CSE 417T
Introduction to Machine Learning

Lecture 20

Instructor: Chien-Ju (CJ) Ho

Logistics

- Homework 5 is due Apr 19 (Tuesday)

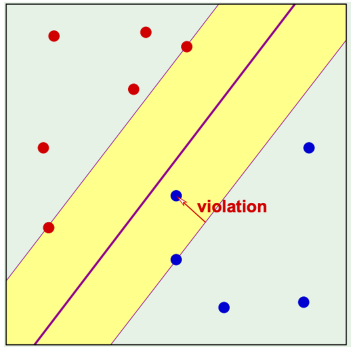
- Exam 2 will be on April 28 (Thursday)
  - Will focus on the topics in the second half of the semester
  - Format / logistics will be similar to Exam 1
  - More details to come

Recap

Support Vector Machines

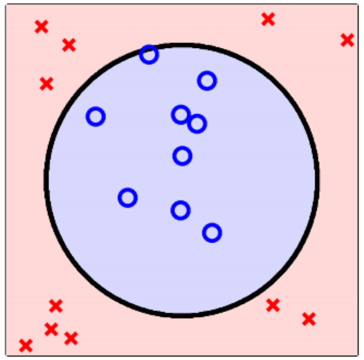
- Soft-margin SVM (approximates hard-margin SVM with $C \to \infty$)

$$\begin{aligned}&\text{minimize}_{\vec{w},b,\vec{\xi}} && \frac{1}{2}\vec{w}^T\vec{w} + C\sum_{n=1}^{N}\xi_n \\ &\text{subject to} && y_n(\vec{w}^T\vec{x}_n + b) \geq 1 - \xi_n, \forall n \\ &&& \xi_n \geq 0, \forall n\end{aligned}$$



- Kernel version of the soft-margin SVM (with Kernel K_Φ)

$$\begin{aligned}&\text{maximize}_{\vec{\alpha}} \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}\alpha_n\alpha_m y_n y_m K_\Phi(\vec{x}_n, \vec{x}_m) \\ &\text{subject to } \sum_{n=1}^{N}\alpha_n y_n = 0 \\ &\qquad\qquad\quad 0 \leq \alpha_n \leq C, \forall n\end{aligned}$$



  - Solve for $\vec{\alpha}^*$ in the kernel SVM using QP

$$\begin{aligned}g(\vec{x}) &= sign({\vec{w}^*}^T\Phi(\vec{x}) + b^*) \\ &= \boldsymbol{sign}\left(\sum_{\alpha_n^*>0}\alpha_n^* y_n K_\Phi(\vec{x}_n, \vec{x}) + b^*\right),\end{aligned}$$

where $b^* = y_m - \sum_{\alpha_n^*>0}\alpha_n^* y_n K_\Phi(\vec{x}_n, \vec{x}_m)$ for some $\alpha_m^* > 0$

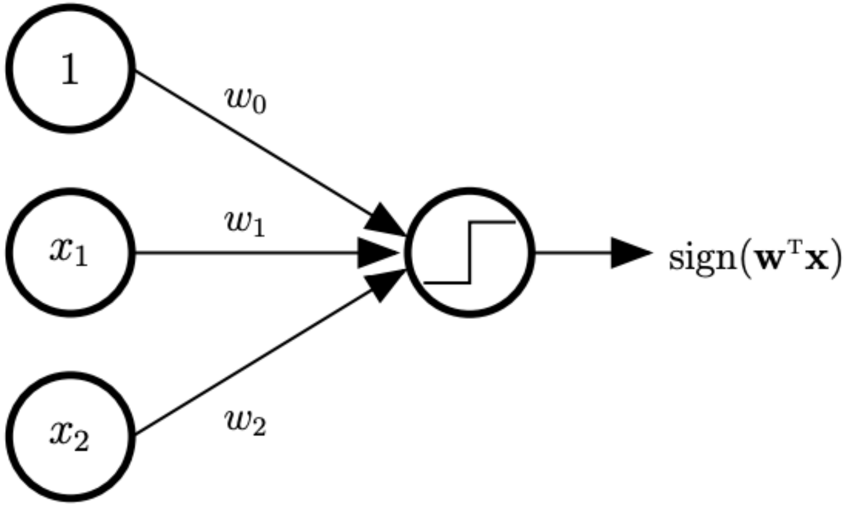
Neural Networks

Perceptron

- A hypothesis in Perceptron

$$h(\vec{x}) = sign(\vec{w}^T \vec{x})$$

- Graphical representation of Perceptron

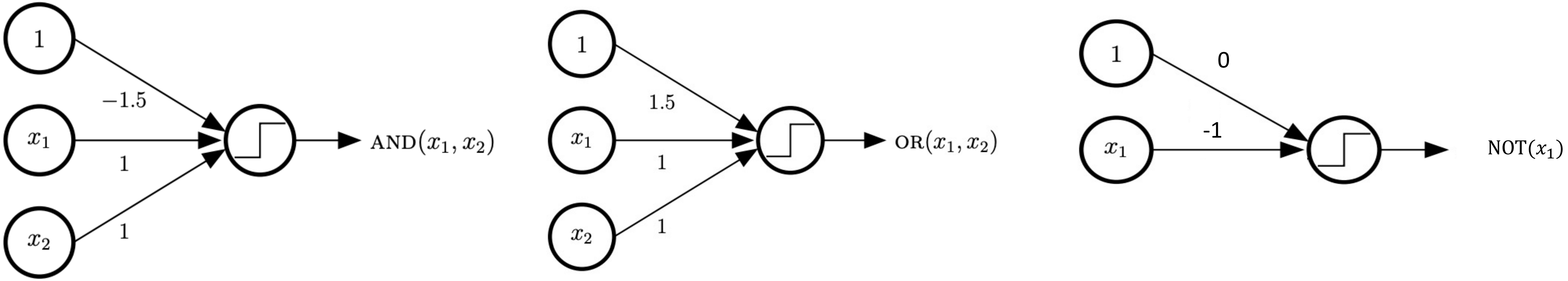


- Notations
  - $\vec{x} = (x_0, x_1, \ldots, x_d)$
  - $\vec{w} = (w_0, w_1, \ldots, w_d)$
  - Linear separator

    $h(\vec{x}) = sign(\vec{w}^T \vec{x})$

Inspired by neurons:
The output signal is triggered when the weighted combination of the inputs is larger than some threshold

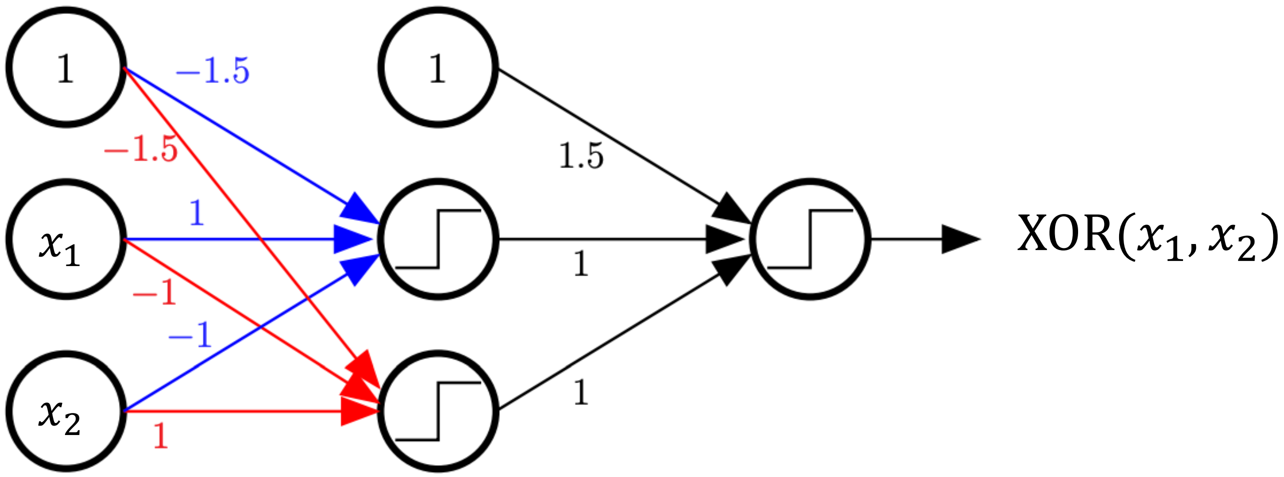
Implementing Logic Gates with Perceptron



