Machine Learning
(機器學習)

Lecture 14: From Neural Net. to Deep Learning

Hsuan-Tien Lin (林軒田)
htlin@csie.ntu.edu.tw

Department of Computer Science
& Information Engineering

National Taiwan University
(國立台灣大學資訊工程系)

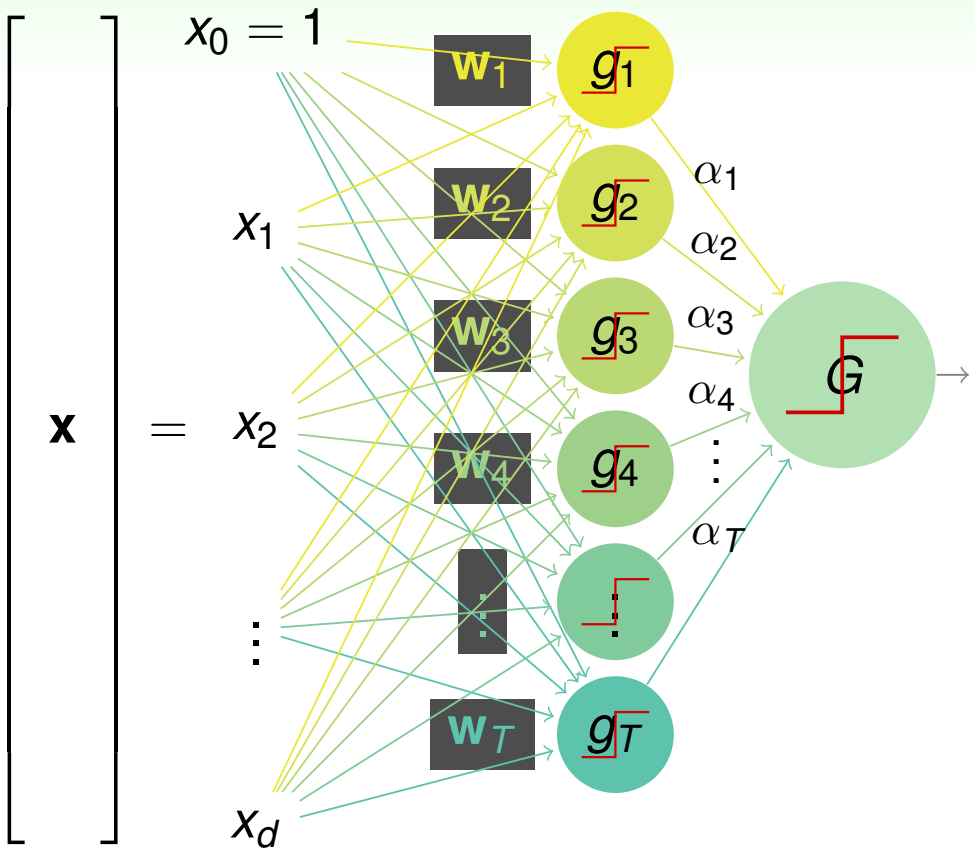
Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn Better?
5. Embedding Numerous Features: Kernel Models
6. Combining Predictive Features: Aggregation Models
7. Distilling Implicit Features: Extraction Models

Lecture 14: From Neural Net. to Deep Learning

- Motivation
- Neural Network Hypothesis
- Neural Network Learning
- Deep Neural Network
- Vanishing Gradient Issue
- Modern Activation Functions

Linear Aggregation of Perceptrons: Pictorial View

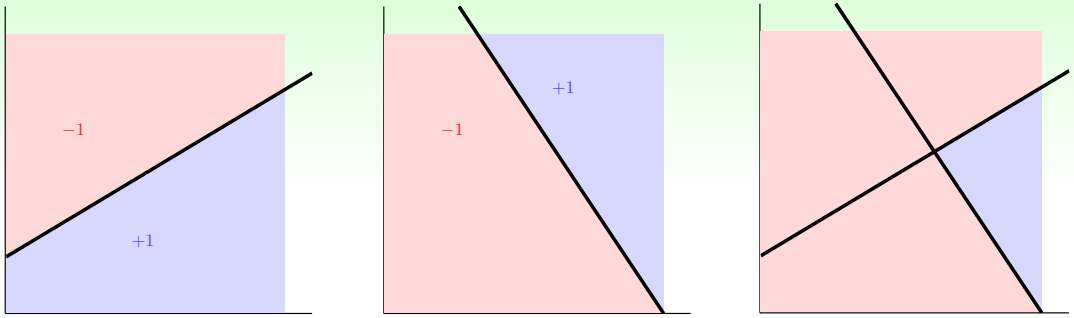


$$G(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t \underbrace{\text{sign}\left(\mathbf{w}_t^T \mathbf{x}\right)}_{g_t(\mathbf{x})}\right)$$

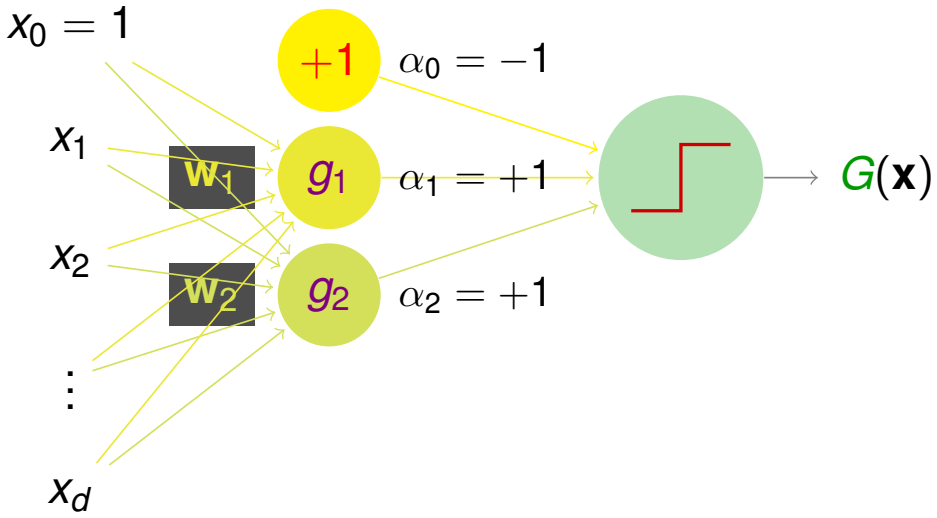
- two layers of weights: $\mathbf{w}_t$ and α
- two layers of sign functions: in g_t and in G

what boundary can G **implement**?

