

CSE 417T

Introduction to Machine Learning

Lecture 20

Instructor: Chien-Ju (CJ) Ho

Logistics

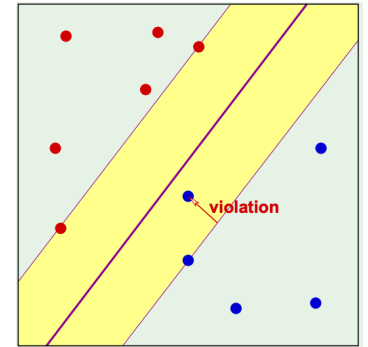
- Homework 5 is due December 2 (Friday)
- Exam 2 will be on December 8 (Thursday)
 - Topics
 - The focus is on the topics in the second half of the semester, starting from decision trees
 - Knowledge is cumulative, so you are still assumed to know the key concepts earlier
 - Format / logistics will be similar to what we did in Exam 1
 - More details to come

Recap

Support Vector Machines

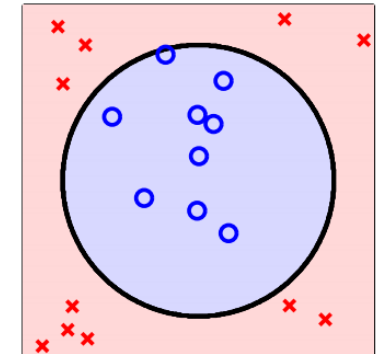
- Soft-margin SVM (approximates hard-margin SVM with $C \rightarrow \infty$)

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



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

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



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

$$\begin{aligned} g(\vec{x}) &= \text{sign}(\vec{w}^{*T} \Phi(\vec{x}) + b^*) \\ &= \text{sign}(\sum_{\alpha_n^* > 0} \alpha_n^* y_n K_\Phi(\vec{x}_n, \vec{x}) + b^*), \\ &\quad \text{where } b^* = y_m - \sum_{\alpha_n^* > 0} \alpha_n^* y_n K_\Phi(\vec{x}_n, \vec{x}_m) \text{ for some } \alpha_m^* > 0 \end{aligned}$$

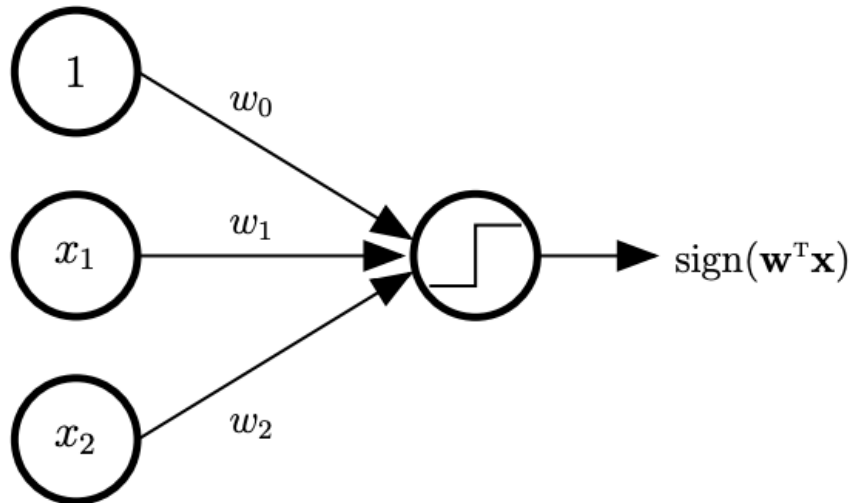
Neural Networks

Perceptron

- A hypothesis in Perceptron

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

- Graphical representation of Perceptron



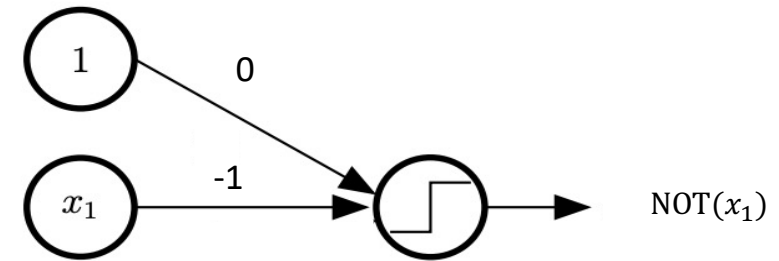
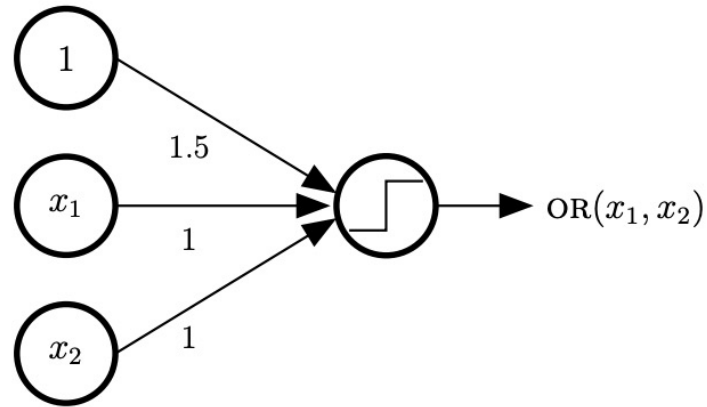
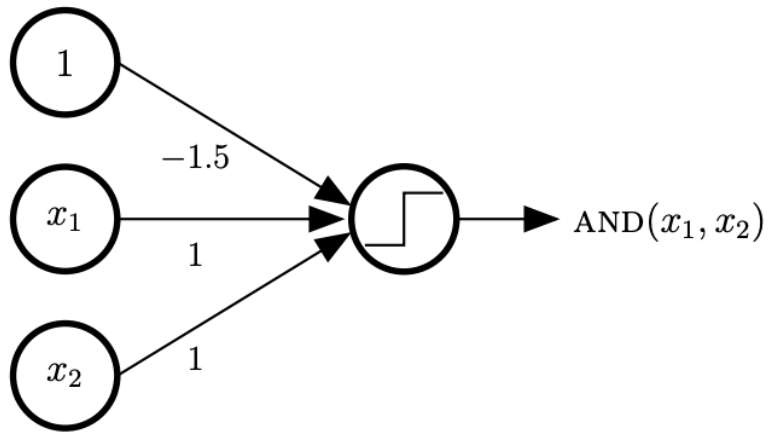
- Notations

- $\vec{x} = (x_0, x_1, \dots, x_d)$
- $\vec{w} = (w_0, w_1, \dots, w_d)$
- Linear separator
 $h(\vec{x}) = \text{sign}(\vec{w}^T \vec{x})$

Inspired by [neurons](#):

The output signal is triggered when the weighted combination of the inputs is larger than some threshold

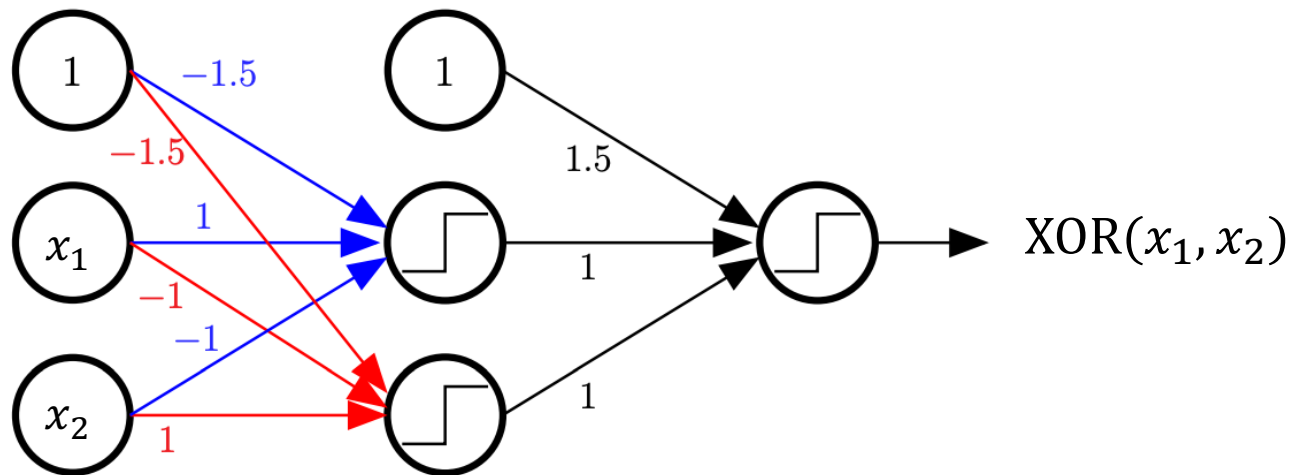
Implementing Logic Gates with Perceptron