Impossible to implement XOR using a single perceptron

Multi-Layer Perceptron

- $\text{XOR}(x_1, x_2) \rightarrow x_1\bar{x}_2 + \bar{x}_1 x_2$



- Note: you are asked to create a neural network with one hidden layer that implements $\text{XOR}(\text{AND}\,(x_1, x_2), x_3)$ in HW5
  - Hint: Try to operate the Boolean algebra first
  - Using sign as the activation function would make sense

Universal Approximation Theorem

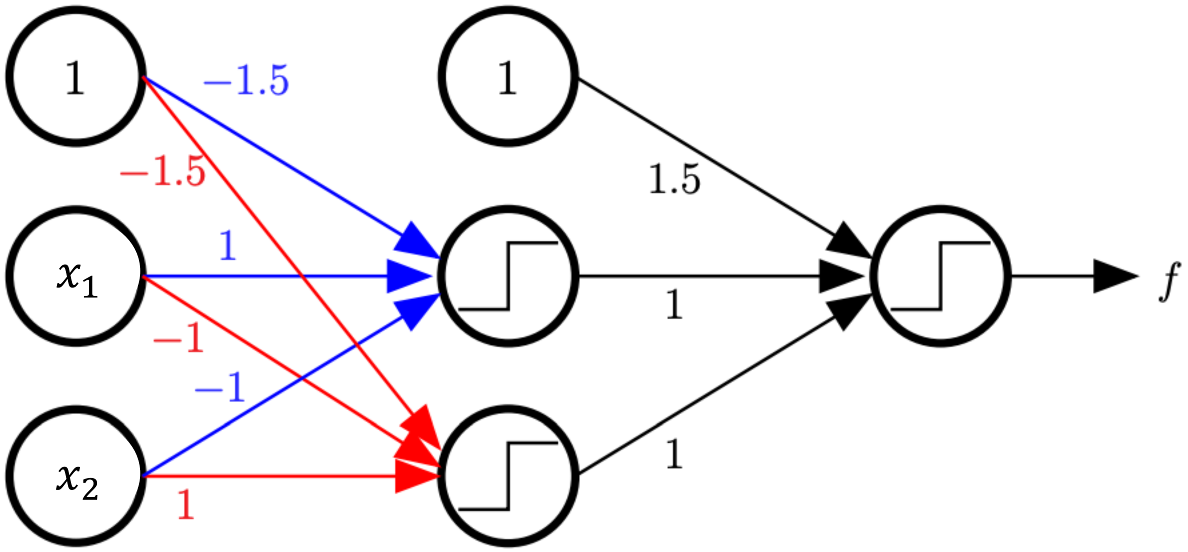
- A feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of $\mathbb{R}^n$, under mild assumptions on the activation function.

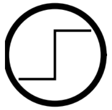
- Three-layer MLP can approximate ANY continuous target function!

- What about overfitting?
  - We'll talk about regularization methods in the next lecture

Learn MLP From Data?

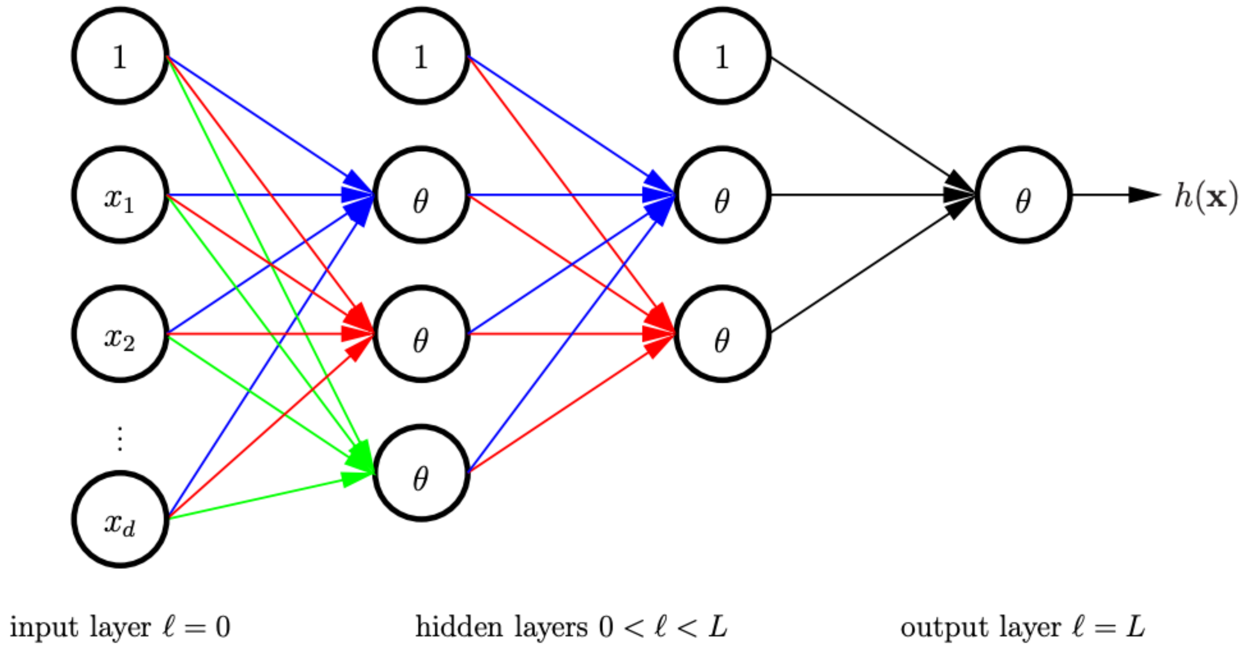
- Given D and the network structure, how to learn the "weights" (i.e., the weight vectors of every Perceptron)?



- Computationally challenging due to the "sign" function 

Neural Networks

- A softened version of multi-layer Perceptron (MLP)



θ: activation function

(Specify the "activation" of the neuron)

(The activation function in the output layer is often separately considered)

Today’s Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.

