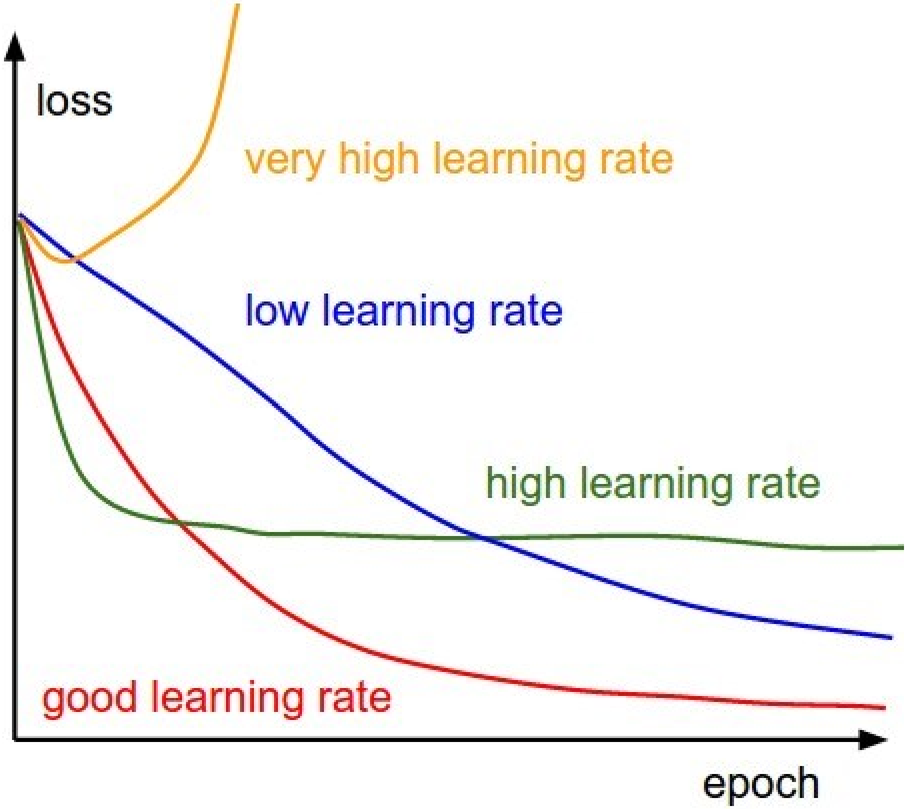
Lecture 6 Recap

Learning Rate: Implications

- What if too high?
- What if too low?



Source: http://cs231n.github.io/neural-networks-3/

Training Schedule

Manually specify learning rate for entire training process

- Manually set learning rate every $\boldsymbol{n}$-epochs
- How?
  - Trial and error (the hard way)
  - Some experience (only generalizes to some degree)

Consider: #epochs, training set size, network size, etc.

Basic Recipe for Training

- Given dataset with ground truth labels
  - $\{\boldsymbol{x}_i, y_i\}$
    - $\boldsymbol{x}_i$ is the $\boldsymbol{i}^{\boldsymbol{th}}$ training image, with label $\boldsymbol{y}_i$
    - Often $\mathbf{dim}(\boldsymbol{X}) \gg \mathbf{dim}(\boldsymbol{y})$ (e.g., for classification)
    - $\boldsymbol{i}$ is often in the 100-thousands or millions
  - Take network $\boldsymbol{f}$ and its parameters $\boldsymbol{W}, \boldsymbol{b}$
  - Use SGD (or variation) to find optimal parameters $\boldsymbol{W}, \boldsymbol{b}$
    - Gradients from backprop

Basic Recipe for Machine Learning

- Split your data

60%	20%	20%
train	validation	test

Example scenario

Ground truth error 1%

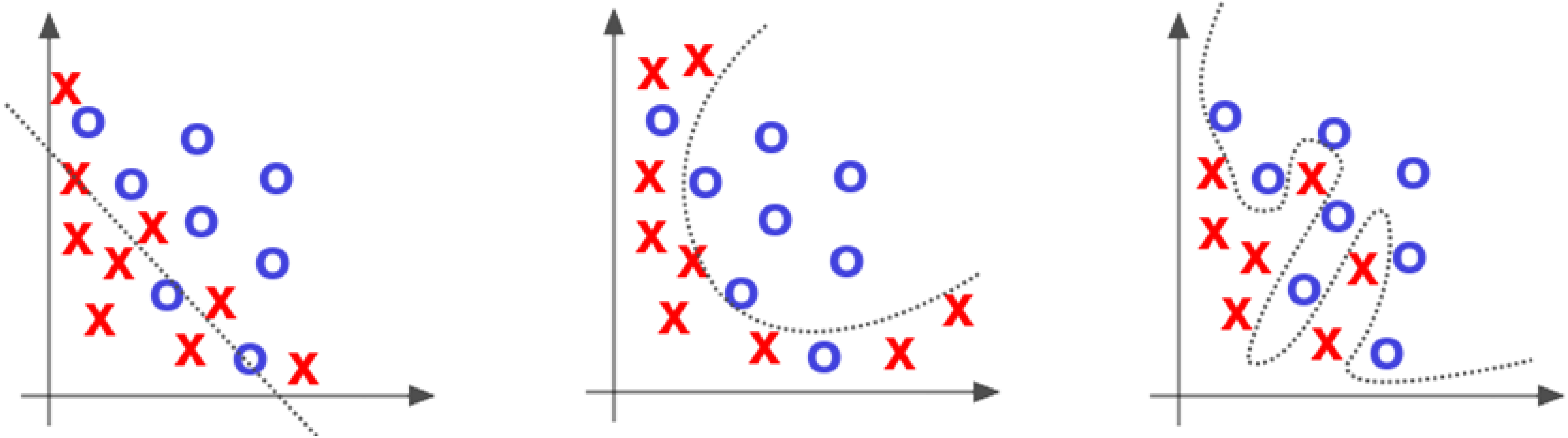
Training set error 5%

Val/test set error 8%

Bias (or underfitting)

Variance (overfitting)

Over and Underfitting



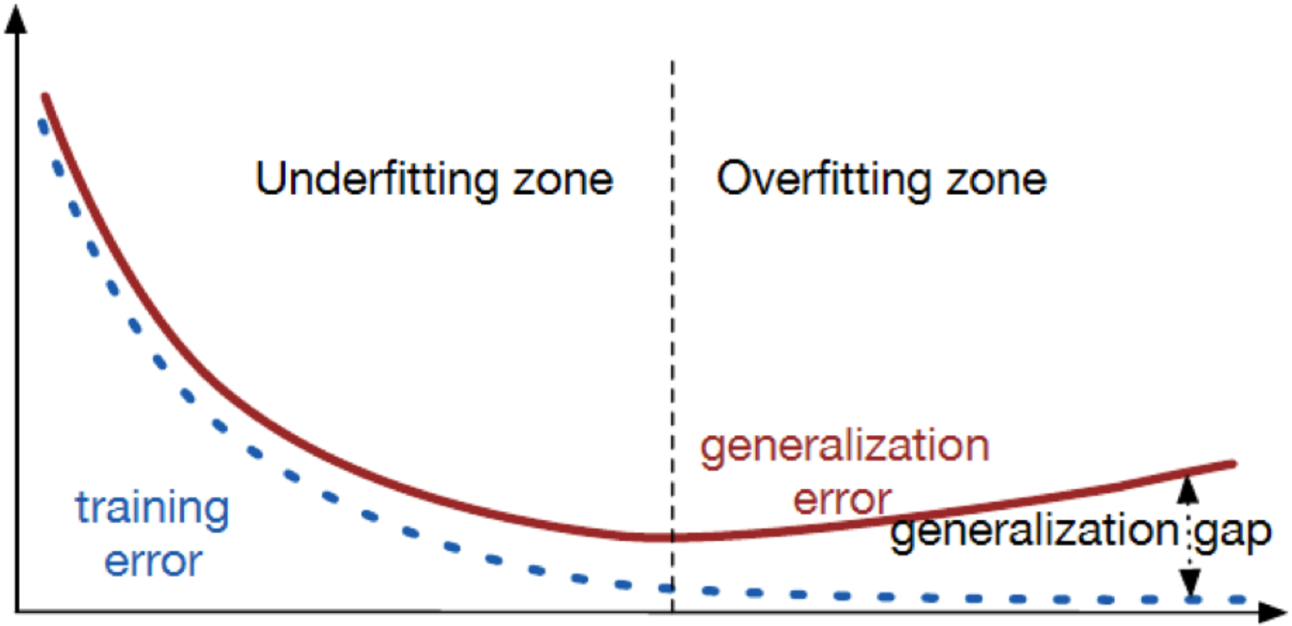
Underfitted

Appropriate

Overfitted

Source: Deep Learning by Adam Gibson, Josh Patterson, O'Reily Media Inc., 2017

Over and Underfitting



Source:
https://srdas.github.io/DLBook/ImprovingModelGeneralization.html

Hyperparameters

- Network architecture (e.g., num layers, #weights)
- Number of iterations
- Learning rate(s)   (i.e., solver parameters, decay, etc.)
- Regularization (more later next lecture)
- Batch size
- …
- Overall: learning setup + optimization = hyperparameters

Hyperparameter Tuning

- Methods:
  - Manual search: most common ☺
  - Grid search (structured, for 'real' applications)
    - Define ranges for all parameters spaces and select points
    - Usually pseudo-uniformly distributed

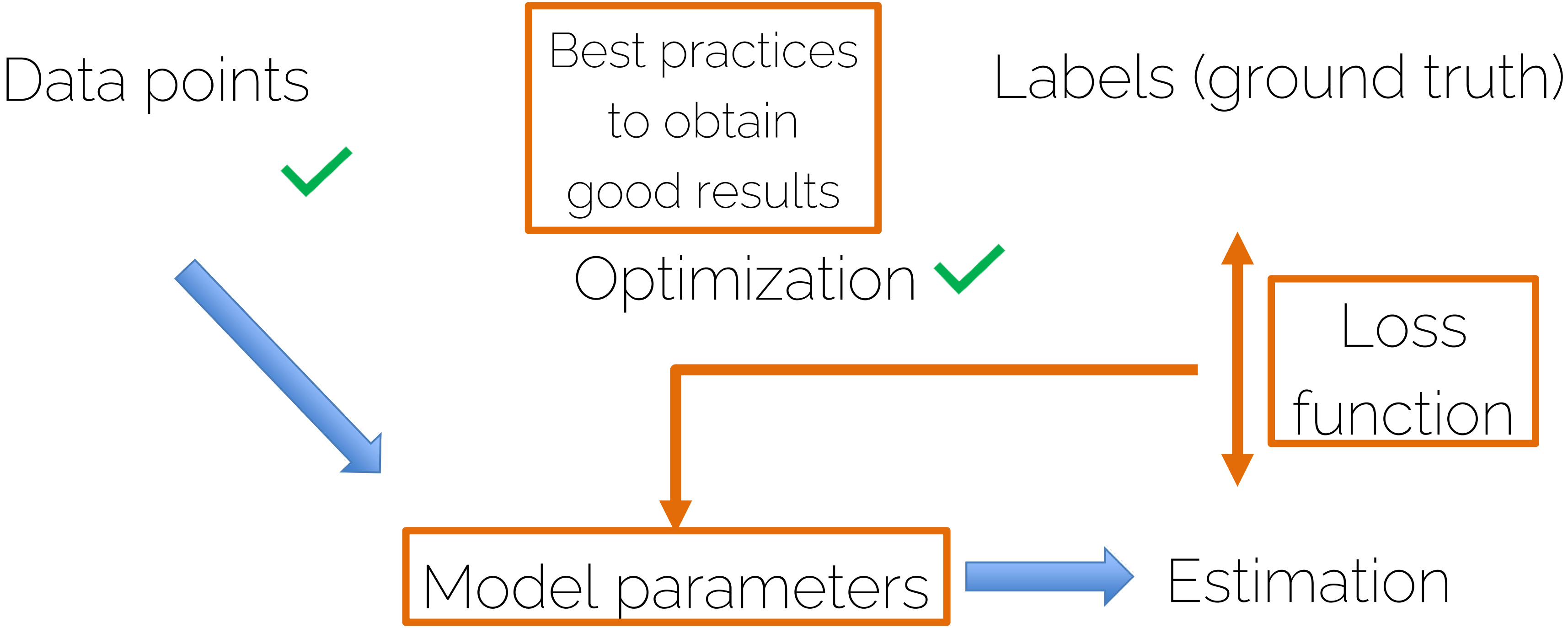
    → Iterate over all possible configurations
  - Random search:

    Like grid search but one picks points at random in the predefined ranges
  - Auto-ML:

    Bayesian, gradient-based etc

Lecture 7
Training NN (part 2)