Impossible to implement XOR using a single perceptron

Multi-Layer Perceptron

- $\text{XOR}(x_1, x_2) \rightarrow x_1\bar{x}_2 + \bar{x}_1x_2$



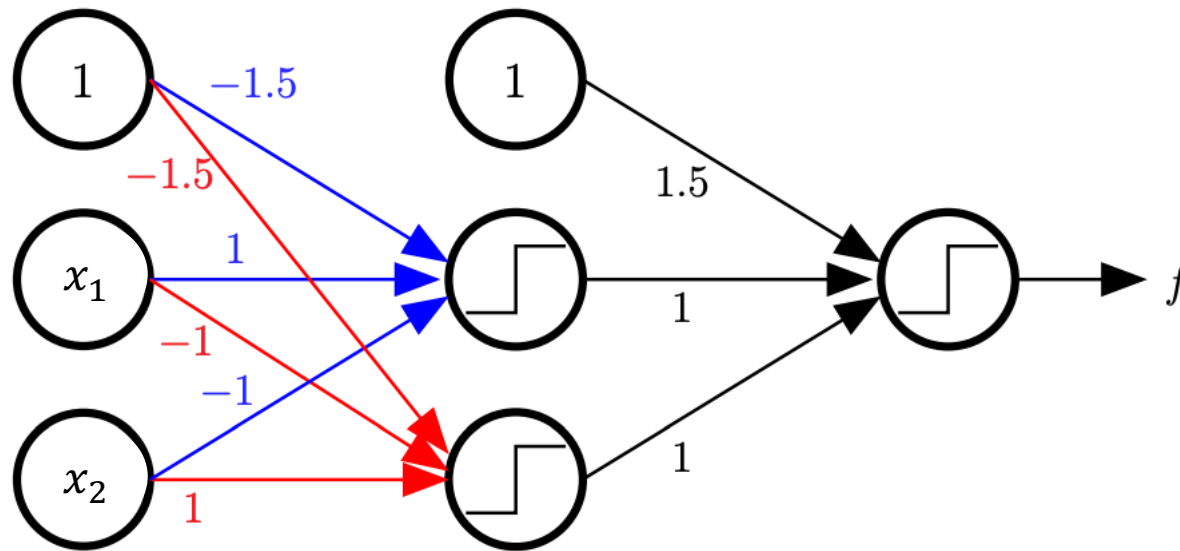
- Note: you are asked to create a neural network with one hidden layer that implements $\text{XOR}(\text{AND}(x_1, x_2), x_3)$ in HW5
- Hint: Try to operate the Boolean algebra first (e.g., applying De Morgan's laws)
 - Using **sign** as the activation function would make sense

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**.
- Single-hidden-layer MLP can **approximate ANY continuous target function!**
- What about overfitting?
 - We'll discuss regularization methods later

Learn MLP From Data?

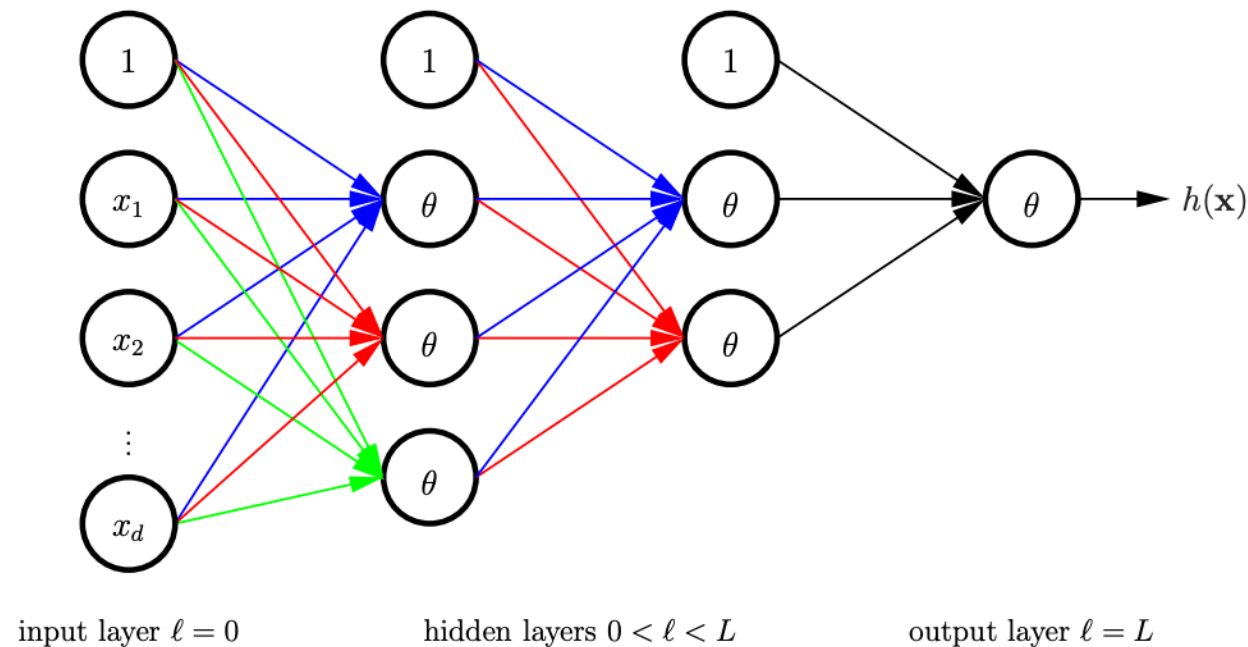
- Given D and the network structure, how to learn the “weights” (i.e., the weight vectors of every Perceptron)?



- 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)

Activation Function

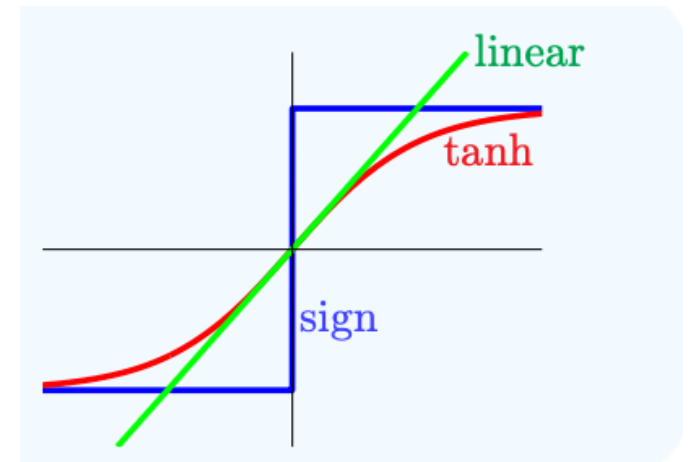
- Activation functions in Neural Networks
 - sign function: hard to optimize
 - linear function: the entire neural network is linear
 - tanh: a softened version of sign

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

- Examine $\tanh(s)$

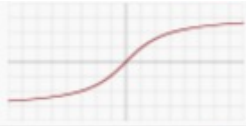




- $\tanh(s) = \begin{cases} 1 & \text{when } s \rightarrow \infty \\ 0 & \text{when } s = 0 \\ -1 & \text{when } s \rightarrow -\infty \end{cases}$

- 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		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$

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.