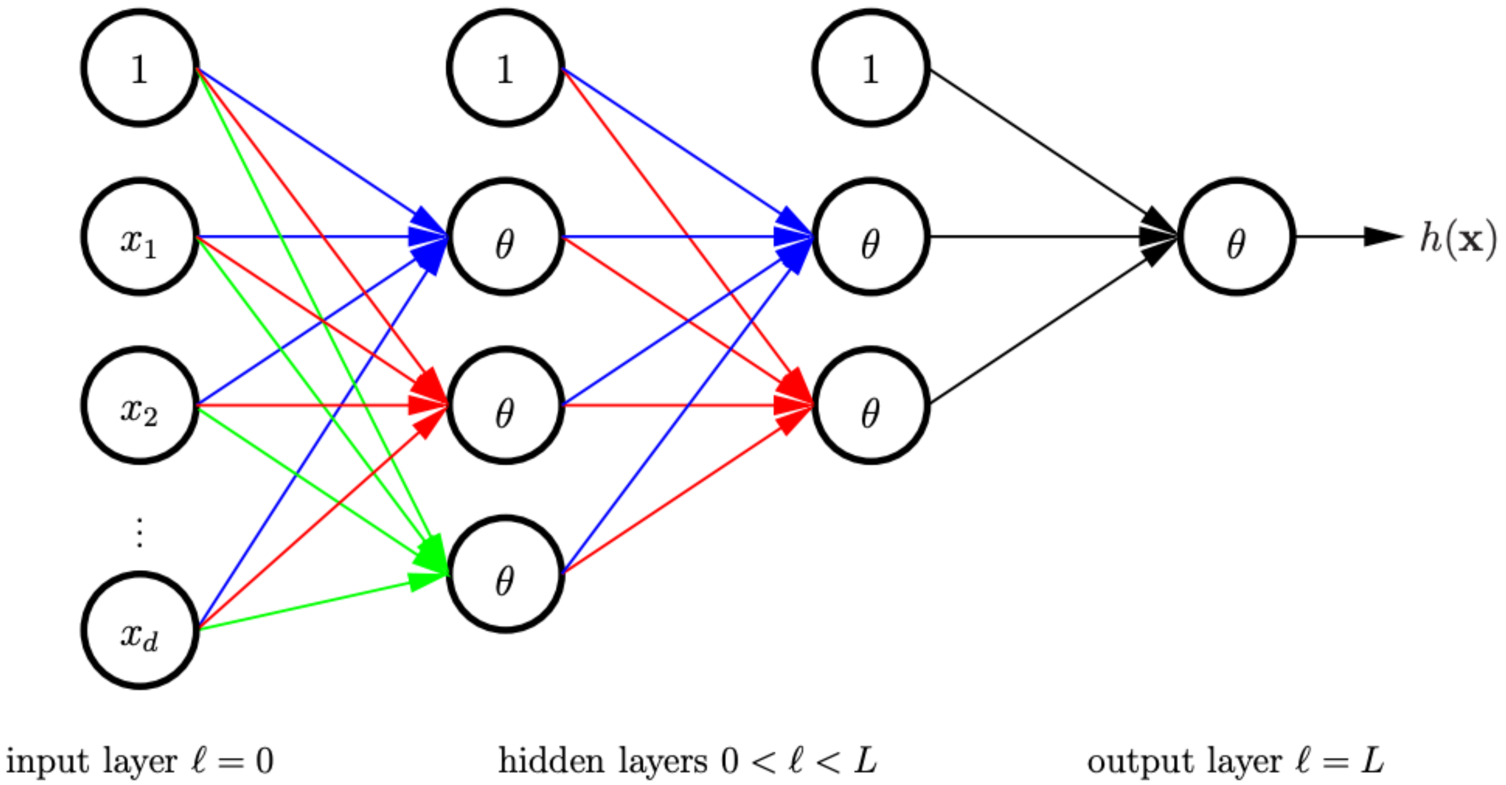
Let me know if you spot errors.

Goal of Today

- Formally characterize Neural Networks (introduce notations)
- Given a Neural Network hypothesis h, how do we make prediction $h(\vec{x})$
- Given D, how do we learn a Neural Network hypothesis

Notations of Neural Networks (NN)

Neural Networks

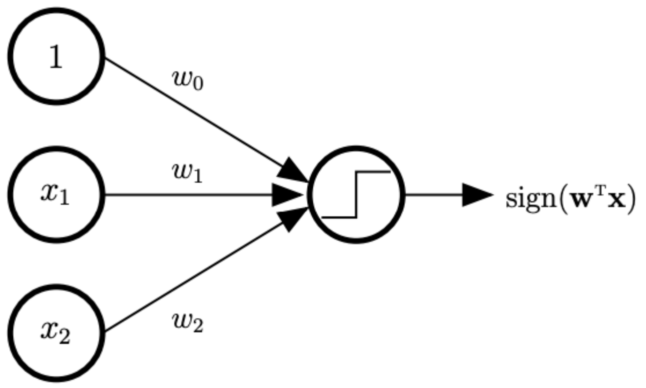


θ: activation function

(Specify the “activation” of the neuron)

We mostly focus on feed-forward network structure

Activation Function



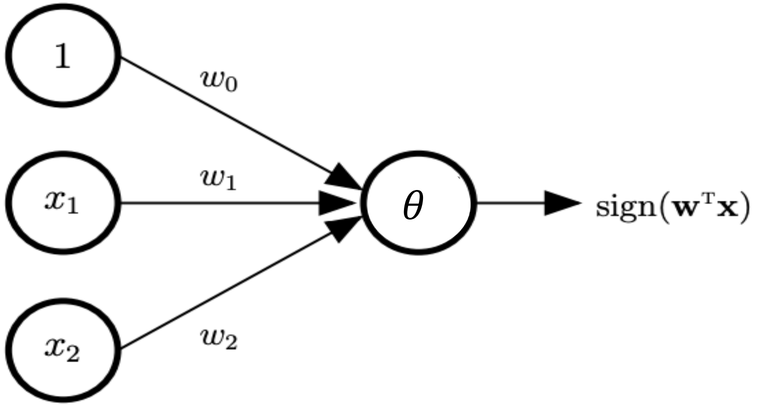
- Think about a single neuron (linear model)
  - Compute the linear signal $s = \vec{w}^T\vec{x}$
  - Transform it to what we need in the output (sign, linear, or sigmoid)

	Domain	Model
Linear Classification	$y \in \{-1, +1\}$	$H = \{h(\vec{x}) = sign(\vec{w}^T\vec{x})\}$
Linear Regression	$y \in \mathbb{R}$	$H = \{h(\vec{x}) = \vec{w}^T\vec{x}\}$
Logistic Regression	$y \in [0,1]$	$H = \{h(\vec{x}) = \theta(\vec{w}^T\vec{x})\}$

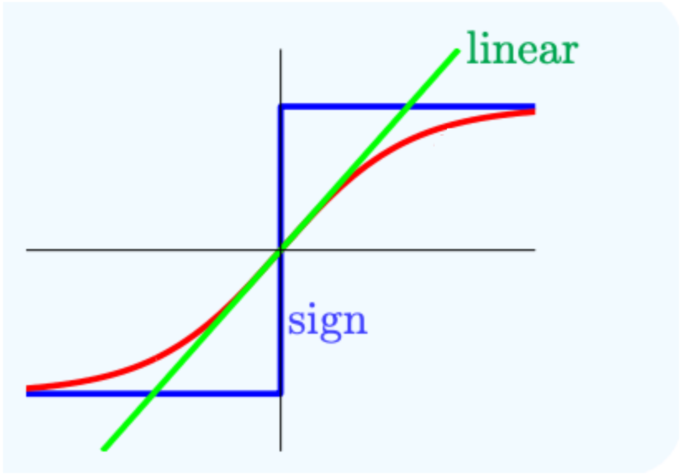
$$\theta(s) = \frac{e^s}{1 + e^s}$$

- In Neural networks, outputs of some nodes are inputs of some others
  - Activation function decides how to do this transformation

