CS 559 Machine Learning

Lecture 13: Neural Networks

Ping Wang
Department of Computer Science
Stevens Institute of Technology

STEVENS INSTITUTE *of* TECHNOLOGY
THE INNOVATION UNIVERSITY®

Today’s Lecture

- Summary and review
- Neural networks
- Implementation

Reviews

- Unsupervised learning:
  - Density estimation
  - K-means
  - Gaussian mixture models
  - Graphical models
- Supervised learning:
  - Classification
  - Regression

Supervised Learning

$$\underbrace{w^T x + b}_{\text{score}}$$

	Classification	Regression
Predictor	Sign	Score
Relate to y	Margin(score, y)	Residual(score,y)
Loss	Zero-one, hinge, logistic	Squared, absolute
Algorithm	Gradient descent	Gradient descent

Review: Optimization Problem

Minimize Training Loss

$$\min_{w \in \mathbb{R}^d} TrainLoss(w) = \frac{1}{N} \sum_{n=1}^{N} L(x_n, y_n, w)$$

Review: Optimization Problem

- Gradient descent:

$$w \leftarrow w - \boxed{\eta} * \boxed{\nabla_w TrainLoss(w)}$$

Step size **Gradient**

$\nabla_w TrainLoss(w)$ denotes the gradient of the (average) total training loss with respect to w

- Stochastic Gradient Descent (SGD):

For each $(x, y) \in D_{train}$,

$$w \leftarrow w - \eta \nabla_w Loss(x, y, w)$$

$\nabla_w Loss(x, y, w)$ denotes the gradient of one example loss with respect to w.

Neural Networks

Everything Has AI Now!

Image Classification

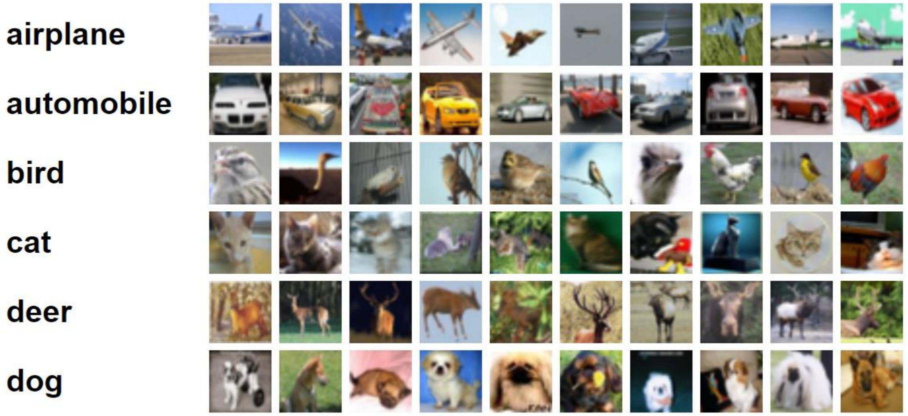


Image Captioning

Speech Recognition

Machine Translation

Deep Learning Breakthrough

- Large high-quality labeled data sets
- Parallel computing with GPUs
- Backprop-friendly activation functions (ReLu)
- Improved model architectures
- Software platforms
- New regularization techniques
- Robust optimization (momentum, RMSprop, ADAM)

2016: YEAR of Deep Learning (and AI)

- DeepMind's AlphaGo beat South Korean professional Go player Lee Sedol.
- Out of five matches, Lee lost 4-1.

2019: Turing Award in Artificial Intelligence

Turing Award Won by 3
Pioneers in Artificial Intelligence

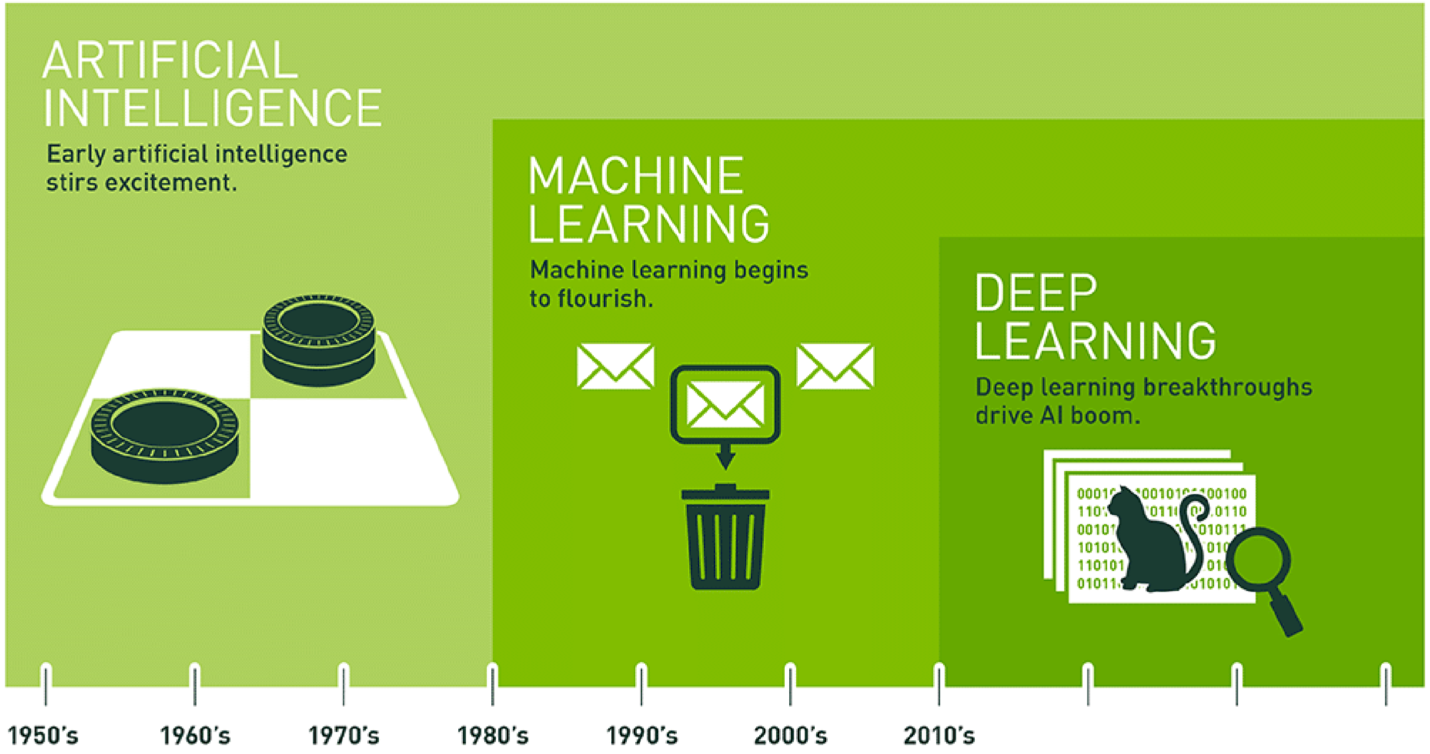
From left, Yann LeCun, Geoffrey Hinton and Yoshua Bengio. The researchers worked on key developments for neural networks, which are reshaping how computer systems are built.

https://www.nytimes.com/2019/03/27/technology/turing-award-ai.html

Myths about Deep Learning

- Deep learning mimics human brain.
  - Deep learning is only “loosely” inspired by the workings of the human brain.
- Deep learning is “magical” and the rest of machine learning models are completely “useless”.
  - The main power of deep learning comes from the fact that deep models can learn efficient representations.
- Any problem can be solved using deep learning.
  - Only in the presence of sufficient data to learn from.
- Deep learning replaces human jobs.
  - It creates more new interesting jobs for humans than it takes.
- Many others …

Deep Learning is Only a Small Part!!



Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

Figure: Nvidia blog about “What’s the Difference Between Artificial Intelligence, Machine Learning and Deep Learning?”.

What is Neural Network?

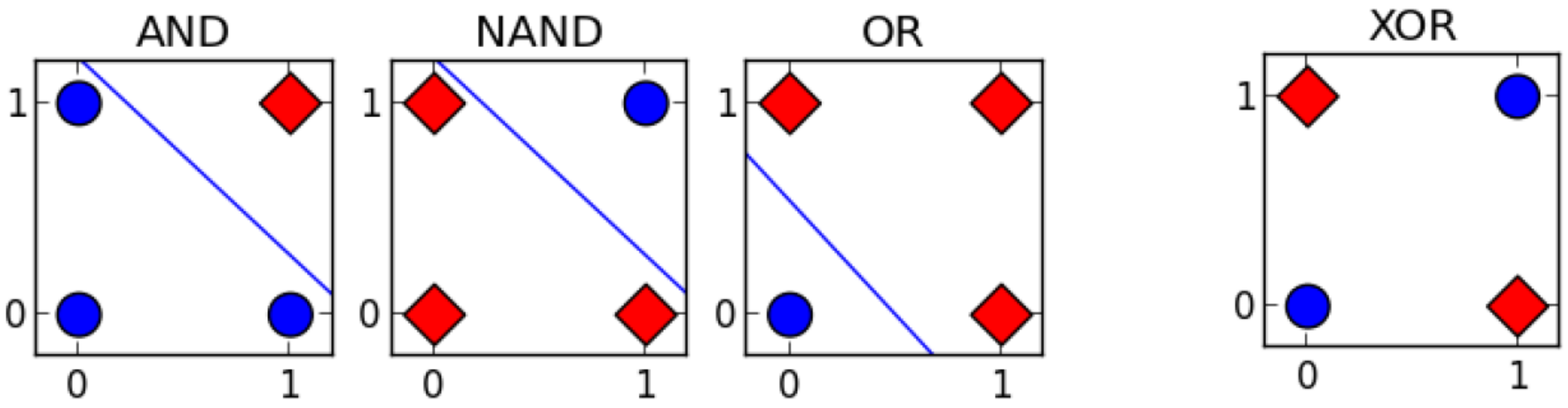
- Often associated with biological devices (brains), electronic devices, or network diagrams;
- But the best conceptualization for this presentation is none of these: think of a neural network as a mathematical function.

The pros of Neural Network

- Successfully used on a variety of domains: computer vision, speech recognition, gaming etc.
- Can provide solutions to very complex and nonlinear problems.
- If provided with sufficient amount of data, can solve classification and forecasting problems accurately and easily.
- Once trained, prediction is fast.

Motivation of Neural Network

- Perceptron: First learning algorithm for neural networks. (Frank Rosenblatt, 1957)
- Limitations: Marvin Minsky and Seymour Papert, “Perceptrons" 1969: The perceptron can only solve problems with linearly separable classes.
  - The functions can be drawn in 2-dim graph and a single straight line separates values in two parts.
  - The perceptron cannot model the non-linearly separable functions: Logical XOR function (computes the logical exclusive).