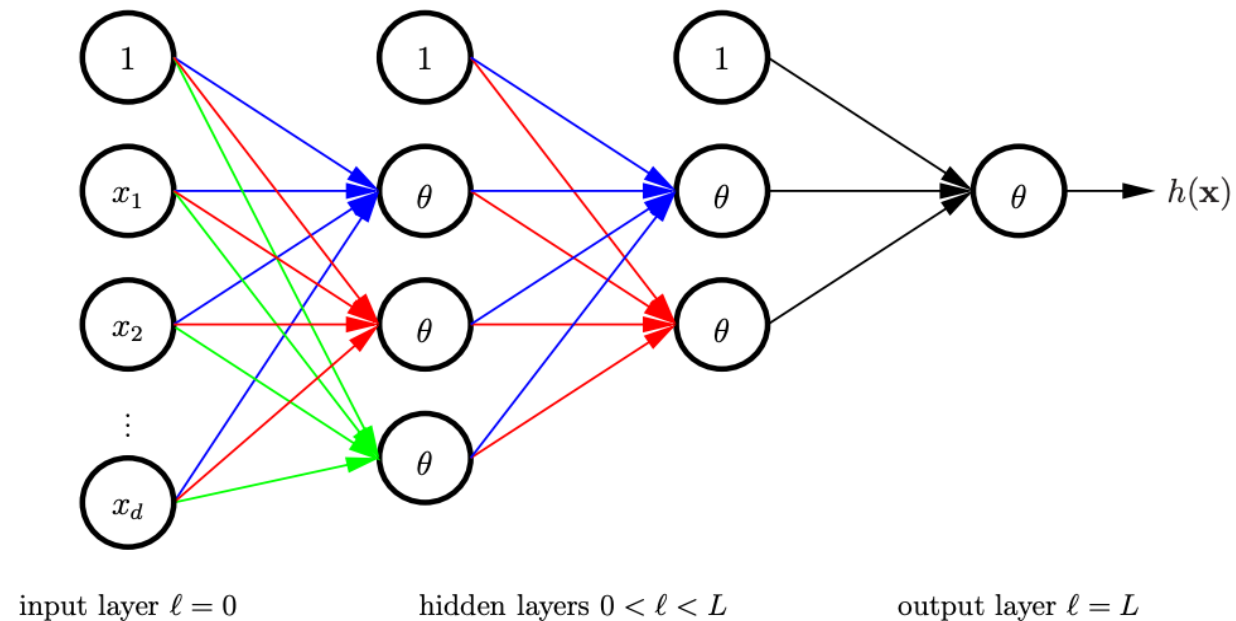
Goal of Today

- 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)

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)

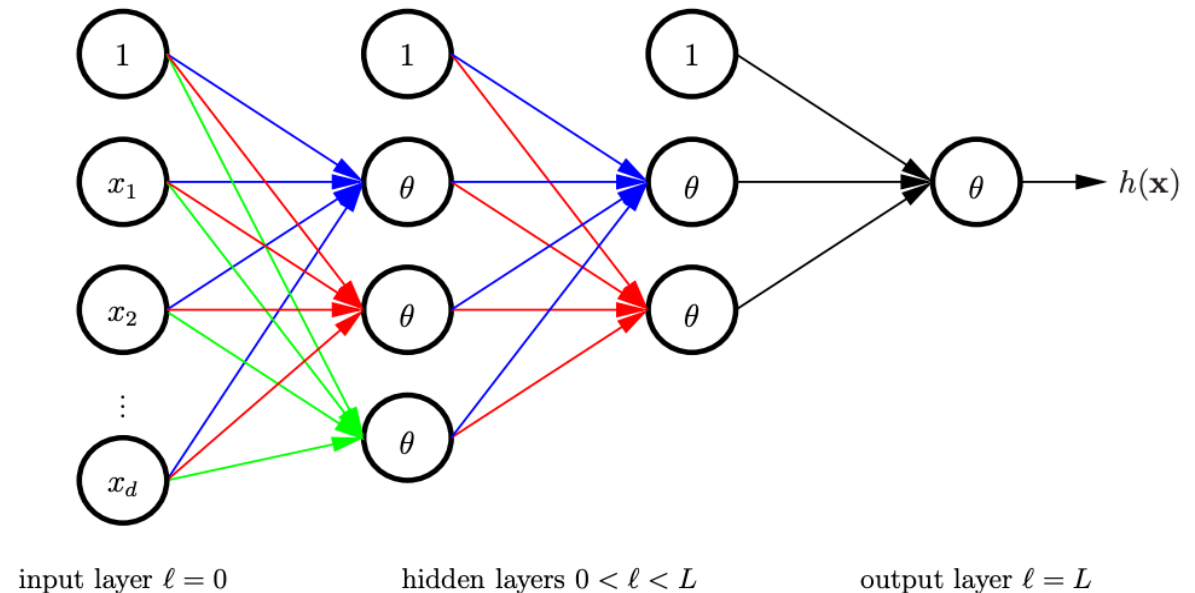
- A hypothesis in linear model is specified by the weights $\{w_i\}$
- Similarly, a hypothesis in NN is characterized by the weights $\{w_{i,j}^{(\ell)}\}$

- $1 \leq \ell \leq L$
- $0 \leq i \leq d^{(\ell-1)}$
- $1 \leq j \leq d^{(\ell)}$

layers

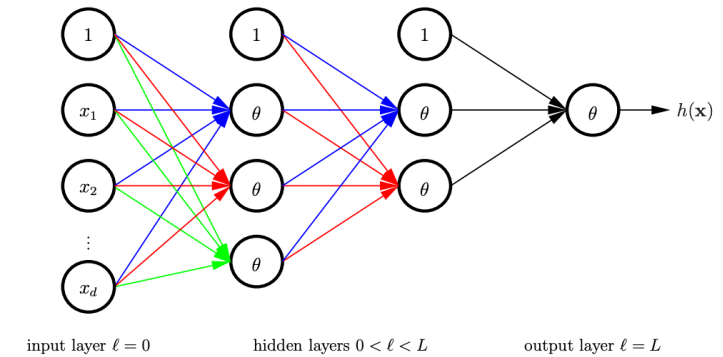
inputs

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

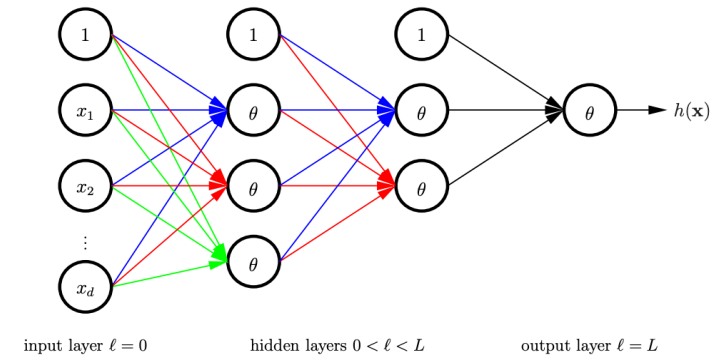


- Lastly, linear signal $s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{i,j}^{(\ell)} x_i^{(\ell-1)}$
 - By definition: $x_j^{(\ell)} = \theta(s_j^{(\ell)})$

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

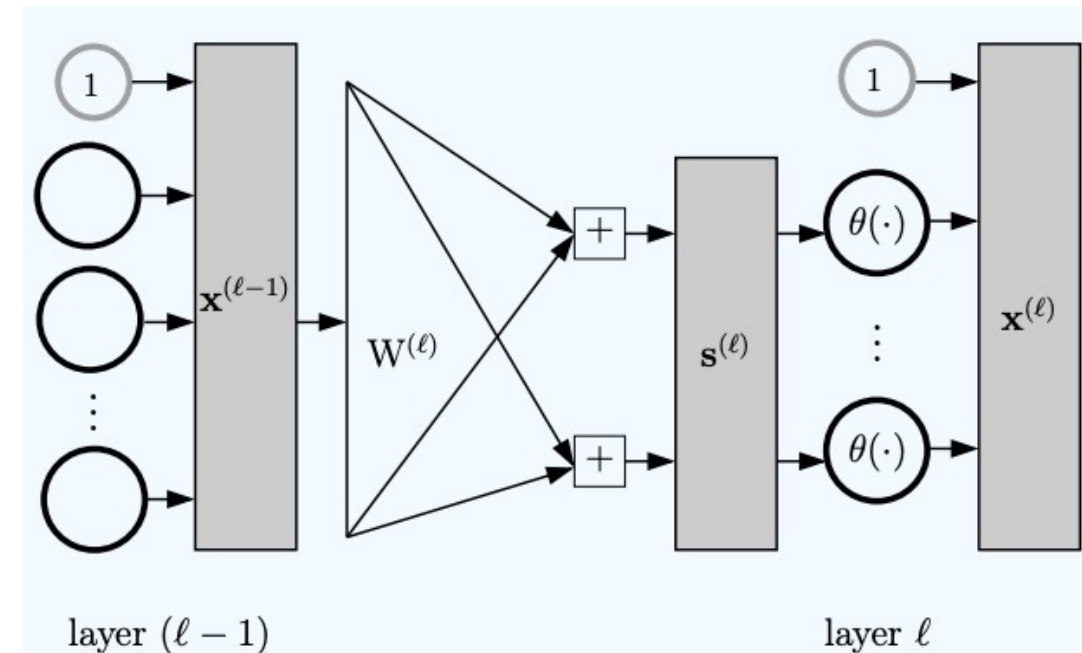
Notations of Neural Networks (NN)