Activation Function



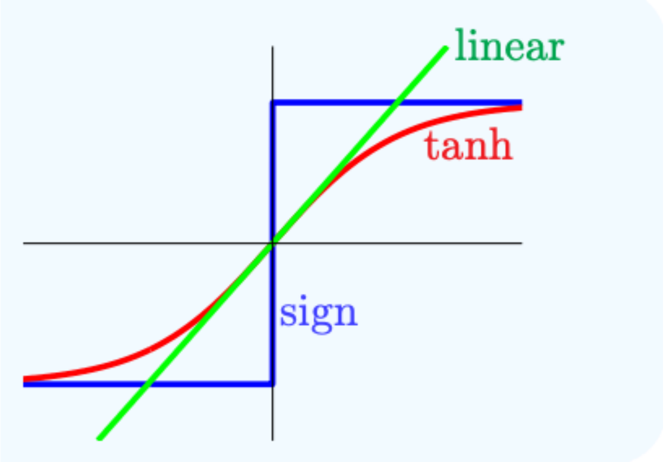
- Activation functions in Neural Networks
  - sign function:
    - hard to optimize
  - linear function:
    - the entire neural network is linear
  - One potential option: having a “softened” version of sign function



Activation Function

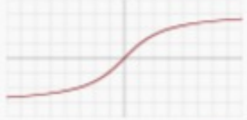
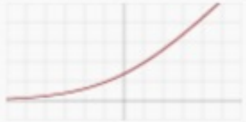
- Activation functions in Neural Networks
  - sign function: hard to optimize
  - linear function: the entire neural network is linear
  - tanh: a softened version of sign
    - $\tanh(s) = \frac{e^{s}-e^{-s}}{e^{s}+e^{-s}}$

- Examine $\tanh(s)$
  - $\tanh(s) = \begin{cases} 1 \text{ when } s \to \infty \\ 0 \text{ when } s = 0 \\ -1 \text{ when } s \to \infty \end{cases}$
  - For $\theta(s) = \tanh(s)$, $\theta'(s) = 1 - \theta(s)^2$



Activation Function

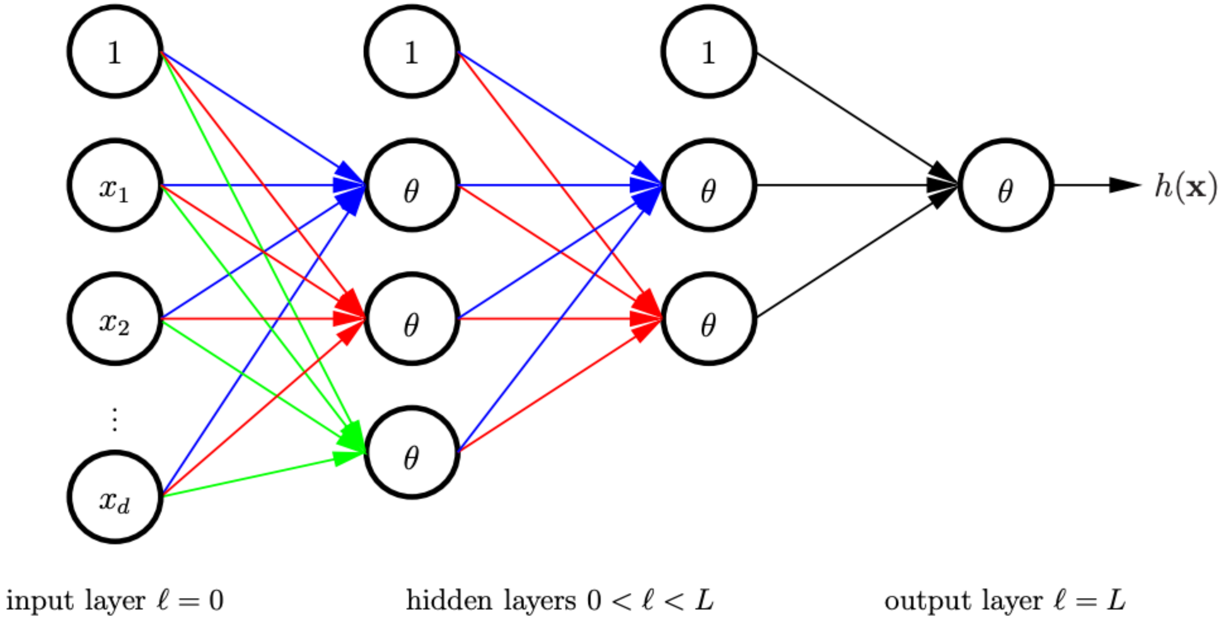
- There are other activation functions with different benefits. However, it doesn't impact our discussions, and we'll focus on $\tanh()$ as the activation function
- A few more examples

ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1+e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$

https://towardsdatascience.com/activation-functions-neural-networks-1cbd9f8d91d6

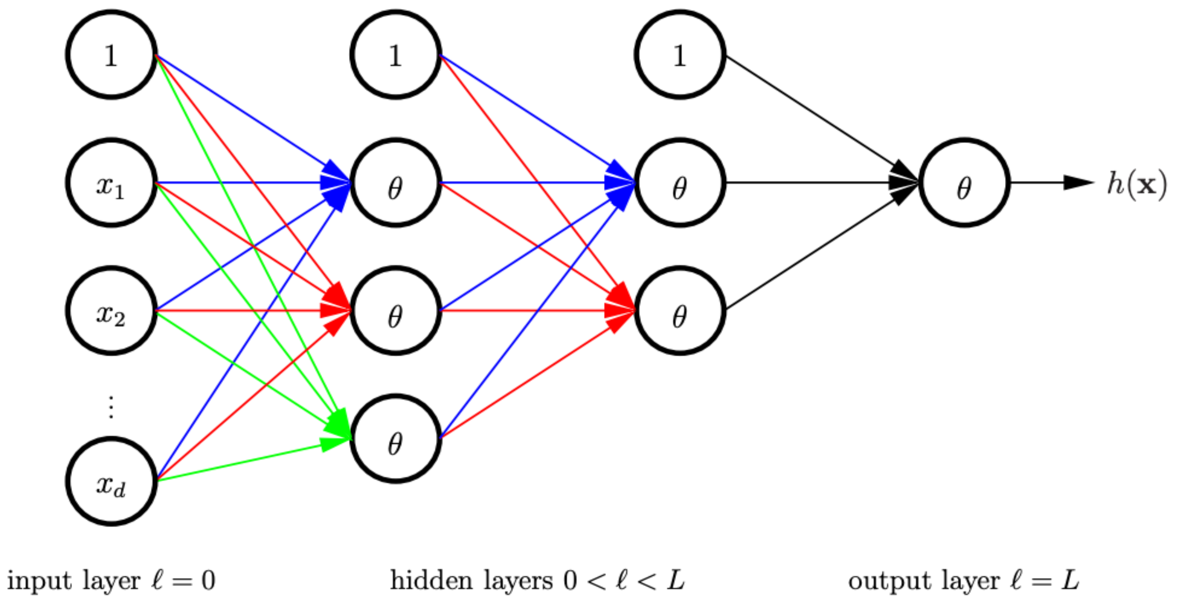
Notations of Neural Networks (NN)