Logic Operations with Aggregation



g_1 g_2 $\texttt{AND}(g_1, g_2)$

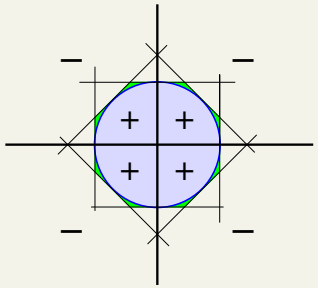


$G(\mathbf{x}) = \text{sign}\left(-1 + g_1(\mathbf{x}) + g_2(\mathbf{x})\right)$

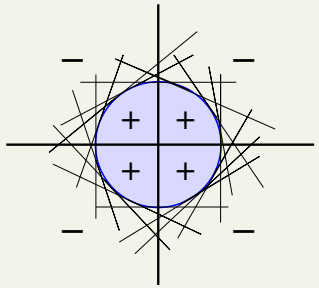
- $g_1(\mathbf{x}) = g_2(\mathbf{x}) = +1$ (TRUE): $G(\mathbf{x}) = +1$ (TRUE)
- otherwise: $G(\mathbf{x}) = -1$ (FALSE)
- $G \equiv \texttt{AND}(g_1, g_2)$

OR, NOT can be **similarly implemented**

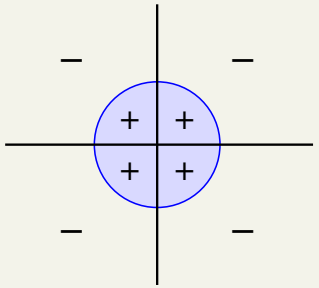
Powerfulness and Limitation



8 perceptrons

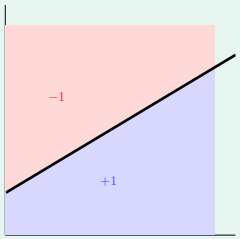


16 perceptrons

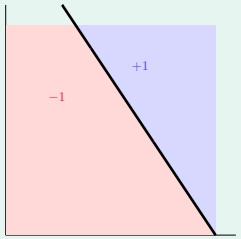


target boundary

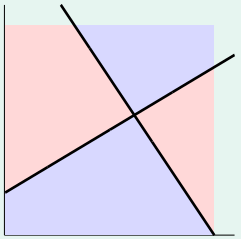
- 'convex set' hypotheses implemented: $d_{\text{VC}} \to \infty$, **remember? :-)**
- powerfulness: enough perceptrons $\approx$ **smooth boundary**



g_1



g_2



$\texttt{XOR}(g_1, g_2)$

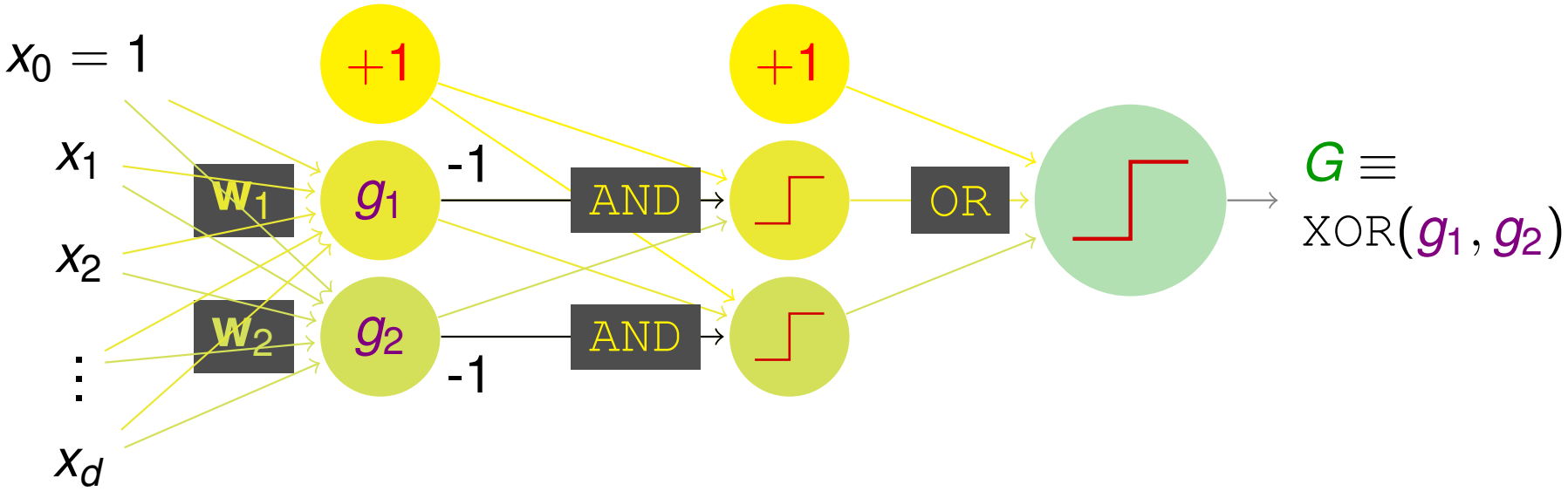
- limitation: XOR **not 'linear separable'** under $\phi(\mathbf{x}) = (g_1(\mathbf{x}), g_2(\mathbf{x}))$

how to implement $\texttt{XOR}(g_1, g_2)$?

