# Machine Learning
# (機器學習)

## Lecture 14: Deep Learning Fundamentals

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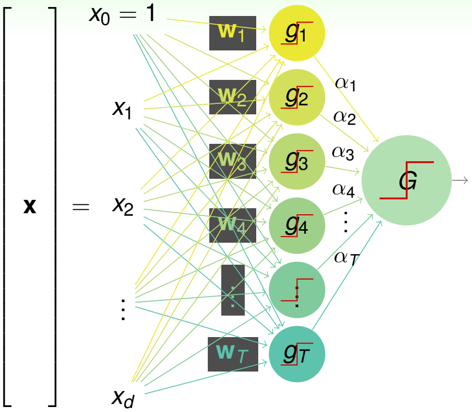
# Roadmap

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: Deep Learning Fundamentals

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

# Linear Aggregation of Perceptrons: Pictorial View

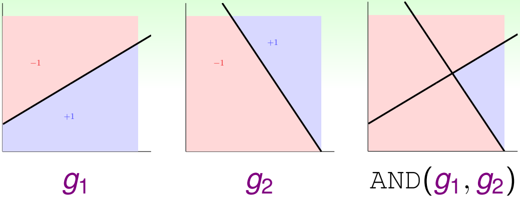


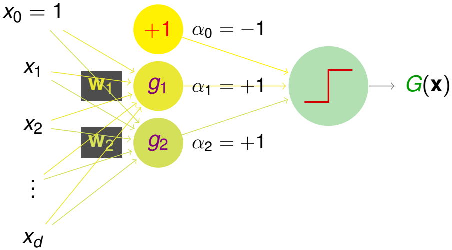

$$G(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t \underbrace{\text{sign}\left(\mathbf{w}_t^T \mathbf{x}\right)}_{g_t(\mathbf{x})}\right)$$

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

what boundary can $G$ **implement**?

# Logic Operations with Aggregation



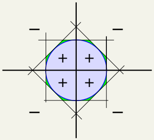




$G(\mathbf{x}) = \mathrm{sign}\left(-1 + g_1(\mathbf{x}) + g_2(\mathbf{x})\right)$

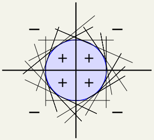
- $g_1(\mathbf{x}) = g_2(\mathbf{x}) = +1$ (TRUE): $G(\mathbf{x}) = +1$ (TRUE)
- otherwise: $G(\mathbf{x}) = -1$ (FALSE)
- $G \equiv \mathrm{AND}(g_1, g_2)$

OR, NOT can be **similarly implemented**

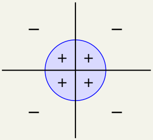
# Powerfulness and Limitation



8 perceptrons

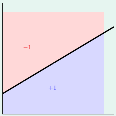


16 perceptrons

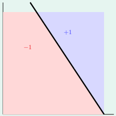


target boundary

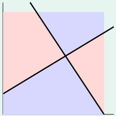
- 'convex set' hypotheses implemented: $d_{\text{VC}} \to \infty$, **remember? :-)**
- powerfulness: enough perceptrons $\approx$ **smooth boundary**




$g_1$




$g_2$



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

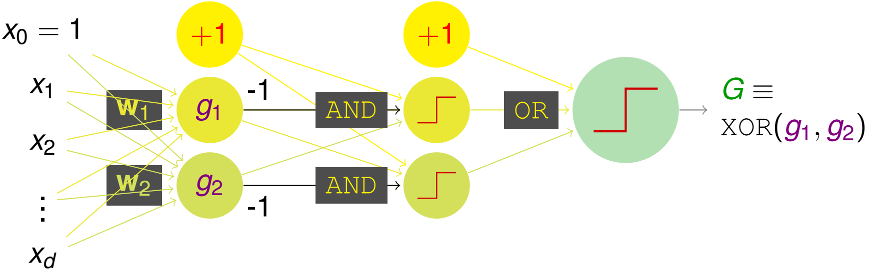
- limitation: XOR **not 'linear separable'** under $\phi(\mathbf{x}) = (g_1(\mathbf{x}), g_2(\mathbf{x}))$

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

# Multi-Layer Perceptrons: Basic Neural Network

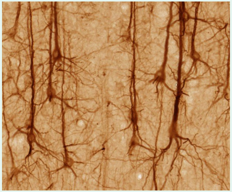
- non-separable data: can use more **transform**
- how about one more layer of **AND transform**?