- Layers $\ell = 0$ to L
  - Layer 0: input layer
  - Layer 1 to $L - 1$: hidden layers
  - Layer L: output layer
- $d^{(\ell)}$: dimension of layer ℓ
  - # nodes (excluding 1s) in the layer
- $\vec{x}^{(\ell)}$: the nodes in layer ℓ
  - $\vec{x}^{(0)}$ is the input feature $\vec{x}$
  - $x_i^{(\ell)}$ is the i-th node in layer ℓ



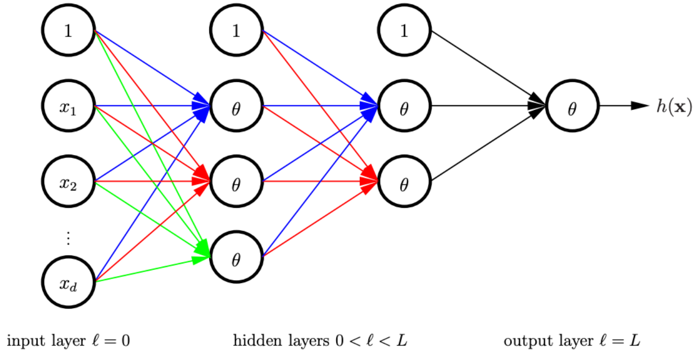
Notations of Neural Networks (NN)

- A hypothesis in linear model is specified by the weights $\{w_i\}$
- Similarly, a hypothesis in NN is characterized by the weights $\{w_{i,j}^{(\ell)}\}$
  - $1 \leq \ell \leq L$ layers
  - $0 \leq i \leq d^{(\ell-1)}$ inputs
  - $1 \leq j \leq d^{(\ell)}$ outputs



Notations of Neural Networks (NN)

- Notations so far:
  - $d^{(\ell)}$: dimension of layer ℓ
  - $\vec{x}^{(\ell)}$: the nodes in layer ℓ
  - $w_{i,j}^{(\ell)}$: weights; characterize hypothesis in NN



- Lastly, linear signal $s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{i,j}^{(\ell)} x_i^{(\ell-1)}$
  - By definition: $x_j^{(\ell)} = \theta\left(s_j^{\ell}\right)$

$$\mathbf{s}^{(\ell)} \xrightarrow{\quad\theta\quad} \mathbf{x}^{(\ell)}$$

Notations of Neural Networks (NN)

- Notations so far:
  - $d^{(\ell)}$: dimension of layer ℓ
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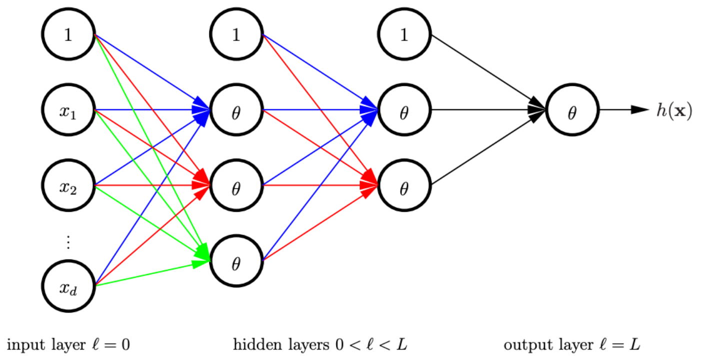

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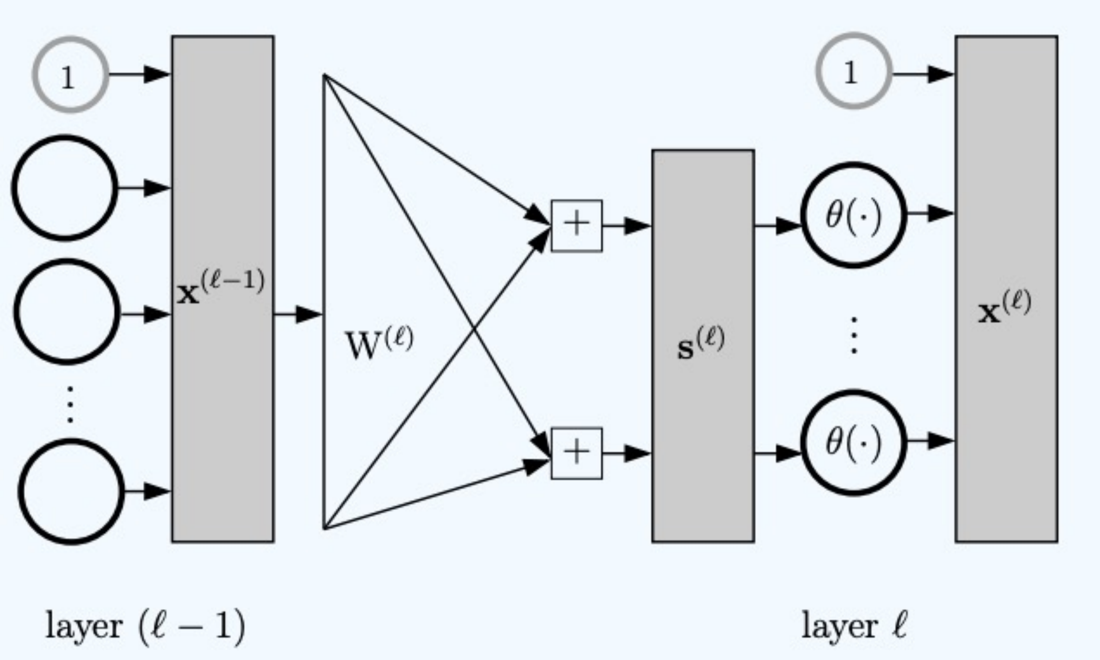
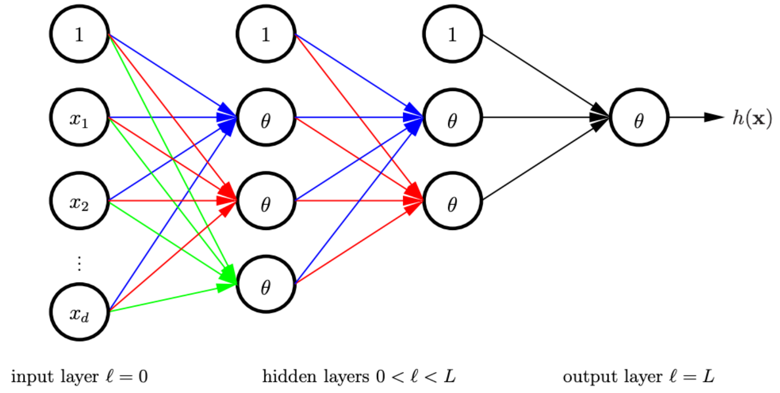


Short Break and Q&A

Practice:

For a neural network with $L = 2$, $d^{(0)} = 3$, $d^{(1)} = 2$, $d^{(2)} = 1$, what is the total # weights?