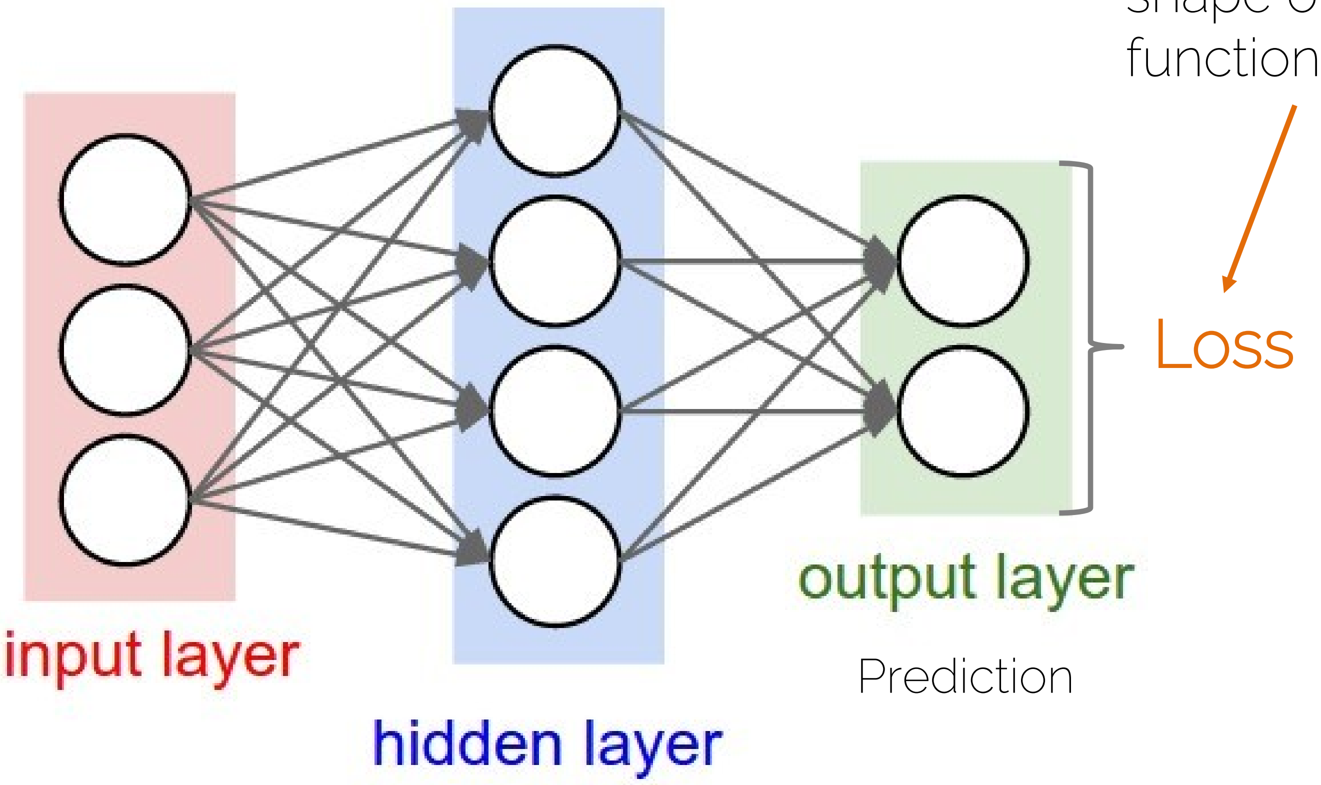
What we have seen so far



Output and Loss Functions

Neural Networks

What is the shape of this function?



Prediction

Regression Losses

- L2 Loss: $L^2 = \sum_{i=1}^{n} \left(y_i - f(\boldsymbol{x}_i)\right)^2$
- L1 Loss: $L^1 = \sum_{i=1}^{n} |y_i - f(\boldsymbol{x}_i)|$

training pairs $[\boldsymbol{x}_i; y_i]$
(input and labels)

$f(\boldsymbol{x}_i)$:

12	24	42	23
34	32	5	2
12	31	12	31
31	64	5	13

y_i:

15	20	40	25
34	32	5	2
12	31	12	31
31	64	5	13

$$L^2(x, y) = 9 + 16 + 4 + 4 + 0 + \cdots + 0 = 33$$

$$L^1(x, y) = 3 + 4 + 2 + 2 + 0 + \cdots + 0 = 11$$

Regression Losses: L2 vs L1

- L2 Loss:

$$L^2 = \sum_{i=1}^{n} \left(y_i - f(\boldsymbol{x}_i)\right)^2$$

  - Sum of squared differences (SSD)
  - Prone to outliers
  - Compute-efficient optimization
  - Optimum is the mean

- L1 Loss:

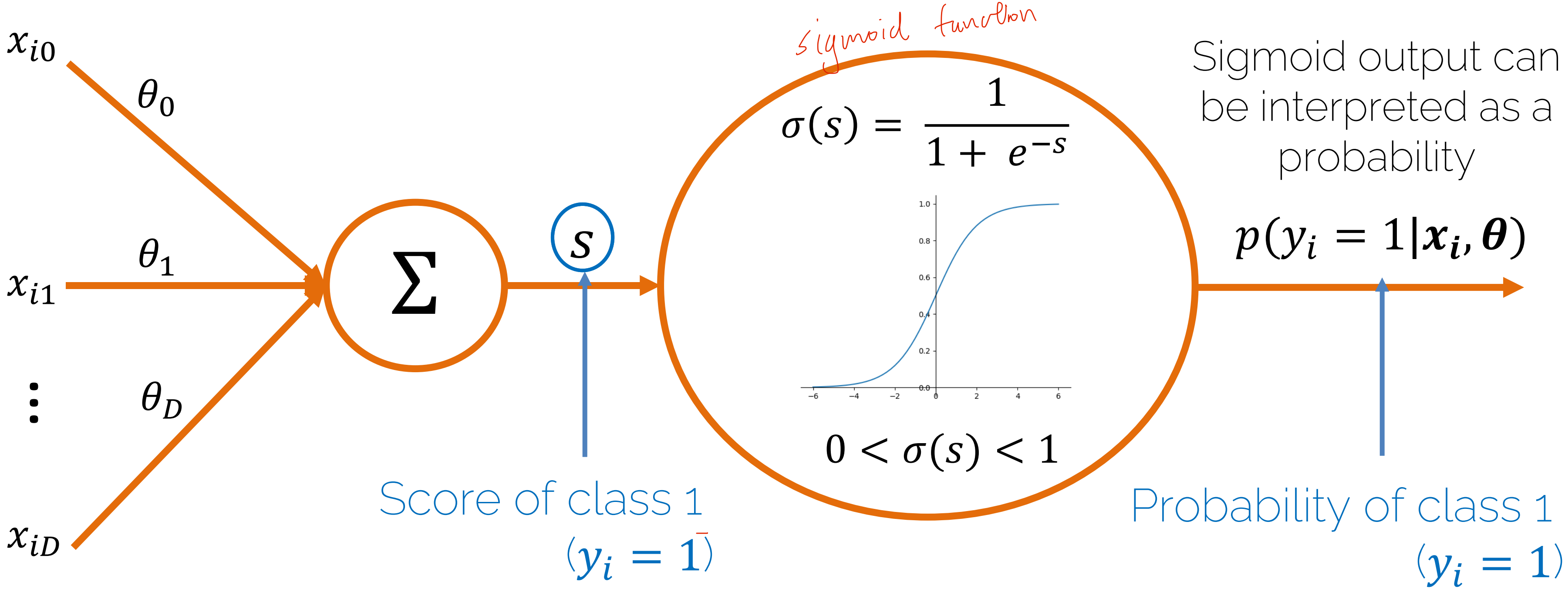
$$L^1 = \sum_{i=1}^{n} |y_i - f(\boldsymbol{x}_i)|$$

  - Sum of absolute differences
  - Robust (cost of outliers is linear)
  - Costly to optimize
  - Optimum is the median

Binary Classification: Sigmoid

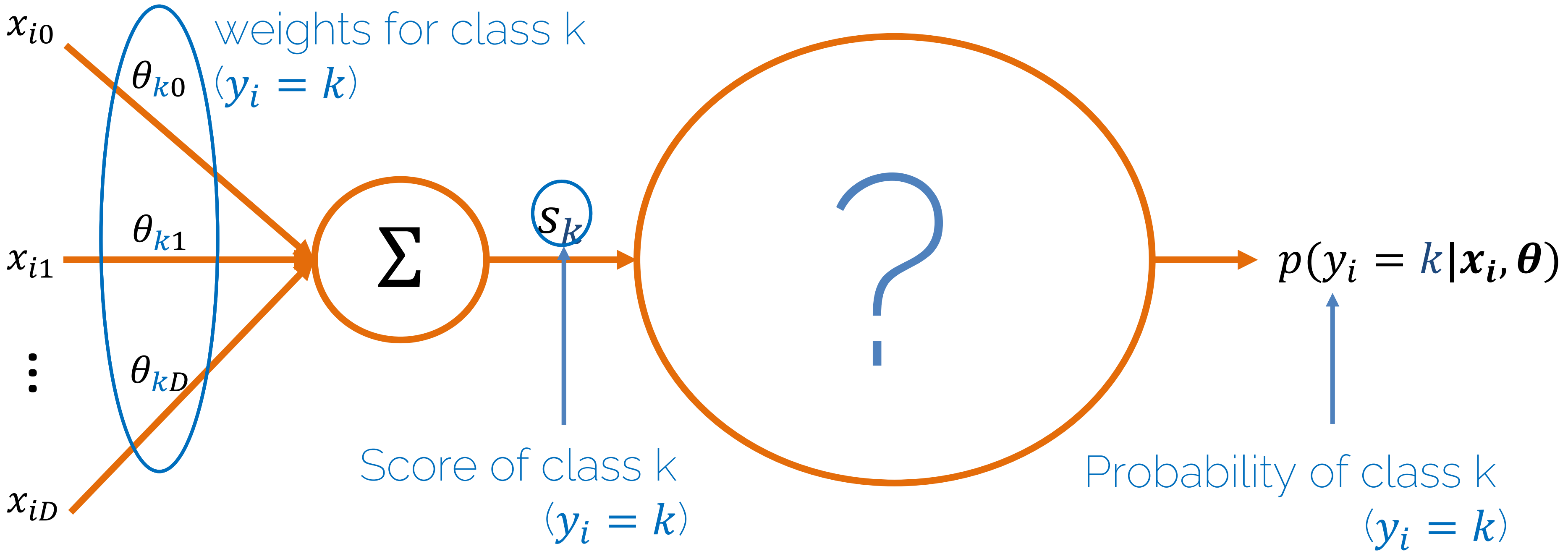
training pairs $[\boldsymbol{x}_i; y_i]$,
$\boldsymbol{x}_i \in \mathbb{R}^D, y_i \in \{1,0\}$ (2 classes)

$$p(y_i = 1|\boldsymbol{x_i}, \boldsymbol{\theta}) = \sigma(s) = \frac{1}{1 + e^{-\sum_{d=0}^{D} \theta_d x_{id}}}$$



Multiclass Classification: Softmax

training pairs $[\boldsymbol{x}_i; y_i]$,
$\boldsymbol{x}_i \in \mathbb{R}^D, y_i \in \{1,2 \ldots C\}$ (C classes)



Multiclass Classification: Softmax

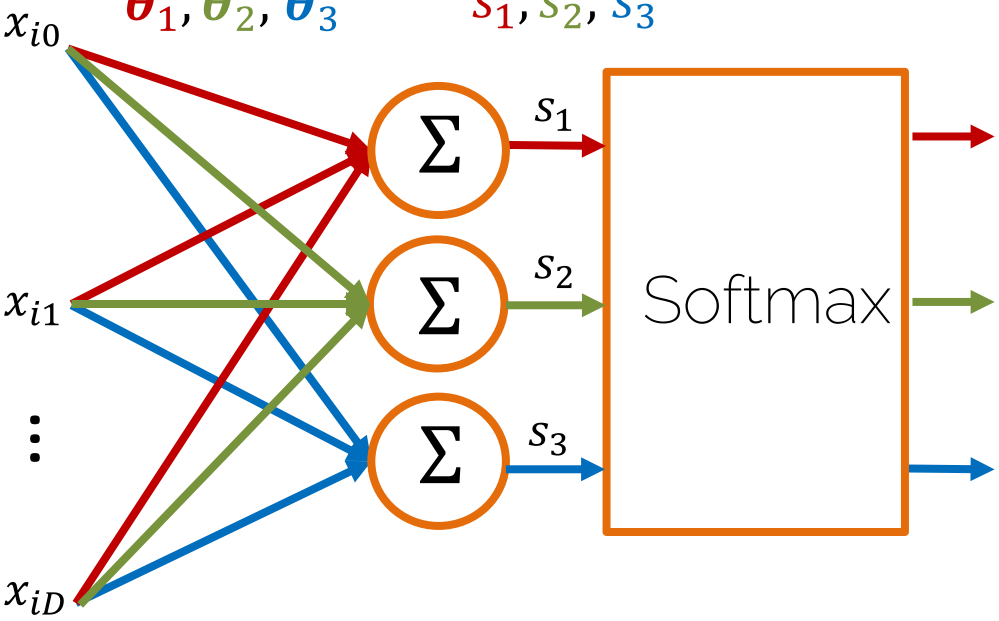
Weights for each class

$\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3$

Scores for each class

s_1, s_2, s_3

Probabilities for each class



$$p(y_i = 1 | \boldsymbol{x_i}, \boldsymbol{\Theta}) = \frac{e^{\boldsymbol{x_i \theta_1}}}{e^{\boldsymbol{x_i \theta_1}} + e^{\boldsymbol{x_i \theta_2}} + e^{\boldsymbol{x_i \theta_3}}}$$

$$p(y_i = 2 | \boldsymbol{x_i}, \boldsymbol{\Theta}) = \frac{e^{\boldsymbol{x_i \theta_2}}}{e^{\boldsymbol{x_i \theta_1}} + e^{\boldsymbol{x_i \theta_2}} + e^{\boldsymbol{x_i \theta_3}}}$$

$$p(y_i = 3 | \boldsymbol{x_i}, \boldsymbol{\Theta}) = \frac{e^{\boldsymbol{x_i \theta_3}}}{e^{\boldsymbol{x_i \theta_1}} + e^{\boldsymbol{x_i \theta_2}} + e^{\boldsymbol{x_i \theta_3}}}$$

Multiclass Classification: Softmax

- Softmax

scores

$$p(y_i|\boldsymbol{x_i},\Theta) = \frac{e^{s_{y_i}}}{\sum_{k=1}^{C} e^{s_k}} = \frac{e^{\boldsymbol{x}_i\boldsymbol{\theta}_{y_i}}}{\sum_{k=1}^{C} e^{\boldsymbol{x}_i\boldsymbol{\theta}_k}}$$