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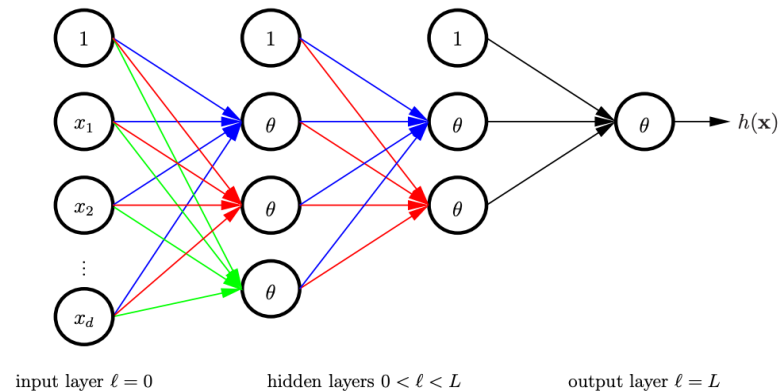
$$\mathbf{s}^{(\ell)} \xrightarrow{\theta} \mathbf{x}^{(\ell)}$$



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

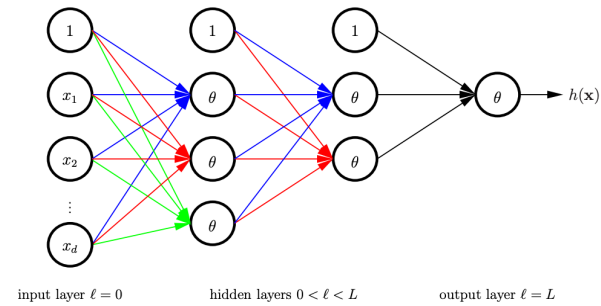
Forward Propagation

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

Backpropagation

Learn a Neural Network hypothesis from data

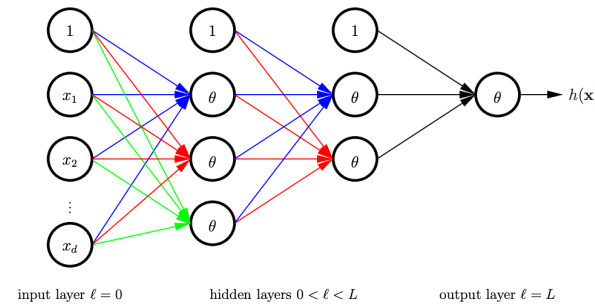
Forward Propagation



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

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{w^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{w^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \dots \xrightarrow{w^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

Forward Propagation



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

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{w^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{w^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \dots \xrightarrow{w^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

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:    $\mathbf{s}^{(\ell)} \leftarrow (W^{(\ell)})^T \mathbf{x}^{(\ell-1)}$ 
4:    $\mathbf{x}^{(\ell)} \leftarrow \begin{bmatrix} 1 \\ \theta(\mathbf{s}^{(\ell)}) \end{bmatrix}$ 
5: end for
6:  $h(\mathbf{x}) = \mathbf{x}^{(L)}$  [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 $W = \{w_{i,j}^{(\ell)}\}$?
- 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

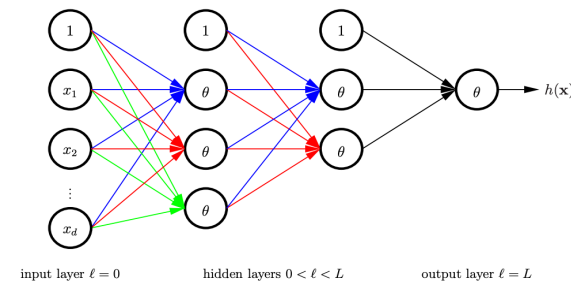
Backpropagation

Use dynamic programming to evaluate the gradient

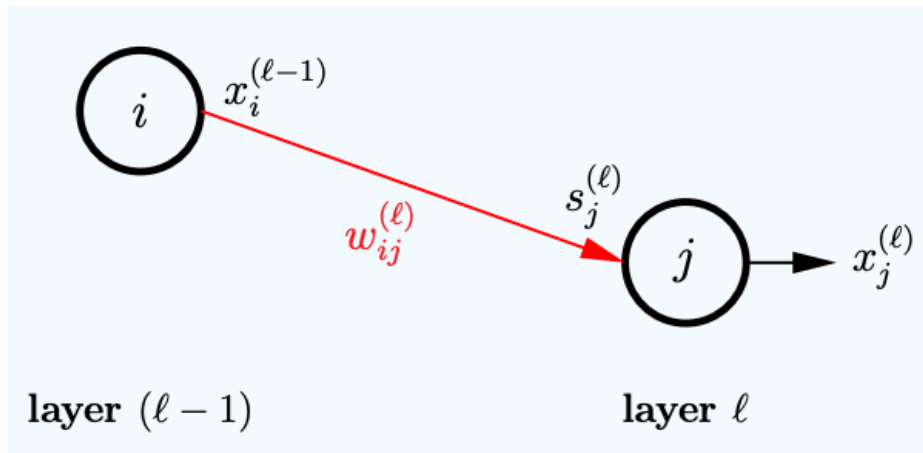
Quick Reminders on Dynamic Programming

- 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, \dots, 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 $w_{i,j}^{(\ell)}$



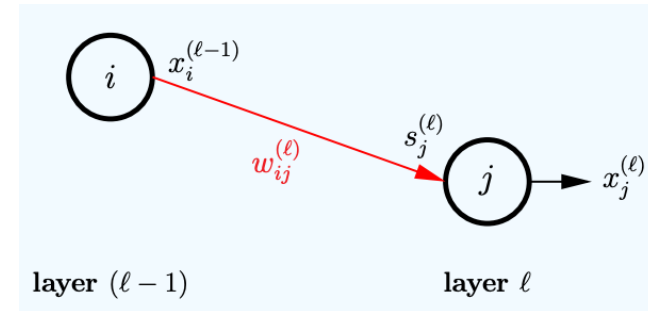
- Apply chain rule

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

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, $\frac{\partial s_j^{(\ell)}}{\partial w_{i,j}^{(\ell)}} = x_i^{(\ell-1)}$

- To sum up

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

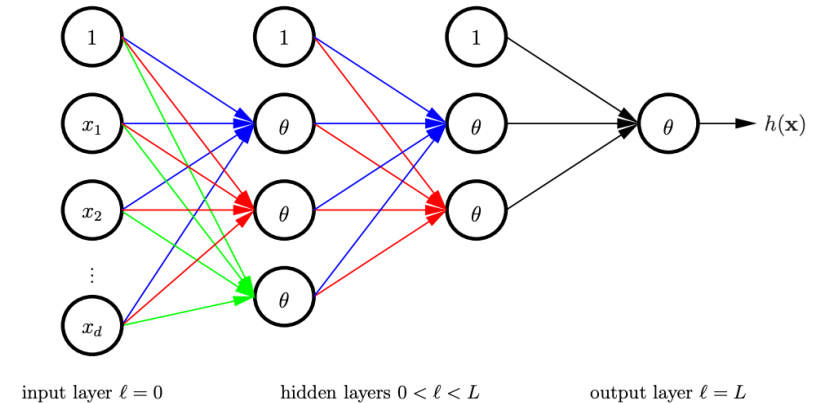
- What about the first term?

- 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

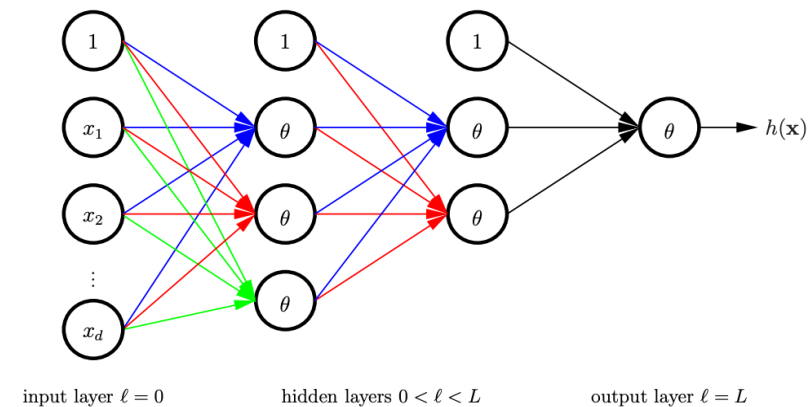
Compute $\delta_j^{(\ell)} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}}$

- 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
 - $e_n(W) = (s_1^{(L)} - y_n)^2$ (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**)