Multi-Layer Perceptrons: Basic Neural Network

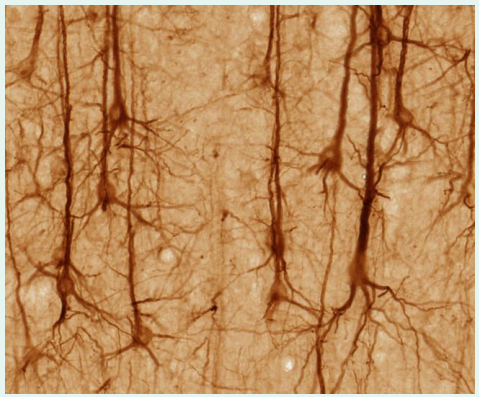
- non-separable data: can use more **transform**
- how about one more layer of **AND transform**?

$$\text{XOR}(g_1, g_2) = \text{OR}(\text{AND}(-g_1, g_2), \text{AND}(g_1, -g_2))$$



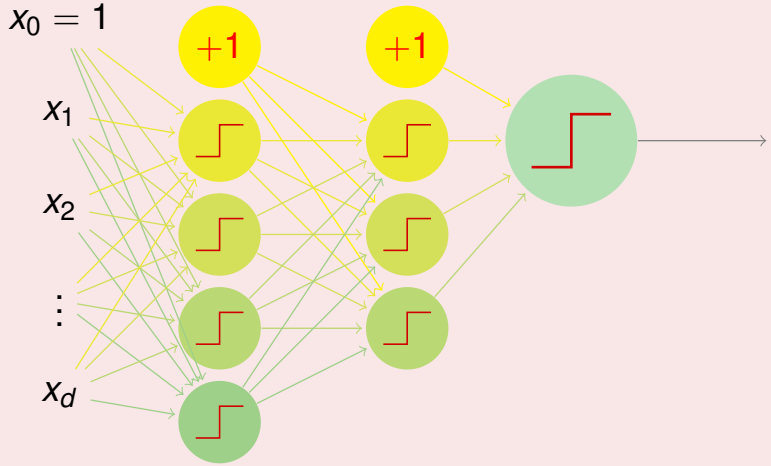
perceptron (simple)
$\Longrightarrow$ aggregation of perceptrons (powerful)
$\Longrightarrow$ **multi-layer perceptrons** (**more powerful**)

Connection to Biological Neurons



by UC Regents Davis campus-brainmaps.org.

Licensed under CC BY 3.0 via Wikimedia Commons



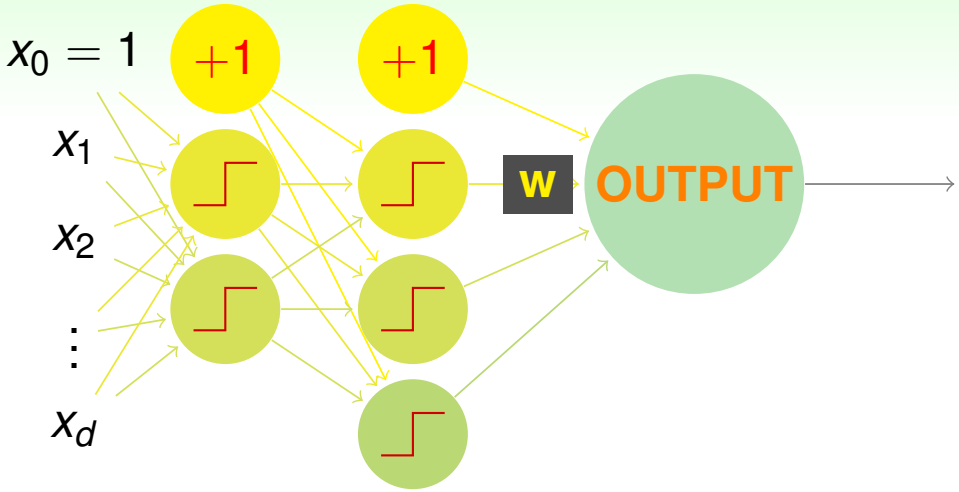
by Lauris Rubenis. Licensed under CC BY 2.0 via https://flic.kr/p/fkVuZX

by Pedro Ribeiro Simões. Licensed under CC BY 2.0 via https://flic.kr/p/adiV7b

neural network: **bio-inspired** model

Questions?

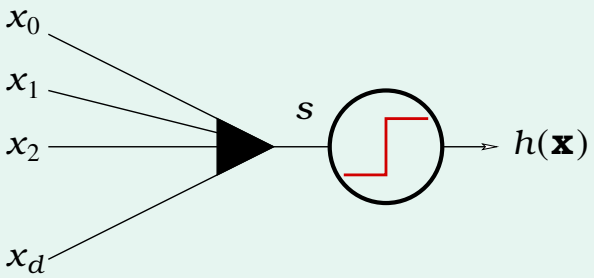
Neural Network Hypothesis: Output



- **OUTPUT**: simply a **linear model** with $s = \mathbf{w}^T \phi^{(2)}(\phi^{(1)}(\mathbf{x}))$
- any linear model can be used—**remember? :-)**