Exp

normalize

Probability of the true class

training pairs $[\boldsymbol{x}_i; y_i]$,
$\boldsymbol{x}_i \in \mathbb{R}^D, y_i \in \{1,2 \dots C\}$
y_i: label (true class)

Parameters:
$\boldsymbol{\Theta} = [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_C]$

$\boldsymbol{C}$: number of classes
$\boldsymbol{s}$: score of the class

1. Exponential operation: make sure probability>0
2. Normalization: make sure probabilities sum up to 1.

Multiclass Classification: Softmax

- Numerical Stability

$$p(y_i|\boldsymbol{x}_i, \Theta) = \frac{e^{s_{y_i}}}{\sum_{k=1}^{C} e^{s_k}} = \frac{e^{s_{y_i} - s_{max}}}{\sum_{k=1}^{C} e^{s_k - s_{max}}}$$

Try to prove it by yourself ☺

- Cross-Entropy Loss (Maximum Likelihood Estimate)

$$L_i = -\log(p(y_i|\boldsymbol{x}_i, \Theta)) = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$$

Example: Cross-Entropy Loss

Cross Entropy $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \dots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_c]$

Suppose: 3 training examples and 3 classes

Given a function with weights $\boldsymbol{\Theta}$, training pairs $[\boldsymbol{x}_i; \boldsymbol{y}_i]$ (input and labels)

$\boldsymbol{\theta}_k = \begin{bmatrix} b_k \\ \boldsymbol{w}_k \end{bmatrix}$ parameters for each class with $\boldsymbol{C}$ classes

scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1

Example: Cross-Entropy Loss

Cross Entropy $L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}}\right)$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

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scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1

Loss 2.04

Image 1

Scores	exp	normalize	-log(x)
3.2	24.5	0.13	2.04
5.1	164.0	0.87	0.14
-1.7	0.18	0.00	6.94

Example: Cross-Entropy Loss

Cross Entropy $L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}}\right)$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \dots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_C]$

Suppose: 3 training examples and 3 classes



scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1
Loss	2.04	0.079	6.156

Given a function with weights $\boldsymbol{\Theta}$, training pairs $[\boldsymbol{x}_i; y_i]$ (input and labels)

$\boldsymbol{\theta}_k = \begin{bmatrix} b_k \\ \boldsymbol{w}_k \end{bmatrix}$ parameters for each class with $\boldsymbol{C}$ classes

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i = \frac{L_1 + L_2 + L_3}{3}$$

$$= \frac{2.04 + 0.079 + 6.156}{3} =$$

$$= \mathbf{2.76}$$

Hinge Loss (SVM Loss)

- Score Function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$
  - e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \dots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_c]$

- Hinge Loss (Multiclass SVM Loss)

$$L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$$

Example: Hinge Loss (SVM Loss)

Multiclass SVM loss $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \ldots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_C]$

Suppose: 3 training examples and 3 classes

Given a function with weights $\boldsymbol{\Theta}$, training pairs $[\boldsymbol{x}_i; y_i]$ (input and labels)

$\boldsymbol{\theta}_k = \begin{bmatrix} b_k \\ \boldsymbol{w}_k \end{bmatrix}$ parameters for each class with $\boldsymbol{C}$ classes

scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1

Loss

Example: Hinge Loss (SVM Loss)

Multiclass SVM loss $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \dots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_C]$

Suppose: 3 training examples and 3 classes

Given a function with weights $\boldsymbol{\Theta}$, training pairs $[\boldsymbol{x}_i; y_i]$ (input and labels)

$\boldsymbol{\theta}_k = \begin{bmatrix} b_k \\ \boldsymbol{w}_k \end{bmatrix}$ parameters for each class with $\boldsymbol{C}$ classes

scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1
Loss	2.9		

$$= \max(0, 5.1 - 3.2 + 1) + \max(0, -1.7 - 3.2 + 1)$$

$$= \max(0, 2.9) + \max(0, -3.9)$$

$$= 2.9 + 0$$

$$= \mathbf{2.9}$$

Example: Hinge Loss (SVM Loss)

Multiclass SVM loss $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \ldots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_C]$

Suppose: 3 training examples and 3 classes

Given a function with weights $\boldsymbol{\Theta}$, training pairs $[\boldsymbol{x}_i; y_i]$ (input and labels)

$\boldsymbol{\theta}_k = \begin{bmatrix} b_k \\ \boldsymbol{w}_k \end{bmatrix}$ parameters for each class with $\boldsymbol{C}$ classes

scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1
Loss	2.9	0	

$$
\begin{aligned}
L_2 &= \max(0, 1.3 - 4.9 + 1) + \\
&\quad \max(0, 2.0 - 4.9 + 1) \\
&= \max(0, -2.6) + \max(0, -1.9) \\
&= 0 + 0 = \mathbf{0}
\end{aligned}
$$

Example: Hinge Loss (SVM Loss)

Multiclass SVM loss $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \ldots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_C]$

Suppose: 3 training examples and 3 classes

Given a function with weights $\boldsymbol{\Theta}$, training pairs $[\boldsymbol{x}_i; y_i]$ (input and labels)

$\boldsymbol{\theta}_k = \begin{bmatrix} b_k \\ \boldsymbol{w}_k \end{bmatrix}$ parameters for each class with $\boldsymbol{C}$ classes



scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1
Loss	2.9	0	12.9

$$
\begin{aligned}
L_3 &= \max(0, 2.2 - (-3.1) + 1) + \\
&\quad \max(0, 2.5 - (-3.1) + 1) \\
&= \max(0, 6.3) + \max(0, 6.6) \\
&= 6.3 + 6.6 \\
&= \mathbf{12.9}
\end{aligned}
$$

Example: Hinge Loss (SVM Loss)

Multiclass SVM loss $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta})$

e.g., $\boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\Theta}) = [x_{i0}, x_{i2}, \dots, x_{id}] \cdot [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_C]$

Suppose: 3 training examples and 3 classes

Given a function with weights $\boldsymbol{\Theta}$, training pairs $[\boldsymbol{x}_i; y_i]$ (input and labels)

$\boldsymbol{\theta}_k = \begin{bmatrix} b_k \\ \boldsymbol{w}_k \end{bmatrix}$ parameters for each class with $\boldsymbol{C}$ classes

scores			
cat	3.2	1.3	2.2
chair	5.1	4.9	2.5
car	-1.7	2.0	-3.1
Loss	2.9	0	12.9

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i = \frac{L_1 + L_2 + L_3}{3}$$

$$= \frac{2.9 + 0 + 12.9}{3}$$

$$= \mathbf{5.3}$$

Multiclass Classification: Hinge vs Cross-Entropy

- Hinge Loss: $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$
- Cross Entropy Loss: $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$

Example: Hinge vs Cross-Entropy

Hinge Loss: $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Cross Entropy : $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$

For image $\boldsymbol{x}_i$ (assume $\boldsymbol{y}_i = \mathbf{0}$):

	Scores	Hinge loss:	Cross Entropy loss:
Model 1	$s = [5, -3, 2]$		
Model 2	$s = [5, 10, 10]$		
Model 3	$s = [5, -20, -20]$		

Example: Hinge vs Cross-Entropy

Hinge Loss: $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Cross Entropy : $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$

For image $\boldsymbol{x_i}$ (assume $\boldsymbol{y_i} = \boldsymbol{0}$):

	Scores	Hinge loss:	Cross Entropy loss:
Model 1	$s = [5, -3, 2]$	$\max(0, -3 - 5 + 1) + \max(0, 2 - 5 + 1) = 0$	
Model 2	$s = [5, 10, 10]$	$\max(0, 10 - 5 + 1) + \max(0, 10 - 5 + 1) = 12$	
Model 3	$s = [5, -20, -20]$	$\max(0, -20 - 5 + 1) + \max(0, -20 - 5 + 1) = 0$	

Apparently Model 3 is better, but losses show no difference between Model 1&3, since they all have same loss=0.

Example: Hinge vs Cross-Entropy

Hinge Loss: $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Cross Entropy : $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$

For image $\boldsymbol{x}_i$ (assume $y_i = 0$):

	Scores	Hinge loss:	Cross Entropy loss:
Model 1	$s = [5, -3, 2]$	$\max(0, -3 - 5 + 1) +$ $\max(0, 2 - 5 + 1) = 0$	$-\ln\left(\frac{e^5}{e^5+e^3+e^2}\right) = 0.05$
Model 2	$s = [5, 10, 10]$	$\max(0, 10 - 5 + 1) +$ $\max(0, 10 - 5 + 1) = 12$	
Model 3	$s = [5, -20, -20]$	$\max(0, -20 - 5 + 1) +$ $\max(0, -20 - 5 + 1) = 0$	$-\ln\left(\frac{e^5}{e^5+e^{-20}+e^{-20}}\right)$ $= 2 * 10^{-11}$

Model 3 has a clearly smaller loss now.

Example: Hinge vs Cross-Entropy

Hinge Loss: $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$

Cross Entropy : $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$

For image $\boldsymbol{x}_i$ (assume $y_i = 0$):

	Scores	Hinge loss:	Cross Entropy loss:
Model 1	$s = [5, -3, 2]$	$\max(0, -3 - 5 + 1) + \max(0, 2 - 5 + 1) = 0$	$-\ln\left(\frac{e^5}{e^5 + e^3 + e^2}\right) = 0.05$
Model 2	$s = [5, 10, 10]$	$\max(0, 10 - 5 + 1) + \max(0, 10 - 5 + 1) = 12$	$-\ln\left(\frac{e^5}{e^5 + e^{10} + e^{10}}\right) = 5.70$
Model 3	$s = [5, -20, -20]$	$\max(0, -20 - 5 + 1) + \max(0, -20 - 5 + 1) = 0$	$-\ln\left(\frac{e^5}{e^5 + e^{-20} + e^{-20}}\right) = 2 * 10^{-11}$

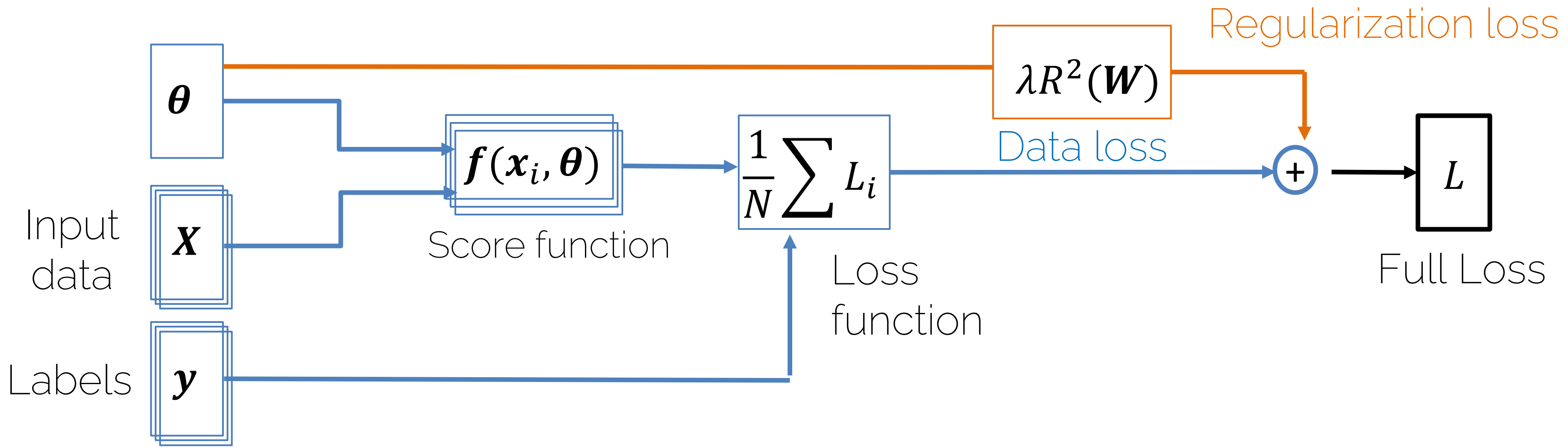
- Cross Entropy *always* wants to improve! (loss never 0)
- Hinge Loss saturates.

Loss in Compute Graph

- How do we combine loss functions with weight regularization?

- How to optimize parameters of our networks according to multiple losses?