Notations so far:

$d^{(\ell)}$: dimension of layer ℓ

$\vec{x}^{(\ell)}$: the nodes in layer ℓ

$w_{i,j}^{(\ell)}$: weights; characterize hypothesis in NN

$s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{i,j}^{(\ell)} x_i^{(\ell-1)}$: linear signal

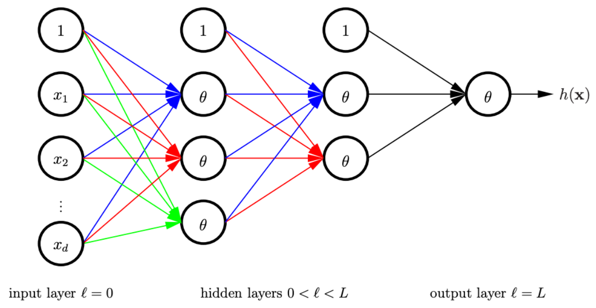
Forward Propagation

Given a NN hypothesis and a point $\vec{x}$, how do we make predictions

Backpropagation

Learn a Neural Network hypothesis from data

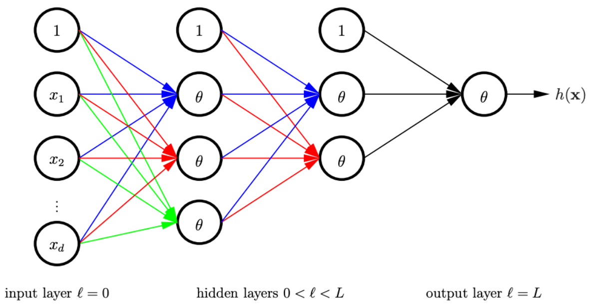
Forward Propagation



- A Neural network hypothesis h is characterized by $\left\{w_{i,j}^{(\ell)}\right\}$
- How to evaluate $h(\vec{x})$?

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{\mathrm{W}^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{\mathrm{W}^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \cdots \xrightarrow{\mathrm{W}^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

Forward Propagation



- A Neural network hypothesis h is characterized by $\left\{w_{i,j}^{(\ell)}\right\}$
- How to evaluate $h(\vec{x})$?

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{\mathrm{W}^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{\mathrm{W}^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \cdots \xrightarrow{\mathrm{W}^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

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

```
x^(0) ← x                                   [Initialization]
for ℓ = 1 to L do                           [Forward Propagation]
    s^(ℓ) ← (W^(ℓ))^T x^(ℓ−1)
    x^(ℓ) ← [ 1 ; θ(s^(ℓ)) ]
end for
h(x) = x^(L)                                [Output]
```

$$\mathbf{x}^{(0)} \leftarrow \mathbf{x} \qquad \text{[Initialization]}$$
$$\text{for } \ell = 1 \text{ to } L \text{ do} \qquad \text{[Forward Propagation]}$$
$$\mathbf{s}^{(\ell)} \leftarrow (\mathrm{W}^{(\ell)})^{\mathrm{T}} \mathbf{x}^{(\ell-1)}$$
$$\mathbf{x}^{(\ell)} \leftarrow \begin{bmatrix} 1 \\ \theta(\mathbf{s}^{(\ell)}) \end{bmatrix}$$
$$\text{end for}$$
$$h(\mathbf{x}) = \mathbf{x}^{(L)} \qquad \text{[Output]}$$

Given weights $w_{i,j}^{(\ell)}$ and $\vec{x}^{(0)} = \vec{x}$, we can calculate all $\vec{x}^{(\ell)}$ and $\vec{s}^{(\ell)}$ through forward propagation.

How to Learn NN From Data?

- Given D, how to learn the weights $W = \left\{w_{i,j}^{(\ell)}\right\}$?
- Intuition: Minimize $E_{in}(W) = \frac{1}{N}\sum_{n=1}^{N} e_n(W)$
- How?
  - Gradient descent: $W(t+1) \leftarrow W(t) - \eta \nabla_W E_{in}(W)$
  - Stochastic gradient descent $W(t+1) \leftarrow W(t) - \eta \nabla_W e_n(W)$
- Key step: we need to be able to evaluate the gradient…
  - Not trivial to do given the network structure
  - Backpropagation is an algorithmic procedure to calculate the gradient

Backpropagation

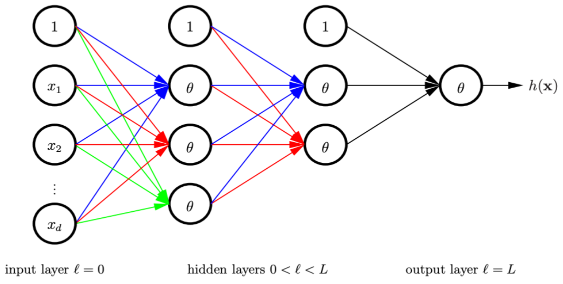
Use dynamic programming to evaluate the gradient

Quick Reminders on Dynamic Programming

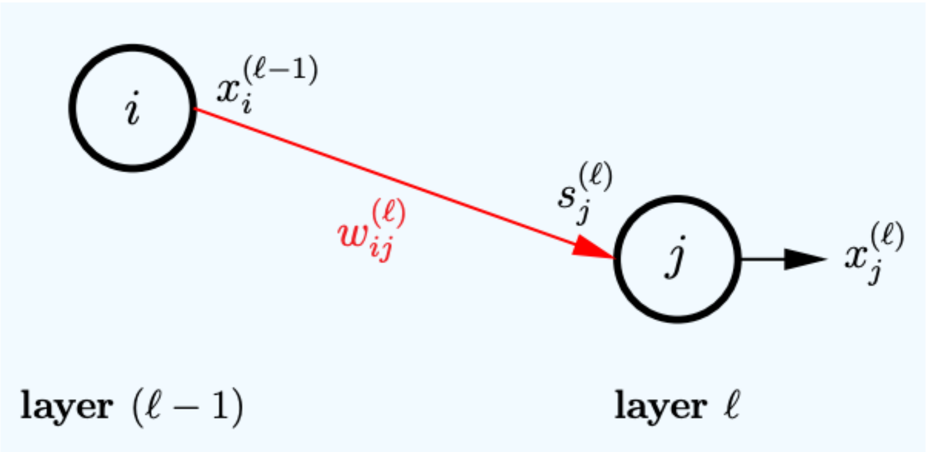
- Example: Fibonacci number
  - $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$
  - $F_0 = 0, F_1 = 1$
  - To evaluate F_N
    - Recursively apply the definition
      - Wasted computation
    - Dynamic programming: evaluate and store $F_0, F_1, \ldots, F_N$
      - Use space to exchange for time

- Key step in backpropagation
  - Find a recursive definition of some key quantities
  - Solve the boundary conditions
  - Adopt dynamic programming

Compute the Gradient $\nabla_W e_n(W)$



- To evaluate $\nabla_W e_n(W)$, we need to calculate $\frac{\partial e_n(W)}{\partial w_{i,j}^{(\ell)}}$ for all (i, j, ℓ)
- Zoom in on the region around $w_{i,j}^{(\ell)}$



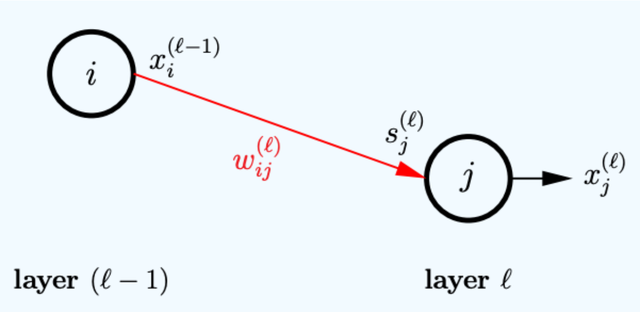
- Apply chain rule

$$\frac{\partial e_n(W)}{\partial w_{i,j}^{(\ell)}} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}} \frac{\partial s_j^{(\ell)}}{\partial w_{i,j}^{(\ell)}}$$