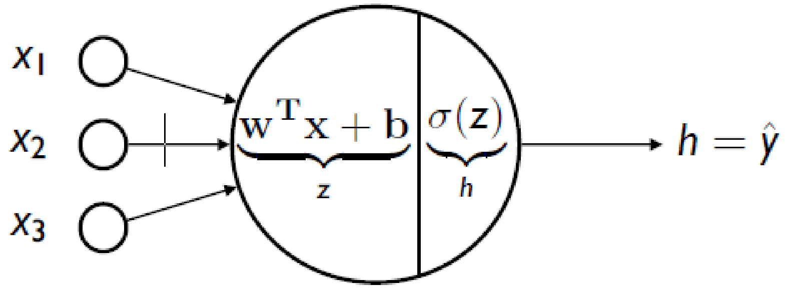


Motivation of Neural Network

- Allow to learn nonlinearly separable transformations from input to output.
- A single hidden layer allows to compute any input/output transformation.

No Hidden Units: Logistic Regression

- Sigmoid activation function:



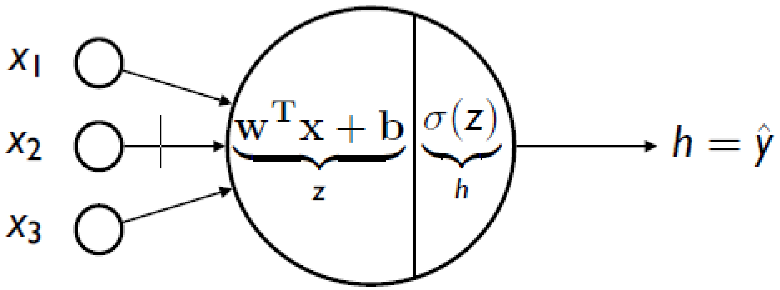
- Output score: sigmoid function $\hat{y} = \sigma(w^T x + b)$
- Recall sigmoid function:

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

Derivative:$\sigma'(z) = \sigma(z)(1 - \sigma(z))$

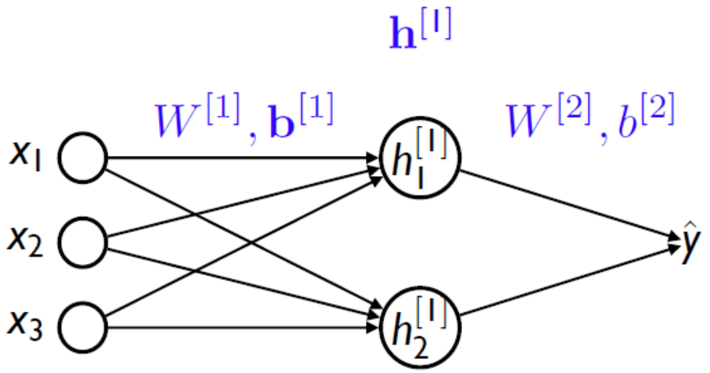
Learning Algorithm: No hidden units

- Logistic loss: $J(x, y, w) = -y\, log\, \hat{y} - (1 - y) \log(1 - \hat{y})$
- $\hat{y} = \frac{1}{1+e^{-w^T x}} = \sigma(w^T x)$
- $\frac{\partial \hat{y}}{\partial w_i} = \hat{y}(1\text{-}\ \hat{y})x_i$
- $\frac{\partial J}{\partial w_i} = \frac{\partial J}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_i} = (\hat{y} - y)x_i$
- Applying gradient descent (η is the learning rate):
- Element (feature) operation: $w_i^{t+1} = w_i^t - \eta \frac{\partial J}{\partial w_i}$
- Vector operation: $w^{t+1} = w^t - \eta \frac{\partial J}{\partial w}$



Neural Networks: One Hidden Layer

- One hidden layer:



- Hidden layer representation:

$$z_1^{[1]} = \mathbf{w}_1^{[1]T}\mathbf{x} + b_1^{[1]}, h_1^{[1]} = \sigma(z_1^{[1]})$$

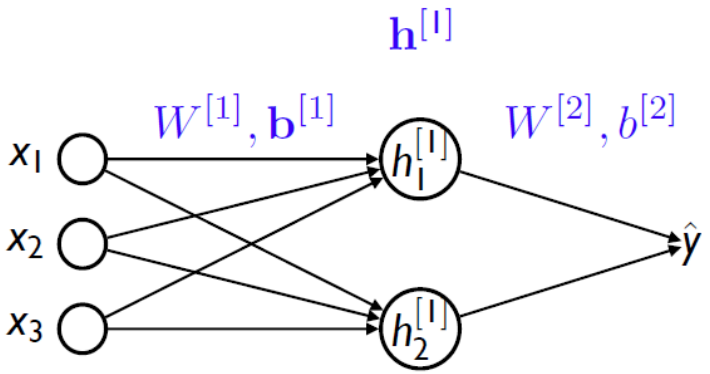
$$z_2^{[1]} = \mathbf{w}_2^{[1]T}\mathbf{x} + b_2^{[1]}, h_2^{[1]} = \sigma(z_2^{[1]})$$

$\Rightarrow$

$$\mathbf{z}^{[1]} = \underbrace{W^{[1]}}_{2\times 3}\underbrace{\mathbf{x}}_{3\times 1} + \underbrace{\mathbf{b}^{[1]}}_{2\times 1}$$

Neural Networks: One Hidden Layer

- One hidden layer:



- Output layer:

$$z^{[2]} = \underbrace{W^{[2]}}_{1\times 2}\,\underbrace{\mathbf{h}^{[1]}}_{2\times 1} + b^{[2]}$$

$$\hat{y} = \sigma(z^{[2]})$$

Neural Networks: One Hidden Layer

- Think of intermediate hidden units as learned features of a linear predictor.
- Feature learning: manually specified features:

$$\mathbf{x}$$

automatically learned features:

$$h(\mathbf{x}) = [h_1(\mathbf{x}), \dots, h_k(\mathbf{x})]$$

Loss Minimization

- Optimization problem

$$TrainLoss(W, b) = \frac{1}{|D_{train}|} \sum_{(x,y) \in D_{train}} L(x, y, W, b)$$

$$L(x, y, W, b) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$\hat{y} = h^{[2]}$$

- Goal: compute gradient

$$\nabla_{W,b} L(W, b)$$

Stochastic Gradient Descent

- Goal: compute gradient

$$\nabla_{W,b} L(W, b)$$

- Repeat, given a sample $(x^{(i)}, y^{(i)})$

$$dW^{[1]} = \frac{\partial L}{\partial W^{[1]}}, \qquad W^{[1]} = W^{[1]} - \eta dW^{[1]}$$

$$db^{[1]} = \frac{\partial L}{\partial b^{[1]}}, \qquad b^{[1]} = b^{[1]} - \eta db^{[1]}$$

$$dW^{[2]} = \frac{\partial L}{\partial W^{[2]}}, \qquad W^{[2]} = W^{[2]} - \eta dW^{[2]}$$

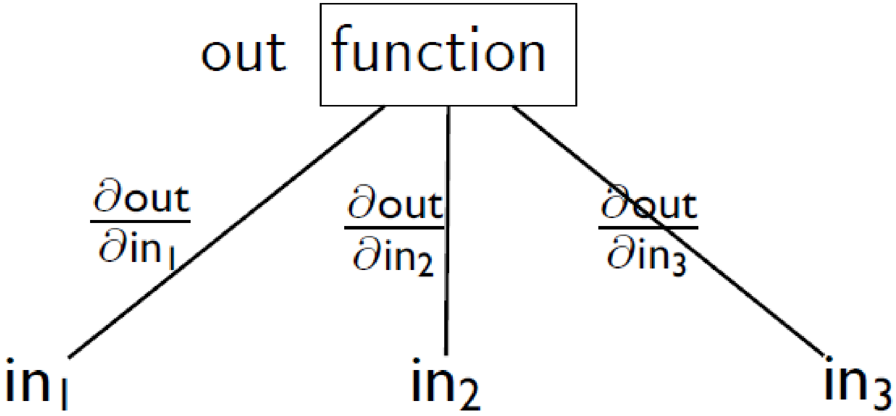
$$db^{[2]} = \frac{\partial L}{\partial b^{[2]}}, \qquad b^{[2]} = b^{[2]} - \eta db^{[2]}$$

Approach

- Mathematical: chain rule
- Next: visualize the computation using a computation graph
- Advantages:
  - Avoid long equations
  - Reveal structure of computations (modularity, efficiency, dependencies)

Functions As Boxes

- Partial derivatives (gradients): how much does the output change if an input changes?

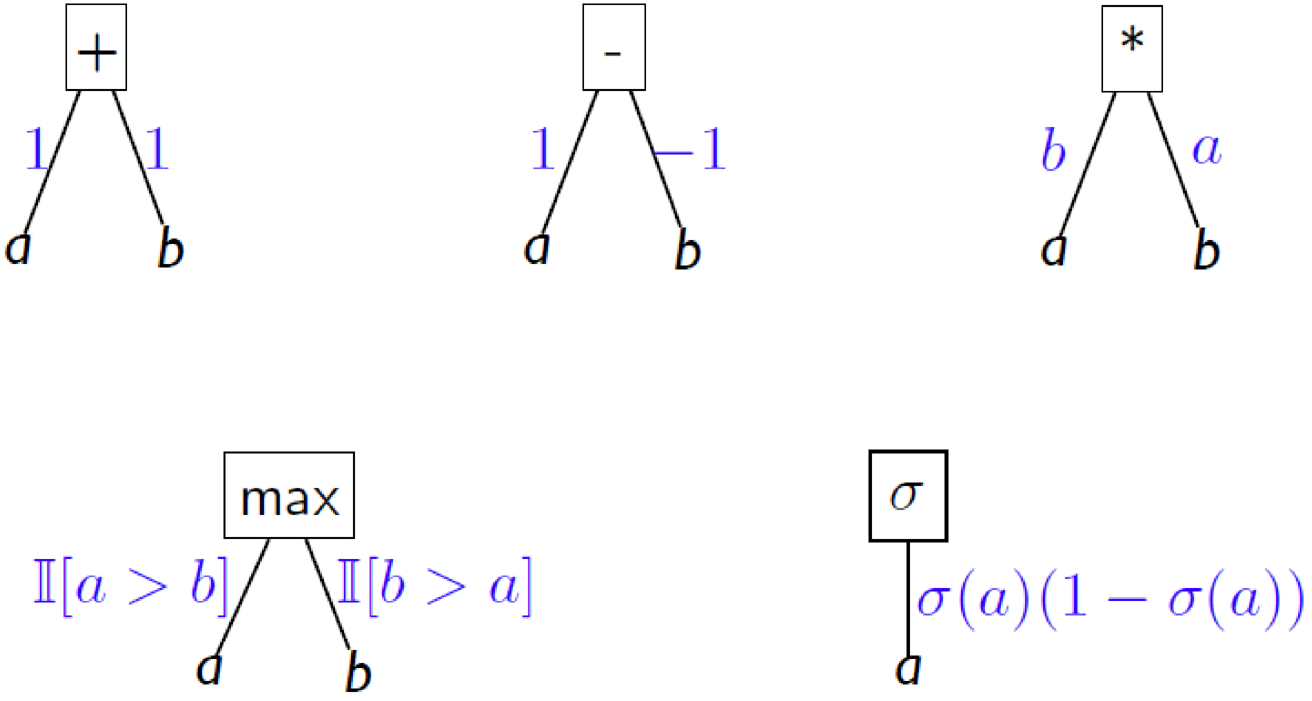


- Example:

