

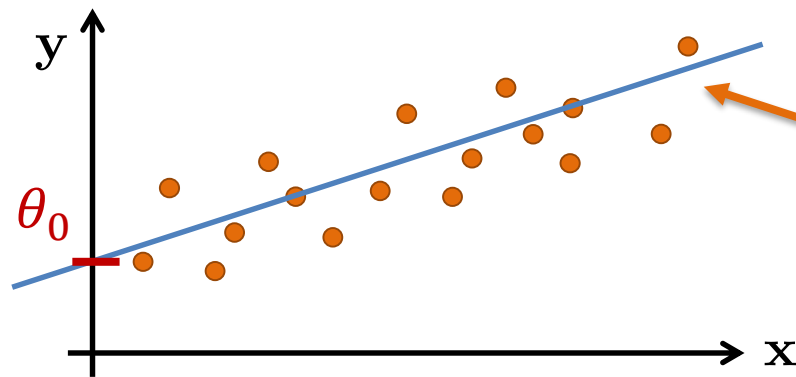
# Introduction to Neural Networks

# From Linear and Logistic Regression to Neural Networks

# Linear Regression

= a supervised learning method to find a linear model of the form

$$\hat{y}_i = \theta_0 + \sum_{j=1}^d x_{ij}\theta_j = \theta_0 + x_{i1}\theta_1 + x_{i2}\theta_2 + \cdots + x_{id}\theta_d$$



Goal: find a model that explains a target  $y$  given the input  $x$

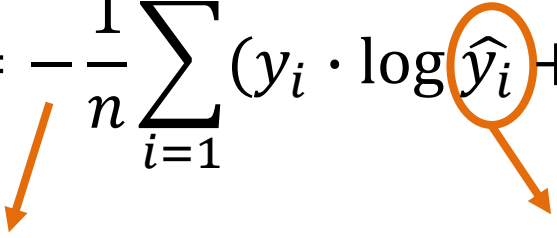
# Logistic Regression

- Loss per training sample

$$\mathcal{L}(\hat{y}_i, y_i) = -[y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)]$$

- Overall loss

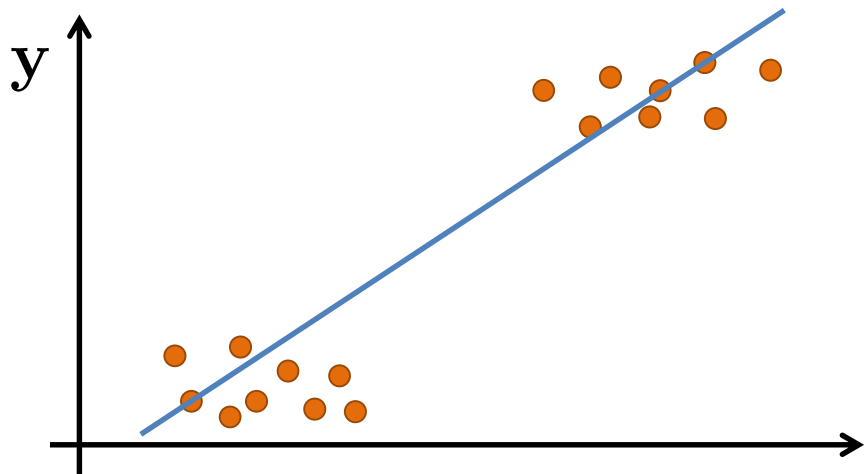
$$\mathcal{C}(\boldsymbol{\theta}) = -\frac{1}{n} \sum_{i=1}^n (y_i \cdot \log \hat{y}_i + (1 - y_i) \cdot \log[1 - \hat{y}_i])$$



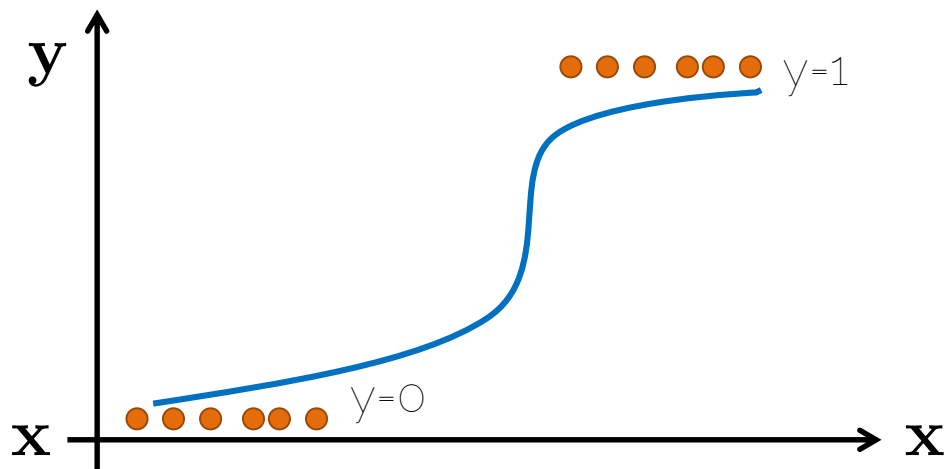
Minimization

$\hat{y}_i = \sigma(x_i \boldsymbol{\theta})$

# Linear vs Logistic Regression

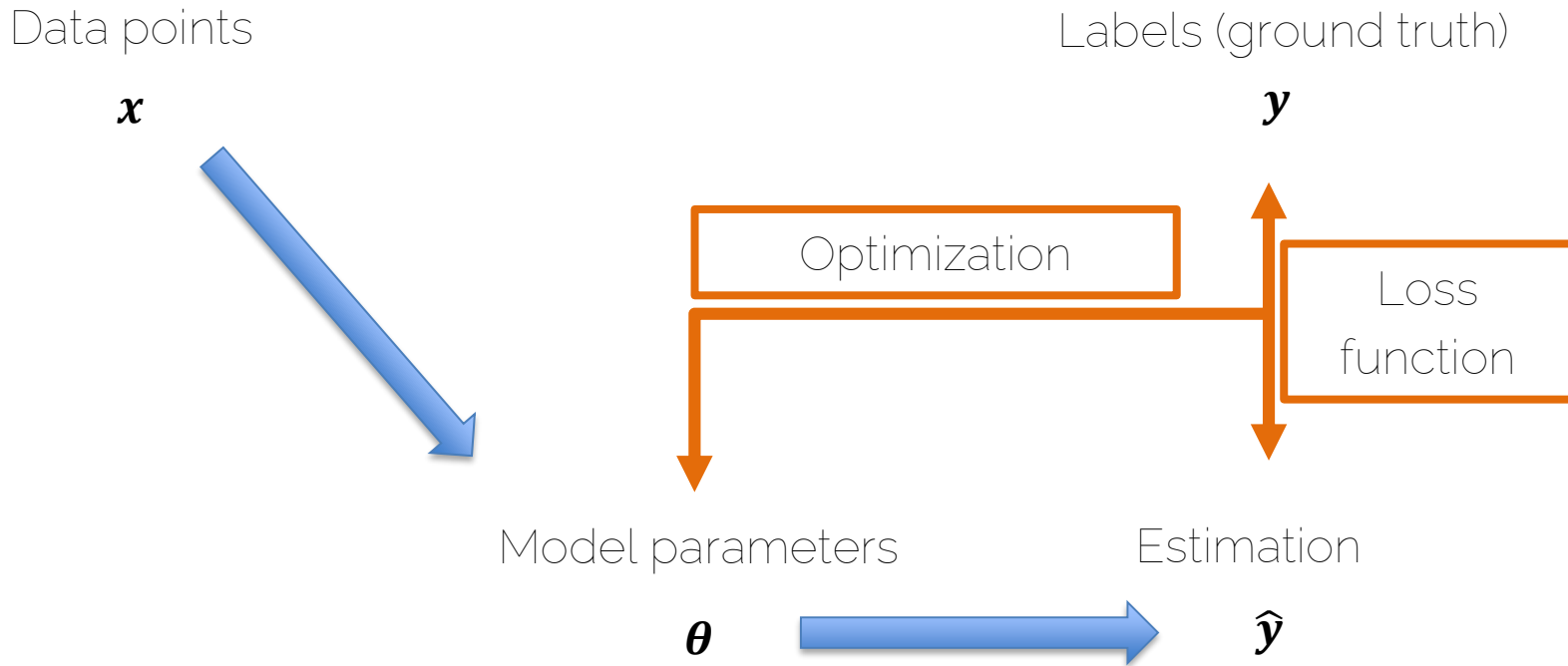


Predictions can exceed the range of the training samples  
→ in the case of classification  $[0;1]$  this becomes a real issue



Predictions are guaranteed to be within  $[0;1]$

# How to obtain the Model?



# Linear Score Functions

- Linear score function as seen in linear regression

$$f_i = \sum_j w_{i,j} x_j$$

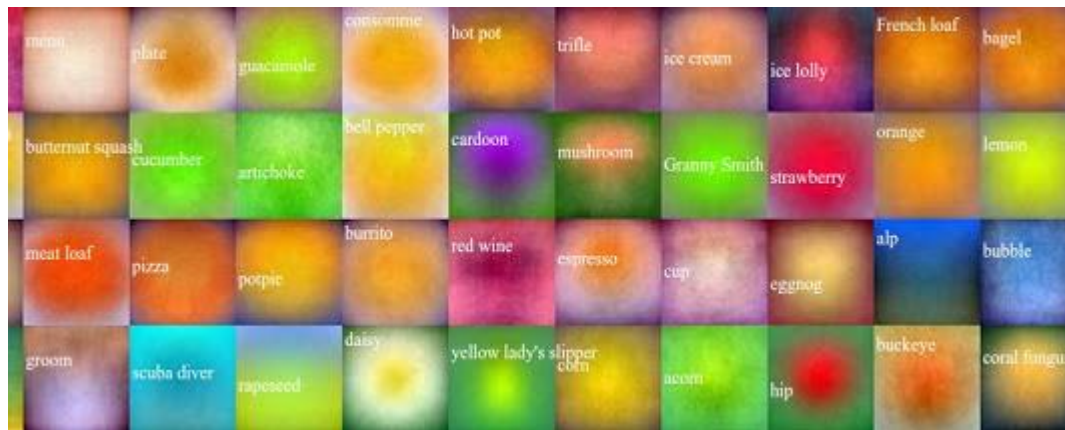
$$\mathbf{f} = \mathbf{W} \mathbf{x} \quad (\text{Matrix Notation})$$

# Linear Score Functions on Images

- Linear score function  $f = Wx$



On CIFAR-10



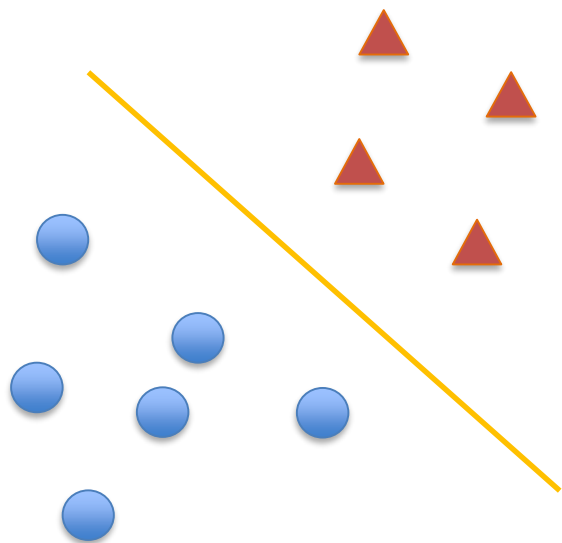
On ImageNet

Source: Li/Karpathy/Johnson

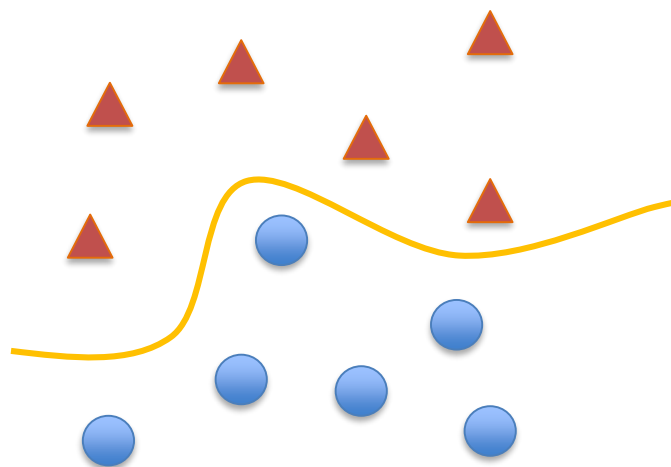


# Linear Score Functions?

Logistic Regression



Linear Separation Impossible!