Loss in Compute Graph



Want to find optimal $\boldsymbol{\theta}$. (weights are unknowns of optimization problem)

- Compute gradient w.r.t. $\boldsymbol{\theta}$.
- Gradient $\nabla_{\boldsymbol{\theta}} \boldsymbol{L}$ is computed via backpropagation

Loss in Compute Graph

Given a function with weights $\boldsymbol{\theta}$,
Training pairs $[\boldsymbol{x}_i; y_i]$ (input and labels)

- Score function $\boldsymbol{s} = \boldsymbol{f}(\boldsymbol{x}_i, \boldsymbol{\theta})$
- Data Loss
  - Cross Entropy $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_k e^{s_k}})$
  - SVM $L_i = \sum_{k \neq y_i} \max(0, s_k - s_{y_i} + 1)$
- Regularization Loss: e.g., $L2$-Reg: $R^2(\boldsymbol{W}) = \sum \boldsymbol{w}_i^2$
- Full Loss $L = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda R^2(\boldsymbol{W})$
- Full Loss = Data Loss + Reg Loss

Example: Regularization & SVM Loss

Multiclass SVM loss $L_i = \sum_{k \neq y_i} \max(0, \boldsymbol{f}(\boldsymbol{x}_i; \boldsymbol{\theta})_k - \boldsymbol{f}(\boldsymbol{x}_i; \boldsymbol{\theta})_{y_i} + 1)$

Full loss $L = \frac{1}{N} \sum_{i=1}^{N} \sum_{k \neq y_i} \max(0, \boldsymbol{f}(\boldsymbol{x}_i; \boldsymbol{\theta})_k - \boldsymbol{f}(\boldsymbol{x}_i; \boldsymbol{\theta})_{y_i} + 1) + \lambda R(\boldsymbol{W})$

$L1$-Reg: $R^1(\boldsymbol{W}) = \sum_{i=1}^{D} |\boldsymbol{w}_i|$

$L2$-Reg: $R^2(\boldsymbol{W}) = \sum_{i=1}^{D} \boldsymbol{w}_i^2$

Example:

$\boldsymbol{x} = [1,1,1,1]^T$

$\boldsymbol{w}_1 = [1, 0, 0, 0]^T$

$\boldsymbol{w}_2 = [0.25, 0.25, 0.25, 0.25]^T$

$\boldsymbol{x}^T \boldsymbol{w}_1 = \boldsymbol{x}^T \boldsymbol{w}_2 = 1$

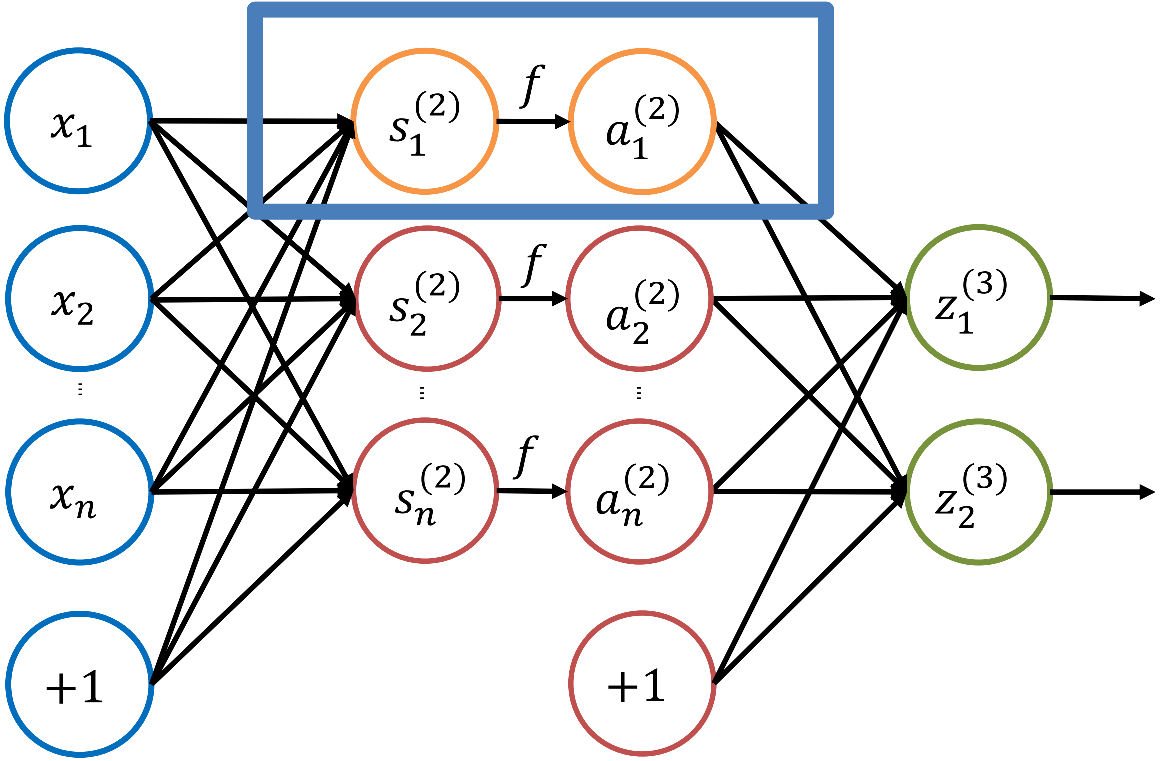
$R^2(\boldsymbol{w}_1) = 1$

$$R^2(\boldsymbol{w}_2) = 0.25^2 + 0.25^2 + 0.25^2 + 0.25^2 = 0.25$$

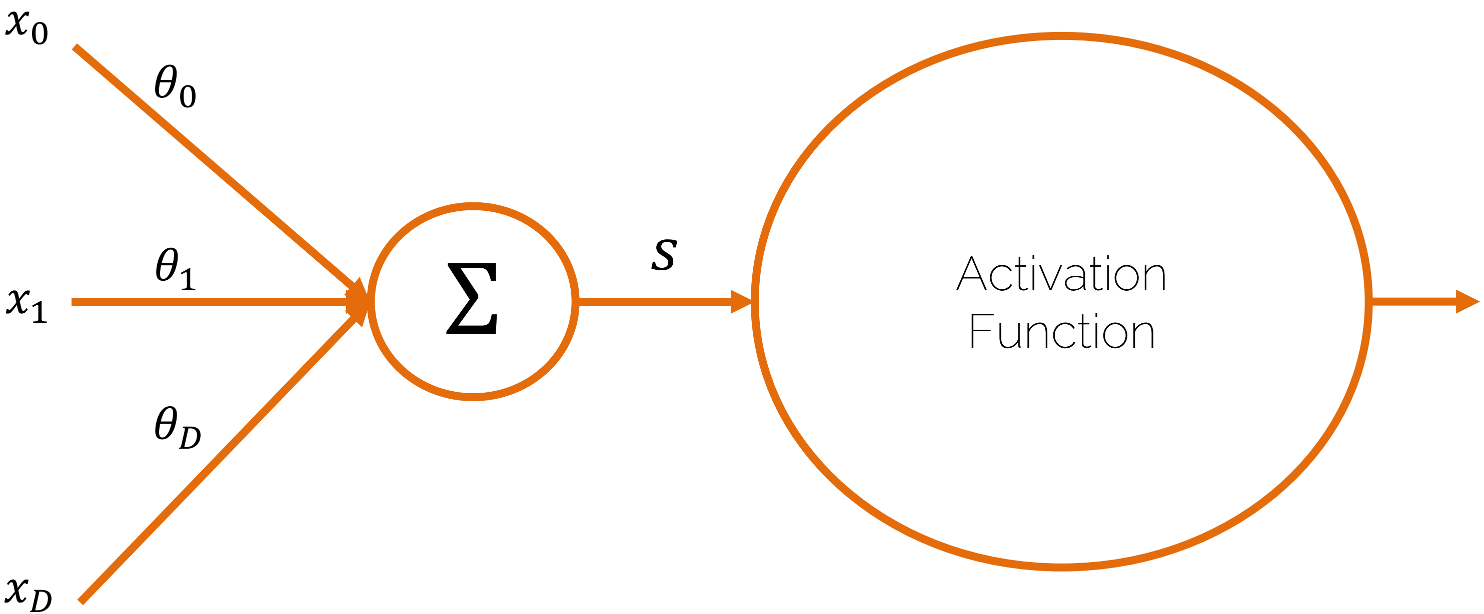
$R^2(\boldsymbol{W}) = 1 + 0.25 = 1.25$

Activation Functions

Neural Networks

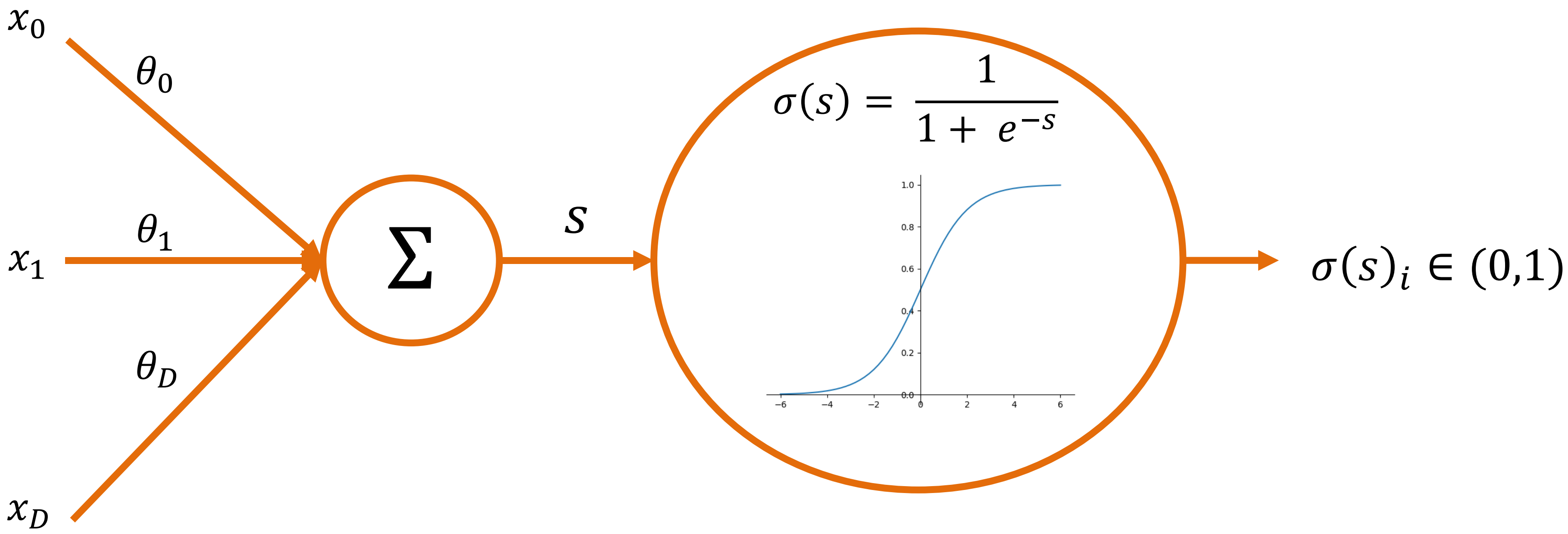


Activation Functions or Hidden Units



Sigmoid Activation

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



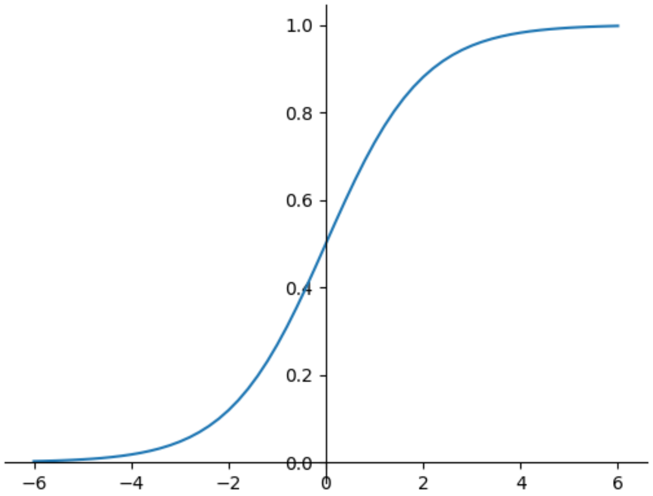
Sigmoid Activation

Forward

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

$$\frac{\partial L}{\partial w} = \frac{\partial s}{\partial w}\frac{\partial L}{\partial s}$$

$\boldsymbol{x}^T$?



$$\frac{\partial L}{\partial s} = \frac{\partial \sigma}{\partial s}\frac{\partial L}{\partial \sigma}$$

$$\frac{\partial \sigma}{\partial s}$$

$$\frac{\partial L}{\partial \sigma}$$

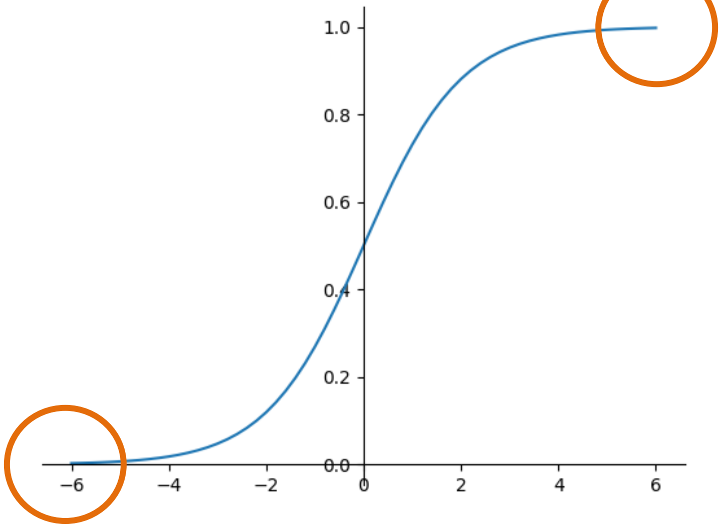
Sigmoid Activation

Forward

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

$\nabla \approx 0.$

$$\cancel{\frac{\partial L}{\partial w}} = \frac{\partial s}{\partial w}\frac{\partial L}{\partial s}$$



✗ Saturated neurons kill the gradient flow

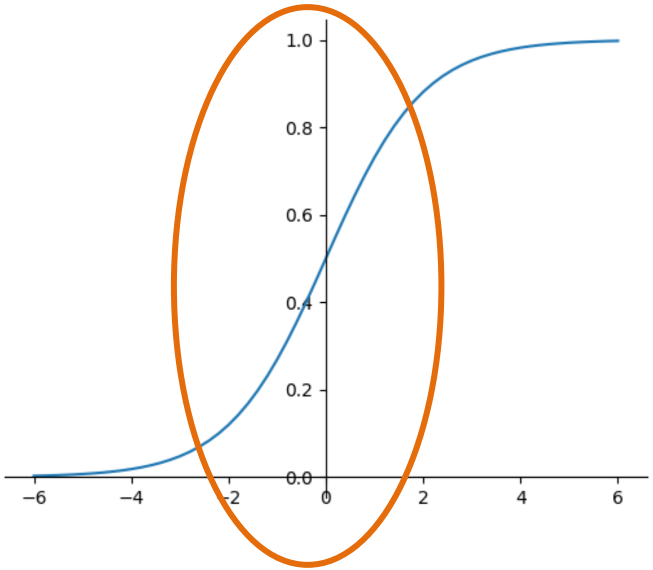
$$\cancel{\frac{\partial L}{\partial s}} = \frac{\partial \sigma}{\partial s}\frac{\partial L}{\partial \sigma} \quad \longleftarrow \quad \cancel{\frac{\partial \sigma}{\partial s}} \quad \longleftarrow \quad \frac{\partial L}{\partial \sigma}$$