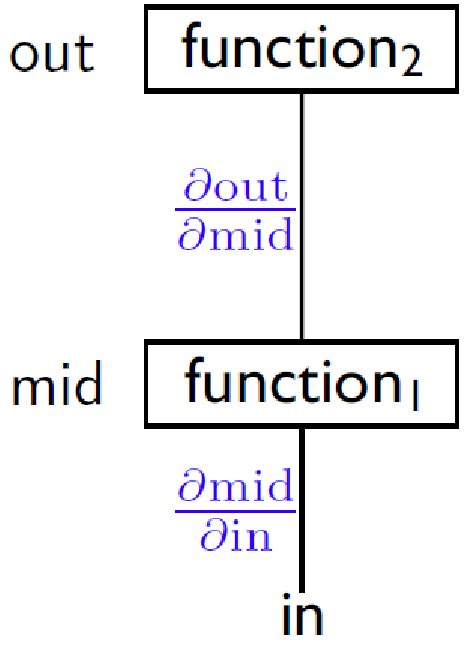
$$out = 2in_1 + in_2 in_3$$
$$2in_1 + (in_2 + \epsilon)in3 = out + \epsilon in3$$

- Partial derivatives (gradients): a measure of sensitivity

Basic Building Blocks



Composing Functions



- Chain rule:

$$\frac{\partial out}{\partial in} = \frac{\partial out}{\partial mid}\frac{\partial mid}{\partial in}$$

Chain Rule

Case 1

$$y = g(x) \qquad z = h(y)$$

$$\Delta x \to \Delta y \to \Delta z \qquad\qquad \frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

Case 2

$$x = g(s) \qquad y = h(s) \qquad z = k(x, y)$$

$$\begin{tikzcd} & \Delta x \arrow[dr] & \\ \Delta s \arrow[ur] \arrow[dr] & & \Delta z \\ & \Delta y \arrow[ur] & \end{tikzcd}$$

$$\frac{\partial z}{\partial s} = \frac{\partial z}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial z}{\partial y}\frac{\partial y}{\partial s}$$

Back Propagation

- Goal: learn the weights so that the loss (error) is minimized.
- It provides an efficient procedure to compute derivatives.
- For a fixed sample (x, y), we want to learn $\hat{y} = f(x)$
- Negative Log-likelihood over input $x_n$is $L_n = -y_n \log \hat{y}_n - (1 - y_n) \log(1 - \hat{y}_n)$
- Total error of training examples is $E = \sum_n L_n$
- Backpropagation: an efficient way to compute the gradients of the network parameters.

Back Propagation

$$
\begin{matrix} W^{[1]}, \mathbf{b}^{[1]} \\ \mathbf{x} \end{matrix} \rightarrow \underbrace{W^{[1]}\mathbf{x} + \mathbf{b}^{[1]}}_{\mathbf{z}^{[1]}} \; \underbrace{\sigma(\mathbf{z}^{[1]})}_{\mathbf{h}^{[1]}} \longrightarrow \underbrace{W^{[2]}\mathbf{h}^{[1]} + \mathbf{b}^{[2]}}_{\mathbf{z}^{[2]}} \; \underbrace{\sigma(\mathbf{z}^{[2]})}_{\mathbf{h}^{[2]} = \hat{\mathbf{y}}} \longrightarrow L(\hat{y}, y)
$$

- Loss function for each data sample: $L_n = -y_n \log \hat{y}_n - (1 - y_n) \log(1 - \hat{y}_n)$

$$
\frac{\partial L}{\partial W^{[1]}} = \frac{\partial L}{\partial z^{[1]}} \frac{\partial z^{[1]}}{\partial W^{[1]}}, \qquad \frac{\partial L}{\partial b^{[1]}} = \frac{\partial L}{\partial z^{[1]}} \frac{\partial z^{[1]}}{\partial b^{[1]}}
$$

$$
\frac{\partial L}{\partial W^{[2]}} = \frac{\partial L}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial W^{[2]}}, \qquad \frac{\partial L}{\partial b^{[2]}} = \frac{\partial L}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial b^{[2]}}
$$

Back Propagation

$$\mathbf{W}^{[1]}, \mathbf{b}^{[1]} \rightarrow \underbrace{\mathbf{W}^{[1]}\mathbf{x} + \mathbf{b}^{[1]}}_{\mathbf{z}^{[1]}} \underbrace{\sigma(\mathbf{z}^{[1]})}_{\mathbf{h}^{[1]}} \rightarrow \underbrace{\mathbf{W}^{[2]}\mathbf{h}^{[1]} + \mathbf{b}^{[2]}}_{\mathbf{z}^{[2]}} \underbrace{\sigma(\mathbf{z}^{[2]})}_{\mathbf{h}^{[2]}=\hat{\mathbf{y}}} \rightarrow L(\hat{y}, y)$$

$$\mathbf{x} \rightarrow$$

$$\frac{\partial L}{\partial z^{[2]}} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{[2]}} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})} \hat{y}(1-\hat{y}) = \hat{y} - y$$

$$\frac{\partial L}{\partial \hat{y}} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})}$$

$$\frac{\partial z^{[2]}}{\partial W^{[2]}} = h^{[1]}, \quad \frac{\partial z^{[2]}}{\partial b^{[2]}} = 1$$

$$\frac{\partial L}{\partial W^{[2]}} = \frac{\partial L}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial W^{[2]}} = (\hat{y} - y)h^{[1]}$$

$$\frac{\partial L}{\partial b^{[2]}} = \frac{\partial L}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial b^{[2]}} = \hat{y} - y$$

Back Propagation

$$\begin{matrix} W^{[1]}, \mathbf{b}^{[1]} \\ \mathbf{x} \end{matrix} \rightarrow \underbrace{W^{[1]}\mathbf{x} + \mathbf{b}^{[1]}}_{\mathbf{z}^{[1]}} \; \underbrace{\sigma(\mathbf{z}^{[1]})}_{\mathbf{h}^{[1]}} \longrightarrow \underbrace{W^{[2]}\mathbf{h}^{[1]} + \mathbf{b}^{[2]}}_{\mathbf{z}^{[2]}} \; \underbrace{\sigma(\mathbf{z}^{[2]})}_{\mathbf{h}^{[2]}=\hat{\mathbf{y}}} \longrightarrow L(\hat{y}, y)$$

$$\frac{\partial L}{\partial z^{[1]}} = \frac{\partial L}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial z^{[1]}} = (\hat{y} - y) W^{[2]} h^{[1]} (1 - h^{[1]})$$

$$\frac{\partial z^{[2]}}{\partial z^{[1]}} = \frac{\partial z^{[2]}}{\partial h^{[1]}} \frac{\partial h^{[1]}}{\partial z^{[1]}} = W^{[2]} h^{[1]} (1 - h^{[1]})$$

$$\frac{\partial z^{[1]}}{\partial W^{[1]}} = \mathrm{x}, \quad \frac{\partial z^{[1]}}{\partial b^{[1]}} = 1$$

$$\frac{\partial L}{\partial W^{[1]}} = \frac{\partial L}{\partial z^{[1]}} \frac{\partial z^{[1]}}{\partial W^{[1]}} = (\hat{y} - y) W^{[2]} h^{[1]} (1 - h^{[1]}) \mathrm{x}$$

$$\frac{\partial L}{\partial b^{[1]}} = \frac{\partial L}{\partial z^{[1]}} \frac{\partial z^{[1]}}{\partial b^{[1]}} == (\hat{y} - y) W^{[2]} h^{[1]} (1 - h^{[1]})$$

Summary: Computing Derivatives

- Forward propagation:

$$z^{[1]} = W^{[1]}x + b^{[1]}$$

$$h^{[1]} = \sigma(z^{[1]})$$

$$z^{[2]} = W^{[2]}h^{[1]} + b^{[2]}$$

$$\hat{y} = h^{[2]} = \sigma(z^{[2]})$$

- Backpropagation:

$$\frac{\partial L}{\partial z^{[2]}} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{[2]}} = \hat{y} - y$$

$$\frac{\partial L}{\partial \hat{y}} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})}$$

$$\frac{\partial z^{[2]}}{\partial W^{[2]}} = h^{[1]}, \ \frac{\partial z^{[2]}}{\partial b^{[2]}} = 1$$

$$\frac{\partial L}{\partial z^{[1]}} = \frac{\partial L}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial z^{[1]}} = (\hat{y} - y)W^{[2]}h^{[1]}(1 - h^{[1]})$$