# Linear Score Functions?

- Can we make linear regression better?
  - Naïve idea: Multiply with another weight matrix  $\mathbf{W}_2$

$$\hat{\mathbf{f}} = \mathbf{W}_2 \cdot \mathbf{W}_1 \cdot \mathbf{x}$$

- Operation remains linear:

$$\mathbf{W} = \mathbf{W}_2 \cdot \mathbf{W}_1$$

$$\hat{\mathbf{f}} = \mathbf{W}\mathbf{x}$$

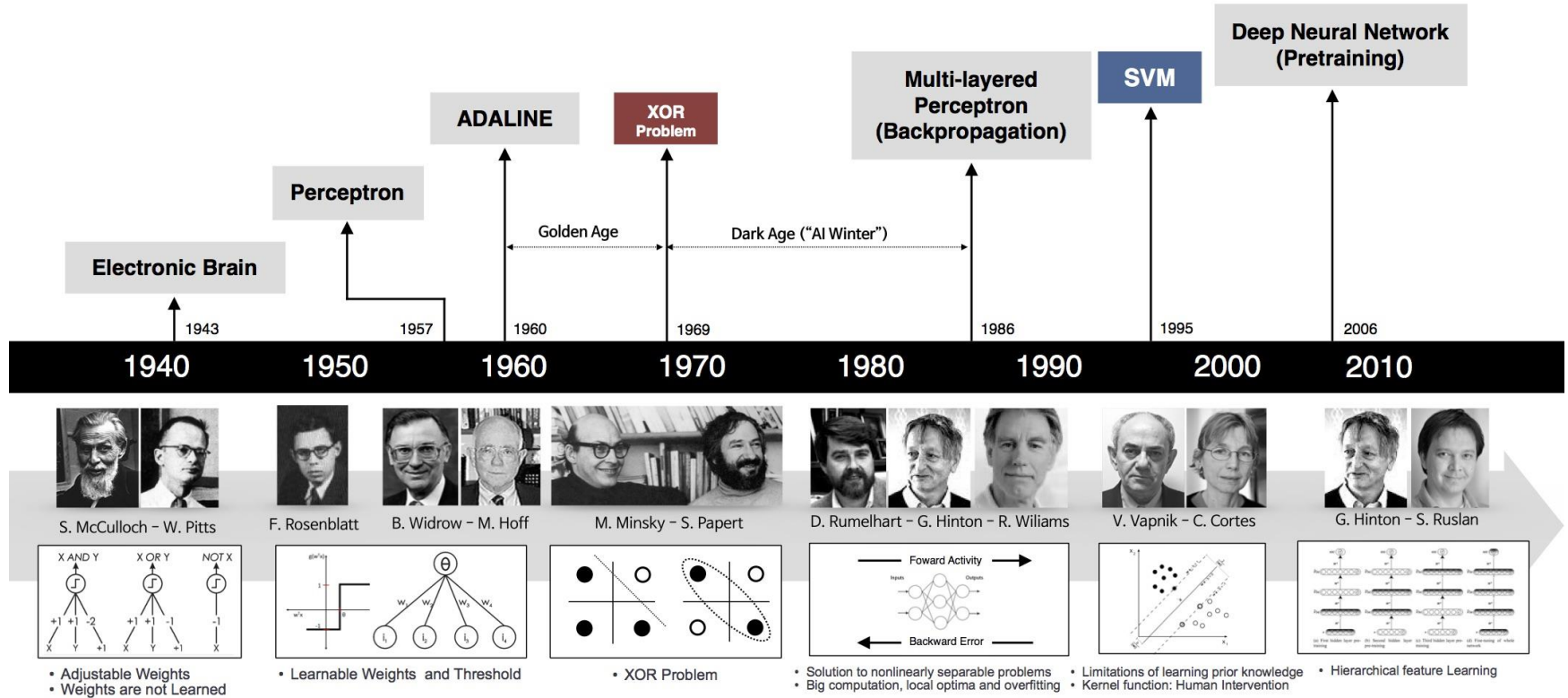
- Solution  $\rightarrow$  add non-linearity!!

# Neural Network

- Linear score function  $\mathbf{f} = \mathbf{W}\mathbf{x}$
- Neural network is a nesting of 'functions'
  - 2-layers:  $\mathbf{f} = \mathbf{W}_2 \max(\mathbf{0}, \mathbf{W}_1 \mathbf{x})$
  - 3-layers:  $\mathbf{f} = \mathbf{W}_3 \max(\mathbf{0}, \mathbf{W}_2 \max(\mathbf{0}, \mathbf{W}_1 \mathbf{x}))$
  - 4-layers:  $\mathbf{f} = \mathbf{W}_4 \tanh(\mathbf{W}_3, \max(\mathbf{0}, \mathbf{W}_2 \max(\mathbf{0}, \mathbf{W}_1 \mathbf{x})))$
  - 5-layers:  $\mathbf{f} = \mathbf{W}_5 \sigma(\mathbf{W}_4 \tanh(\mathbf{W}_3, \max(\mathbf{0}, \mathbf{W}_2 \max(\mathbf{0}, \mathbf{W}_1 \mathbf{x}))))$
  - ... up to hundreds of layers

# Introduction to Neural Networks

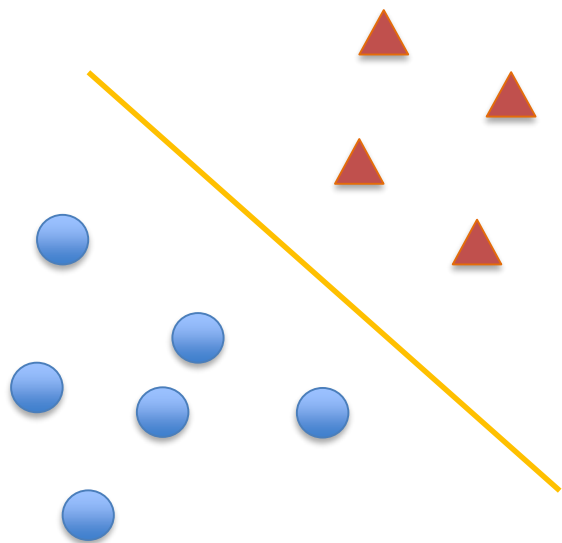
# History of Neural Networks



Source: [http://beamlab.org/deeplearning/2017/02/23/deep\\_learning\\_101\\_part1.html](http://beamlab.org/deeplearning/2017/02/23/deep_learning_101_part1.html)

# Neural Network

Logistic Regression



Neural Networks

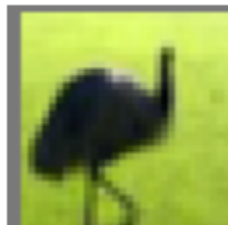


# Neural Network

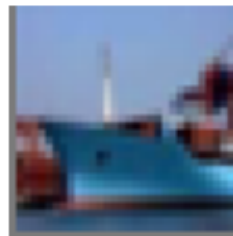
- Non-linear score function  $f = \dots (\max(0, \mathbf{W}_1 \mathbf{x}))$



truck  
ship  
airplane

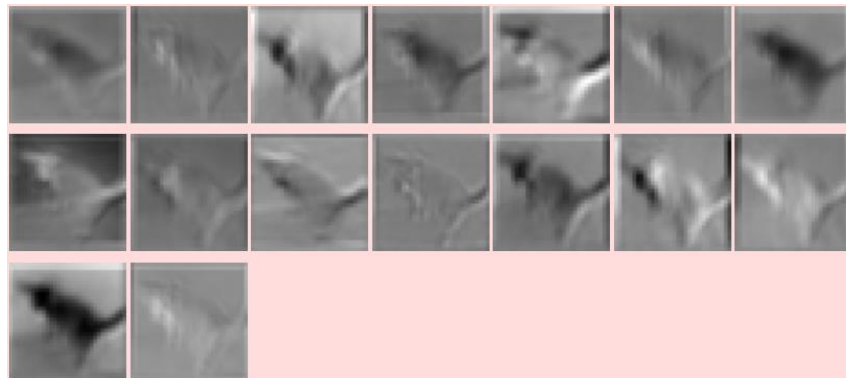
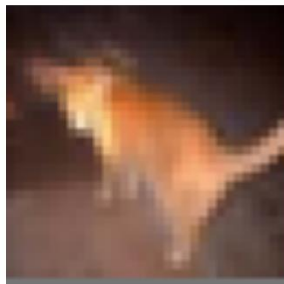


bird  
deer  
frog



ship  
airplane  
truck

On CIFAR-10

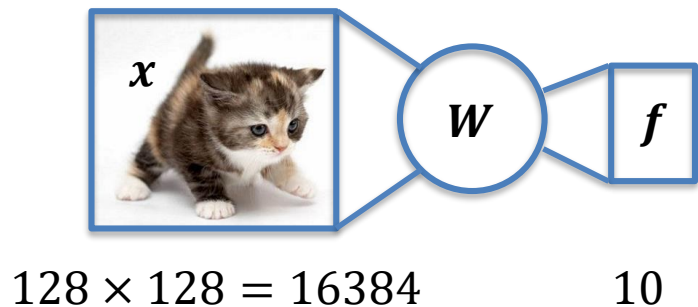


Visualizing activations of the first layer.