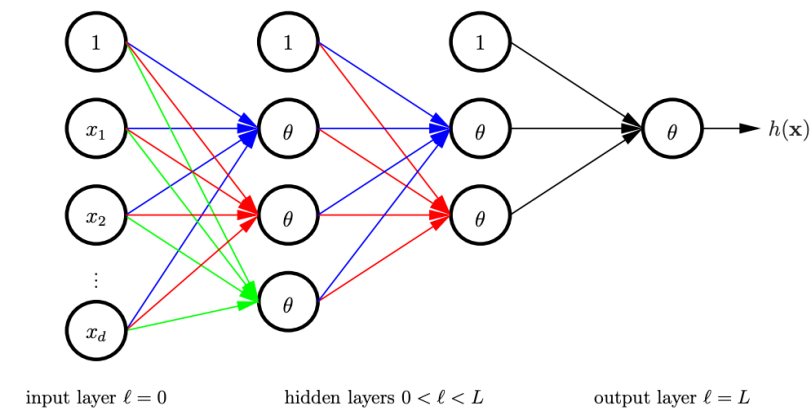
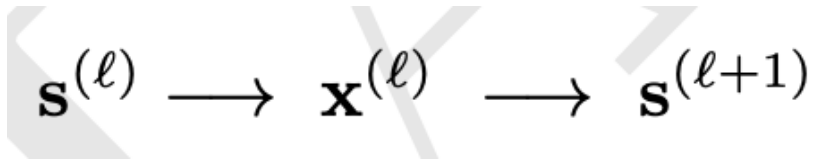
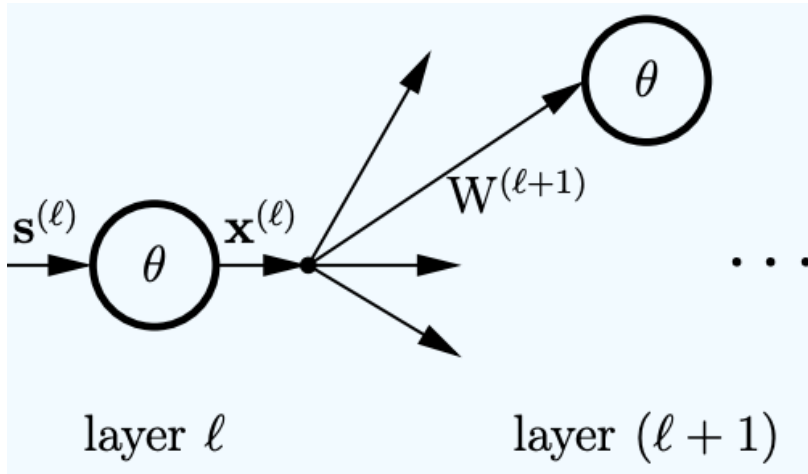
Compute $\delta_j^{(\ell)} = \frac{\partial e_n(W)}{\partial s_j^{(\ell)}}$

- Zoom in to see the chain of dependencies



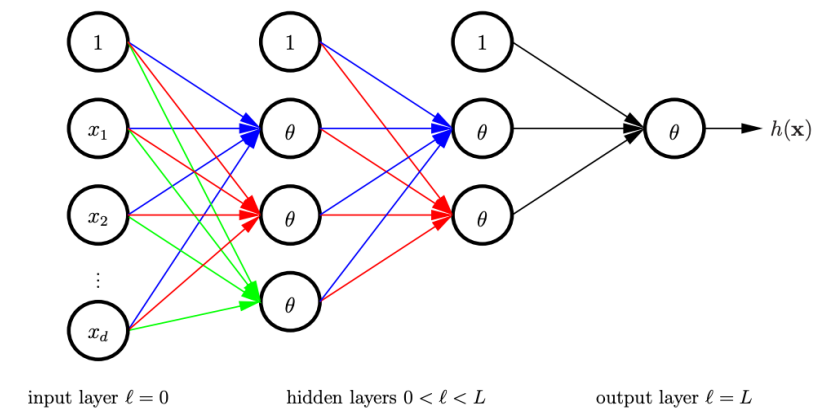
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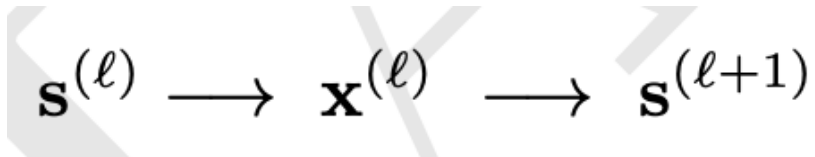
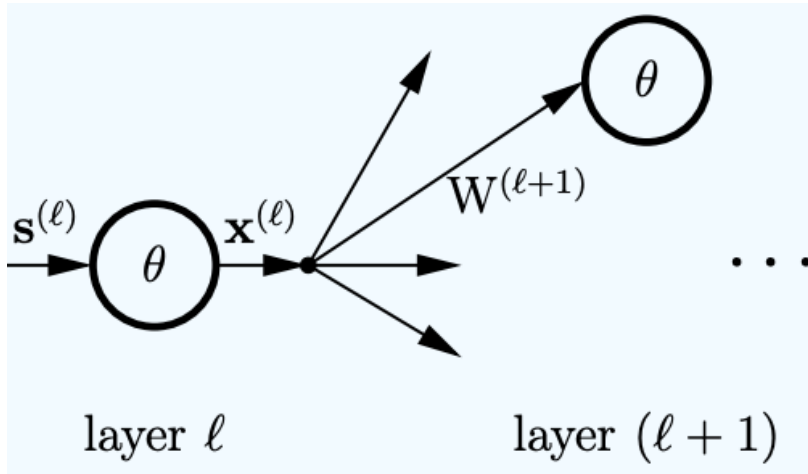


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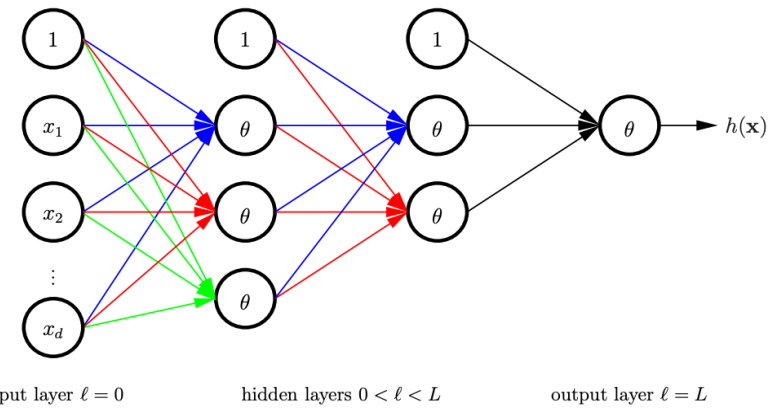
For $\theta(s) = \tanh(s)$,
 $\theta'(s) = 1 - \theta(s)^2$



$$\begin{aligned} \delta_j^{(\ell)} &= \frac{\partial e_n(W)}{\partial s_j^{(\ell)}} \\ &= \sum_{k=1}^{d^{(\ell+1)}} \frac{\partial e_n(W)}{\partial s_k^{(\ell+1)}} \frac{\partial s_k^{(\ell+1)}}{\partial x_j^{(\ell)}} \frac{\partial x_j^{(\ell)}}{\partial s_j^{(\ell)}} \\ &= \sum_{k=1}^{d^{(\ell+1)}} \delta_k^{(\ell+1)} w_{j,k}^{(\ell+1)} \theta' \left(s_j^{(\ell)} \right) \end{aligned}$$

We have the backward recurse definition!

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



- 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?

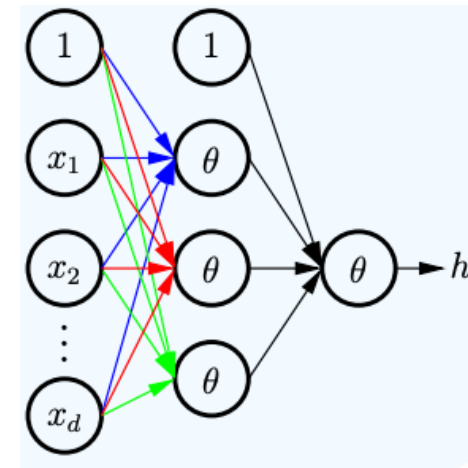
$$\begin{aligned} \bullet \quad h(\vec{x}) &= \theta \left(w_{0,1}^{(2)} + \sum_{j=1}^{d^{(1)}} w_{j,1}^{(2)} x_j^{(1)} \right) \\ &= \theta \left(w_{0,1}^{(2)} + \sum_{j=1}^{d^{(1)}} w_{j,1}^{(2)} \theta \left(\sum_{i=0}^{d^{(0)}} w_{i,j}^{(1)} x_i \right) \right) \end{aligned}$$

- How do we write a Kernel SVM hypothesis
(linear model with nonlinear transformation)

$$\bullet \quad g(\vec{x}) = \theta \left(b^* + \sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x}) \right)$$

- Interpretation:

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



Neural Network is Expressive

- 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.
 - A single-hidden-layer NN can approximate ANY continuous target function!
- We also seem to only discuss how to minimize E_{in}

What about overfitting?