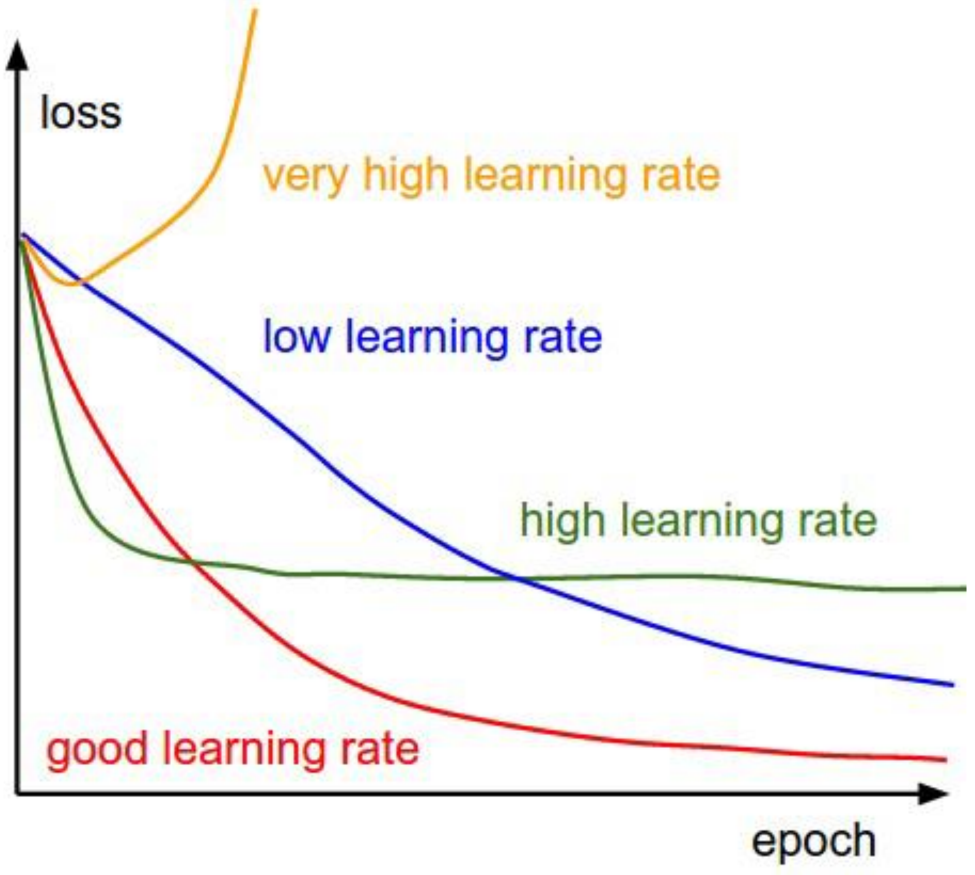
$$\frac{\partial z^{[2]}}{\partial z^{[1]}} = \frac{\partial z^{[2]}}{\partial h^{[1]}} \frac{\partial h^{[1]}}{\partial z^{[1]}} = W^{[2]}h^{[1]}(1 - h^{[1]})$$

$$\frac{\partial z^{[1]}}{\partial W^{[1]}} = \mathrm{x}, \ \frac{\partial z^{[1]}}{\partial b^{[1]}} = 1$$

Learning Rate

Set the learning rate carefully:

- If there are more than 3 parameters, it is hard to visualize the loss w.r.t the parameters.
- But you can visualize the loss w.r.t the # of parameter updates (epoch).
  - If the loss increases, we need to decrease the value of the learning rate.
  - If the loss is decreasing at a very slow rate, we need to increase the value of the learning rate.

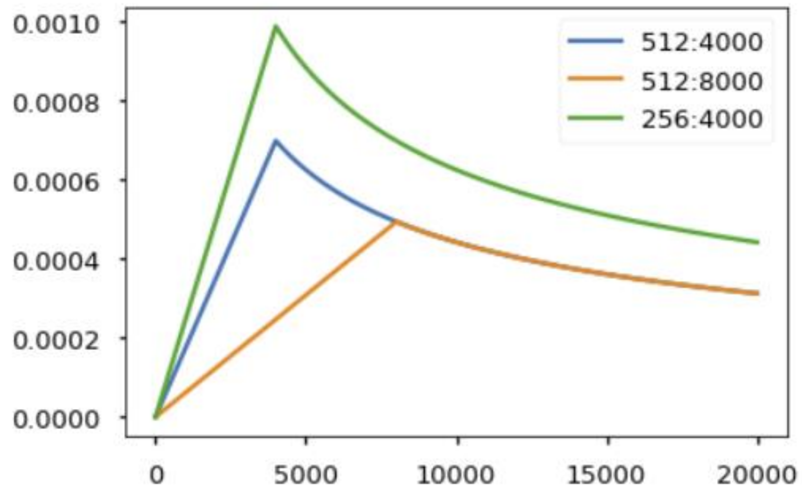


Adaptive Learning Rates

- Popular & Simple Idea: Reduce the learning rate by some factor every few epochs.
  - At the beginning, we are far from the destination, so we use larger learning rate
  - After several epochs, we are close to the destination, so we reduce the learning rate
  - For example: $\frac{1}{t}$ decay, $\eta^{(t)} = \frac{\eta}{\sqrt{t+1}}$
- Learning rate cannot be one-size-fits-all
  - Giving different parameters different learning rates
  - Adagrad, RMSprop, Adam etc

Warm-up Learning Rate

- **Motivation**: At the beginning of training, the weights of the model are randomly initialized. If you choose a larger learning rate, it may lead to instability (oscillation) of the model.
- **Solution**: At the beginning of training, it uses a small learning rate to train some epochs or steps, and then modifies it to the preset learning for training.
- The model can gradually become stable, which makes the convergence speed of the model become faster and the model effect is better.

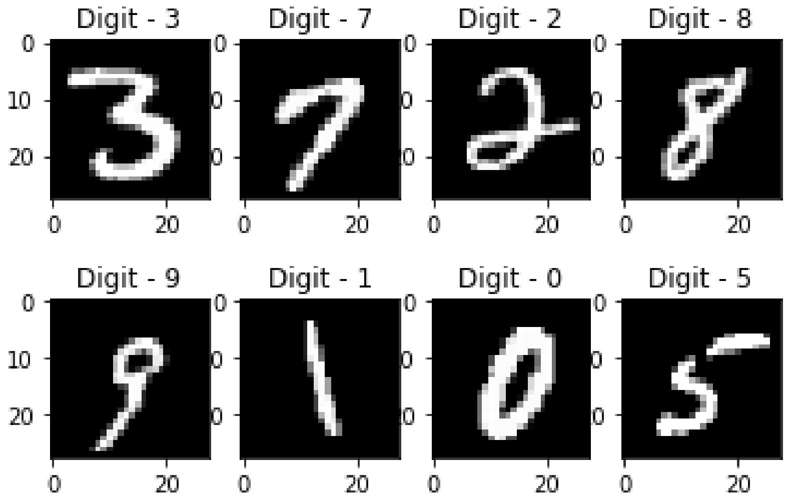


Optimization

- Gradient descent
- Stochastic gradient descent: faster and better
- Mini-batch gradient descent