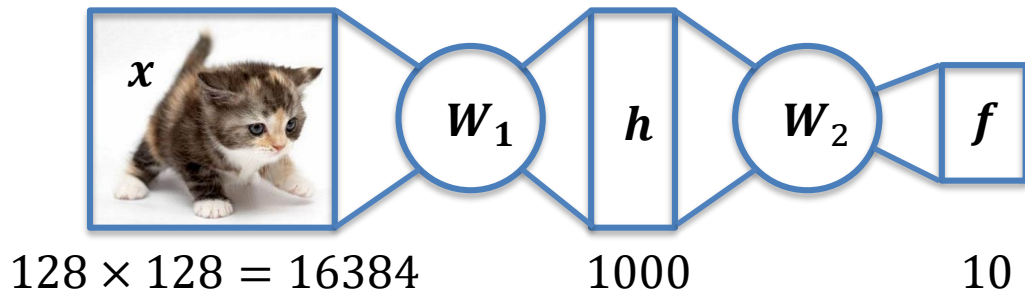
Source: ConvNetJS

# Neural Network

1-layer network:  $f = Wx$



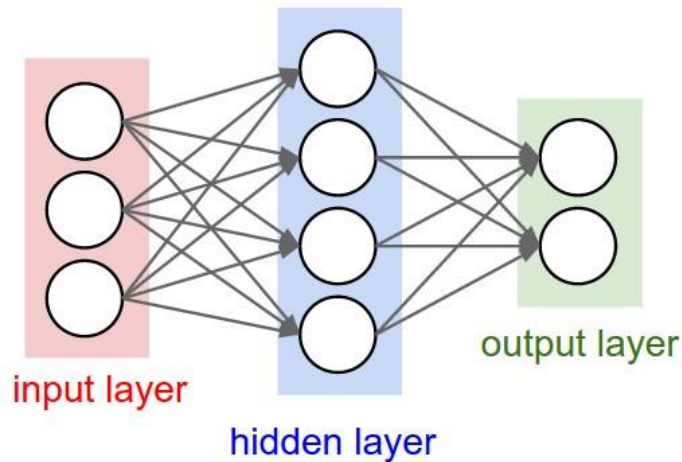
2-layer network:  $f = W_2 \max(0, W_1 x)$



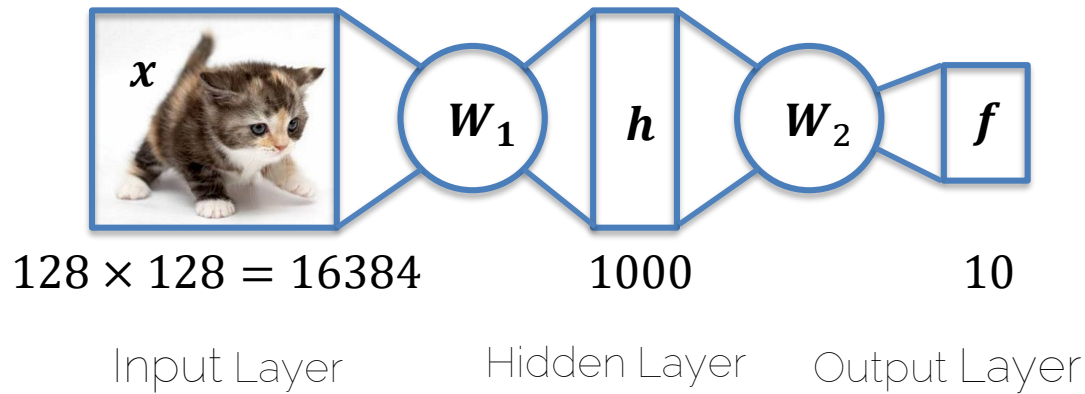
Why is this structure useful?



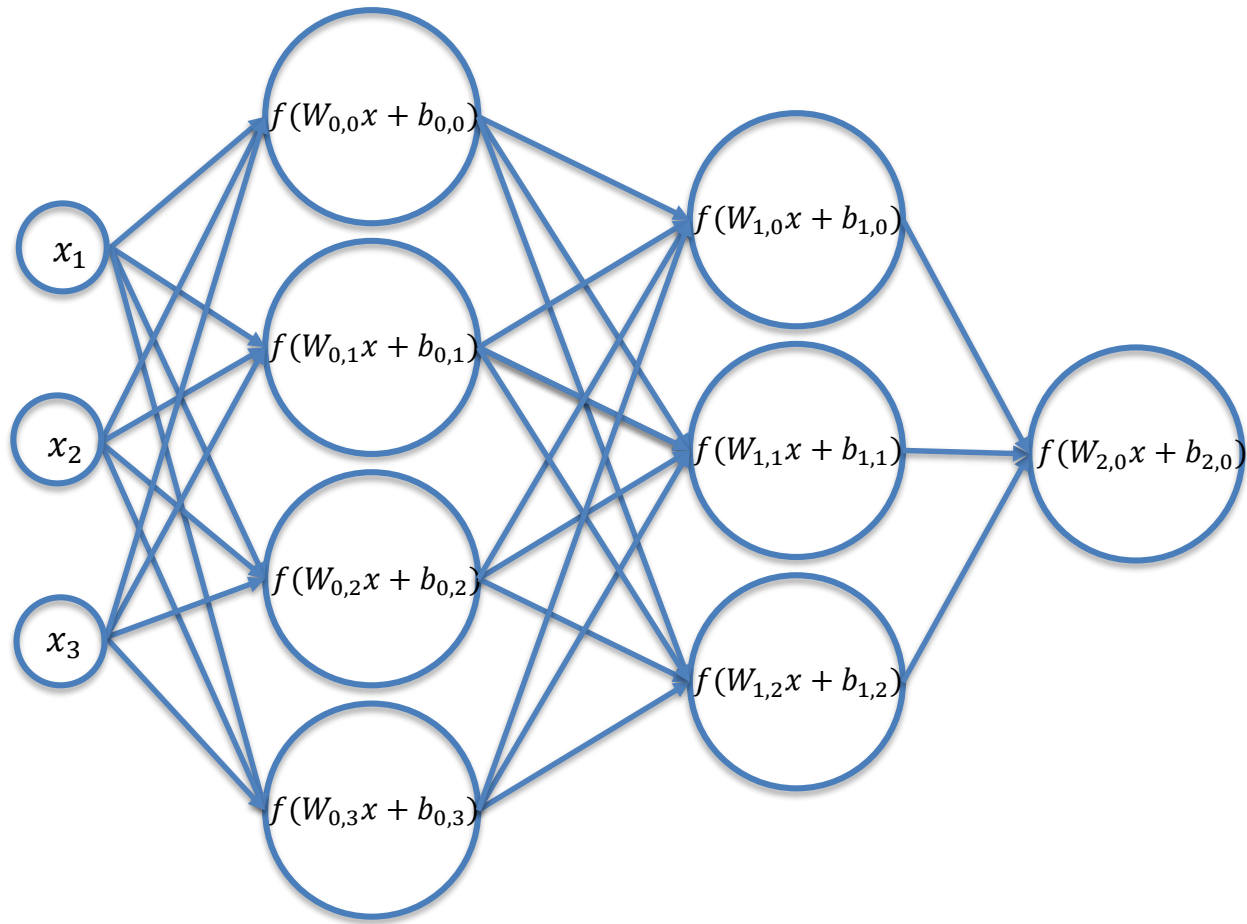
# Neural Network



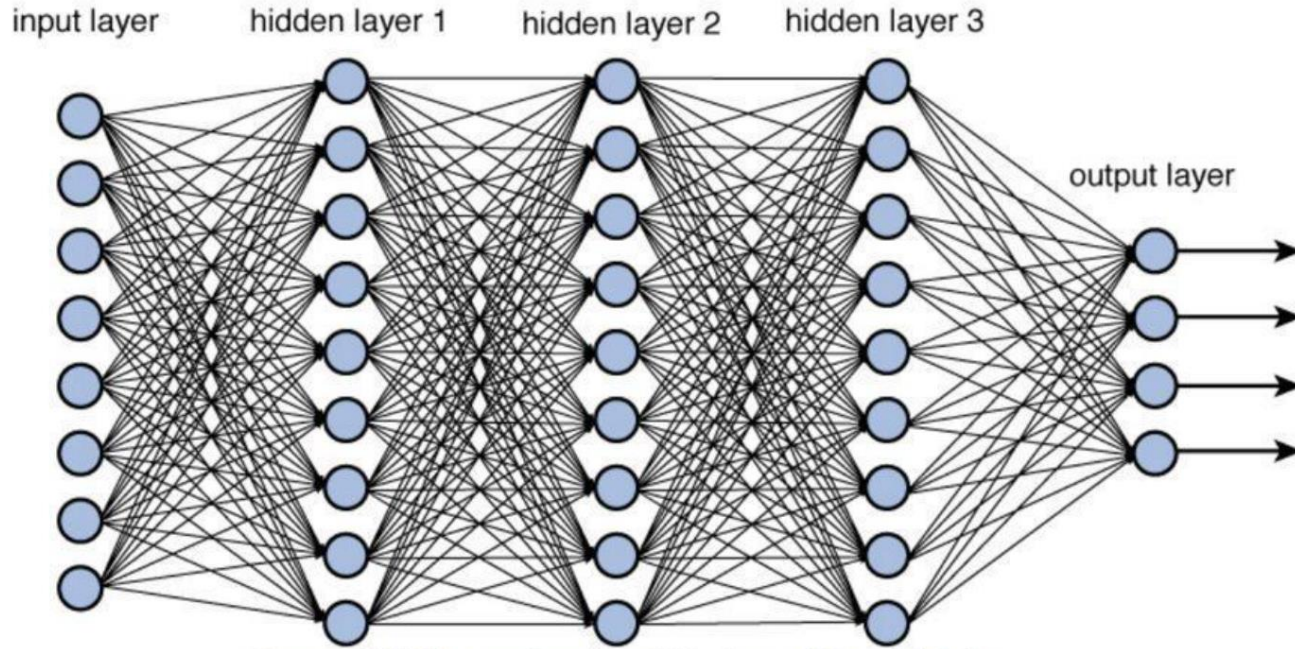
2-layer network:  $f = W_2 \max(0, W_1 x)$



# Net of Artificial Neurons



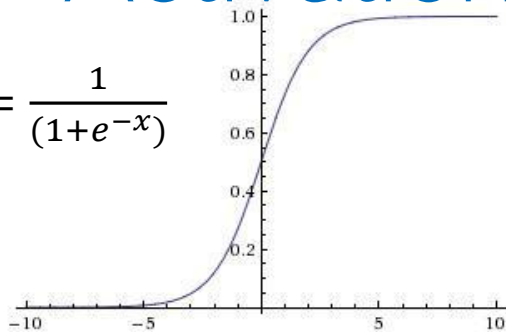
# Neural Network



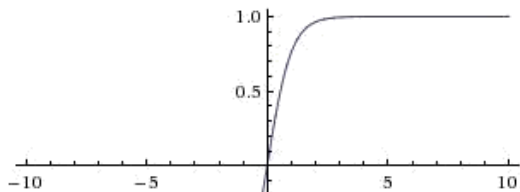
Source: <https://towardsdatascience.com/training-deep-neural-networks-gfdb1964b964>

# Activation Functions

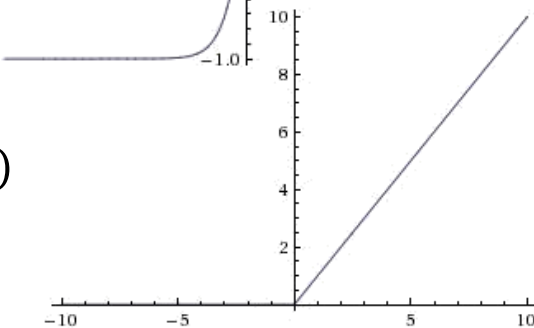
Sigmoid:  $\sigma(x) = \frac{1}{1+e^{-x}}$