linear classification

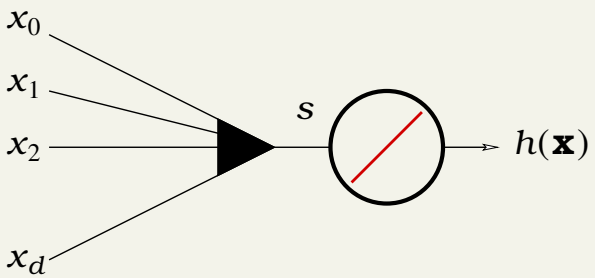
$h(\mathbf{x}) = \text{sign}(s)$



err = 0/1

linear regression

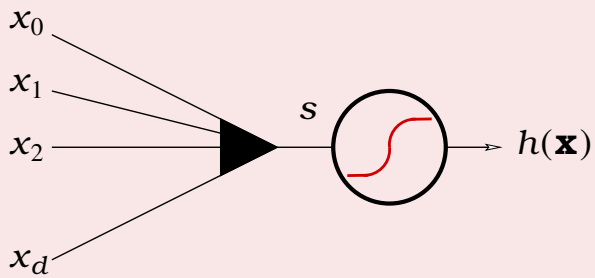
$h(\mathbf{x}) = s$



err = squared

logistic regression

$h(\mathbf{x}) = \theta(s)$

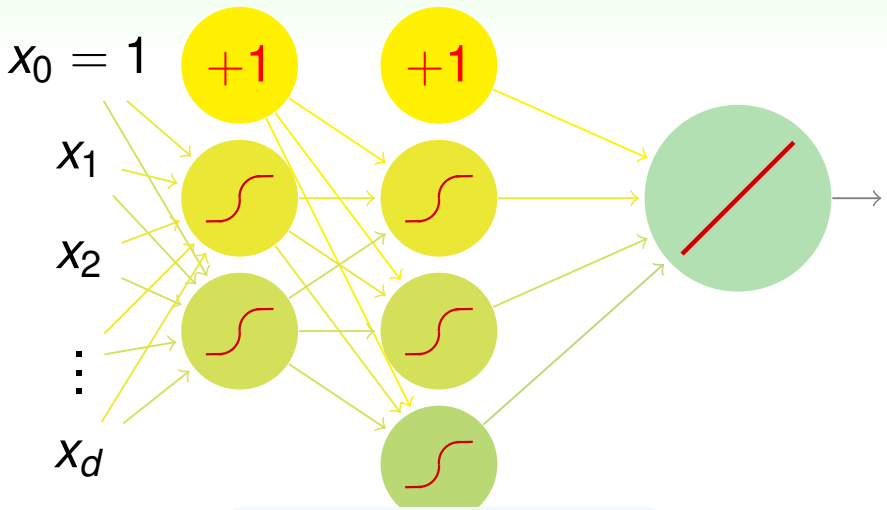


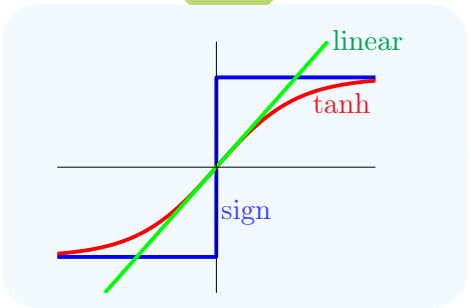
err = cross-entropy

will discuss **'regression' with squared error**

Neural Network Hypothesis: Transformation

- $\sqcap\!\!\!\!\sqcup$: **transformation** function of score (signal) s
- any transformation?
  - $\diagup$: whole network linear & thus **less useful**
  - $\sqcap\!\!\!\!\sqcup$: discrete & thus **hard to optimize** for $\mathbf{w}$
- traditional choice of transformation: $\int$ $= \tanh(s)$
  - 'analog' approximation of $\sqcap\!\!\!\!\sqcup$: **easier to optimize**
  - somewhat **closer to biological** neuron
  - **not that new! :-)**

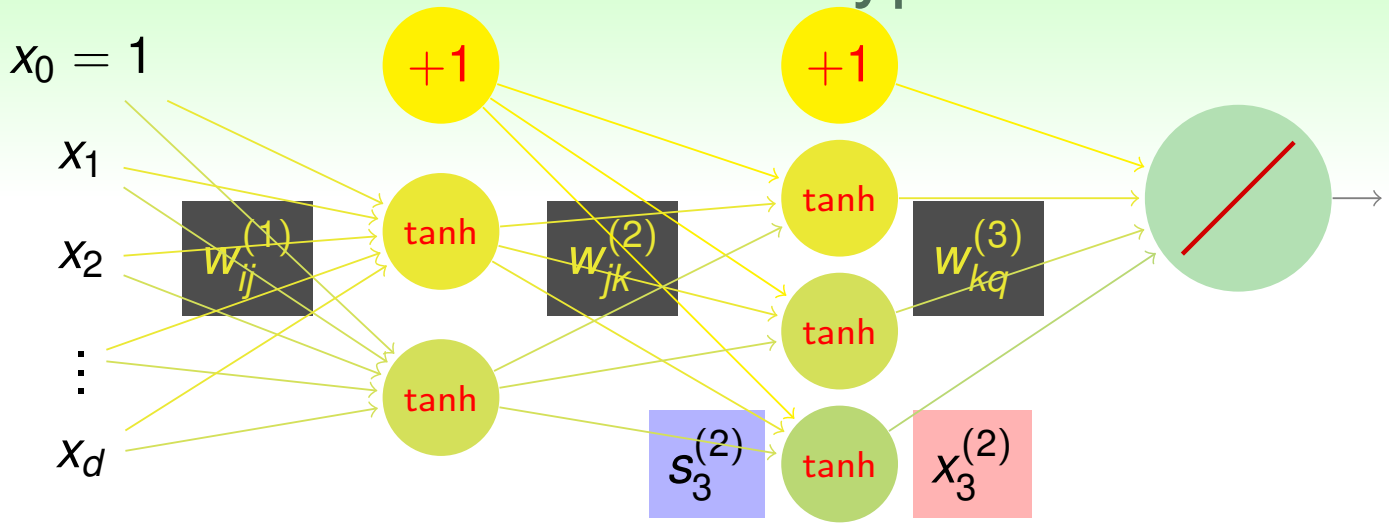




$$\tanh(s) = \frac{\exp(s) - \exp(-s)}{\exp(s) + \exp(-s)} = 2\theta(2s) - 1$$

will discuss with tanh first

Neural Network Hypothesis



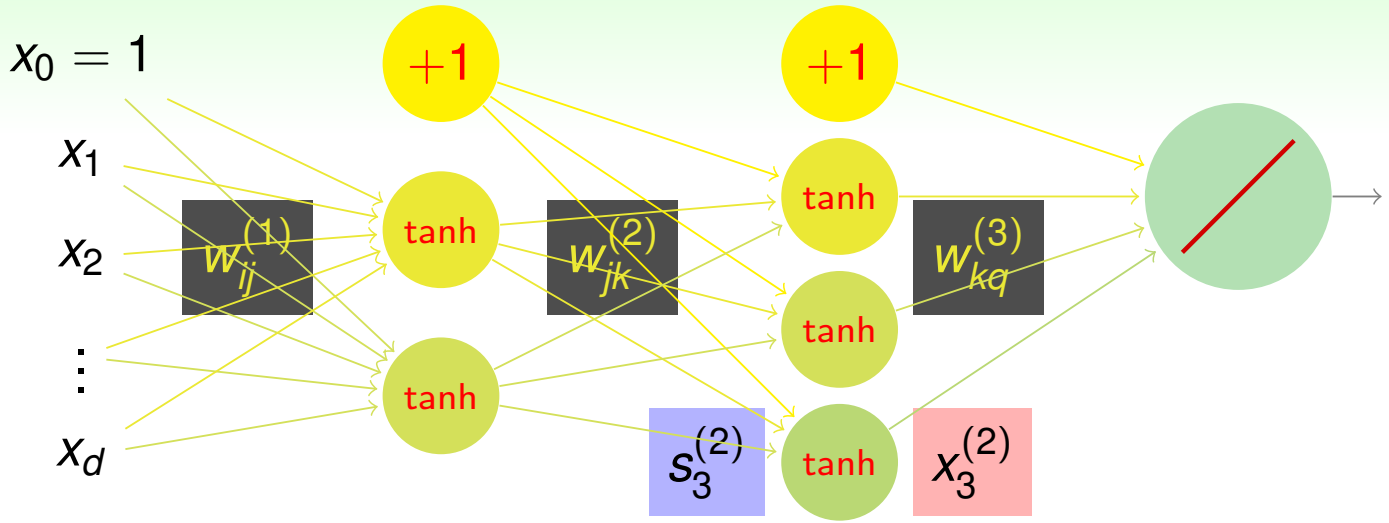
$d^{(0)}$-$d^{(1)}$-$d^{(2)}$-$\cdots$-$d^{(L)}$ Neural Network (NNet)