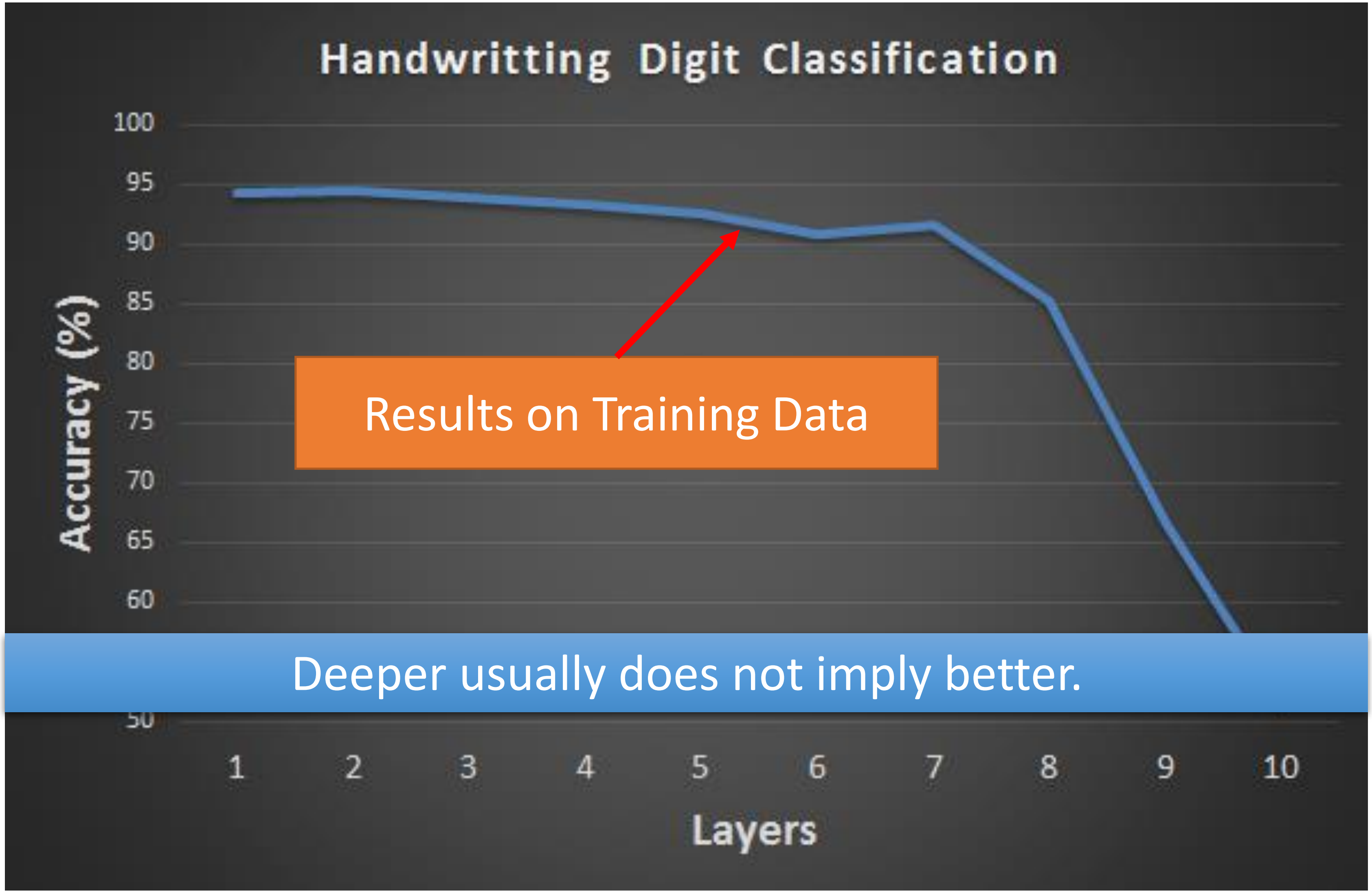
Comparisons

- Handwriting Digit Classification

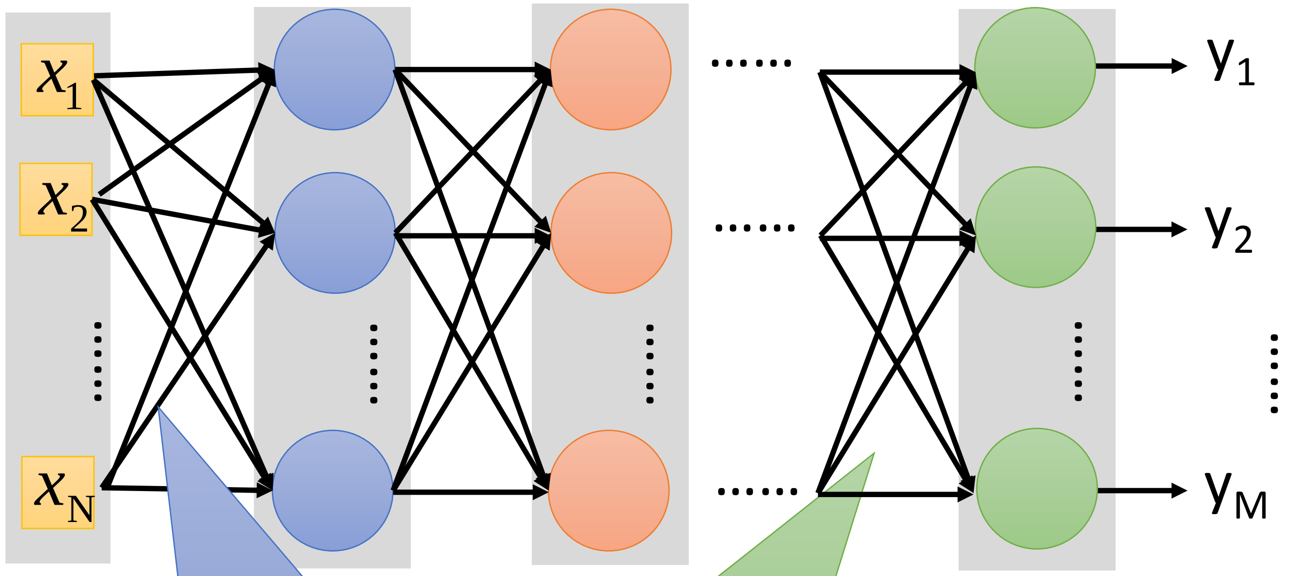


Gradient Descent

Hard to get the power of Deep …



Vanishing Gradient Problem



Smaller gradients

Learn very slow

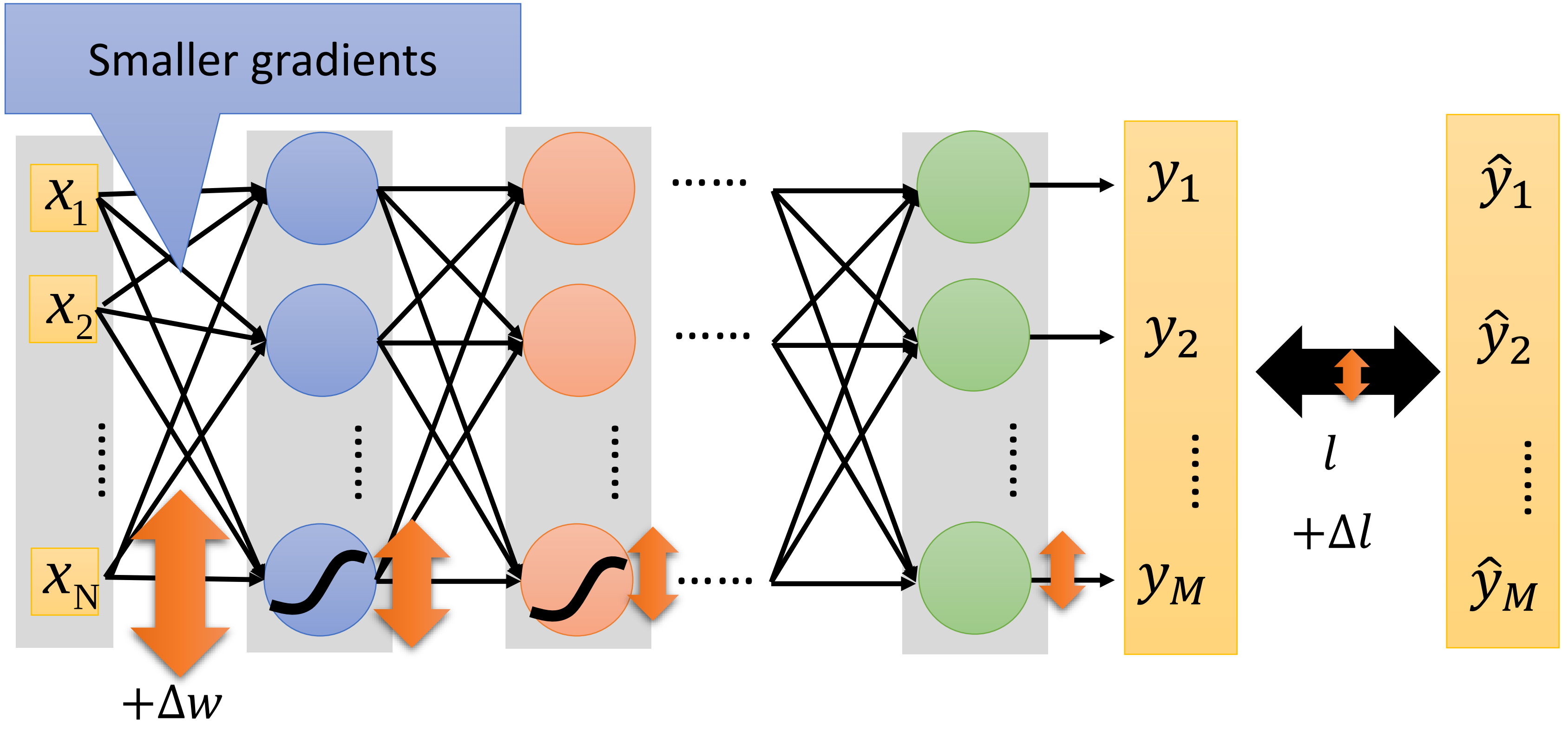
Almost random

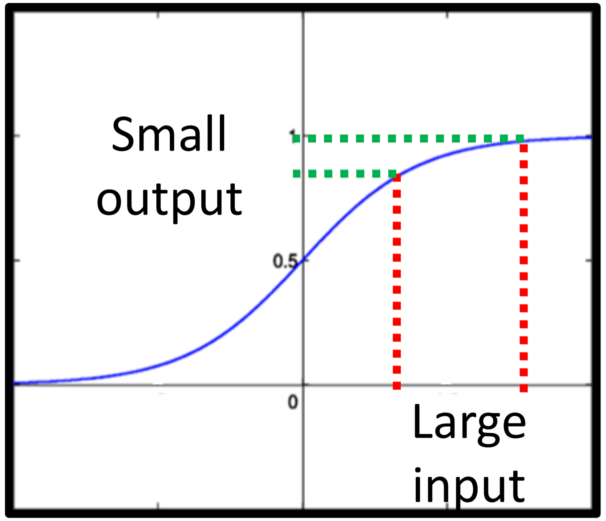
Larger gradients

Learn very fast

Already converge

Vanishing Gradient Problem

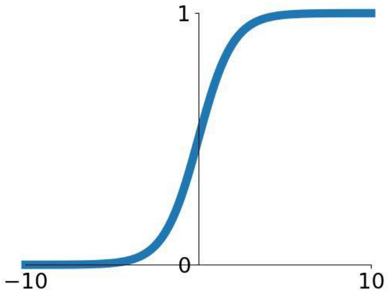




Activation Functions

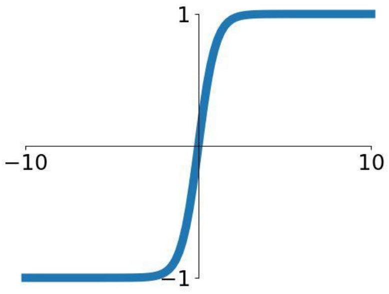
Sigmoid

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



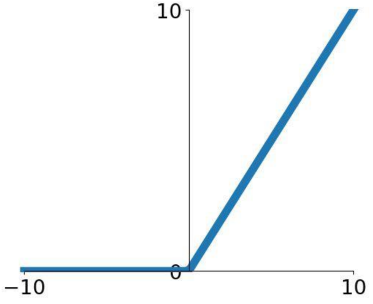
tanh

$$\tanh(x)$$



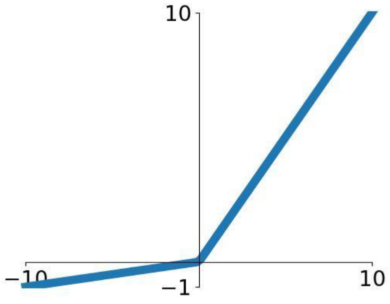
ReLU

$$\max(0, x)$$



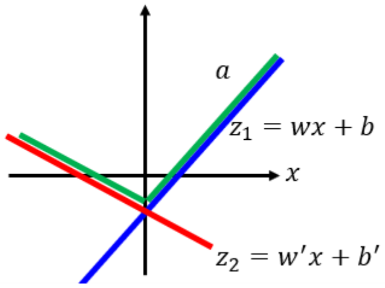
Leaky ReLU

$$\max(0.1x, x)$$



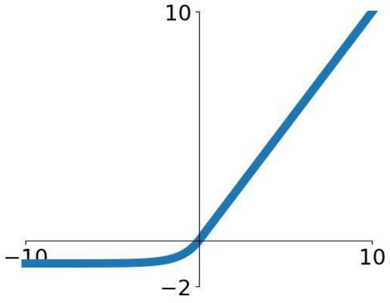
Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

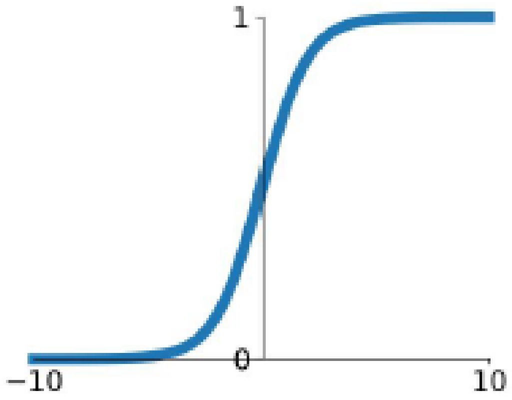


ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$

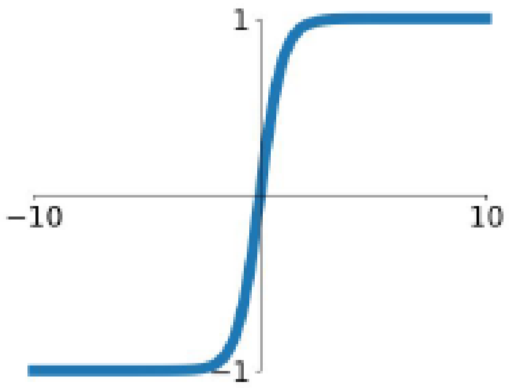


Sigmoid and tanh



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

1. Vanishing gradient problem
2. The output of sigmoid function is not zero centered.
3. It is expensive to calculate e^{-x}.