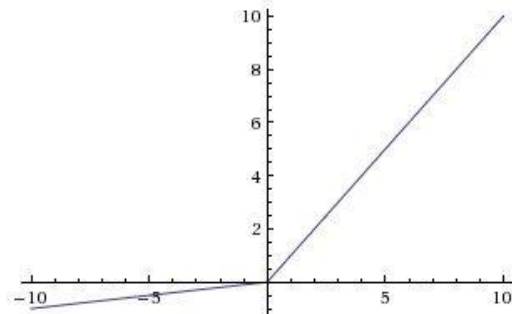
tanh:  $\tanh(x)$



ReLU:  $\max(0, x)$



Leaky ReLU:  $\max(0.1x, x)$



Parametric ReLU:  $\max(\alpha x, x)$

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

ELU  $f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha(e^x - 1) & \text{if } x \leq 0 \end{cases}$

# Neural Network

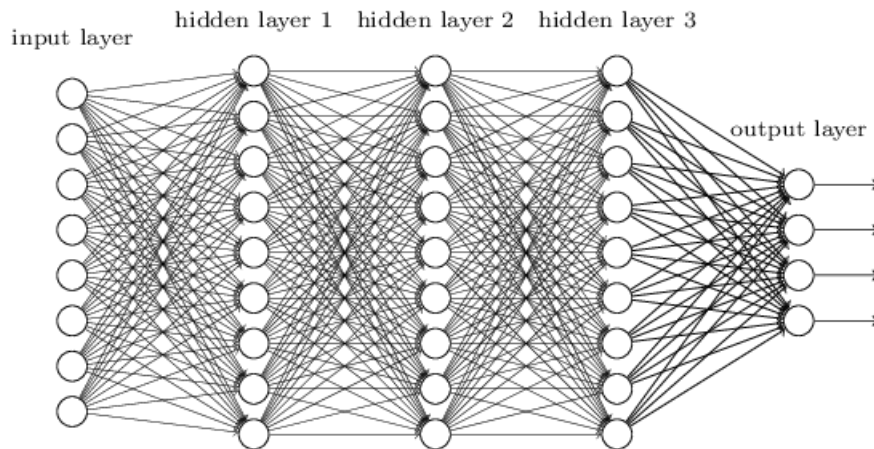
$$\mathbf{f} = \mathbf{W}_3 \cdot (\mathbf{W}_2 \cdot (\mathbf{W}_1 \cdot \mathbf{x}))$$

Why activation functions?

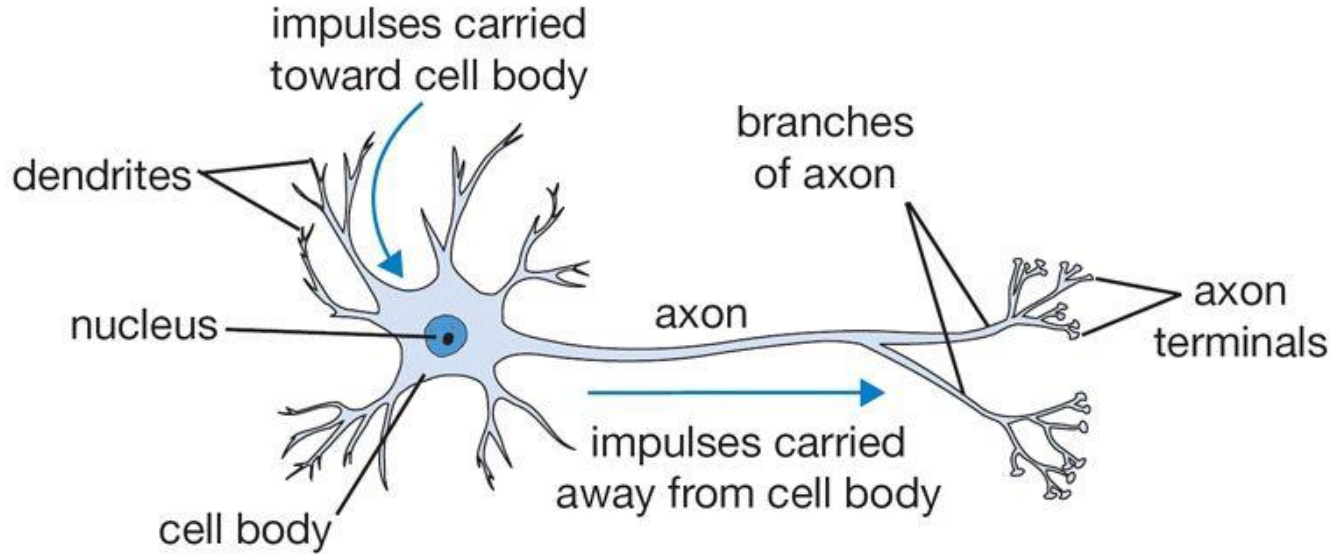
Simply concatenating linear layers would be so much cheaper...

# Neural Network

Why organize a neural network into layers?

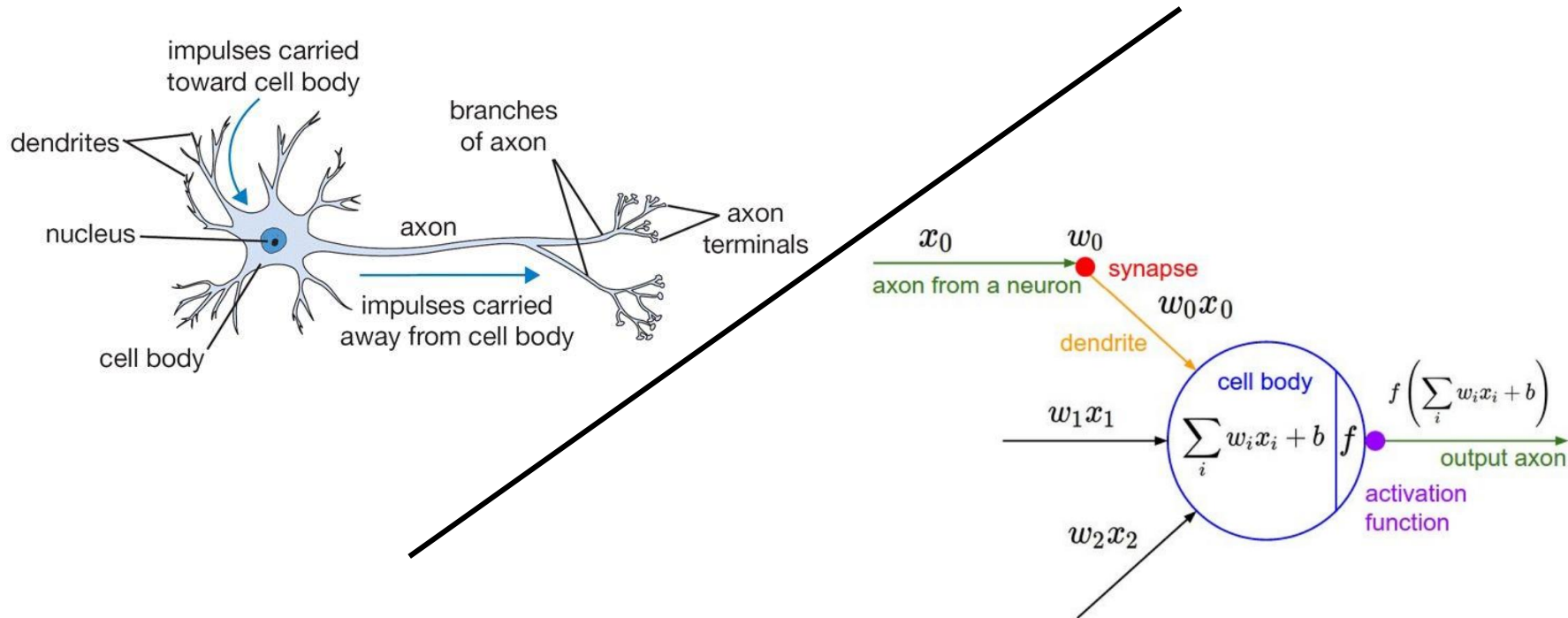


# Biological Neurons



Credit: Stanford CS 231n

# Biological Neurons



Credit: Stanford CS 231n

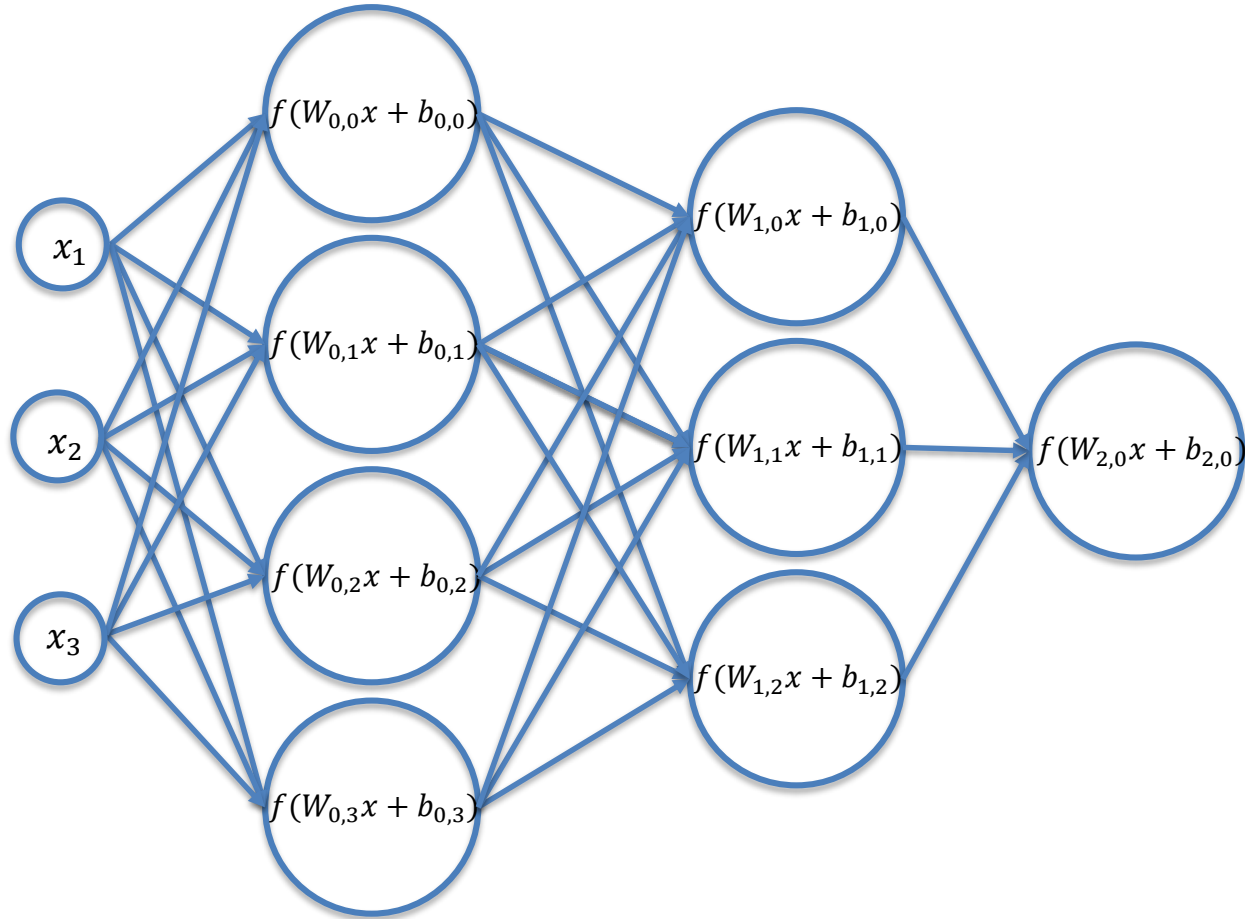


# Artificial Neural Networks vs Brain



Artificial neural networks are **inspired** by the brain,  
but not even close in terms of complexity!  
The comparison is great for the media and news articles though... 😊