Regularization in Neural Networks

Weight-Based Regularization

- Weight decay

$$E_{aug}(W) = E_{in}(W) + \frac{\lambda}{N} \sum_{i,j,\ell} \left(w_{i,j}^{(\ell)} \right)^2$$

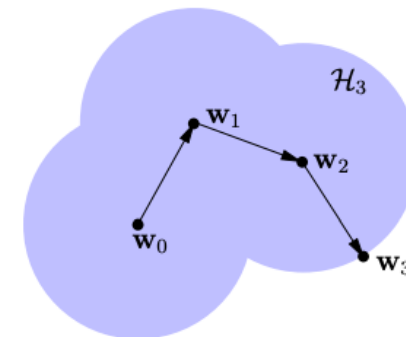
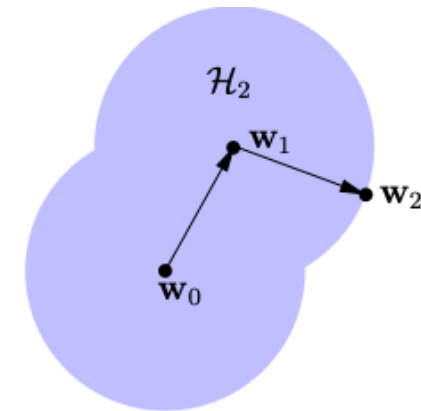
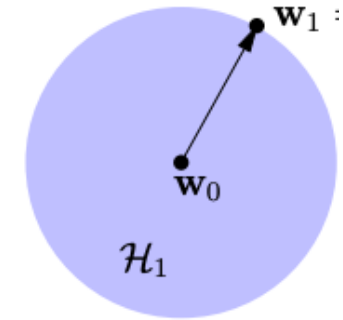
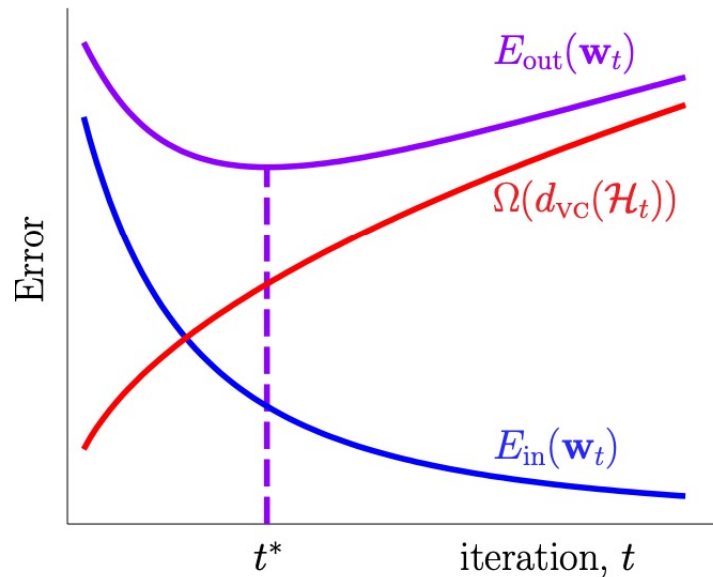
- Weight elimination

$$E_{aug}(W) = E_{in}(W) + \frac{\lambda}{N} \sum_{i,j,\ell} \frac{\left(w_{i,j}^{(\ell)} \right)^2}{1 + \left(w_{i,j}^{(\ell)} \right)^2}$$

- When $w_{i,j}^{(\ell)}$ is small, approximates weight decay
- When $w_{i,j}^{(\ell)}$ is large, approximates adding a constant (no impacts to gradient)
- “Decaying” more on smaller weights (i.e., eliminating small weights)

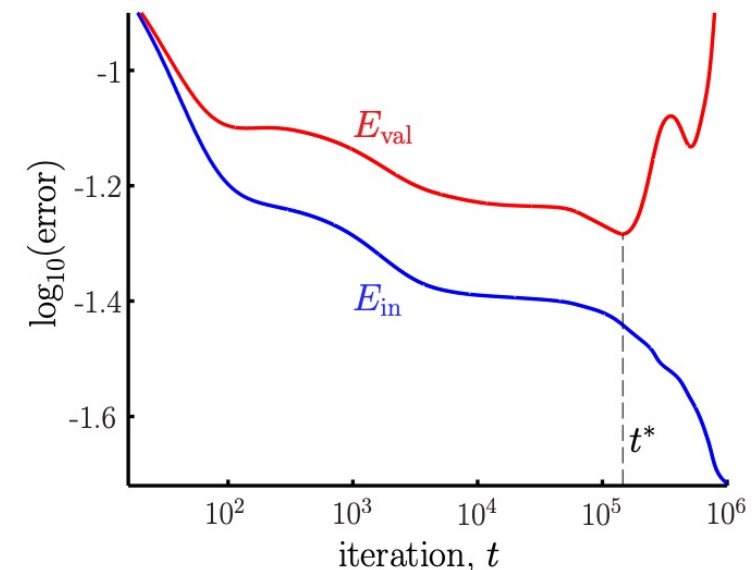
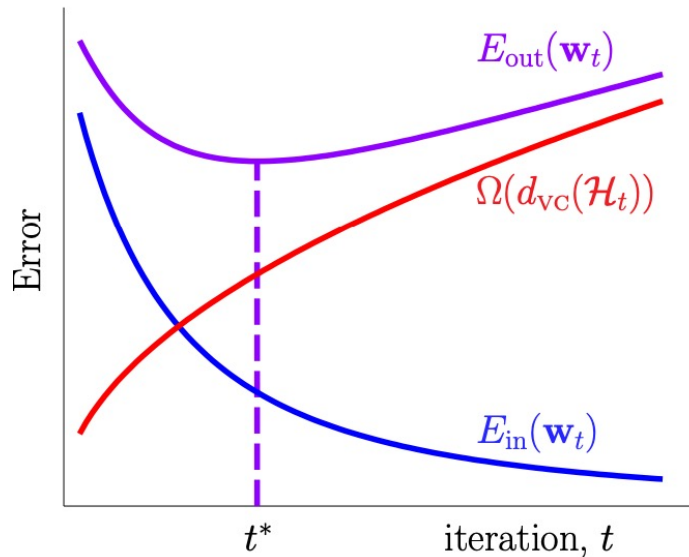
Early Stopping

- Consider gradient descent (GD)
 - H_1 : the set of hypothesis GD can reach at $t = 1$
 - H_2 : the set of hypothesis GD can reach at $t = 2$
 - ...
 - $H_1 \subseteq H_2 \subseteq H_3 \subseteq \dots$



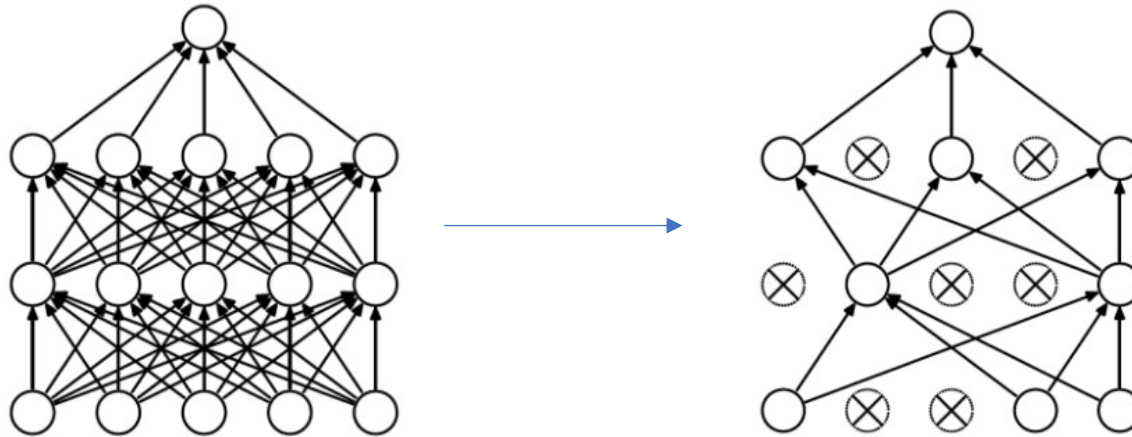
Early Stopping

- Stopping gradient descent early is a regularization method
 - **Constrain** the hypothesis set
- How to find the optimal stopping point t^* ?
 - Using validation is a common approach