Sigmoid Activation

Forward

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

$$\frac{\partial L}{\partial w} = \frac{\partial s}{\partial w}\frac{\partial L}{\partial s}$$



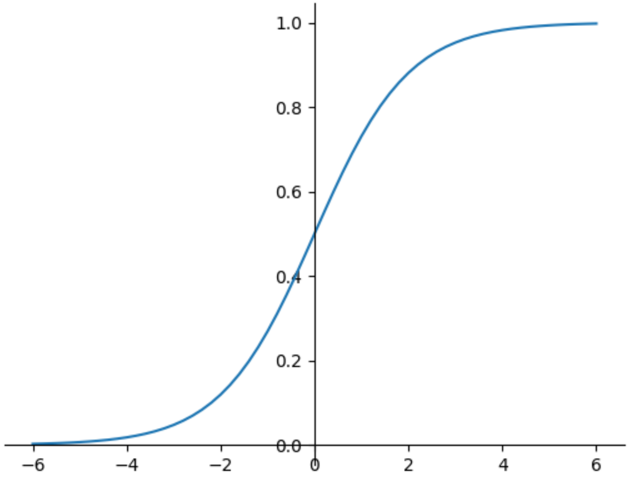
Active region for gradient descent

$$\frac{\partial L}{\partial s} = \frac{\partial \sigma}{\partial s}\frac{\partial L}{\partial \sigma}$$

$$\frac{\partial \sigma}{\partial s}$$

$$\frac{\partial L}{\partial \sigma}$$

Sigmoid Activation



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

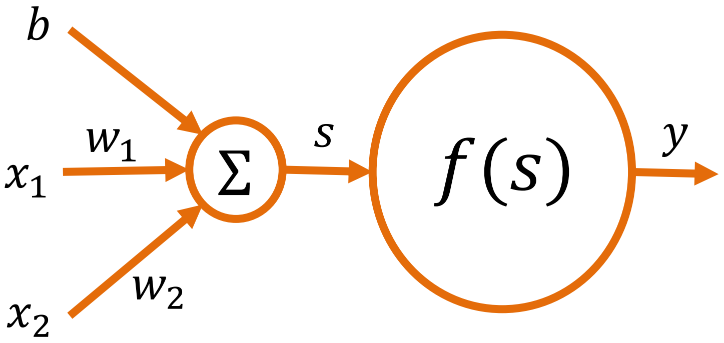
Output is always positive!

- Sigmoid output provides positive input for the next layer

What is the disadvantage of this?

Sigmoid Output not Zero-centered

- We want to compute the gradient w.r.t. the weights



Assume we have all positive data:

$\boldsymbol{x} = (x_1, x_2)^T > 0$

either positive or negative

$x_1 > 0$

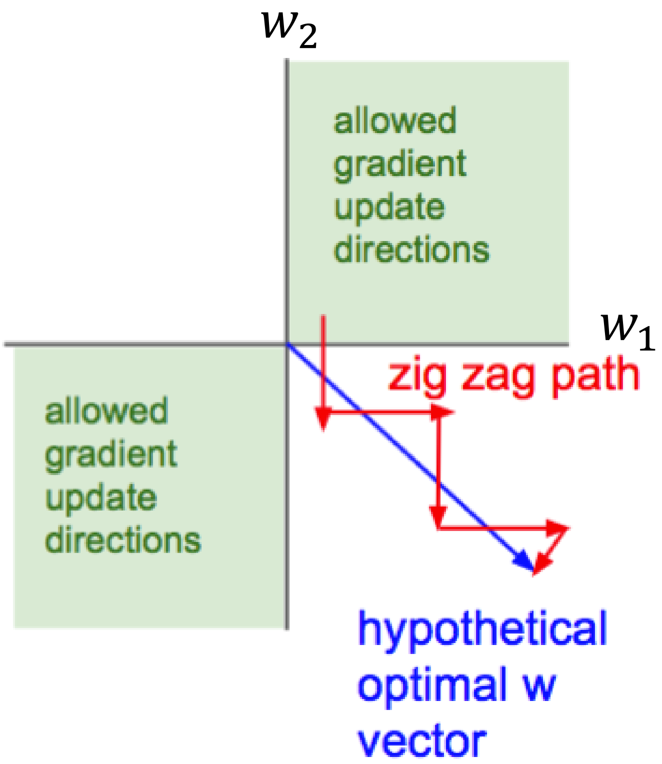
$$\frac{\partial L}{\partial w_1} = \boxed{\frac{\partial L}{\partial y} \cdot \frac{\partial y}{\partial s}} \cdot \frac{\partial s}{\partial w_1}$$

$x_2 > 0$

$$\frac{\partial L}{\partial w_2} = \boxed{\frac{\partial L}{\partial y} \cdot \frac{\partial y}{\partial s}} \cdot \frac{\partial s}{\partial w_2}$$

It is going to be either positive or negative for all weights' update.☹

Sigmoid Output not Zero-centered

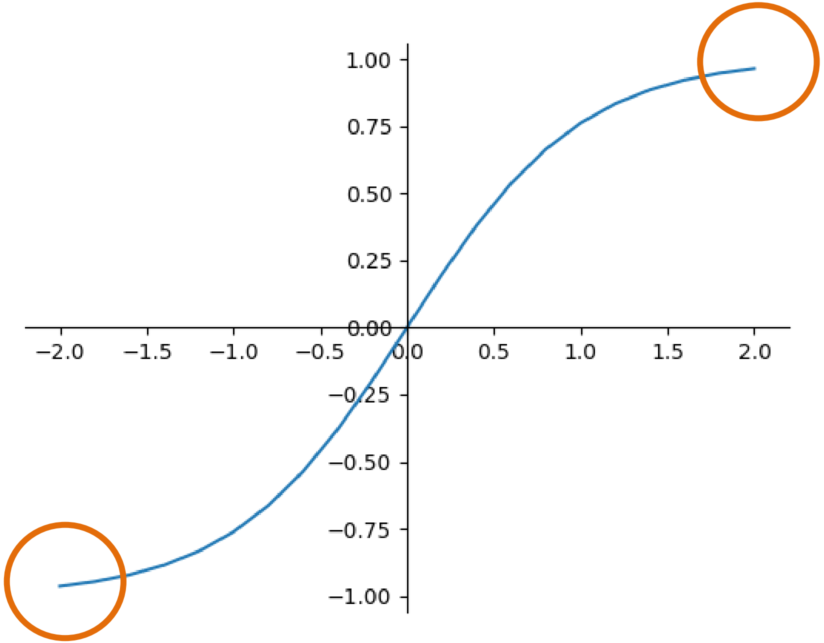


w_1, w_2 can only be increased or decreased at the same time, which is not good for update.

That is also why you need zero-centered data.

Source : http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture6.pdf

TanH Activation



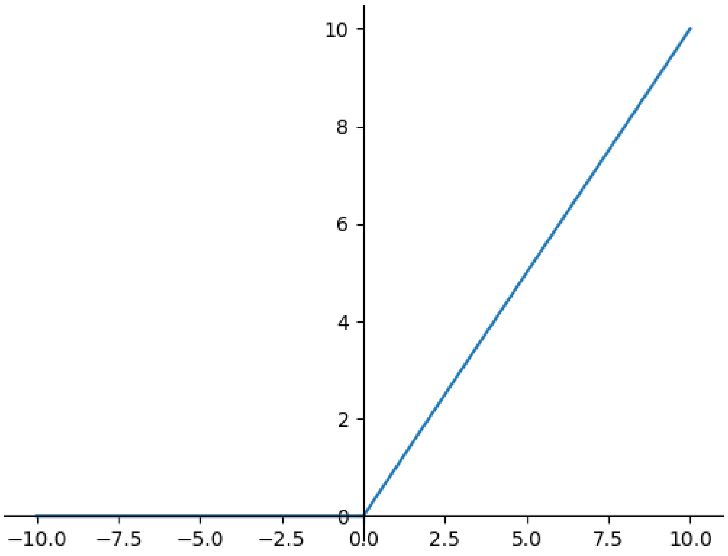
✗ Still saturates

✓Zero-centered

[LeCun et al. 1991] Improving Generalization Performance in Character Recognition

Rectified Linear Units (ReLU)

$$\sigma(x) = \max(0, x)$$



Large and consistent gradients ✓

✓ Fast convergence

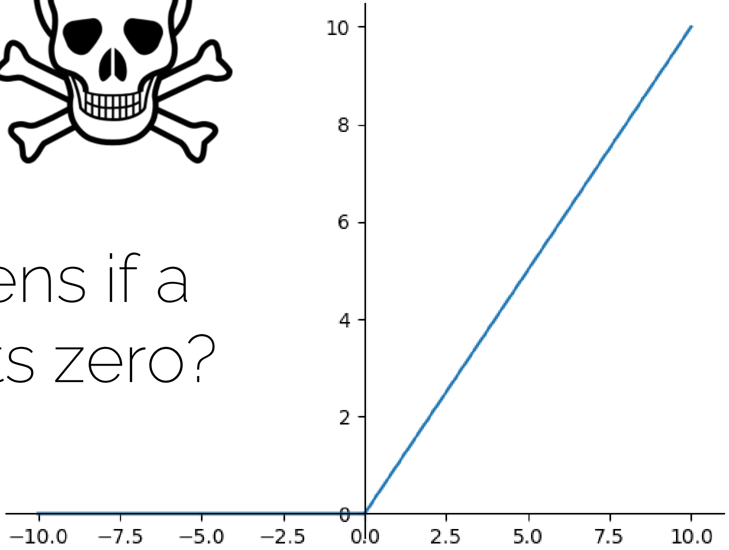
✓ Does not saturate

[Krizhevsky et al. NeurIPS 2012] ImageNet Classification with Deep Convolutional Neural Networks

Rectified Linear Units (ReLU)

✗ Dead ReLU

What happens if a ReLU outputs zero?



Large and consistent gradients ✓

✓ Fast convergence

✓ Does not saturate

[Krizhevsky et al. NeurIPS 2012] ImageNet Classification with Deep Convolutional Neural Networks

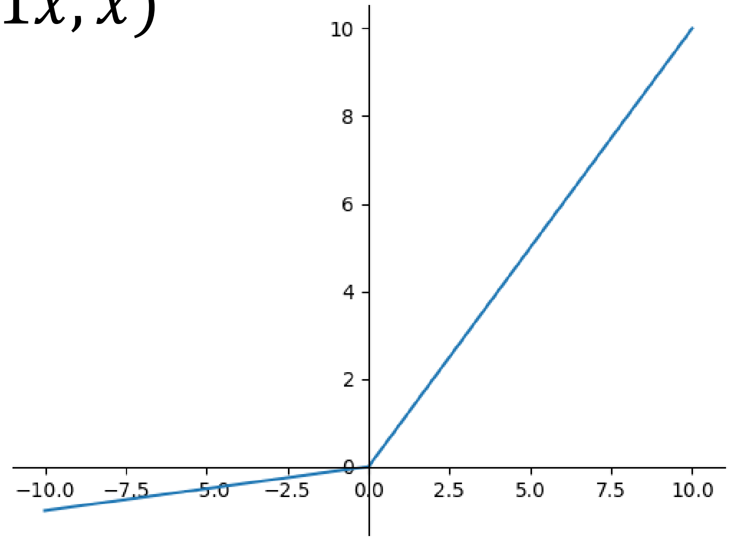
Rectified Linear Units (ReLU)

- Initializing ReLU neurons with slightly positive biases (0.01) makes it likely that they stay active for most inputs

$$f\left(\sum_i w_i x_i + b\right)$$

Leaky ReLU

$$\sigma(x) = \max(0.01x, x)$$



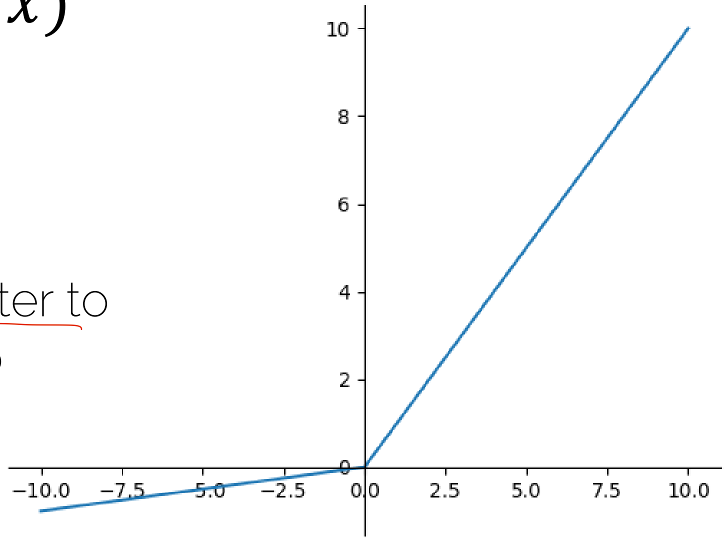
✓ Does not die

[Mass et al., ICML 2013] Rectifier Nonlinearities Improve Neural Network Acoustic Models