# Artificial Neural Network



# Neural Network

- Summary
  - Given a dataset with ground truth training pairs  $[x_i; y_i]$ ,
  - Find optimal weights and biases  $\mathbf{W}$  using stochastic gradient descent, such that the loss function is minimized
    - Compute gradients with backpropagation (use batch-mode; more later)
    - Iterate many times over training set (SGD; more later)

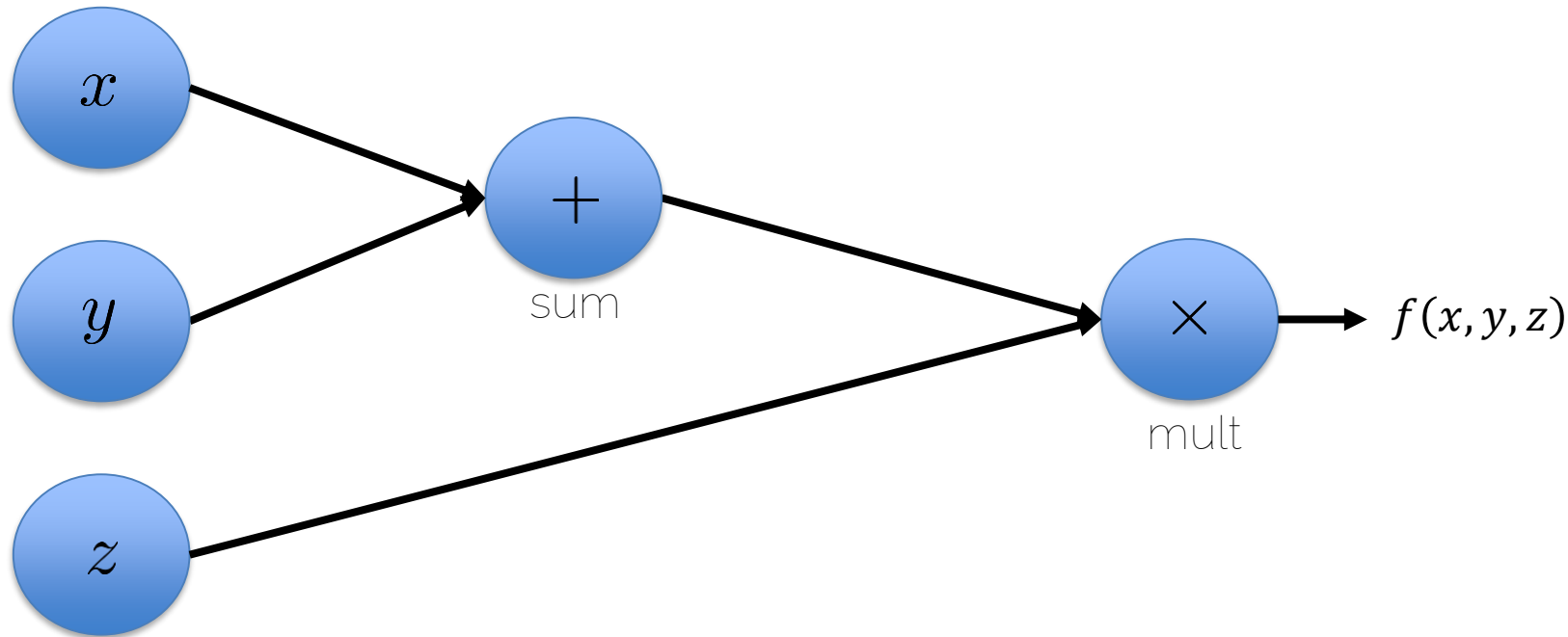
# Computational Graphs

# Computational Graphs

- Directional graph
- Matrix operations are represented as compute nodes.
- Vertex nodes are variables or operators like  $+$ ,  $-$ ,  $*$ ,  $/$ ,  $\log()$ ,  $\exp()$  ...
- Directional edges show flow of inputs to vertices

# Computational Graphs

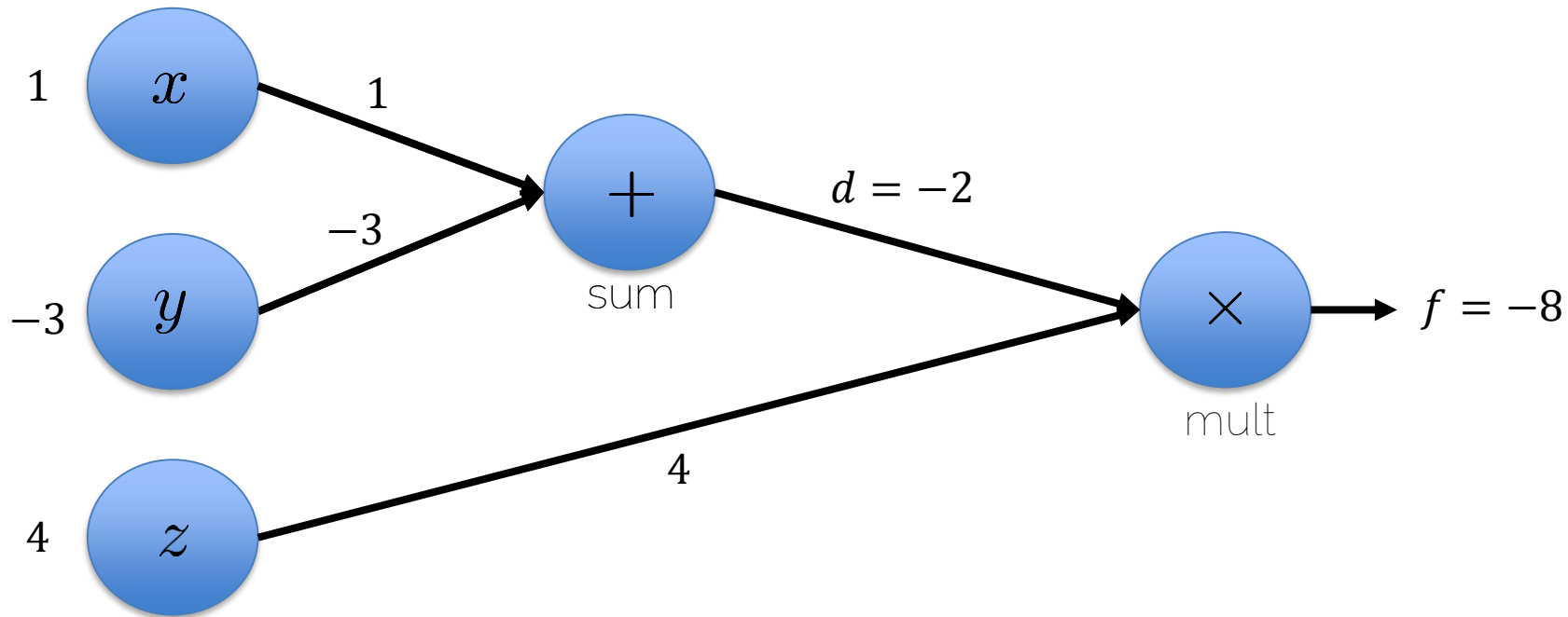
- $f(x, y, z) = (x + y) \cdot z$



# Evaluation: Forward Pass

- $f(x, y, z) = (x + y) \cdot z$

Initialization  $x = 1, y = -3, z = 4$



# Computational Graphs

- Why discuss compute graphs?
- Neural networks have complicated architectures
$$f = W_5 \sigma(W_4 \tanh(W_3, \max(0, W_2 \max(0, W_1 x))))$$
- Lot of matrix operations!
- Represent NN as computational graphs!

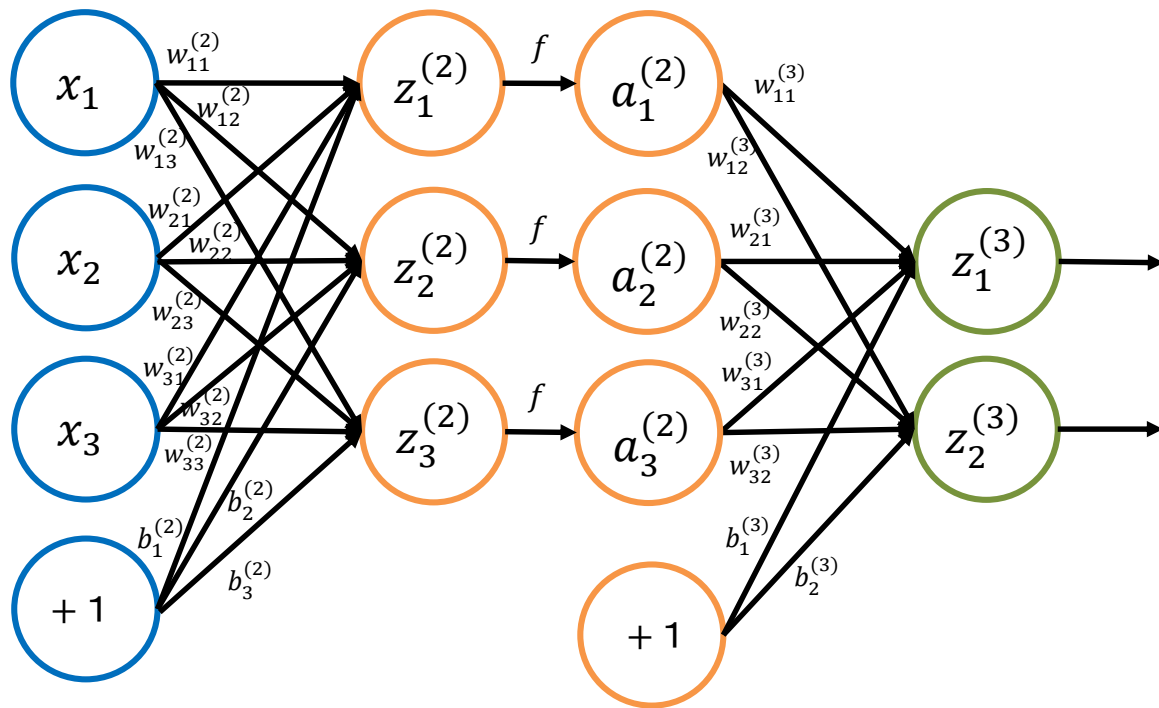


# Computational Graphs

A neural network can be represented as a computational graph...