Compute the Gradient $\nabla_W e_n(W)$

- Apply chain rule

$$\frac{\partial e_n(W)}{\partial w_{i,j}^{(\ell)}} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}} \frac{\partial s_j^{(\ell)}}{\partial w_{i,j}^{(\ell)}}$$



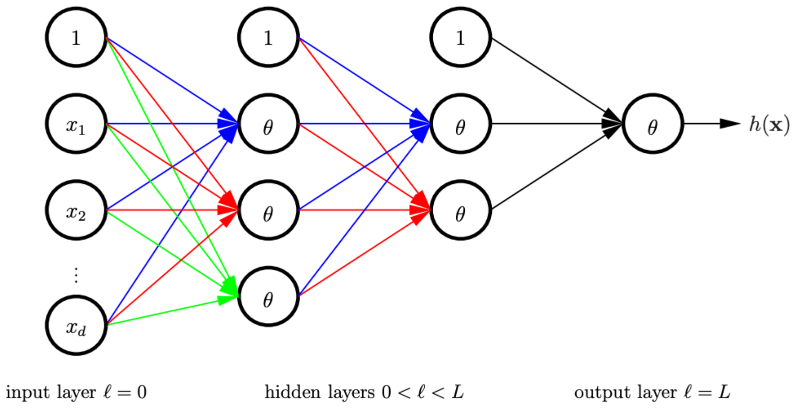
- Let's look at the second term first
  - Remember $s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{i,j}^{(\ell)} x_i^{(\ell-1)}$
  - Therefore, $\frac{\partial s_j^{(\ell)}}{\partial w_{i,j}^{(\ell)}} = x_i^{(\ell-1)}$

- What about the first term?
  - Let's define $\delta_j^{(\ell)} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}}$
  - We'll apply dynamic programming style algorithm to deal with this term

- To sum up

$$\boxed{\frac{\partial e_n(W)}{\partial w_{i,j}^{(\ell)}} = \delta_j^{(\ell)} x_i^{(\ell-1)}}$$

Compute $\delta_j^{(\ell)} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}}$

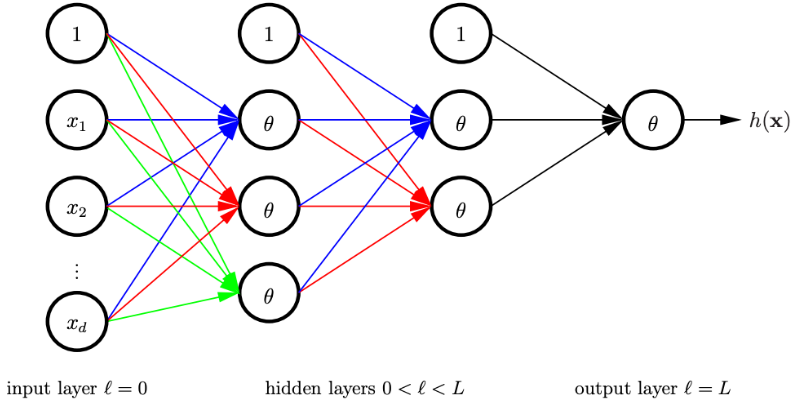


- Using dynamic programming style approach
  - Check boundary case (what is the boundary case?)
  - Write the recursive formulation

- Check boundary case (when $\ell = L$)
  - Output layer
  - For simplicity, assume we are doing regression and the error is squared error
    - $e_n(W) = \left(s_1^{(L)} - y_n\right)^2$ (Usually only one node in the output layer)
  - $\delta_1^{(L)} = 2(s_1^{(L)} - y_n)$ (similar discussion applies for other differentiable error function)

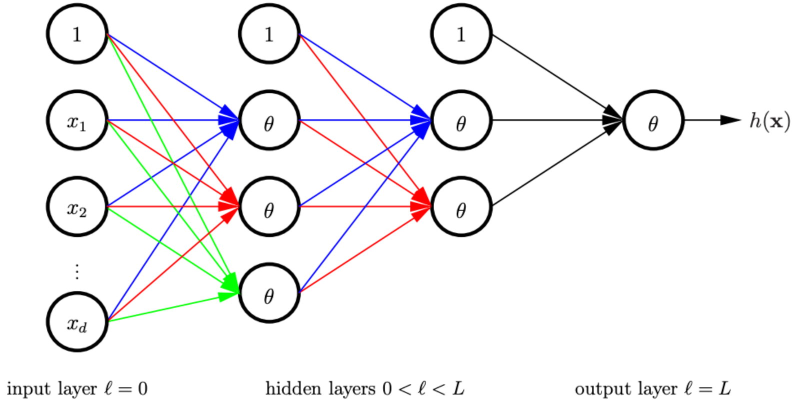
  - So the boundary condition at L is checked.
  - Next we will derive the backward recursive formulation (hence, backpropagation)

Compute $\delta_j^{(\ell)} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}}$



- Zoom in to see the chain of dependencies

Compute $\delta_j^{(\ell)} = \dfrac{\partial e_n(W)}{\partial s_j^{(\ell)}}$



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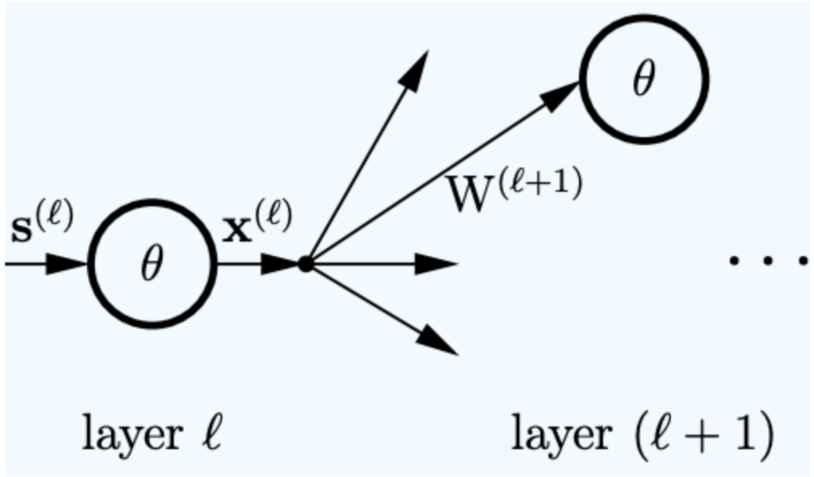
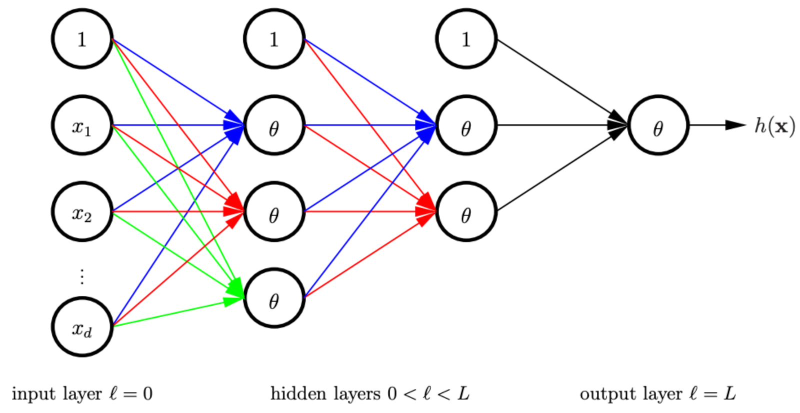