Parametric ReLU

$$\sigma(x) = \max(\alpha x, x)$$

One more parameter to backprop into

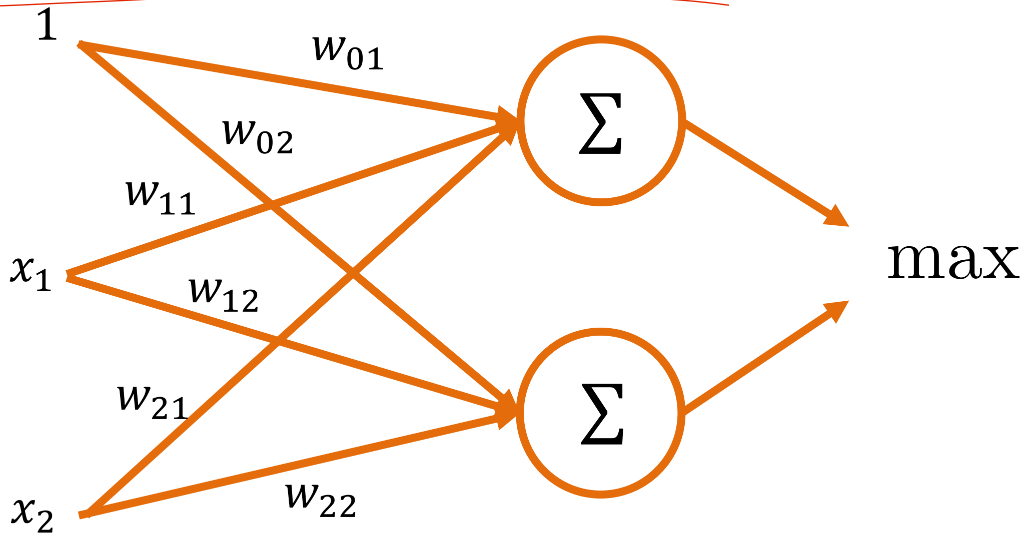


✓ Does not die

[He et al. ICCV 2015] Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification

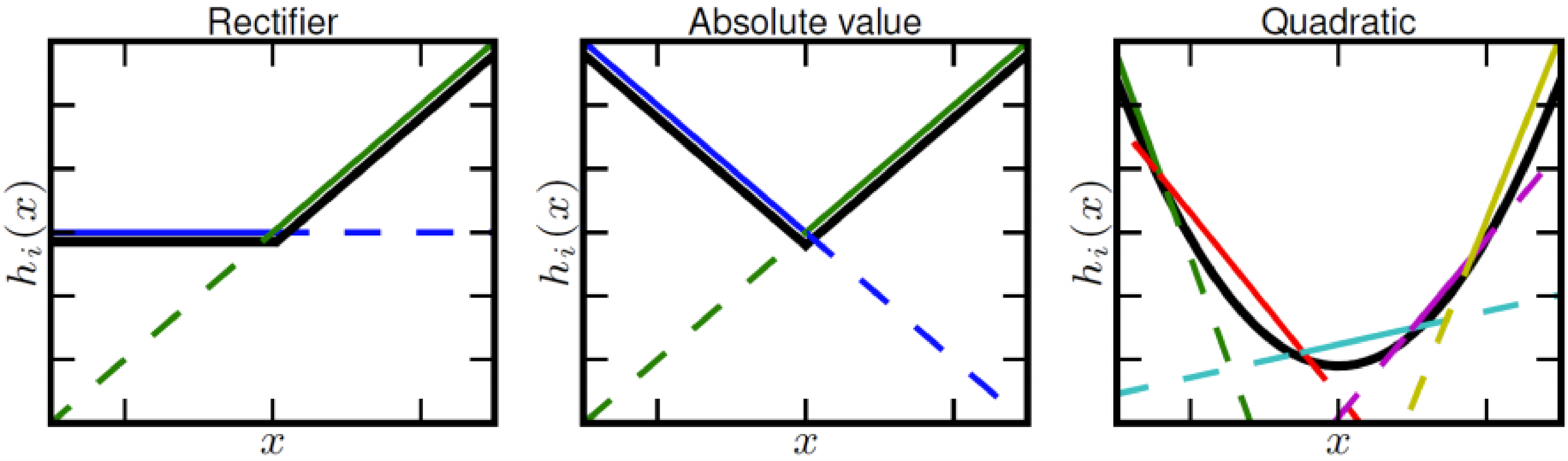
Maxout Units

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



[Goodfellow et al. ICML 2013] Maxout Networks

Maxout Units

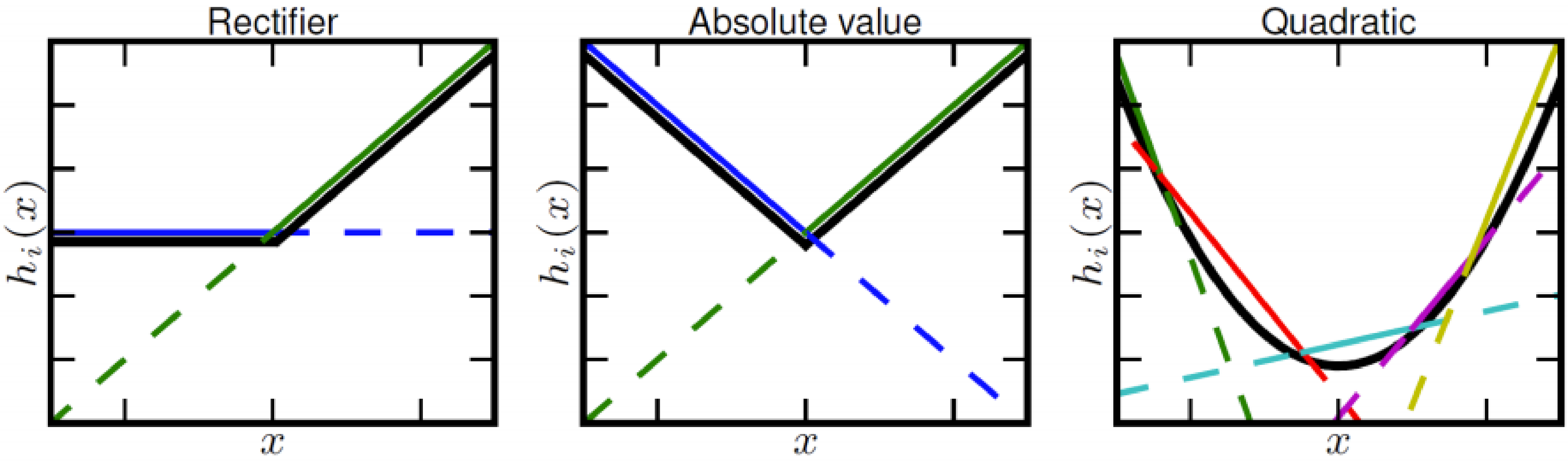


k=2 k=2 k=5

Piecewise linear approximation of
a convex function with N pieces

[Goodfellow et al. ICML 2013] Maxout Networks

Maxout Units

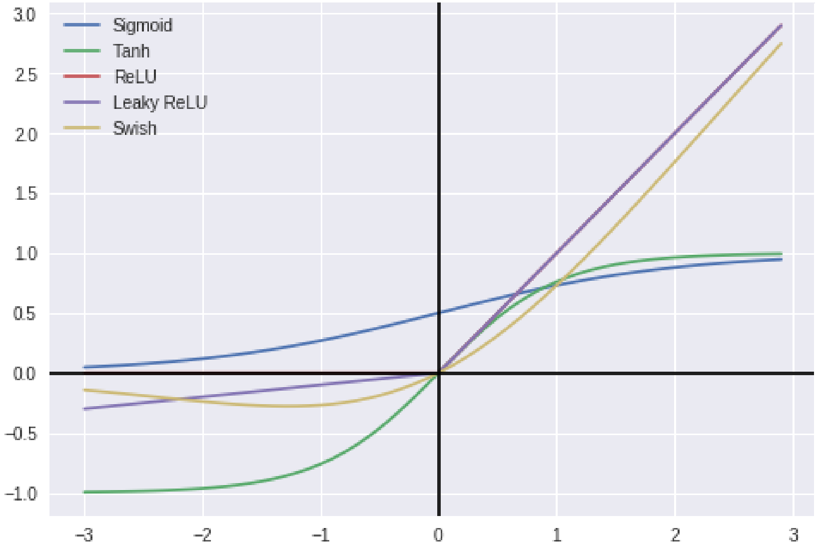


k=2 k=2 k=5

✓ Generalization of ReLUs ✓ Linear regimes ✓ Does not die ✓ Does not saturate

✗ Increases of the number of parameters

In a Nutshell



ACTIVATION FUNCTION	EQUATION	RANGE
Linear Function	$f(x) = x$	$(-\infty, \infty)$
Step Function	$f(x) = \begin{cases} 0 \; for \; x < 0 \\ 1 \; for \; x \geq 0 \end{cases}$	$\{0, 1\}$
Sigmoid Function	$f(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$	$(0, 1)$
Hyperbolic Tanjant Function	$f(x) = \tanh(x) = \frac{(e^{x} - e^{-x})}{(e^{x} + e^{-x})}$	$(-1, 1)$
ReLU	$f(x) = \begin{cases} 0 \; for \; x < 0 \\ x \; for \; x \geq 0 \end{cases}$	$[0, \infty)$
Leaky ReLU	$f(x) = \begin{cases} 0.01 \; for \; x < 0 \\ x \; for \; x \geq 0 \end{cases}$	$(-\infty, \infty)$
Swish Function	$f(x) = 2x\sigma(\beta x) = \begin{cases} \beta = 0 \; for \; f(x) = x \\ \beta \to \infty \; for \; f(x) = 2\max(0, x) \end{cases}$	$(-\infty, \infty)$

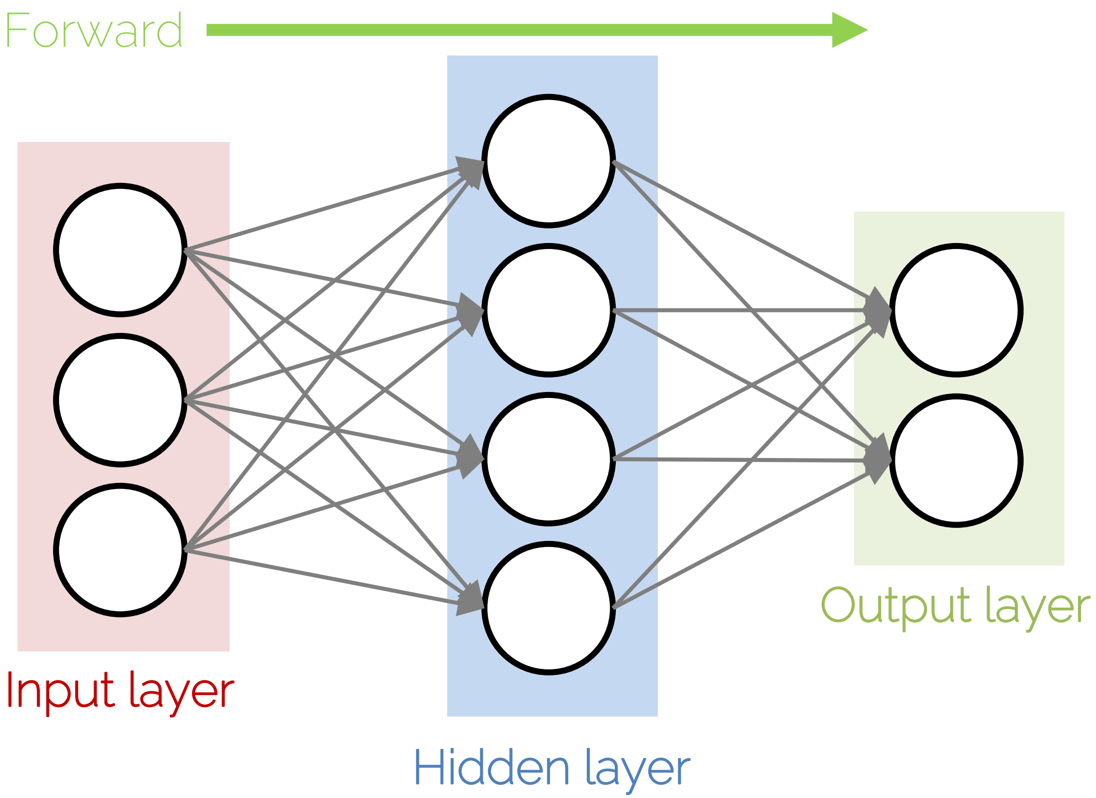
Source : https://towardsdatascience.com/comparison-of-activation-functions-for-deep-neural-networks-706ac4284c8a

Quick Guide

- Sigmoid/TanH are not really used in feedforward nets.
- ReLU is the standard choice.
- Second choice are the variants of ReLU or Maxout.
- Recurrent nets will require Sigmoid/TanH or similar.