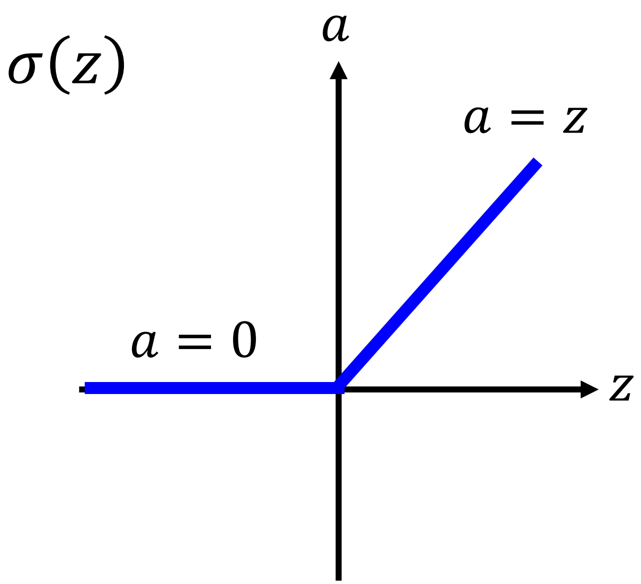


$\tanh(x)$

1. The output is zero centered.
2. Suffer from vanishing gradient problem.

ReLU

- Rectified Linear Unit (ReLU)

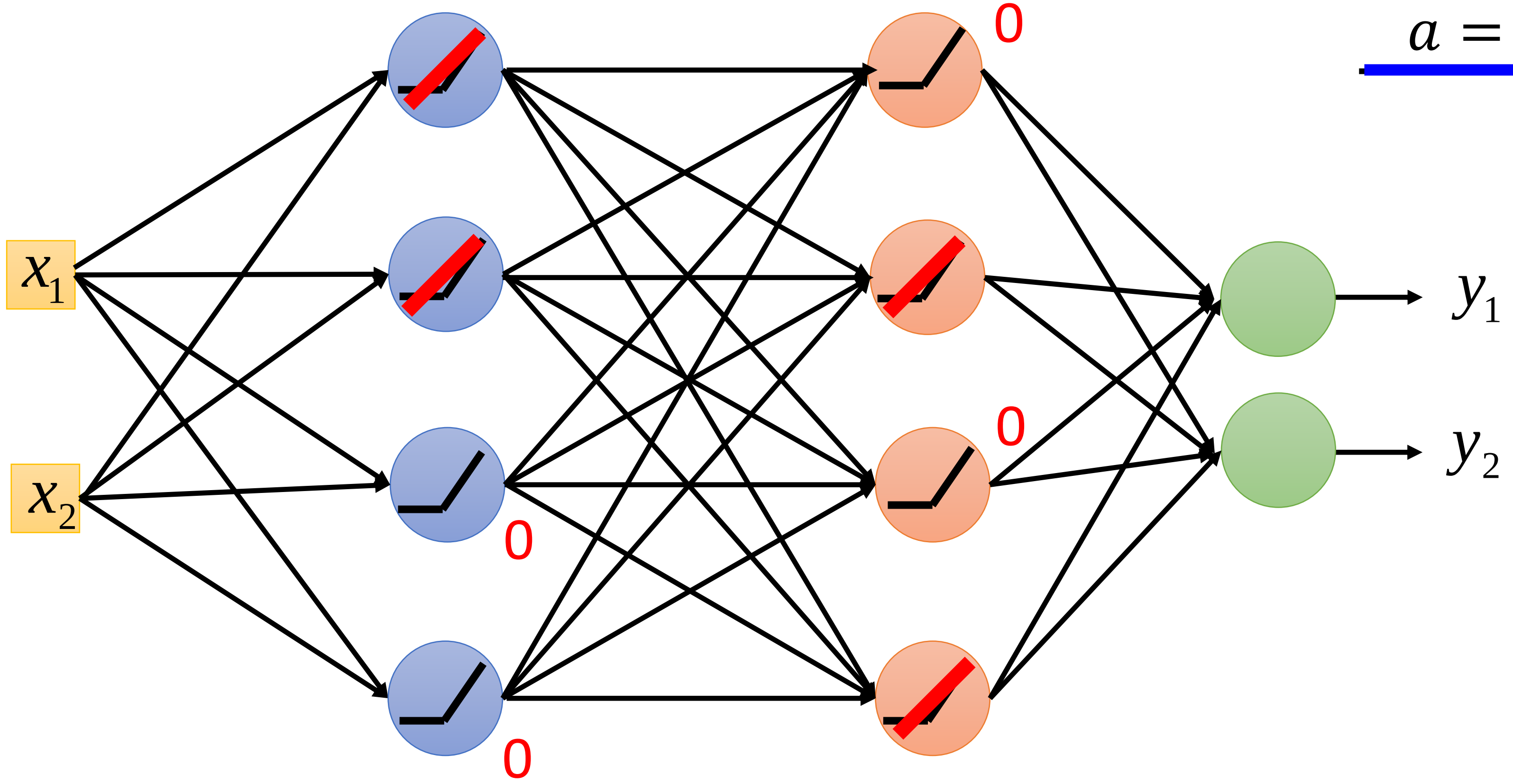


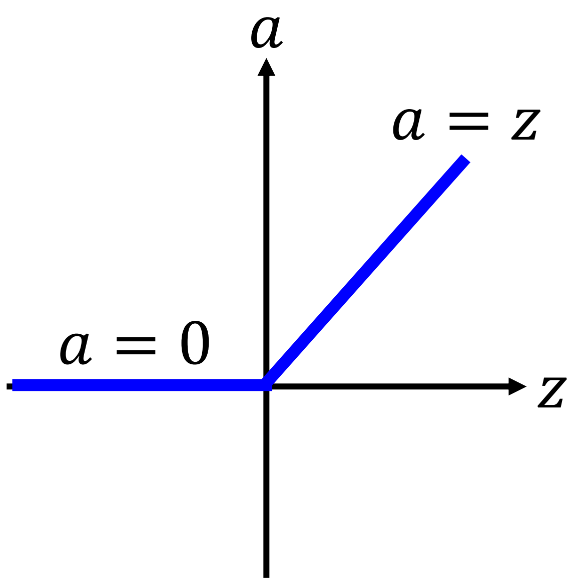
[Xavier Glorot, AISTATS'11]
[Andrew L. Maas, ICML'13]
[Kaiming He, arXiv'15]

Reason:

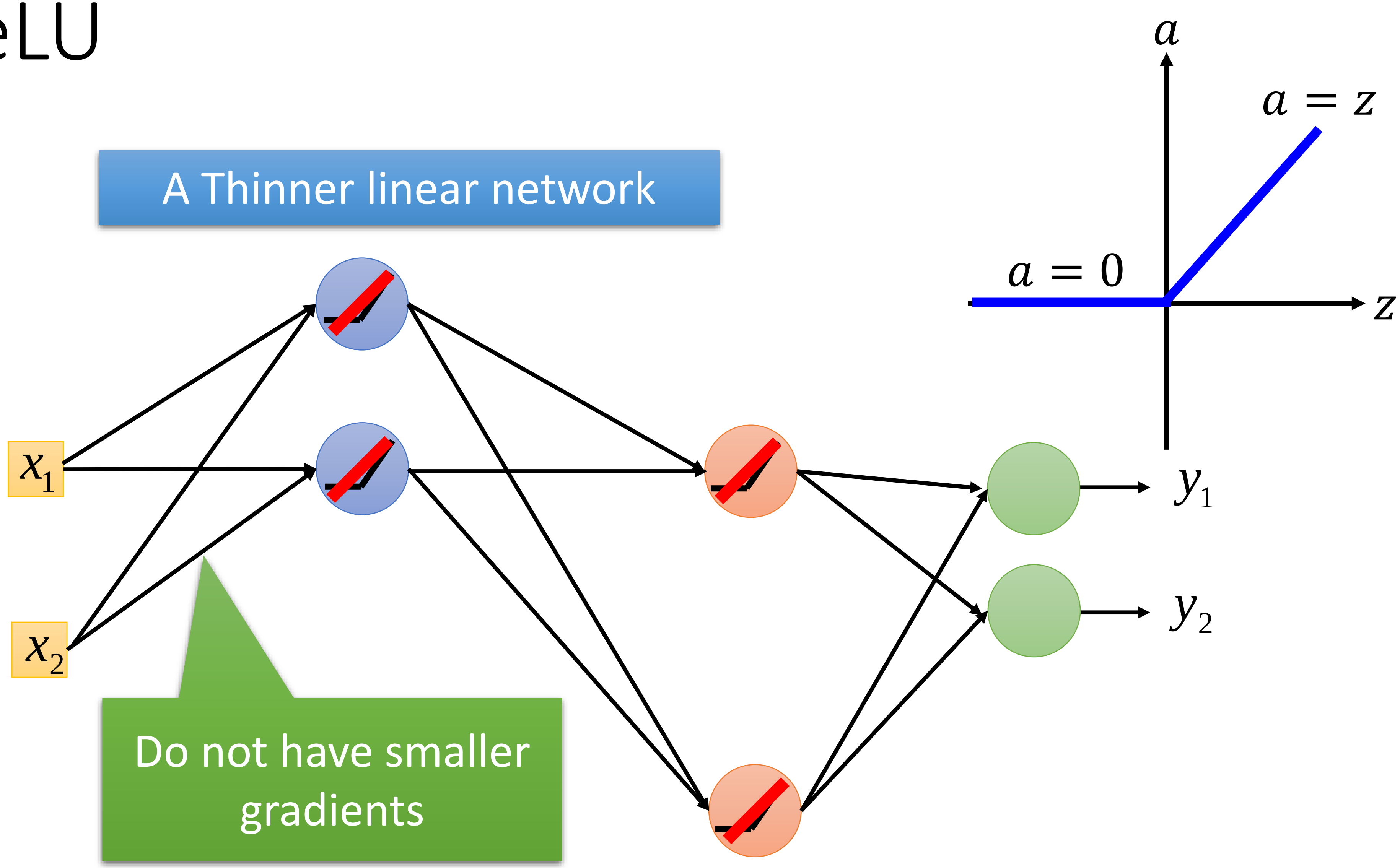
1. Fast to compute: no exponential computations
2. Solves the vanishing gradient problem