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

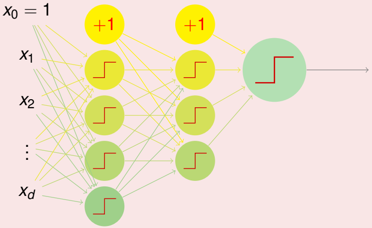



perceptron (simple)
$\Longrightarrow$ aggregation of perceptrons (powerful)
$\Longrightarrow$ **multi-layer perceptrons** (**more powerful**)

# Connection to Biological Neurons







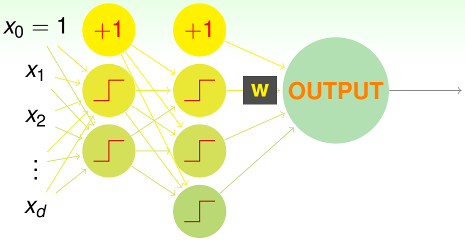





neural network: **bio-inspired** model

# Questions?

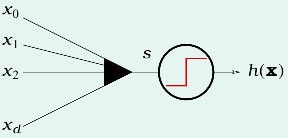
# Neural Network Hypothesis: Output




- **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

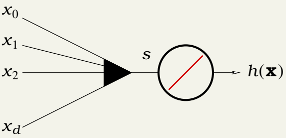
$h(\mathbf{x}) = \text{sign}(s)$




err = 0/1

## linear regression

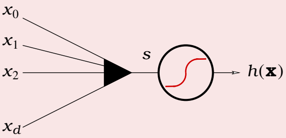
$h(\mathbf{x}) = s$




err = squared

## logistic regression

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

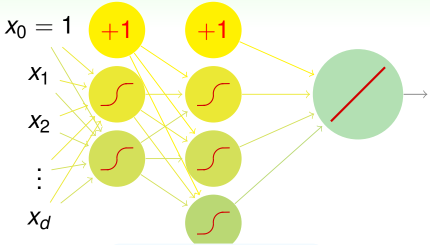


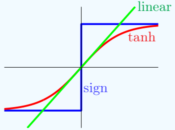

err = cross-entropy

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

# Neural Network Hypothesis: Transformation

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

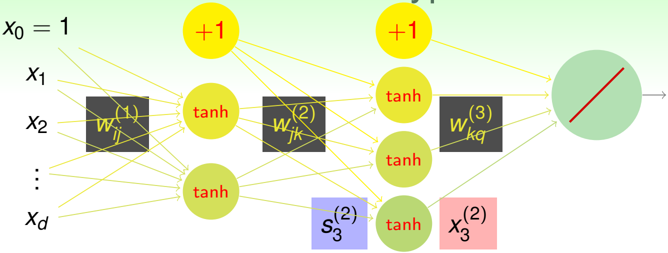



$$\tanh(s) = \frac{\exp(s) - \exp(-s)}{\exp(s) + \exp(-s)} = 2\theta(2s) - 1$$

will discuss with tanh first

# Neural Network Hypothesis



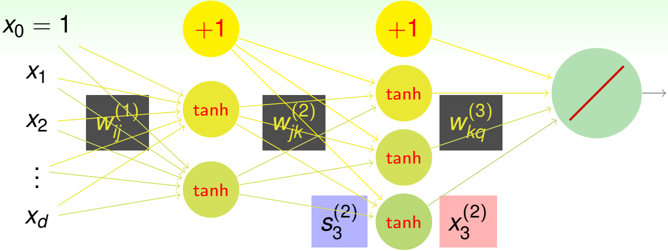

## $d^{(0)}$-$d^{(1)}$-$d^{(2)}$-$\cdots$-$d^{(L)}$ Neural Network (NNet)

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

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

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



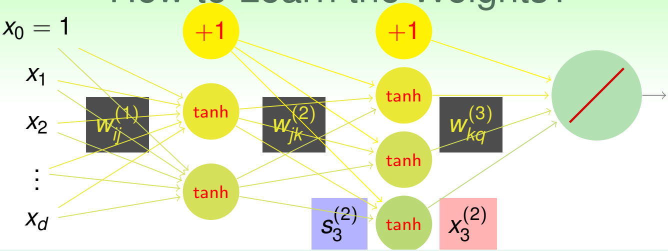

- each layer: **transformation** to be **learned** from data
- $\phi^{(\ell)}(\mathbf{x}) = \tanh\left(\begin{bmatrix} \sum_{i=0}^{d^{(\ell-1)}} w_{i1}^{(\ell)} x_i^{(\ell-1)} \\ \vdots \end{bmatrix}\right)$

  —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) $(0 \le i \le d^{(L-1)})$**

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

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