- it has compute nodes (operations)
- it has edges that connect nodes (data flow)
- it is directional
- it can be organized into 'layers'

# Computational Graphs



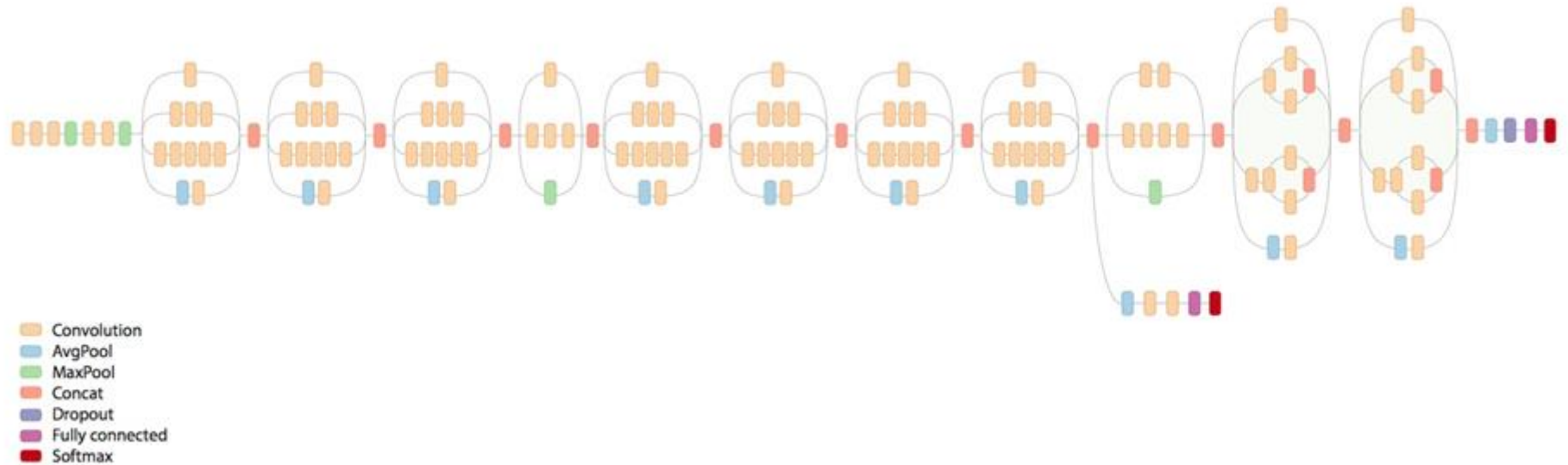
$$z_k^{(2)} = \sum_i x_i w_{ik}^{(2)} + b_k^{(2)}$$

$$a_k^{(2)} = f(z_k^{(2)})$$

$$z_k^{(3)} = \sum_i a_i^{(2)} w_{ik}^{(3)} + b_k^{(3)}$$

# Computational Graphs

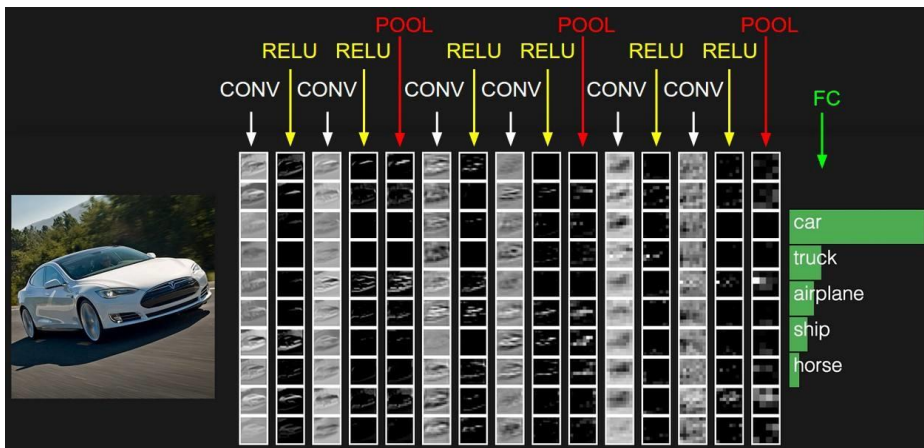
- From a set of neurons to a Structured Compute Pipeline



[Szegedy et al., CVPR'15] Going Deeper with Convolutions

# Computational Graphs

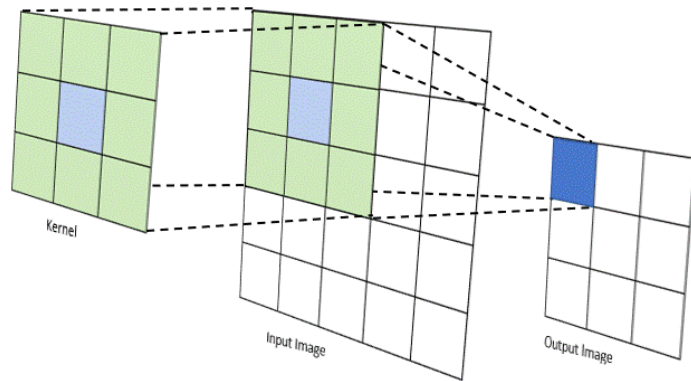
- The computation of Neural Network has further meanings:
  - The multiplication of  $\mathbf{W}$  and  $\mathbf{x}$ : encode input information
  - The activation function: select the key features



Source: <https://www.zybuluo.com/liuhui0803/note/981434>

# Computational Graphs

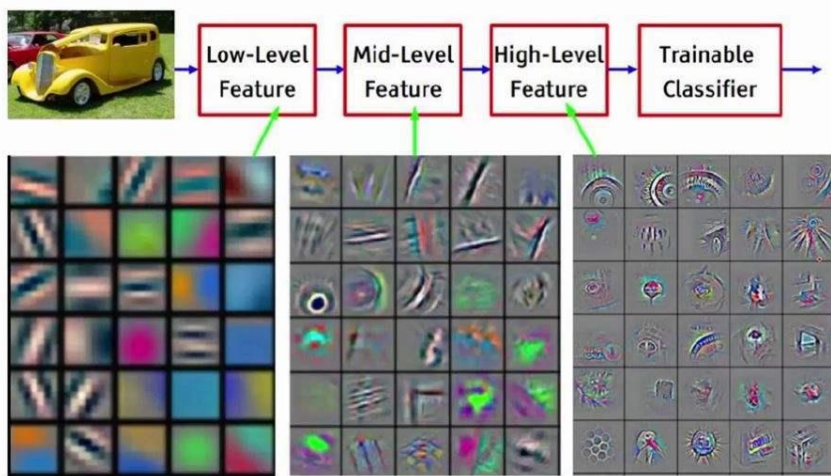
- The computations of Neural Networks have further meanings:
  - The convolutional layers: extract useful features with shared weights



Source: [https://medium.com/@timothy\\_terati/image-convolution-filtering-a54dce7c786b](https://medium.com/@timothy_terati/image-convolution-filtering-a54dce7c786b)

# Computational Graphs

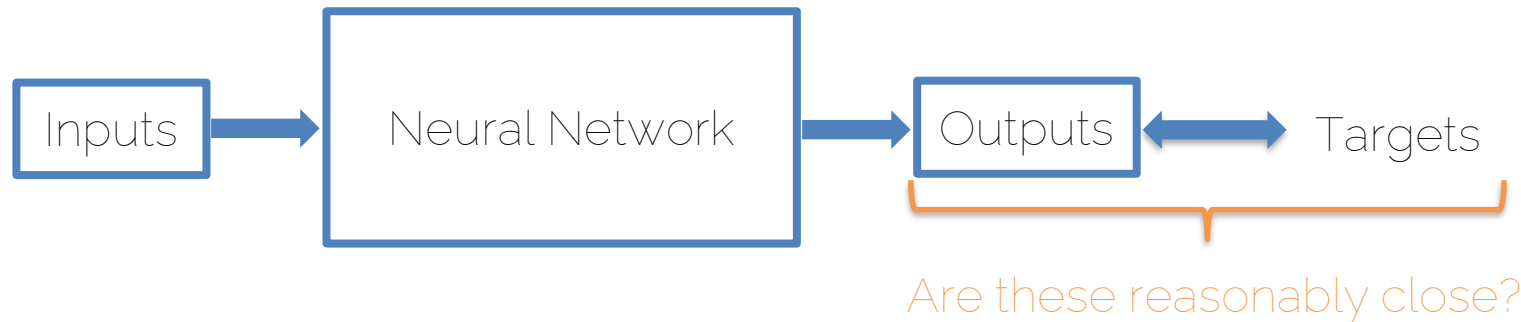
- The computations of Neural Networks have further meanings:
  - The convolutional layers: extract useful features with shared weights



Source: <https://www.zybuluo.com/liuhuio803/note/981434>

# Loss Functions

# What's Next?

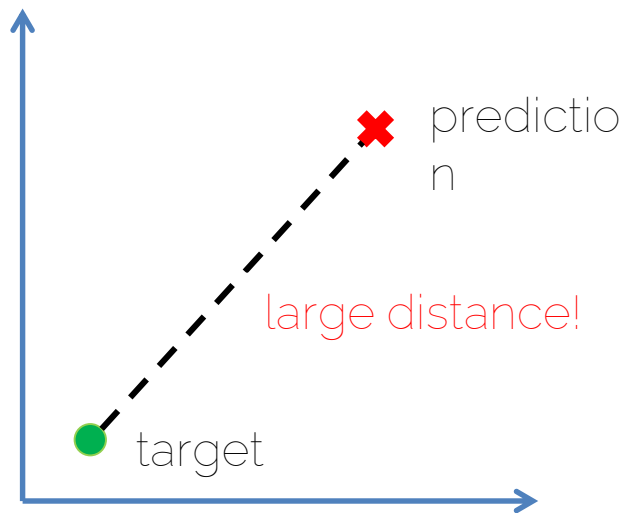


We need a way to describe how close the network's outputs (= predictions) are to the targets!



# What's Next?

Idea: calculate a 'distance' between prediction and target!



bad prediction



good prediction

# Loss Functions

- A function to measure the goodness of the **predictions** (or equivalently, the network's performance)

Intuitively, ...

- a large loss indicates bad predictions/performance (→ performance needs to be improved by training the model)
- the choice of the loss function depends on the concrete problem or the distribution of the target variable

# Regression Loss

- L1 Loss:

$$L(\mathbf{y}, \hat{\mathbf{y}}; \boldsymbol{\theta}) = \frac{1}{n} \sum_i^n \|y_i - \hat{y}_i\|_1$$

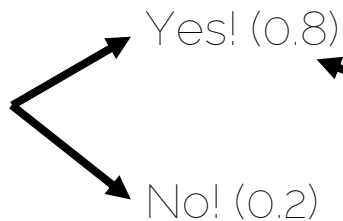
- MSE Loss:

$$L(\mathbf{y}, \hat{\mathbf{y}}; \boldsymbol{\theta}) = \frac{1}{n} \sum_i^n \|y_i - \hat{y}_i\|_2^2$$

# Binary Cross Entropy

- Loss function for binary (yes/no) classification

$$L(\mathbf{y}, \hat{\mathbf{y}}; \boldsymbol{\theta}) = -\frac{1}{n} \sum_i^n [y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)]$$



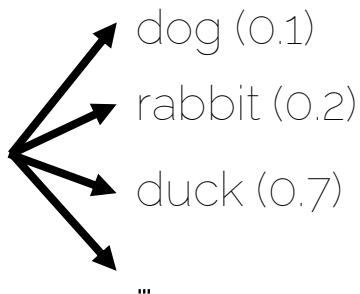
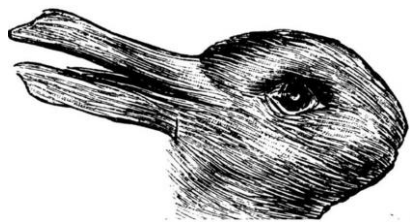
The network predicts the probability of the input belonging to the "yes" class!