$$w_{ij}^{(\ell)}: \begin{cases} 1 \le \ell \le L & \text{layers} \\ 0 \le i \le d^{(\ell-1)} & \text{inputs} \\ 1 \le j \le d^{(\ell)} & \text{outputs} \end{cases}, \quad \text{score } s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{ij}^{(\ell)} x_i^{(\ell-1)},$$

$$\text{transformed } x_j^{(\ell)} = \begin{cases} \tanh\left(s_j^{(\ell)}\right) & \text{if } \ell < L \\ s_j^{(\ell)} & \text{if } \ell = L \end{cases}$$

apply $\mathbf{x}$ as input layer $\mathbf{x}^{(0)}$, go through hidden layers to get $\mathbf{x}^{(\ell)}$, predict at output layer $x_1^{(L)}$

Physical Interpretation



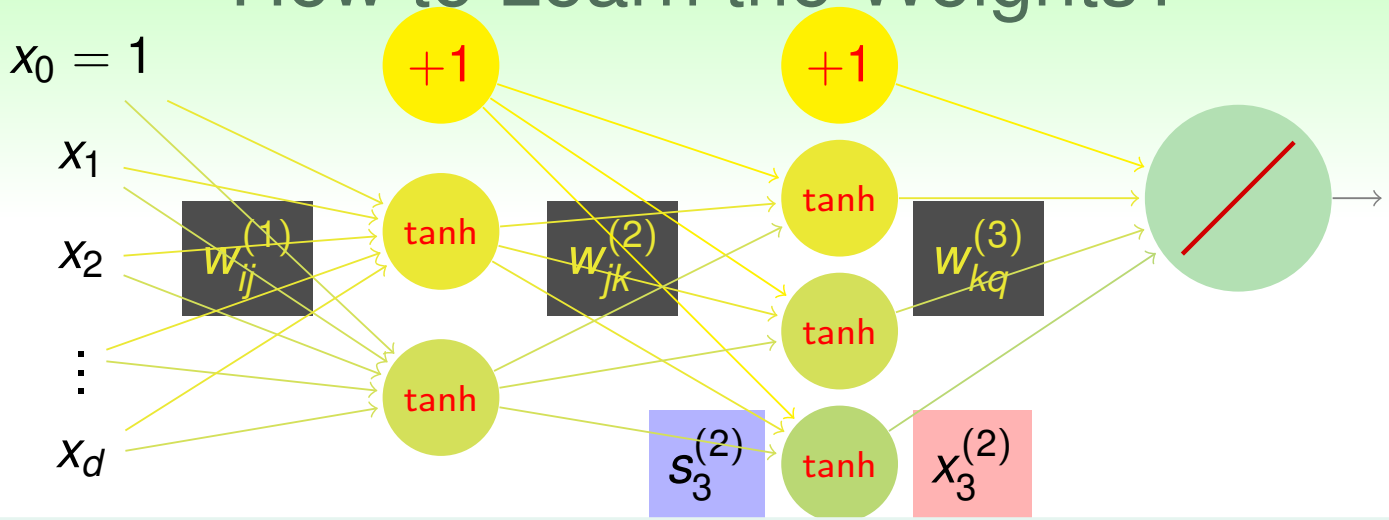
- each layer: **transformation** to be **learned** from data
- $\phi^{(\ell)}(\mathbf{x}) = \tanh\left(\begin{bmatrix} \sum_{i=0}^{d^{(\ell-1)}} w_{i1}^{(\ell)} x_i^{(\ell-1)} \\ \vdots \end{bmatrix}\right)$

  —whether $\mathbf{x}$ 'matches' weight vectors in pattern

NNet: **pattern extraction** with layers of connection weights

Questions?

How to Learn the Weights?



- goal: learning all $\{w_{ij}^{(\ell)}\}$ to **minimize** $E_{\text{in}}\left(\{w_{ij}^{(\ell)}\}\right)$
- one hidden layer: simply **aggregation of perceptrons**
  —**gradient boosting** to determine hidden neuron one by one
- multiple hidden layers? **not easy**
- let $e_n = (y_n - \text{NNet}(\mathbf{x}_n))^2$:
  can apply **(stochastic) GD** after computing $\frac{\partial e_n}{\partial w_{ij}^{(\ell)}}$!

next: efficient computation of $\frac{\partial e_n}{\partial w_{ij}^{(\ell)}}$

Computing $\frac{\partial e_n}{\partial w_{i1}^{(L)}}$ (Output Layer)

$$e_n = (y_n - \text{NNet}(\mathbf{x}_n))^2 = \left(y_n - s_1^{(L)}\right)^2 = \left(y_n - \sum_{i=0}^{d^{(L-1)}} w_{i1}^{(L)} x_i^{(L-1)}\right)^2$$

specially (output layer) $(0 \le i \le d^{(L-1)})$

$$\begin{aligned} & \frac{\partial e_n}{\partial w_{i1}^{(L)}} \\ = & \frac{\partial e_n}{\partial s_1^{(L)}} \cdot \frac{\partial s_1^{(L)}}{\partial w_{i1}^{(L)}} \\ = & -2\left(y_n - s_1^{(L)}\right) \cdot \left(x_i^{(L-1)}\right) \end{aligned}$$

generally $(1 \le \ell < L)$ $(0 \le i \le d^{(\ell-1)}; 1 \le j \le d^{(\ell)})$

$$\begin{aligned} & \frac{\partial e_n}{\partial w_{ij}^{(\ell)}} \\ = & \frac{\partial e_n}{\partial s_j^{(\ell)}} \cdot \frac{\partial s_j^{(\ell)}}{\partial w_{ij}^{(\ell)}} \\ = & \delta_j^{(\ell)} \cdot \left(x_i^{(\ell-1)}\right) \end{aligned}$$

$\delta_1^{(L)} = -2\left(y_n - s_1^{(L)}\right)$, how about **others**?