Dropout

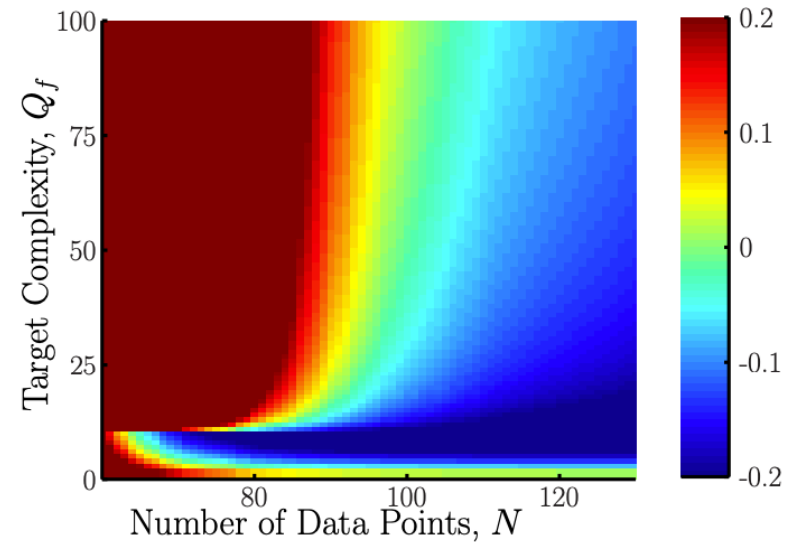
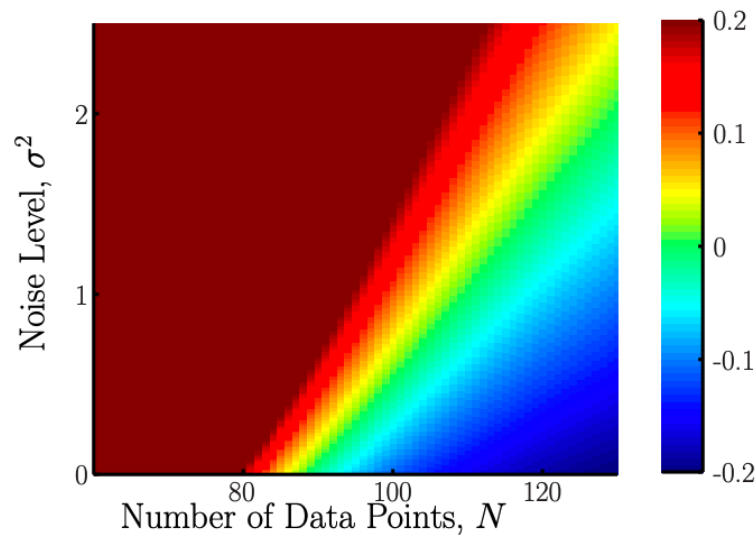
- Neural networks is very expressive (low bias, potentially high variance)
- Dropout
 - Randomly **drop** p portion of the weights during training



- Learn many models with dropout
- **Average** them during prediction (reduce weights by a ratio of p)

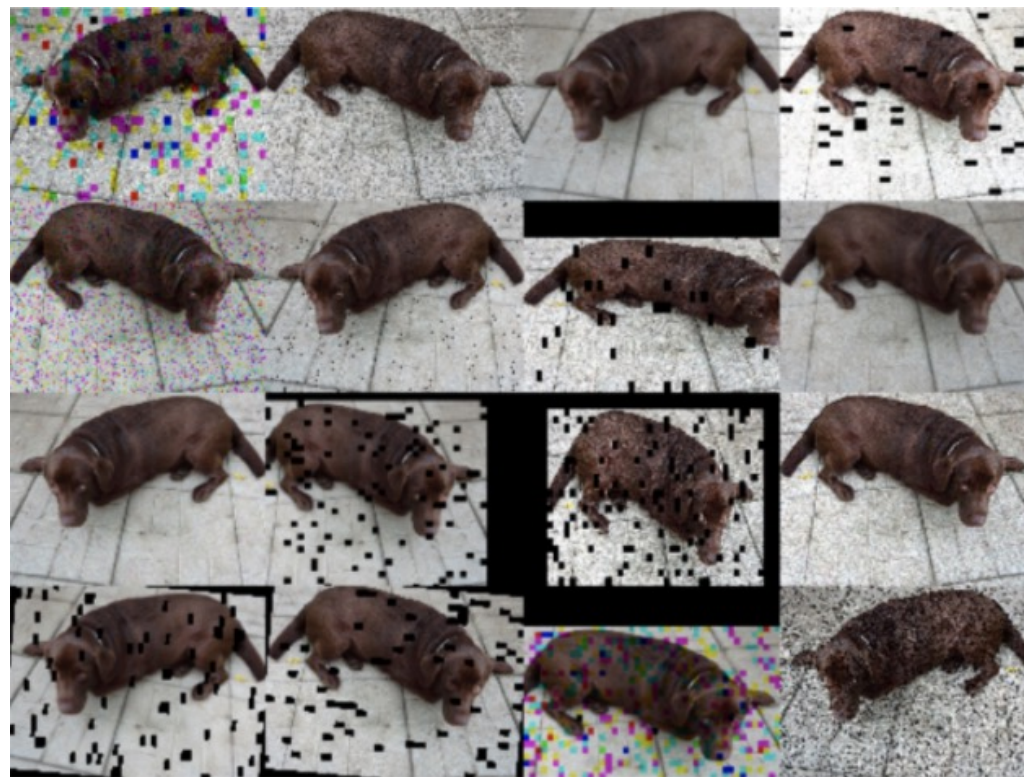
A Nontraditional Method to Avoid Overfitting

- What's the cause of overfitting?



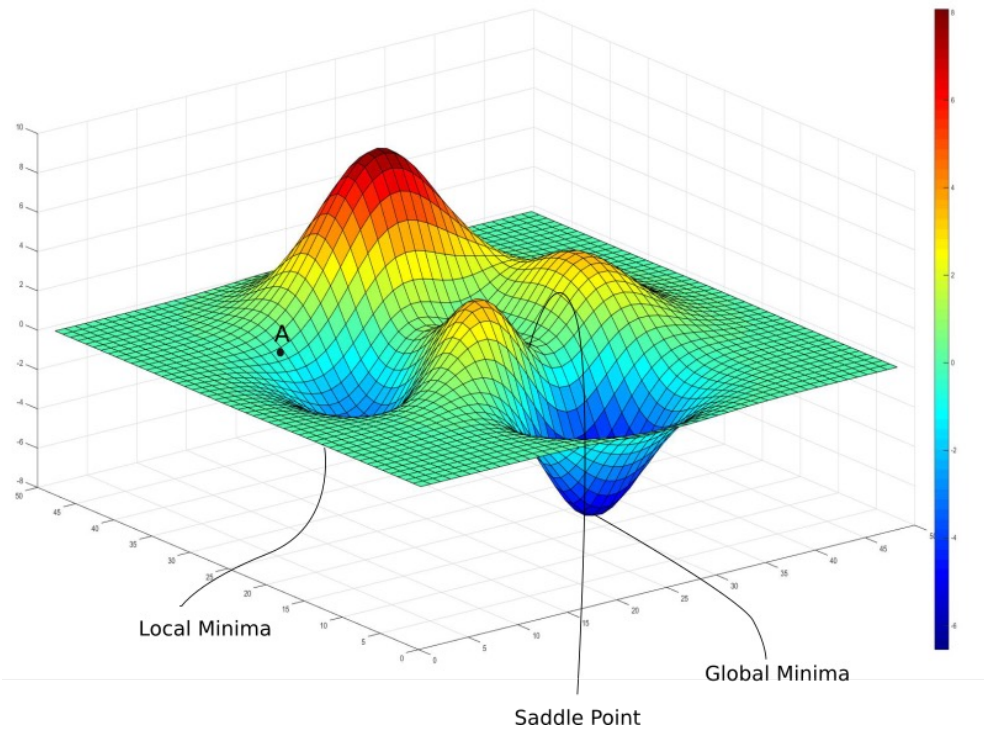
- Fitting the **noise** instead of the target
- Regularization: Constrain H so it's not that powerful to fit noise
- How about **adding noises** to data?

Adding Noises as Regularization



Initialization

Error is Nonconvex in Neural Networks



- We mostly adopt gradient-descent-style algorithms for optimization.
- No guarantee to converge to global optimal.
- Need to run it many times.
- Initialization matters!