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

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

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

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

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

$\delta_j^{(\ell)}$ 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: $w_{ij}^{(\ell)} \leftarrow w_{ij}^{(\ell)} - \eta x_i^{(\ell-1)} \delta_j^{(\ell)}$

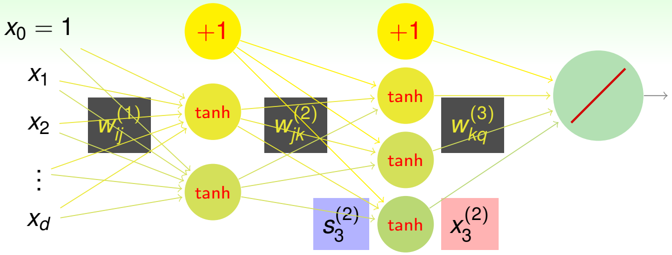
return $g_{\text{NNET}}(\mathbf{x}) = \left( \cdots \tanh\left( \sum_j w_{jk}^{(2)} \cdot \tanh\left( \sum_i w_{ij}^{(1)} x_i \right) \right) \right)$

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

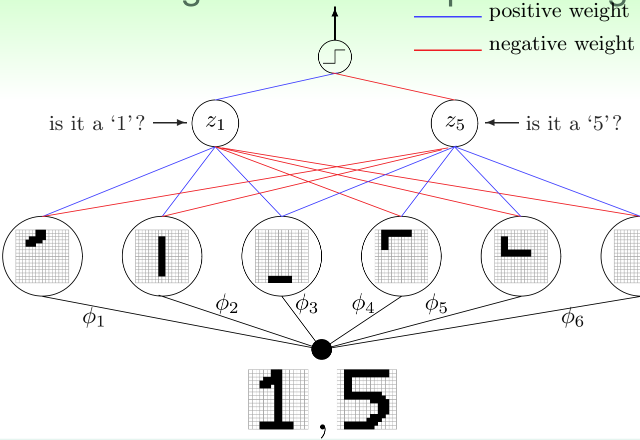
- more **efficient** to train (◯)
- **simpler** structural decisions (◯)
- theoretically **powerful enough** (◯)

## 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/**...

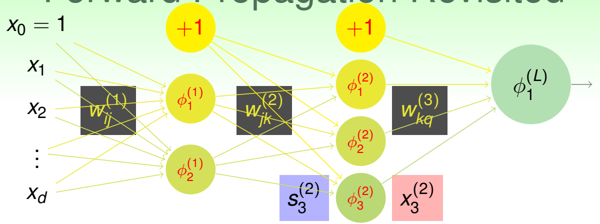
# Challenges and Key Techniques for Deep Learning

- 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




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

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

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

$\phi_j^{(\ell)}$: 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 $\alpha$
- optimizable $\alpha$:

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

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

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: Deep Learning Fundamentals

- Motivation
  multi-layer for power w/ biological inspirations
- Neural Network Hypothesis
  layered pattern extraction + linear hypothesis
- Neural Network Learning
  backprop to compute gradient efficiently
- Deep Neural Network
  many-layer feature extraction
- Vanishing Gradient Issue
  saturated neuron cannot backprop error
- Modern Activation Functions
  ReLU extensions with fewer saturating ends