an automatic way to apply chain rule to compute gradient
- Auto-differentiation (AD) --- as long as we define derivative for each basic function, we can use AD to compute any of their compositions
- Implemented in most deep learning packages (e.g., pytorch, tensorflow)

Neural Network

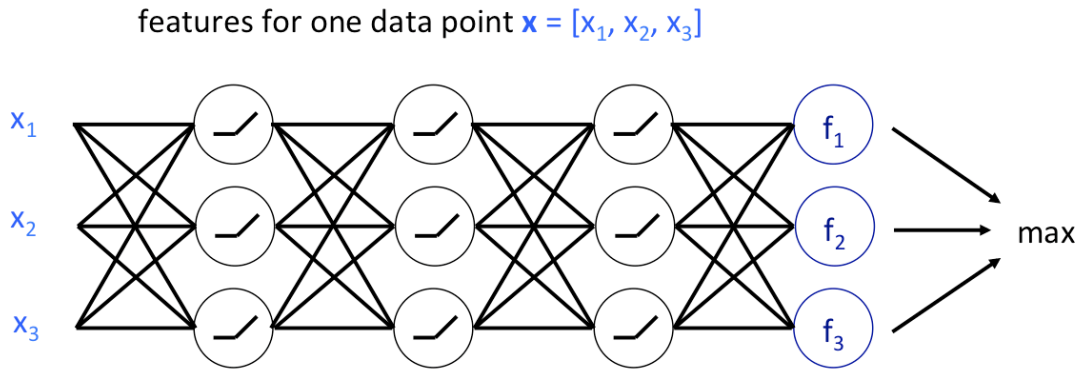
Backpropagation

- Just an automatic way to apply chain rule to compute gradient
- Auto-differentiation (AD) --- as long as we define derivative for each basic function, we can use AD to compute any of their compositions
- Implemented in most deep learning packages (e.g., pytorch, tensorflow)
- Auto-differentiation needs to store all the intermediate nodes of each sample
  - $\Rightarrow$ Memory cost > number of neurons $\times$ batch size
  - $\Rightarrow$ This poses a constraint on the batch size

Neural Network

Multiclass Classification

- K classes: K neurons in the final layer
- Output of each f_i is the score of class i
  - Taking $\arg\max_i f_i(x)$ as the prediction



Neural Network

Multiclass loss

- Softmax function: transform output to probability:
  - $[f_1, \cdots, f_K] \rightarrow [p_i, \cdots, p_K]$
  - Where $p_i = \frac{e^{f_i}}{\sum_{j=1}^{K} e^{f_j}}$
- Cross-entropy loss:
  - $L = -\sum_{i=1}^{K} y_i \log(p_i)$
  - Where y_i is the i-th label