Vanishing Gradient Problem

- Backpropagation

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

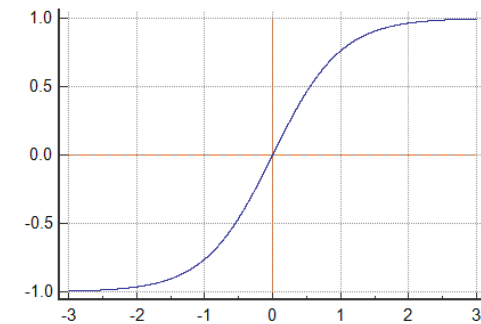
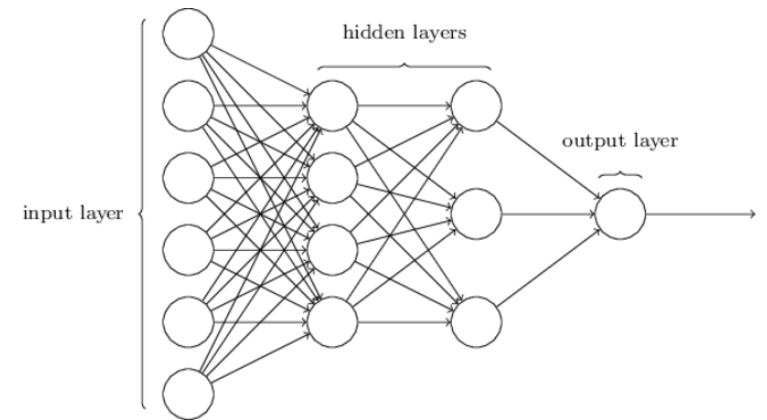
- $\delta_j^{(\ell)} = \theta' \left(s_j^{(\ell)} \right) \sum_{k=1}^{d^{(\ell+1)}} \delta_k^{(\ell+1)} w_{j,k}^{(\ell+1)}$

- If we use activation function $\theta(s) = \tanh(s)$

- $\theta'(s) = 1 - \theta(s)^2 < 1$

- In deep learning with a lot of layers,

- the gradient might vanish
 - hard to update the early layers



Vanishing Gradient Problem

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

- There is also a corresponding “exploding gradient problem”

- What can we do

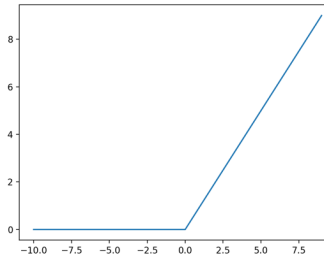
- Choose more suitable activation functions

- One common choice is Rectified Linear Unit (ReLU) and its variant

- $\theta(s) = \max(0, s)$

- Choose better **initialization**

- Many approaches

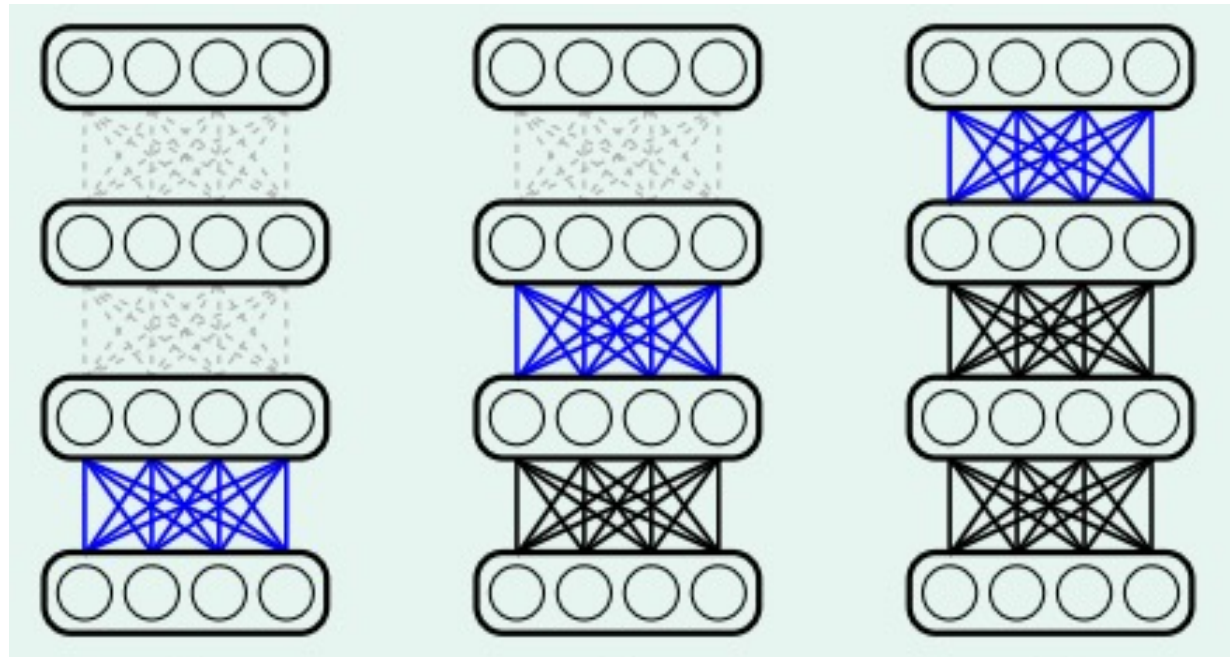


Weight Initialization

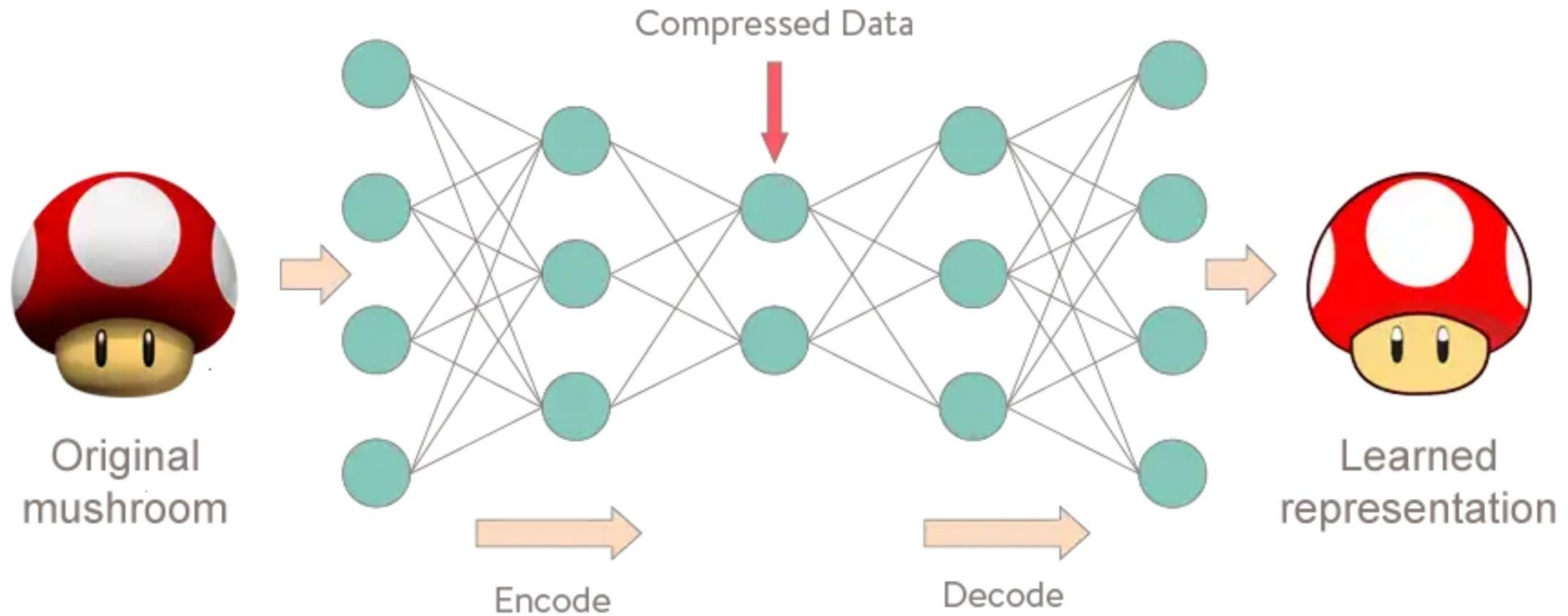
- Initializing weights to 0 is a bad idea
 - Q5 of HW1
- Randomly Initializing weights to regions so that vanishing/exploding gradients are less likely to happen
 - Activation-function dependent
 - e.g., Xavier initialization for tanh
- Learning the initialization
 - E.g., autoencoder

Initialization

- Hard to initialize the entire network well.
- Intuition: Initialize the weights **layer by layer** such that each layer **preserves** the properties of the previous layer.



Autoencoder



Unsupervised learning!