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

$$s_j^{(\ell)} \xrightarrow{\tanh} x_j^{(\ell)} \xrightarrow{w_{jk}^{(\ell+1)}} \begin{bmatrix} s_1^{(\ell+1)} \\ \vdots \\ s_k^{(\ell+1)} \\ \vdots \end{bmatrix} \Longrightarrow \cdots \Longrightarrow e_n$$

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

$$= \sum_k \left(\delta_k^{(\ell+1)}\right) \left(w_{jk}^{(\ell+1)}\right) \left(\tanh'\left(s_j^{(\ell)}\right)\right)$$

$\delta_j^{(\ell)}$ can be computed **backwards** from $\delta_k^{(\ell+1)}$

Backpropagation (Backprop) Algorithm

Backprop on NNet

initialize all weights $w_{ij}^{(\ell)}$

for $t = 0, 1, \ldots, T$

1. stochastic: randomly pick $n \in \{1, 2, \cdots, N\}$
2. forward: compute all $x_i^{(\ell)}$ with $\mathbf{x}^{(0)} = \mathbf{x}_n$
3. backward: compute all $\delta_j^{(\ell)}$ subject to $\mathbf{x}^{(0)} = \mathbf{x}_n$
4. gradient descent: $w_{ij}^{(\ell)} \leftarrow w_{ij}^{(\ell)} - \eta x_i^{(\ell-1)} \delta_j^{(\ell)}$

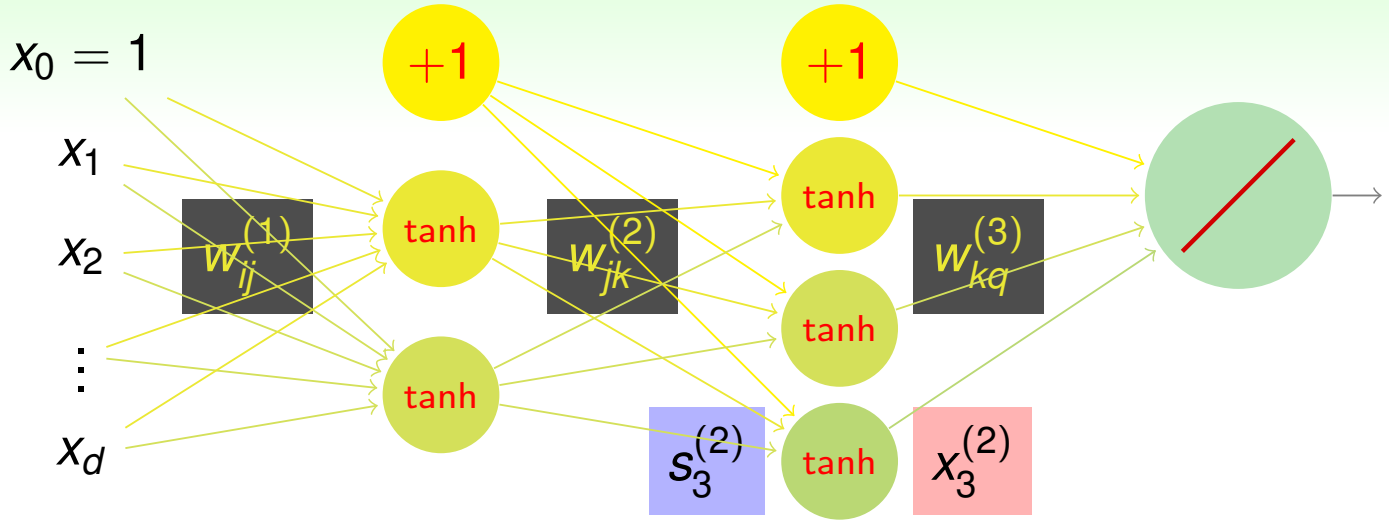
return $g_{\text{NNET}}(\mathbf{x}) = \left(\cdots \tanh \left(\sum_j w_{jk}^{(2)} \cdot \tanh \left(\sum_i w_{ij}^{(1)} x_i \right) \right) \right)$

sometimes (1) to (3) is (parallelly) done many times and average($x_i^{(\ell-1)} \delta_j^{(\ell)}$) taken for update in (4), called **mini-batch**

basic NNet algorithm: backprop to compute the gradient **efficiently**

Questions?

Physical Interpretation of NNet Revisited



- each layer: **pattern feature extracted** from data, **remember? :-)**
- how many neurons? how many layers?
  —more generally, **what structure?**
  - subjectively, **your design!**
  - objectively, **validation, maybe?**