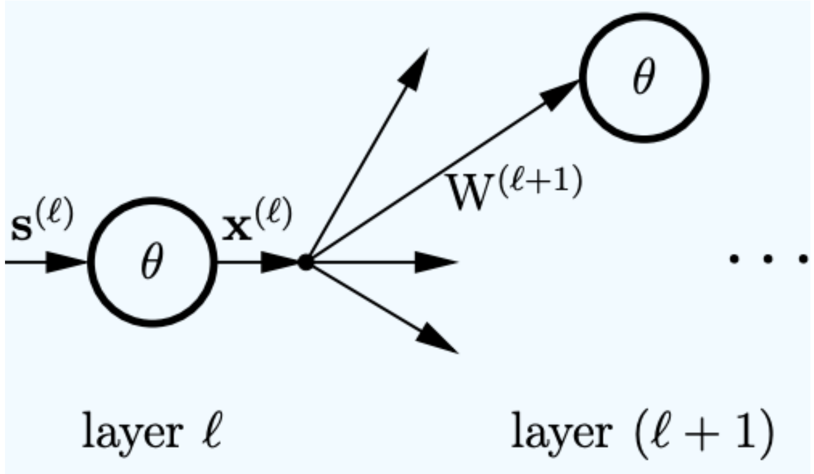
$$\mathbf{s}^{(\ell)} \longrightarrow \mathbf{x}^{(\ell)} \longrightarrow \mathbf{s}^{(\ell+1)}$$

Compute $\delta_j^{(\ell)} = \dfrac{\partial e_n(W)}{\partial s_j^{(\ell)}}$



- Zoom in to see the chain of dependencies

For $\theta(s) = \tanh(s)$,
$\theta'(s) = 1 - \theta(s)^2$



$$\mathbf{s}^{(\ell)} \longrightarrow \mathbf{x}^{(\ell)} \longrightarrow \mathbf{s}^{(\ell+1)}$$

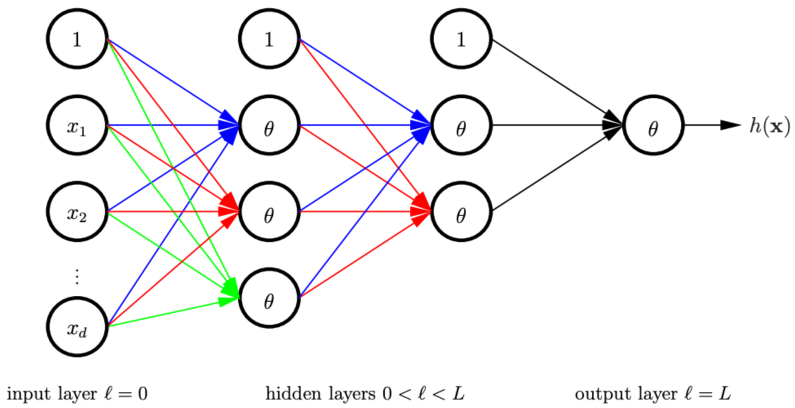
$$\delta_j^{(\ell)} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}}$$

$$= \sum_{k=1}^{d^{(\ell+1)}} \frac{\partial e_n(W)}{\partial s_k^{(\ell+1)}} \frac{\partial s_k^{(\ell+1)}}{\partial x_j^{(\ell)}} \frac{\partial x_j^{(\ell)}}{\partial s_j^{(\ell)}}$$

$$= \sum_{k=1}^{d^{(\ell+1)}} \delta_k^{(\ell+1)} w_{j,k}^{(\ell+1)} \theta'\left(s_j^{(\ell)}\right)$$

We have the backward recurve definition!

Compute $\delta_j^{(\ell)} = \dfrac{\partial e_n(W)}{\partial s_j^{(\ell)}}$



- We can calculate $\delta_j^{(\ell)}$ in a dynamic programming manner:

- Boundary condition: $\delta_1^{(L)} = 2(s_1^{(L)} - y_n)$
- Recursive formulation: $\delta_j^{(\ell)} = \sum_{k=1}^{d^{(\ell+1)}} \delta_k^{(\ell+1)} w_{j,k}^{(\ell+1)} \theta'\left(s_j^{(\ell)}\right)$

- Calculate $\delta_j^{(\ell)}$ for $\ell < L$ in a backward manner

Backpropagation Algorithm

- Recall that $\frac{\partial e_n(W)}{\partial w_{i,j}^{(\ell)}} = \delta_j^{(\ell)} x_i^{(\ell-1)}$
- Backpropagation Algorithm
  - Initialize $w_{i,j}^{(\ell)}$ randomly [You will discuss the impacts of initialization in HW5]
  - For $t = 1$ to T
    - Randomly pick a point from D (for stochastic gradient descent)
    - Forward propagation: Calculate all $x_i^{(\ell)}$ and $s_i^{(\ell)}$
    - Backward propagation: Calculate all $\delta_j^{(\ell)}$
    - Update the weights $w_{i,j}^{(\ell)} \leftarrow w_{i,j}^{(\ell)} - \eta \delta_j^{(\ell)} x_i^{(\ell-1)}$
  - Return the weights

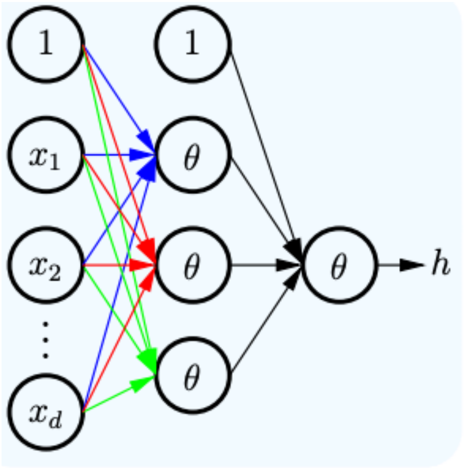
Discussion

- Backpropagation is gradient descent with efficient gradient computation
- Note that the E_{in} is not convex in weights
- Gradient descent doesn’t guarantee to converge to global optimal

- Common approaches:
  - Run it many times
  - Each with a different initialization (the choice of initialization matters)
    - Initialization matters (more discussion next lecture)
    - Initializing at 0 is not a good choice (Q6b of HW5)
    - Initializing at larger weights is not a good idea for tanh as activation function (Q6a of HW5)

Single Hidden-Layer Neural Network

- How do we write a hypothesis in single-hidden layer mathematically?
  - $h(\vec{x}) = \theta\left(w_{0,1}^{(2)} + \sum_{j=1}^{d^{(1)}} w_{j,1}^{(2)} x_j^{(1)}\right)$
    $= \theta\left(w_{0,1}^{(2)} + \sum_{j=1}^{d^{(1)}} w_{j,1}^{(2)} \theta\left(\sum_{i=0}^{d^{(0)}} w_{i,j}^{(1)} x_i\right)\right)$



- How do we write a Kernel SVM hypothesis (linear model with nonlinear transformation)
  - $g(\vec{x}) = \theta\left(b^* + \sum_{\alpha_n^*>0} \alpha_n^* y_n K(\vec{x}_n, \vec{x})\right)$

- Interpretation:
  - The hidden layer is like "feature transform"
  - Shallow learning vs. deep learning
  - More discussion on neural networks and deep learning next lecture