# Cross Entropy

Generalizes to multi-class classification:

$$L(\mathbf{y}, \hat{\mathbf{y}}; \boldsymbol{\theta}) = - \sum_{i=1}^n \sum_{k=1}^k (y_{ik} \cdot \log \hat{y}_{ik})$$

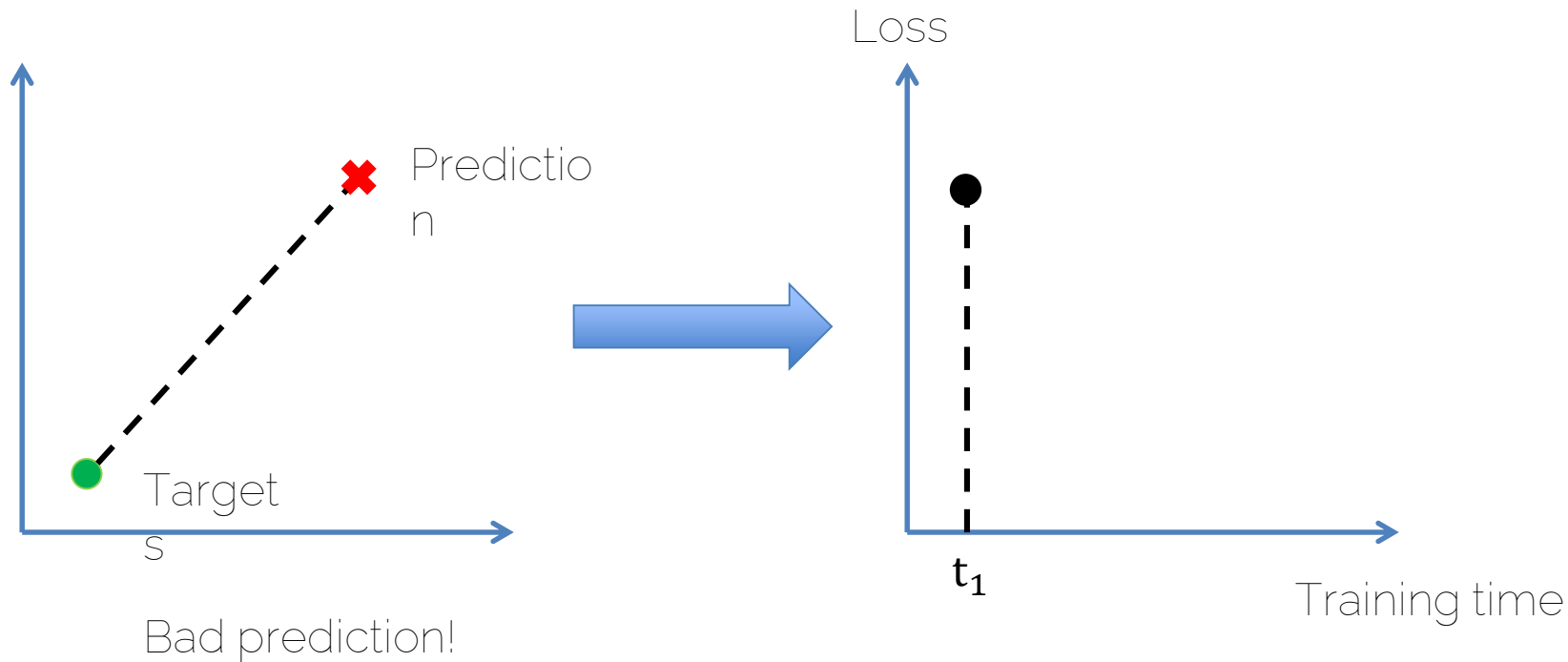
$y_{ik} = \begin{cases} 1 & \text{if } x_i \in \text{class } k \\ 0 & \text{else} \end{cases}$



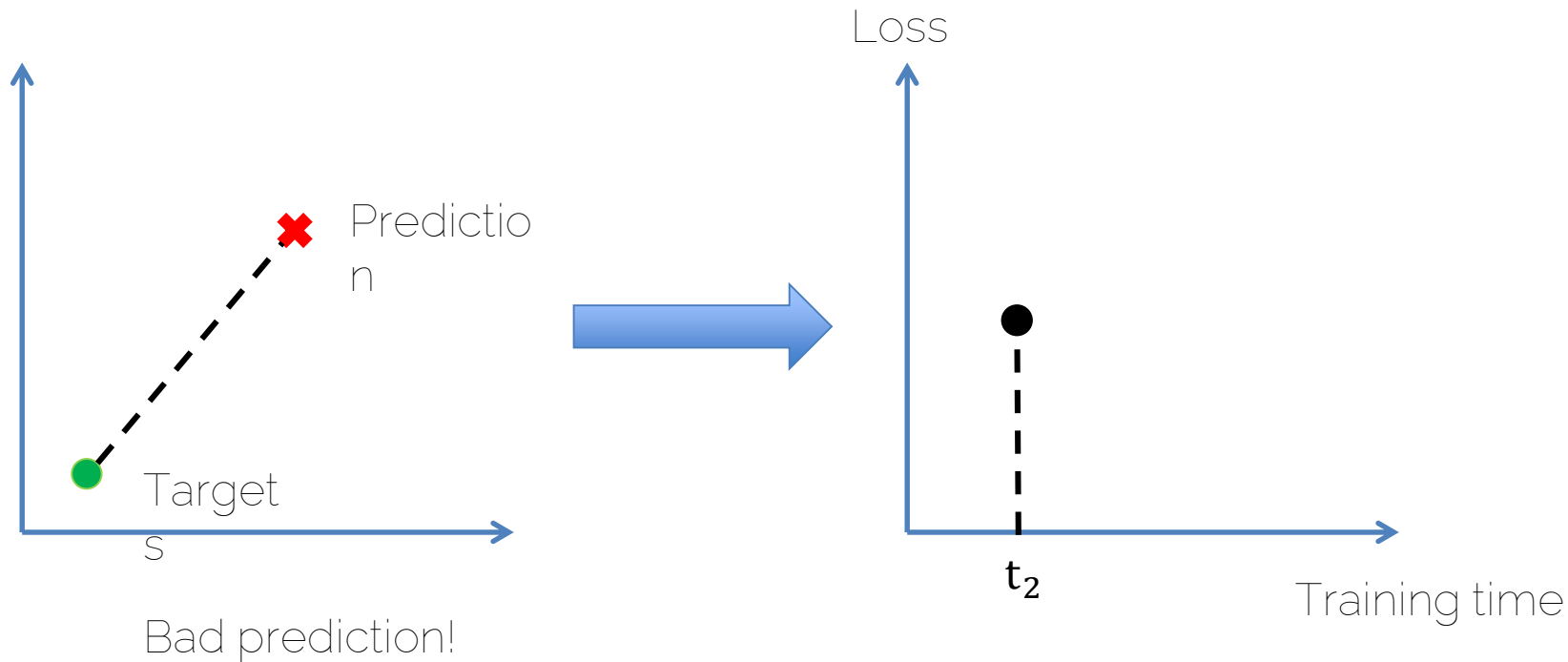
# More General Case

- Ground truth:  $\mathbf{y}$
- Prediction:  $\hat{\mathbf{y}}$
- Loss function:  $L(\mathbf{y}, \hat{\mathbf{y}})$
- Motivation:
  - minimize the loss  $\Leftrightarrow$  find better predictions
  - predictions are generated by the NN
  - find better predictions  $\Leftrightarrow$  find better NN