structural decisions:
key issue for applying NNet

Shallow versus Deep Neural Networks

shallow: few (hidden) layers; deep: many layers

Shallow NNet

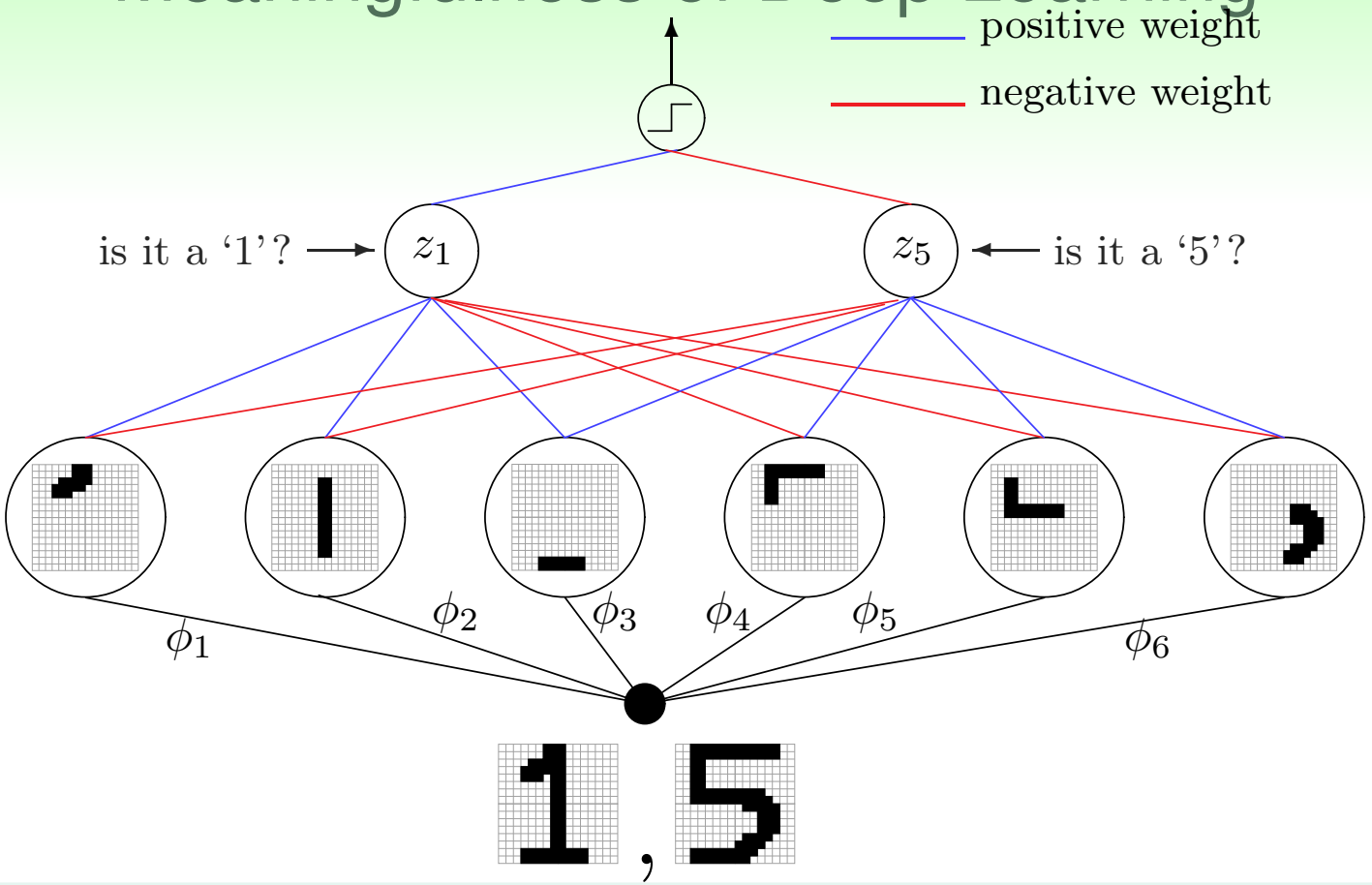
- more **efficient** to train (◯)
- **simpler** structural decisions (◯)
- theoretically **powerful enough** (◯)

Deep NNet

- **challenging** to train (×)
- **sophisticated** structural decisions (×)
- **'arbitrarily' powerful** (◯)
- more **'meaningful'?** (see next slide)

deep NNet (**deep learning**)
gaining attention in recent years

Meaningfulness of Deep Learning



- **'less burden'** for each layer: **simple** to **complex** features
- natural for **difficult** learning task with **raw features**, like **vision**

deep NNet: currently popular in **vision/speech/. . .**

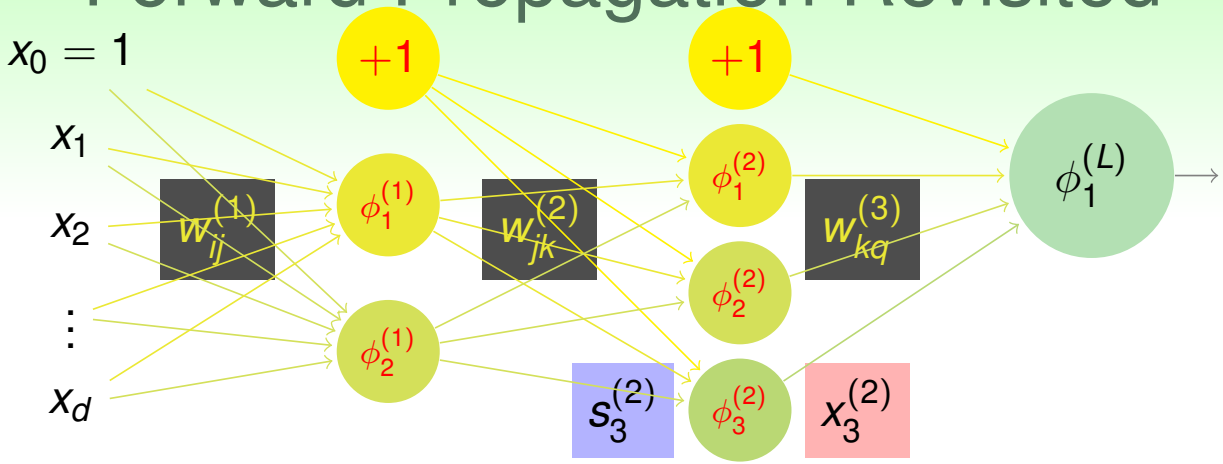
Challenges and Key Techniques for Deep Learning

- difficult **structural decisions**:
  - subjective with **domain knowledge**: like **convNet** for images
- high **model complexity**:
  - no big worries if **big enough data**
  - **regularization** towards noise-tolerant: like
    - **dropout** (tolerant when network corrupted)
    - **denoising** (tolerant when input corrupted)
- hard **optimization problem**:
  - **change optimization landscape**
  - **careful initialization**
  - **higher-order optimization** beyond SGD/backprop
- huge **computational complexity** (worsen with **big data**):
  - novel hardware/architecture: like **mini-batch with GPU**

IMHO, careful **regularization** and **optimization** are key techniques

Questions?