Weight Initialization

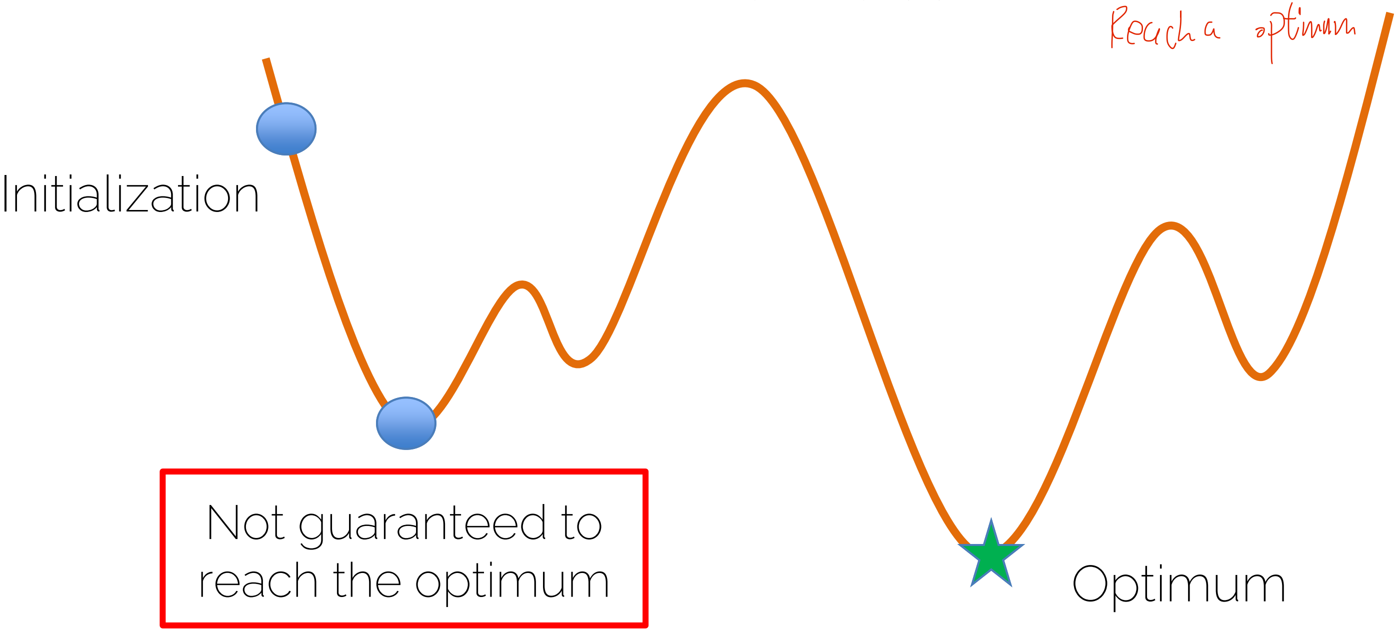
How do I start?



Initialization is Extremely Important!

$$x^* = \arg\min f(x)$$

Reach a optimum

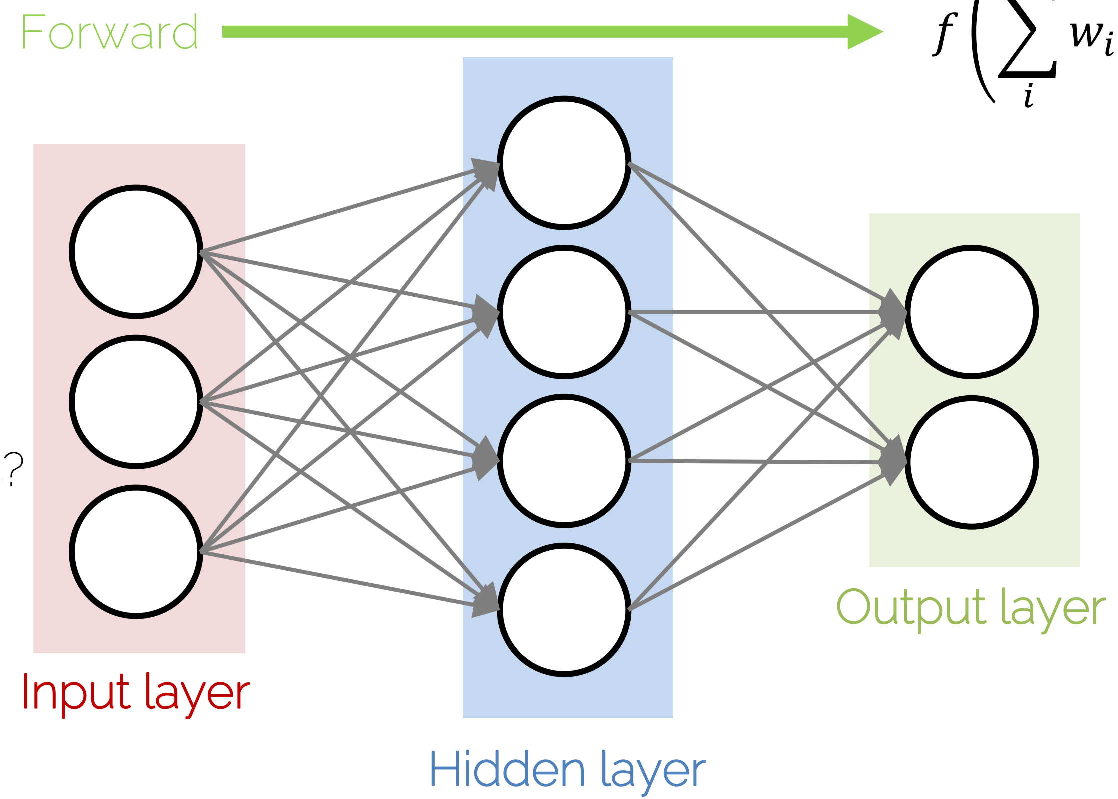


How do I start?

$$f\left(\sum_i w_i x_i + b\right)$$

$w = 0$

What happens to the gradients?



All Weights Zero

- What happens to the gradients?

- The hidden units are all going to compute the same function, gradients are going to be the same
  - No symmetry breaking

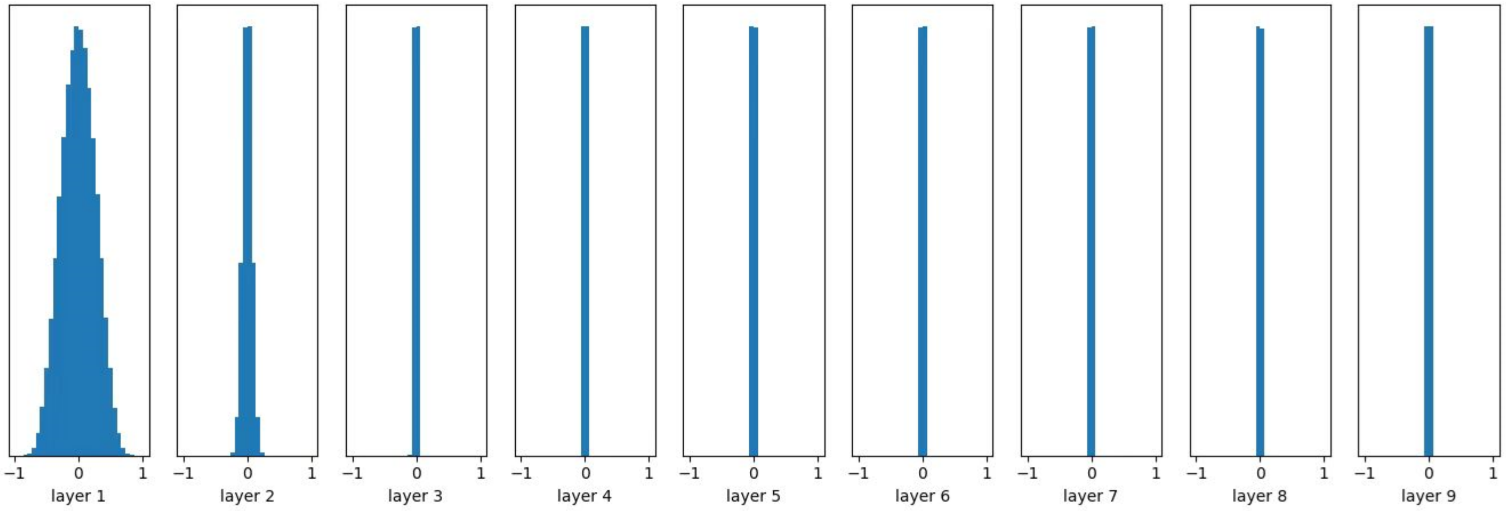
Small Random Numbers

- Gaussian with zero mean and standard deviation 0.01

- Let's see what happens:
  - Network with 10 layers with 500 neurons each
  - Tanh as activation functions
  - Input unit Gaussian data

Small Random Numbers

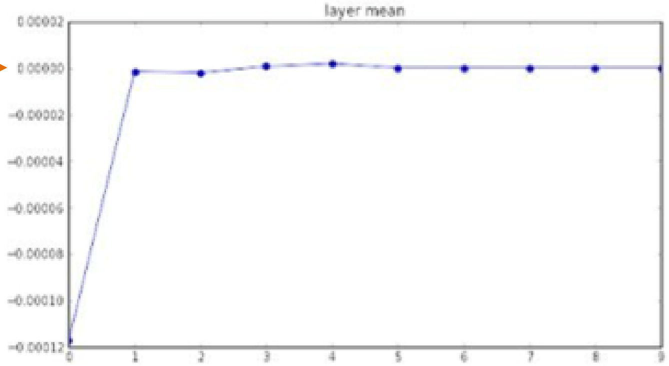
tanh as activation functions

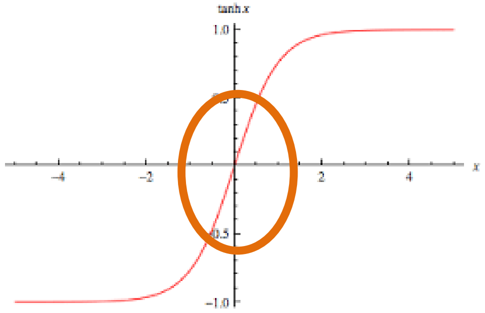


Output goes to zero

Forward

Small Random Numbers





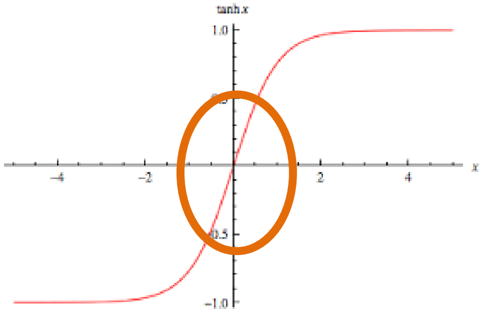
Small w_i^l cause small output for layer l:

$$f_l\left(\sum_i w_i^l x_i^l + b^l\right) \approx \mathbf{0}$$

Forward

Small Random Numbers

Even activation function's gradient is ok, we still have vanishing gradient problem.



Small outputs of layer l (input of layer $l+1$) cause small gradient w.r.t to the weights of layer $l+1$:

$$f_{l+1}\left(\sum_i w_i^{l+1} x_i^{l+1} + b^{l+1}\right)$$

$$\frac{\partial L}{\partial w_i^{l+1}} = \frac{\partial L}{\partial f_{l+1}} \cdot \frac{\partial f_{l+1}}{\partial w_i^{l+1}} = \frac{\partial L}{\partial f_{l+1}} \cdot x_i^{l+1} \approx 0$$

Vanishing gradient, caused by small output

Backward

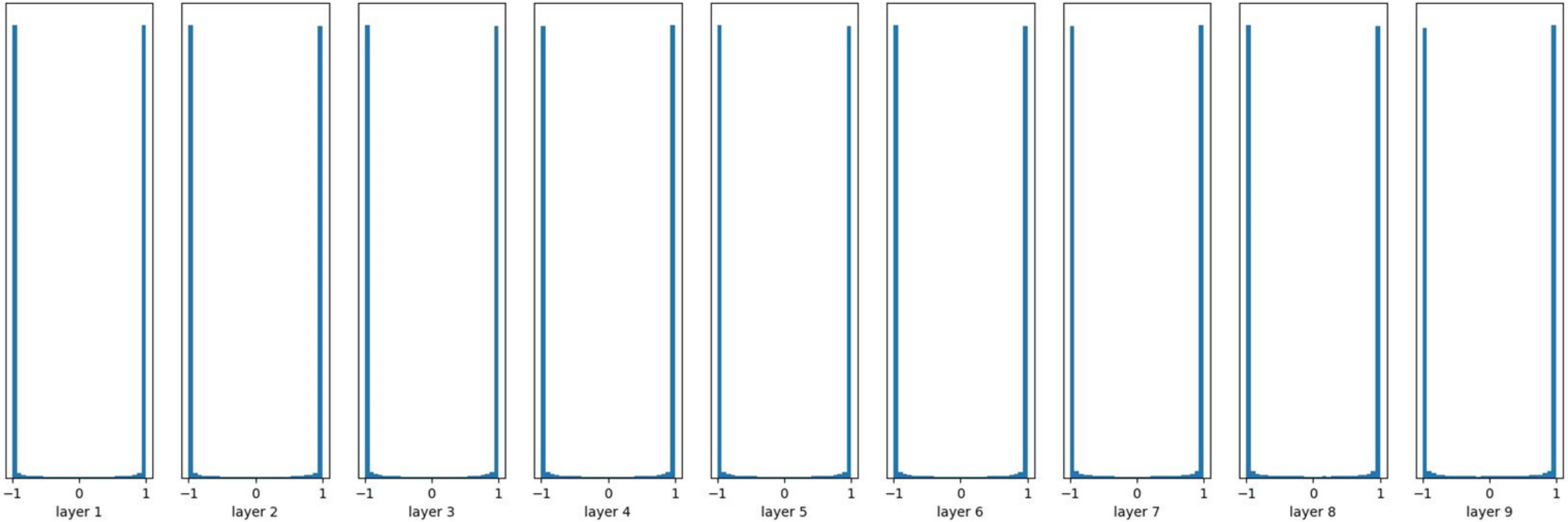
Big Random Numbers

- Gaussian with zero mean and standard deviation 1

- Let us see what happens:
  - Network with 10 layers with 500 neurons each
  - Tanh as activation functions
  - Input unit Gaussian data

Big Random Numbers

tanh as activation functions

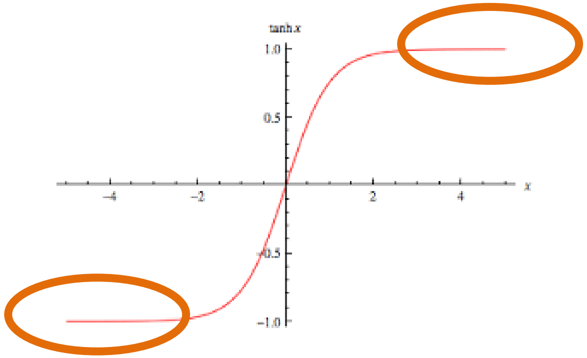


Output saturated to -1 and 1

Big Random Numbers

Output saturated to -1 and 1.
Gradient of the activation function becomes close to 0.

$$f(s) = f\left(\sum_i w_i x_i + b\right)$$



$$\frac{\partial L}{\partial w_i} = \frac{\partial L}{\partial f} \cdot \frac{\partial f}{\partial s} \cdot \frac{\partial s}{\partial w_i} \approx 0$$

Vanishing gradient, caused by saturated activation function.