ReLU



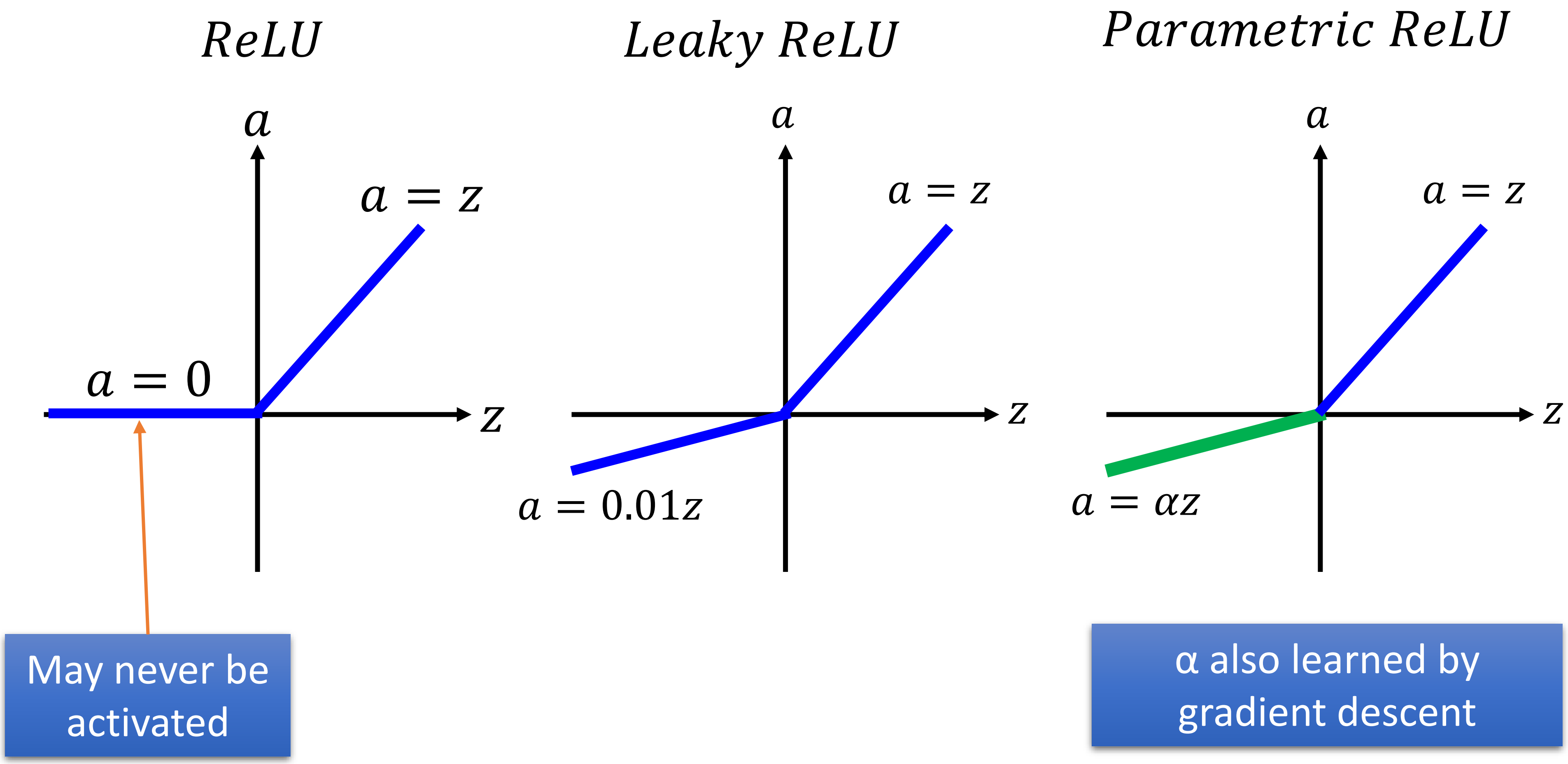


ReLU



A Thinner linear network
x_1
x_2
y_1
y_2
Do not have smaller gradients
a
$a = z$
$a = 0$
z

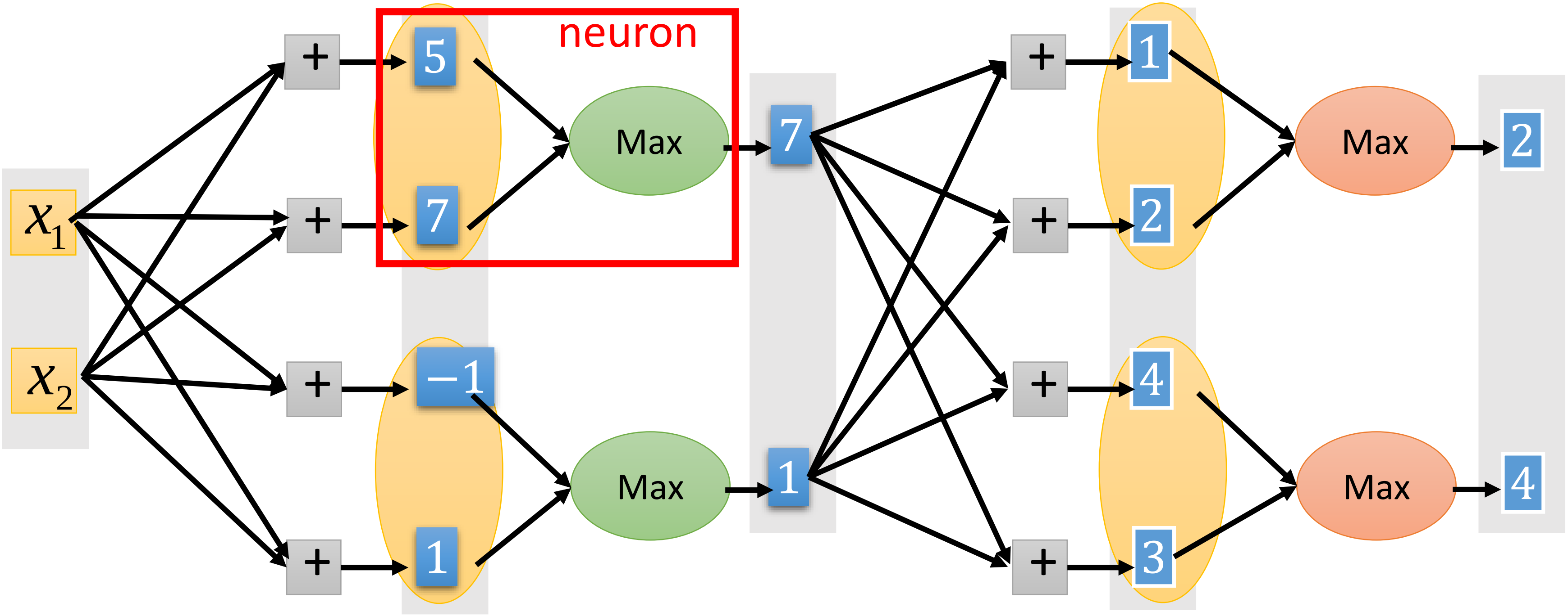
ReLU: Variant



Maxout

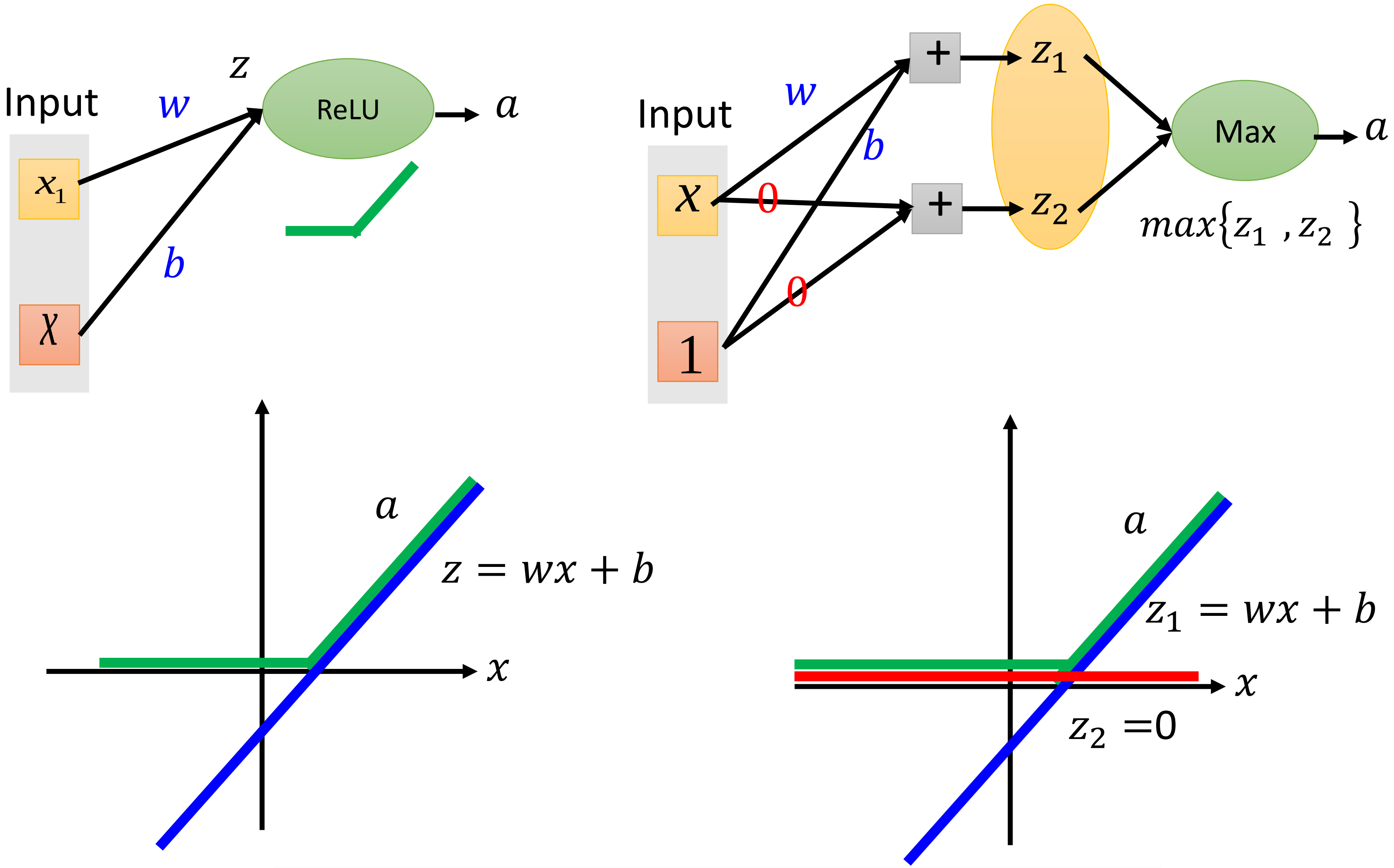
- Learnable activation function [Ian J. Goodfellow, ICML’13]

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$



You can have more than 2 elements in a group.