Forward Propagation Revisited



$d^{(0)}$-$d^{(1)}$-$d^{(2)}$-...-$d^{(L)}$ Neural Network (NNet)

$w_{ij}^{(\ell)}$: $\left(1 + d^{(\ell-1)}\right) \times \left(d^{(\ell)}\right)$ matrix before layer ℓ

score $s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{ij}^{(\ell)} \cdot x_i^{(\ell-1)}$, transformed $x_j^{(\ell)} = \phi_j^{(\ell)}\left(s_j^{(\ell)}\right)$

$\phi_j^{(\ell)}$: transformation (activation) function, e.g.

$\phi_1^{(L)} = /$ for regression;

$\phi_j^{(\ell)} = \tanh$ for traditional NNet

Backpropagation Revisited

$$
\begin{aligned}
\delta_j^{(\ell)} &= \frac{\partial e_n}{\partial s_j^{(\ell)}} \\
&= \sum_{k=1}^{d^{(\ell+1)}} \frac{\partial e_n}{\partial s_k^{(\ell+1)}} \frac{\partial s_k^{(\ell+1)}}{\partial x_j^{(\ell)}} \frac{\partial x_j^{(\ell)}}{\partial s_j^{(\ell)}} \\
&= \sum_k \left(\delta_k^{(\ell+1)}\right) \left(w_{jk}^{(\ell+1)}\right) \left(\phi'\left(s_j^{(\ell)}\right)\right) \\
&= \sum_k \left(\sum_m \left(\delta_m^{(\ell+2)}\right) \left(w_{km}^{(\ell+2)}\right) \phi'\left(s_k^{(\ell+1)}\right)\right) \left(w_{jk}^{(\ell+1)}\right) \left(\phi'\left(s_j^{(\ell)}\right)\right)
\end{aligned}
$$

$\delta_i^{(1)}$: $\delta_1^{(L)}$ multiplied by many $w_{??}^{(\ell+1)}$ and $\phi'(s_?^{(\ell)})$ for $\ell = 1, 2, \ldots, L-1$

The Vanishing Gradient Issue

gradient $\nabla_{ij}^{(\ell)} = x_i^{(\ell-1)} \cdot \delta_j^{(\ell)} = x_i^{(\ell-1)} \sum\sum\sum \delta_1^{(L)} www\phi'\phi'\phi'$

when $\phi = \tanh \Rightarrow x_i^{(\ell-1)} \in (-1, 1)$

- $\phi(s) \to \pm 1$ when $s \to \pm\infty$: saturation
- $\phi'(s) = 1 - \tanh^2(s)$
  - $\to 0$ when $s \to \pm\infty$
- vanishing gradient: $w_{??}^{(\ell)}$ too big $\Rightarrow |s|$ too big
  $\Rightarrow \phi'(s)$ too small $\Rightarrow \delta_?^{(1)}$ too small $\Rightarrow \nabla_{??}^{(1)}$ too small

vanishing gradient: early weights not updated
$\Rightarrow$ cannot train 'deep' network

Possible Cures for Vanishing Gradient

- better-behaved network
  - skip connection (escape some $w\phi'$)
- better-behaved weights
  - small-random initialization (to be discussed)
- better-behaved network + better-behaved weights
  - layer-wise pre-training (see MLTech Lecture 213)
- better-behaved (hidden) inputs
  - internal normalization (scale $x_j^{(\ell)}$)
- better-behaved gradient
  - gradient normalization (to be discussed)
- better-behaved activation functions (to be discussed)

vanishing/varying gradients: difficulty of deep learning optimization

Questions?

Rectified Linear Unit

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

- Rectified Linear Unit (ReLU):
  $\phi(s) = s$ for $s > 0$, 0 for $s = 0$, 0 for $s < 0$
  —continuous
- $\phi'(s) = 1$ for $s > 0$, 0 for $s < 0$
  —**less gradient vanishing** ($\approx$ 'half' of the time)
- $\phi'(s) =$ undefined for $s = 0$
  —floating point 0.0 hardly encountered, replace by 'sub-gradient' usually okay
- **sparse** network per example
- **fast** arithmetic computation

ReLU (with or without some $\tanh$): arguably the most widely-used for deep learning

Dead Neuron Issue

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

- $s < 0$: $\phi(s) = 0$ and $\phi'(s) = 0$ per example
- $s < 0$ for every example (dead neuron) if
  - very negative $w_{0?}^{(\ell)}$ (e.g. update from a very big gradient step)
  - all positive $x_i^{(0)}$ (e.g. images without shifting) + negative weights $w_{ij}^{(1)}$

dead neurons worrisome (but not always serious)

Leaky Rectified Linear Unit

$$\phi(s) = \max(s, 0.01s) = \max(s, 0) + 0.01 \min(s, 0)$$

- $s > 0$: $\phi(s) = s$ and $\phi'(s) = 1$ per example
- $s < 0$: $\phi(s) = 0.01s$ and $\phi'(s) = 0.01$ per example

less likely to have dead neurons, but why 0.01?

Parametric Rectified Linear Unit

$$\phi(\alpha, s) = \max(s, \alpha \cdot s)$$

- ReLU: $\alpha = 0$, Leaky ReLU: fixed α
- optimizable α:

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

$$= \sum_k \left(\delta_k^{(\ell+1)}\right) \left(w_{jk}^{(\ell+1)}\right) \left(\frac{\partial \phi(\alpha_j^{(\ell)}, s_j^{(\ell)})}{\partial \alpha_j^{(\ell)}}\right)$$

with $\frac{\partial \phi(\alpha,s)}{\partial \alpha} = s$ if $\alpha s > s$, or 0 otherwise.

'power' of deep learning: anything (loosely) differentiable is 'learnable'

Questions?

Summary

1. Distilling Implicit Features: Extraction Models

Lecture 14: From Neural Net. to Deep Learning

- Motivation

multi-layer for power with biological inspirations

- Neural Network Hypothesis

layered pattern extraction until linear hypothesis

- Neural Network Learning

backprop to compute gradient efficiently

- Deep Neural Network

difficult hierarchical feature extraction problem

- Vanishing Gradient Issue

saturated neuron cannot backprop error signal

- Modern Activation Functions

ReLU extensions with fewer saturating ends