How to solve this?

- Working on the initialization
- Working on the output generated by each layer

Xavier Initialization

- Gaussian with zero mean, but what standard deviation?

$$Var(s) = Var\left(\sum_{i}^{n} w_i x_i\right) = \sum_{i}^{n} Var(w_i x_i)$$

Notice: $\boldsymbol{n}$ is the number of input neurons for the layer of weights you want to initialized. This $\boldsymbol{n}$ is not the number N of input data $X \in R^{N \times D}$. For the first layer $\boldsymbol{n} = D$.

Tips:

$$E[X^2] = Var[X] + E[X]^2$$

If X, Y are independent:

$$Var[XY] = E[X^2Y^2] - E[XY]^2$$

$$E[XY] = E[X]E[Y]$$

[Glorot and Bengio, AISTATS'10] Xavier Initialization

Xavier Initialization

- Gaussian with zero mean, but what standard deviation?

$$Var(s) = Var\left(\sum_i^n w_i x_i\right) = \sum_i^n Var(w_i x_i)$$

$$= \sum_i^n [E(w_i)]^2 Var(x_i) + E[(x_i)]^2 Var(w_i) + Var(x_i)Var(w_i)$$

Zero mean Zero mean

[Glorot and Bengio, AISTATS'10] Xavier Initialization

Xavier Initialization

- Gaussian with zero mean, but what standard deviation?

$$Var(s) = Var\left(\sum_{i}^{n} w_i x_i\right) = \sum_{i}^{n} Var(w_i x_i)$$

$$= \sum_{i}^{n} [E(w_i)]^2 Var(x_i) + E[(x_i)]^2 Var(w_i) + Var(x_i) Var(w_i)$$

$$= \sum_{i}^{n} Var(x_i) Var(w_i) = n(Var(w) Var(x))$$

Identically distributed
(each random variable has the same distribution)

[Glorot and Bengio, AISTATS'10] Xavier Initialization

Xavier Initialization

- How to ensure the variance of the output is the same as the input?

Goal:

$$Var(s) = Var(x) \longrightarrow \underbrace{n \cdot Var(w)}_{=1} Var(x) = Var(x)$$

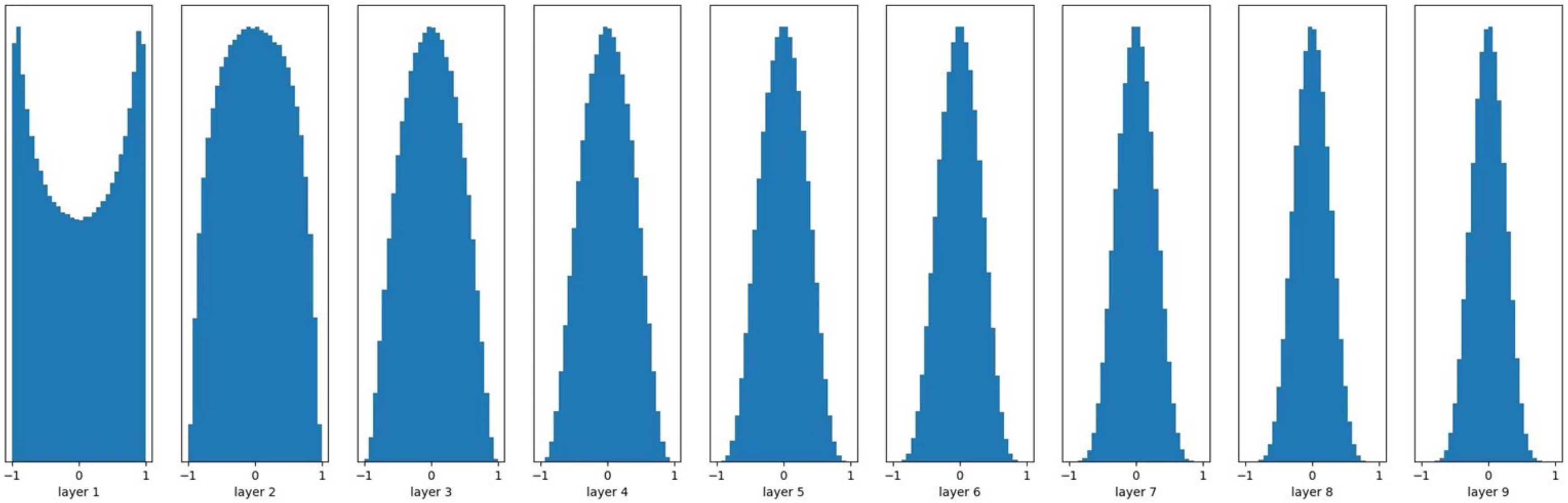
$$\longrightarrow Var(w) = \frac{1}{n}$$

n: number of input neurons

Xavier Initialization

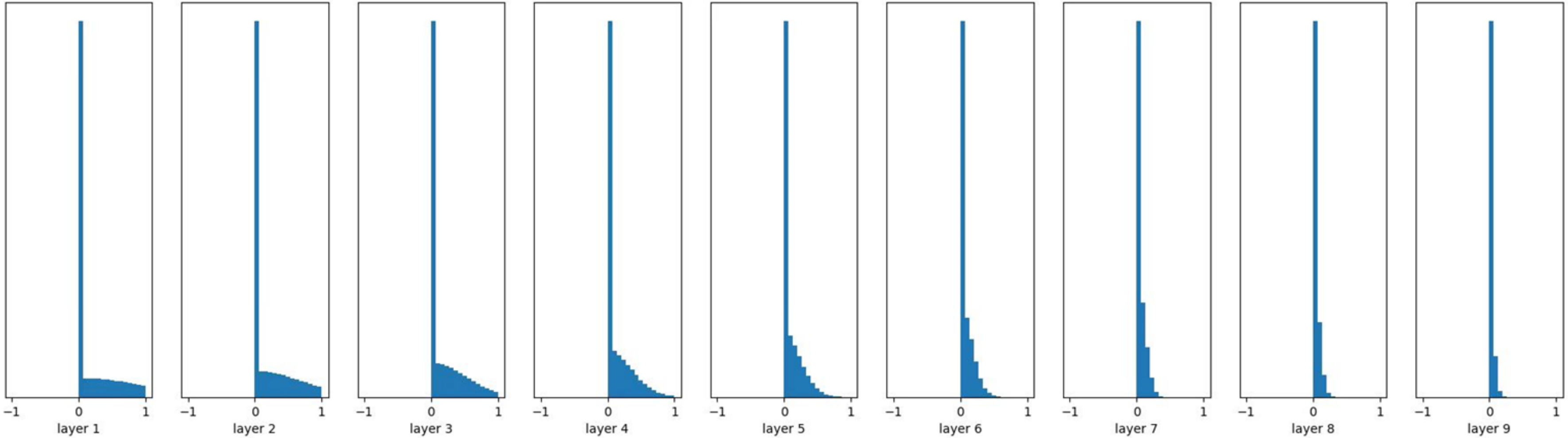
$$\boxed{Var(w) = \frac{1}{n}}$$

tanh as activation functions



Xavier Initialization with ReLU (Kaiming Initialization)

$$\boxed{Var(w) = \frac{1}{n}}$$



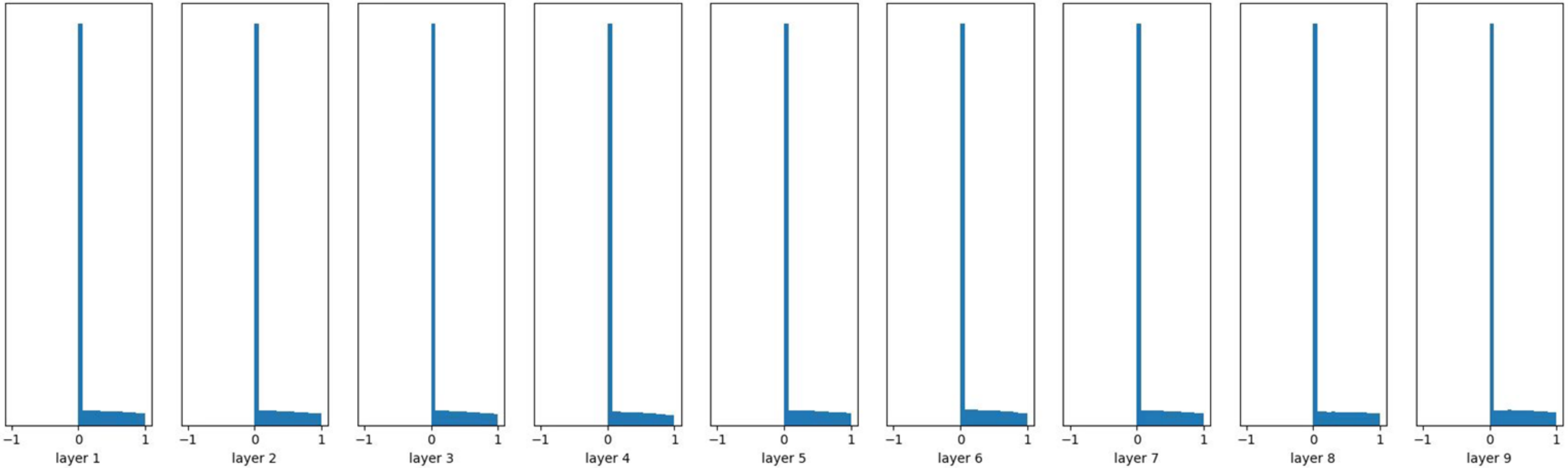
ReLU kills Half of the Data

What's the solution?

When using ReLU, output close to zero again ☹

Kaiming Initialization with ReLU

$$\boxed{Var(w) = \frac{1}{n/2} = \boxed{\frac{2}{n}}}$$

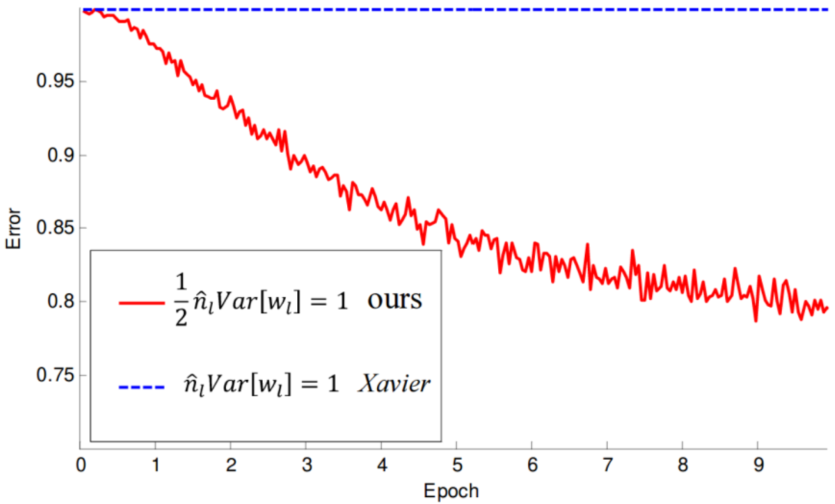


[He et al., ICCV'15] He Initialization

Kaiming Initialization with ReLU

$$\boxed{Var(w) = \frac{2}{n}}$$

It makes a huge difference!



- Use ReLU and Xavier/2 initialization

[He et al., ICCV'15] He Initialization

Summary

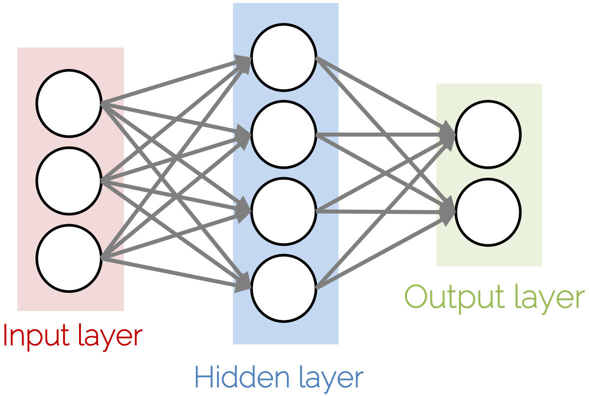


Image Classification	Output Layer	Loss function
Binary Classification	Sigmoid	Binary Cross entropy
Multiclass Classification	Softmax	Cross entropy

Other Losses:
SVM Loss (Hinge Loss), L1/L2-Loss

Initialization of optimization

- How to set weights at beginning

Next Lecture

- Next lecture
  - More about training neural networks: regularization, dropout, data augmentation, batch normalization, etc.
  - Followed by CNNs

See you next week!

References

- Goodfellow et al. “Deep Learning” (2016),
  – Chapter 6: Deep Feedforward Networks

- Bishop “Pattern Recognition and Machine Learning” (2006),
  – Chapter 5.5: Regularization in Network Nets

- http://cs231n.github.io/neural-networks-1/

- http://cs231n.github.io/neural-networks-2/

- http://cs231n.github.io/neural-networks-3/