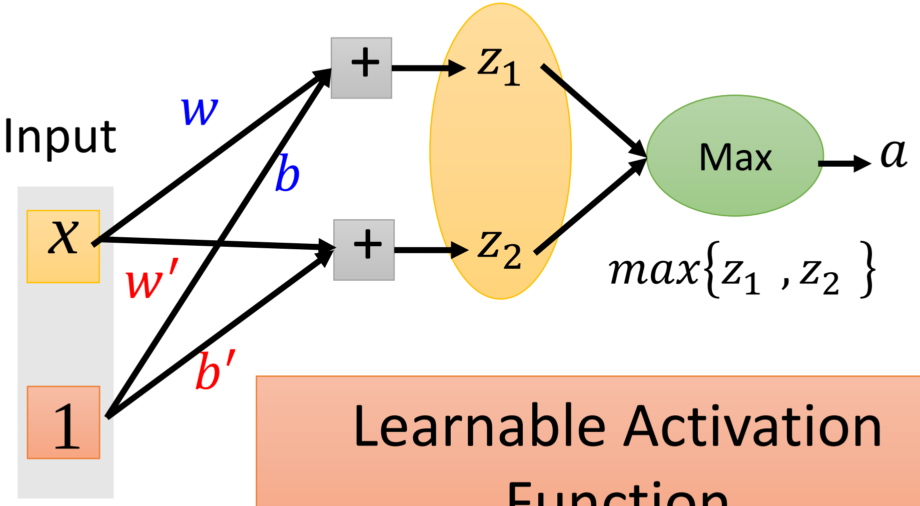
Maxout



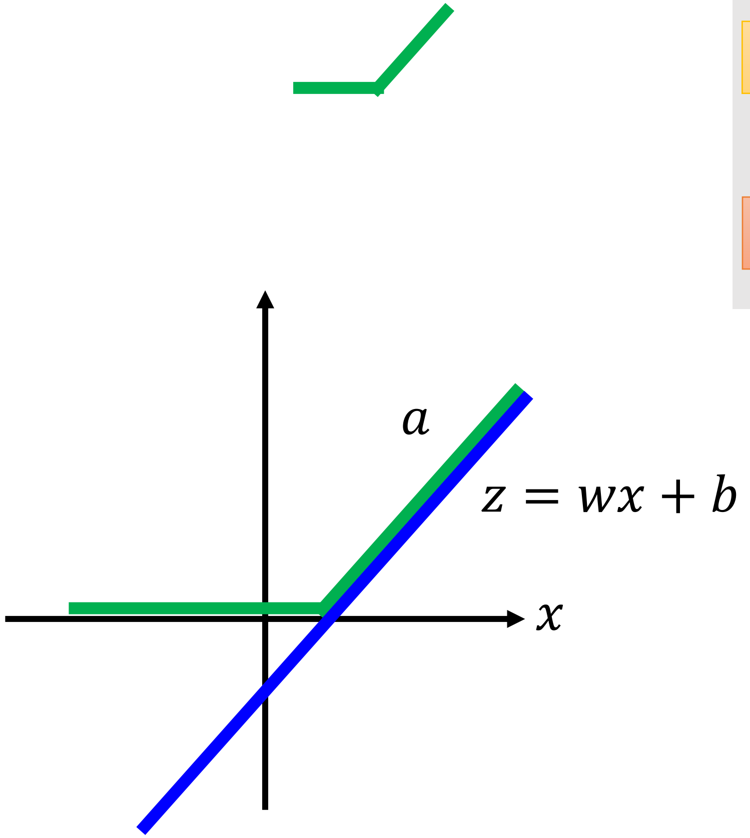
ReLU is a special cases of Maxout

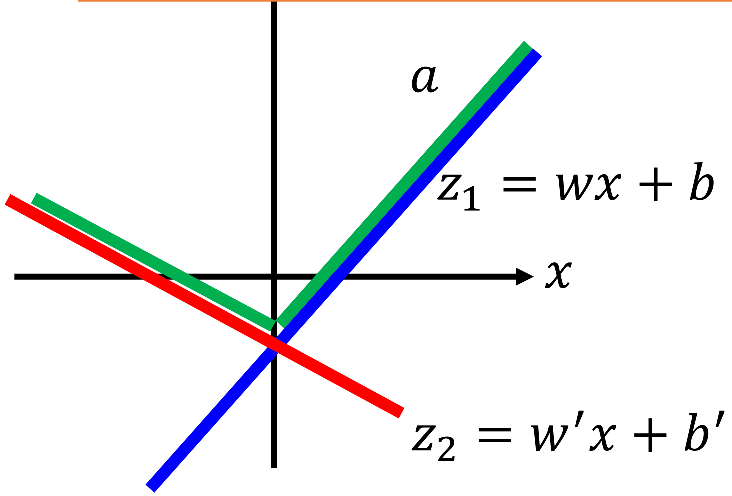
Maxout

More than ReLU



Learnable Activation Function

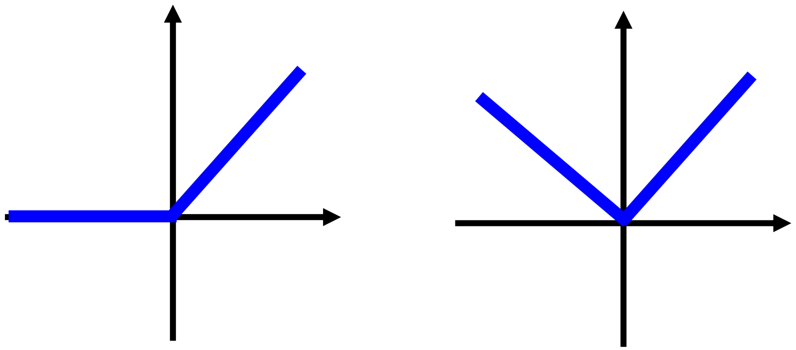




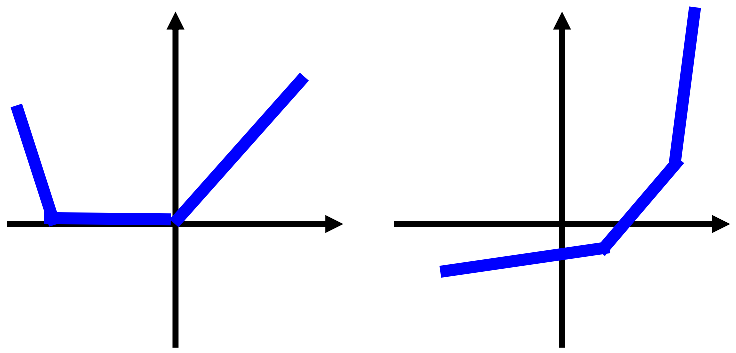
Maxout

- Learnable activation function [Ian J. Goodfellow, ICML'13]
  - Activation function in maxout network can be any piecewise linear convex function
  - How many pieces depending on how many elements in a group

2 elements in a group



3 elements in a group



Problem: The number of parameters are doubled.

Regularization

- New loss function to be minimized
- Find a set of weight not only minimizing original cost but also close to zero

$$\mathrm{L}'(\theta) = \underline{L(\theta)} + \lambda \frac{1}{2} \underline{\|\theta\|_2}$$

→ Regularization term

$$\theta = \{w_1, w_2, \ldots\}$$

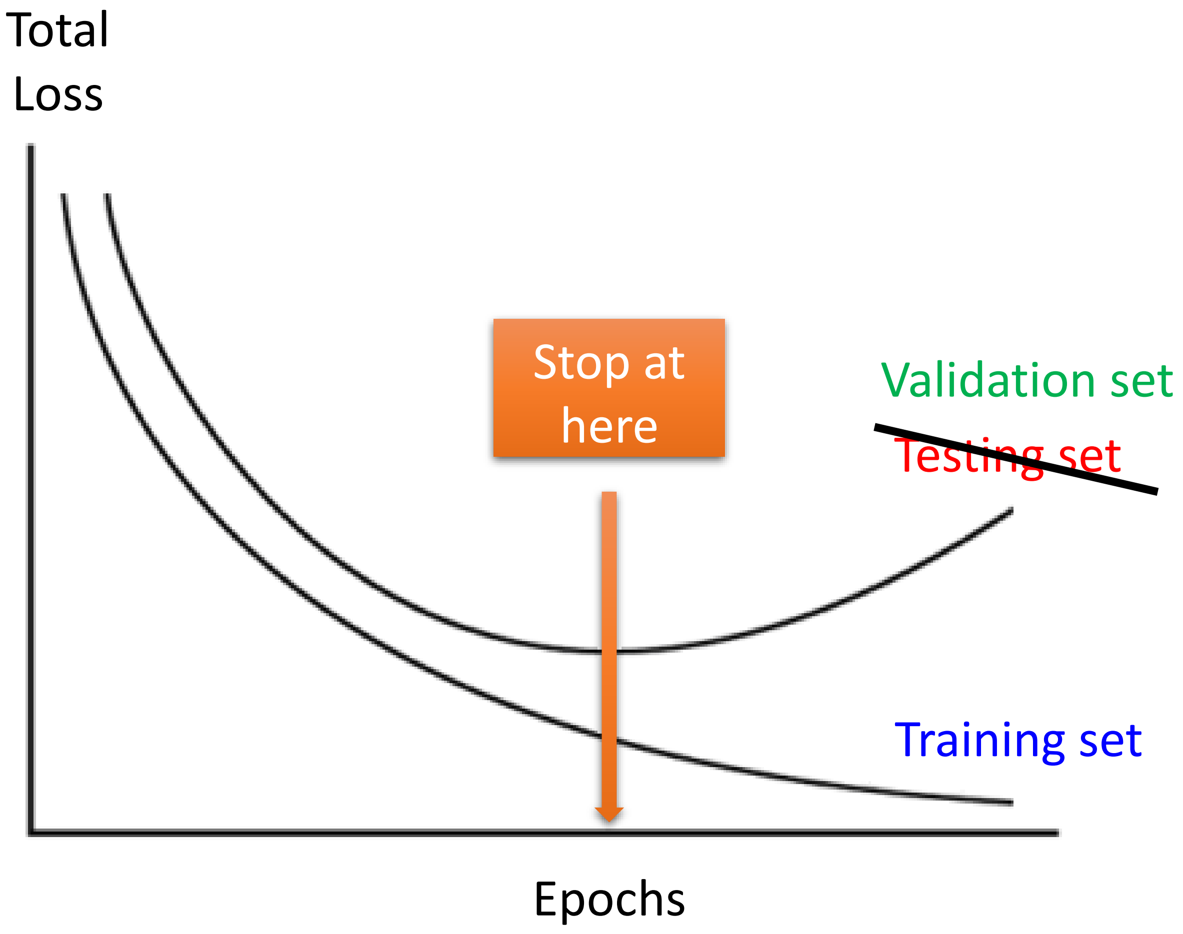
L2 regularization: $\|\theta\|_2 = (w_1)^2 + (w_2)^2 + \ldots$

L1 regularization: $\|\theta\|_1 = |w_1| + |w_2| + \ldots$

Original loss
(e.g. minimize square error,
cross entropy …)

Early Stopping

- One of the most widely used regularization techniques to overcome the overfitting issue.
- Monitors the performance of the model for every epoch on the validation set during the training.
- Terminates the training as soon as the validation error reaches A minimum.



Implementation

- Deep learning packages: Tensorflow, Pytorch …
- Visualization of Learning a Neural Network
- Implementation of a 1-hidden layer Neural Network

Summary of Today's Lecture

- Summary and review
- Neural networks
- Implementation