# Initially

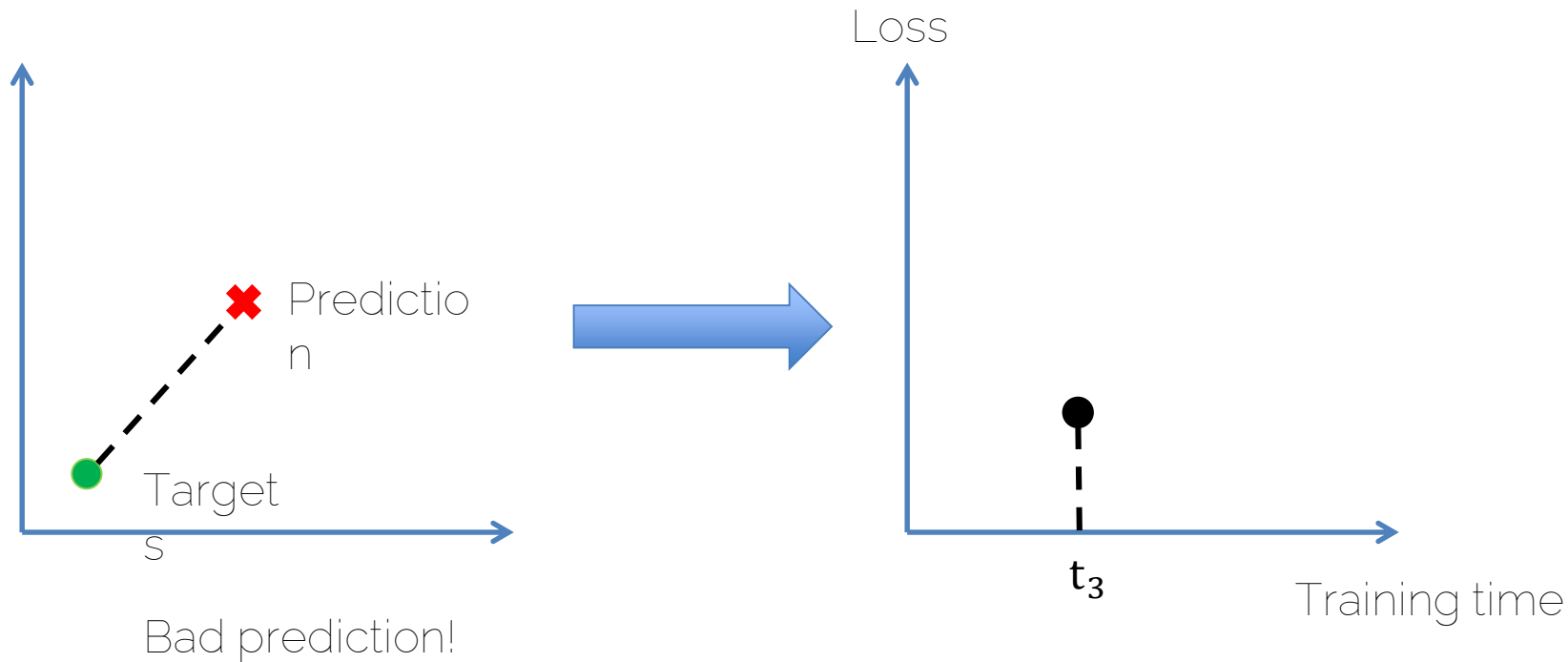


# During Training...

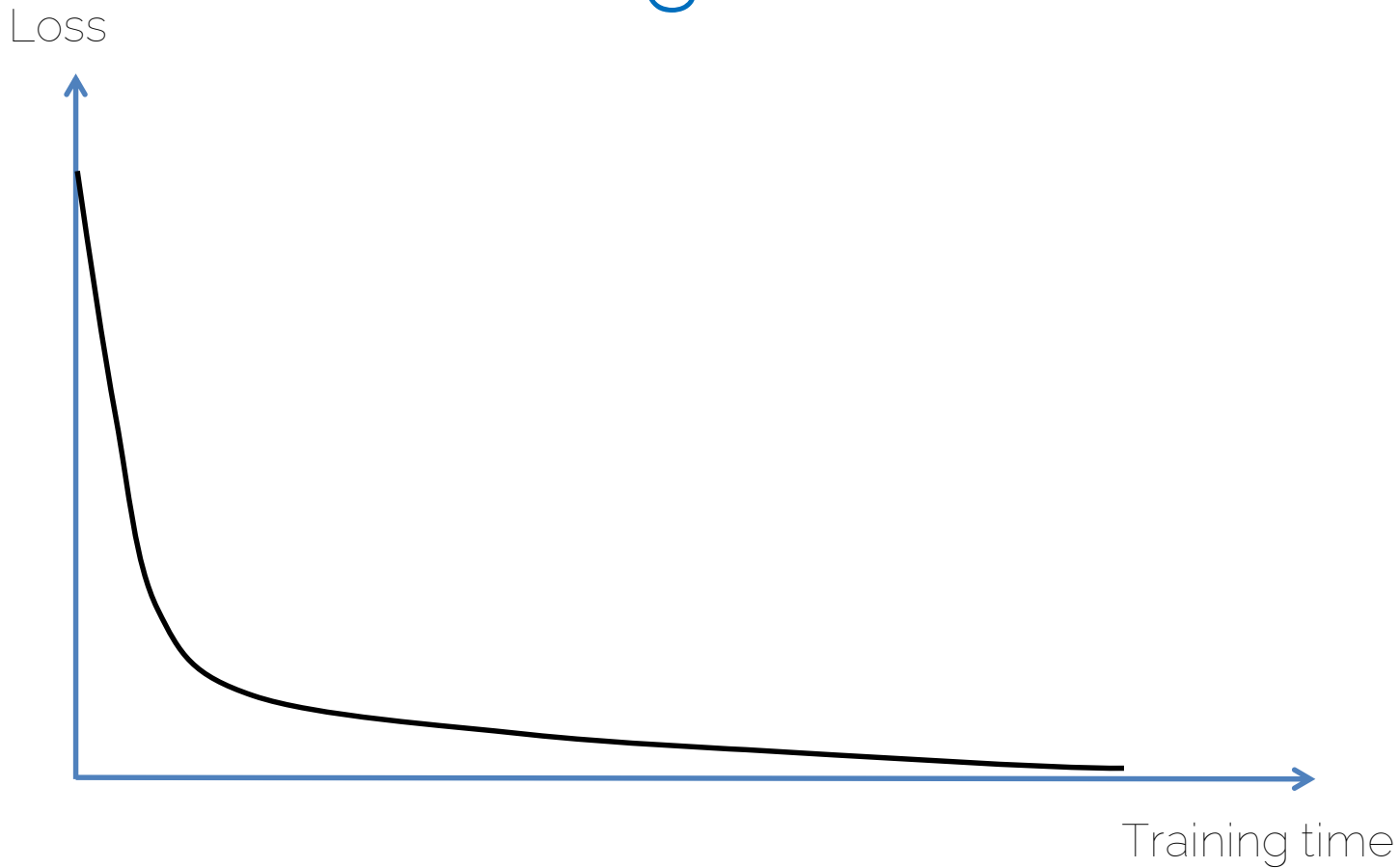




# During Training...

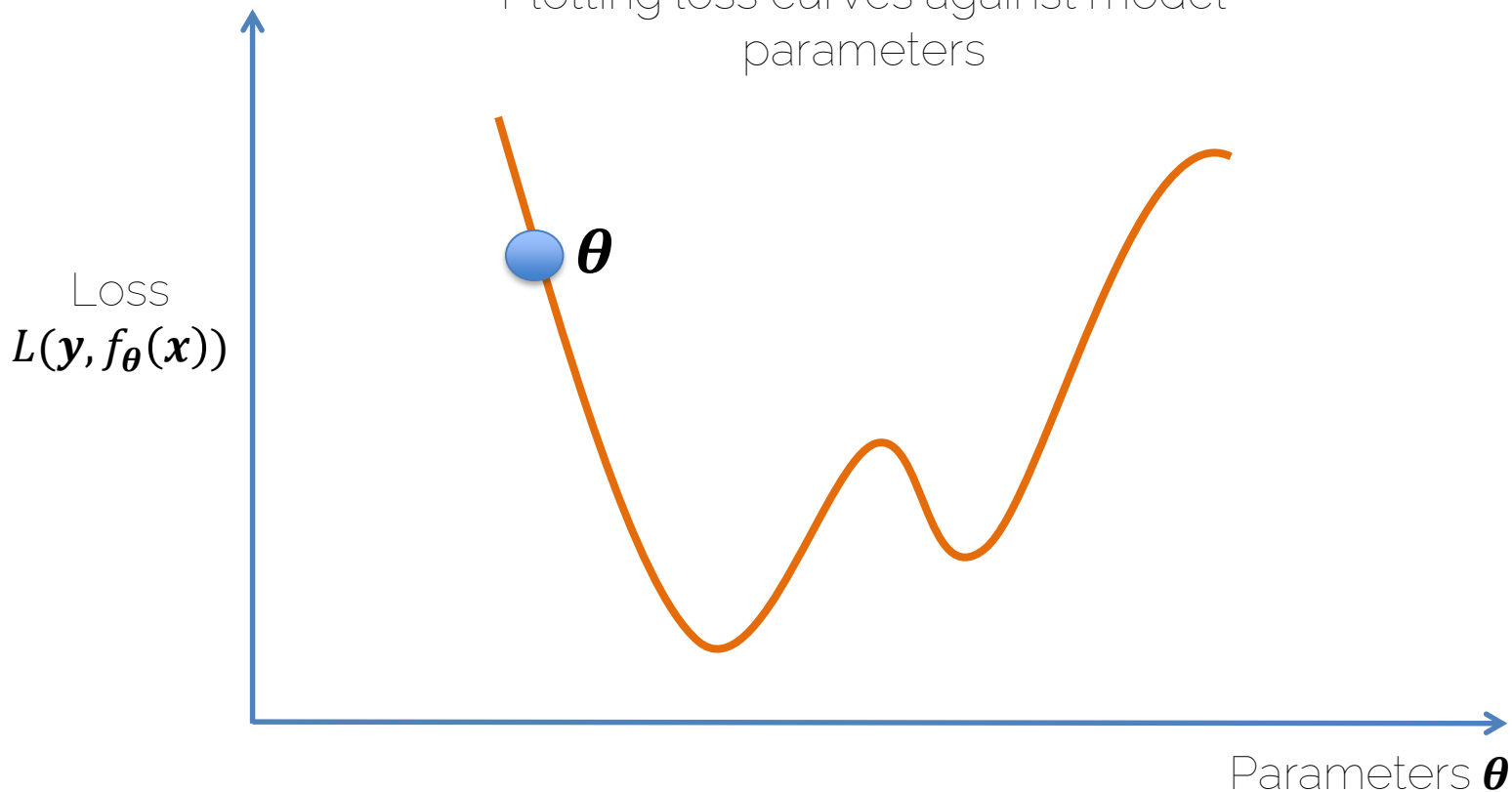


# Training Curve



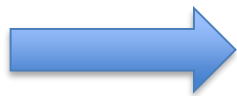
# How to Find a Better NN?

Plotting loss curves against model parameters



# How to Find a Better NN?

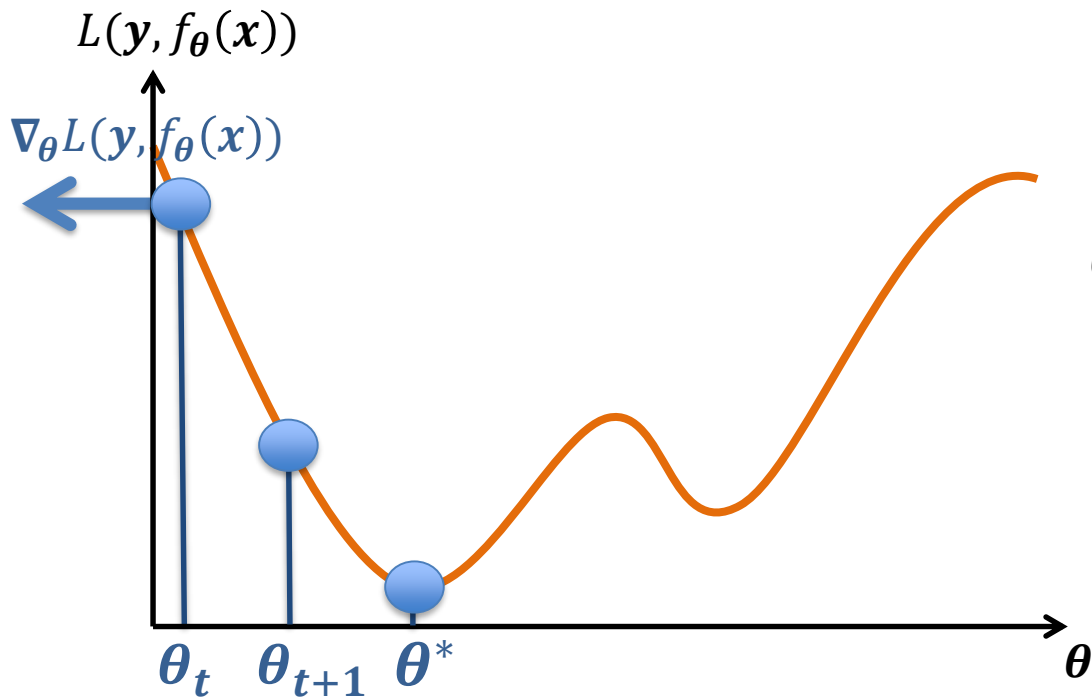
- Loss function:  $L(\mathbf{y}, \hat{\mathbf{y}}) = L(\mathbf{y}, f_{\boldsymbol{\theta}}(\mathbf{x}))$
- Neural Network:  $f_{\boldsymbol{\theta}}(\mathbf{x})$
- Goal:
  - minimize the loss w. r. t.  $\boldsymbol{\theta}$



Optimization! We train compute graphs with some optimization techniques!

# Gradient Descent

Minimize loss  $L(\mathbf{y}, f_{\boldsymbol{\theta}}(\mathbf{x}))$  w.r.t.  $\boldsymbol{\theta}$ :



step size / learning rate

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \alpha \nabla_{\boldsymbol{\theta}} L(\mathbf{y}, f_{\boldsymbol{\theta}}(\mathbf{x})) \big|_{\boldsymbol{\theta}_t}$$

$t \rightarrow \infty$

$$\boldsymbol{\theta}^* = \arg \min L(\mathbf{y}, f_{\boldsymbol{\theta}}(\mathbf{x}))$$

# How to Find a Better NN?

- Given inputs  $\mathbf{x}$  and targets  $\mathbf{y}$
- Given one layer NN with no activation function

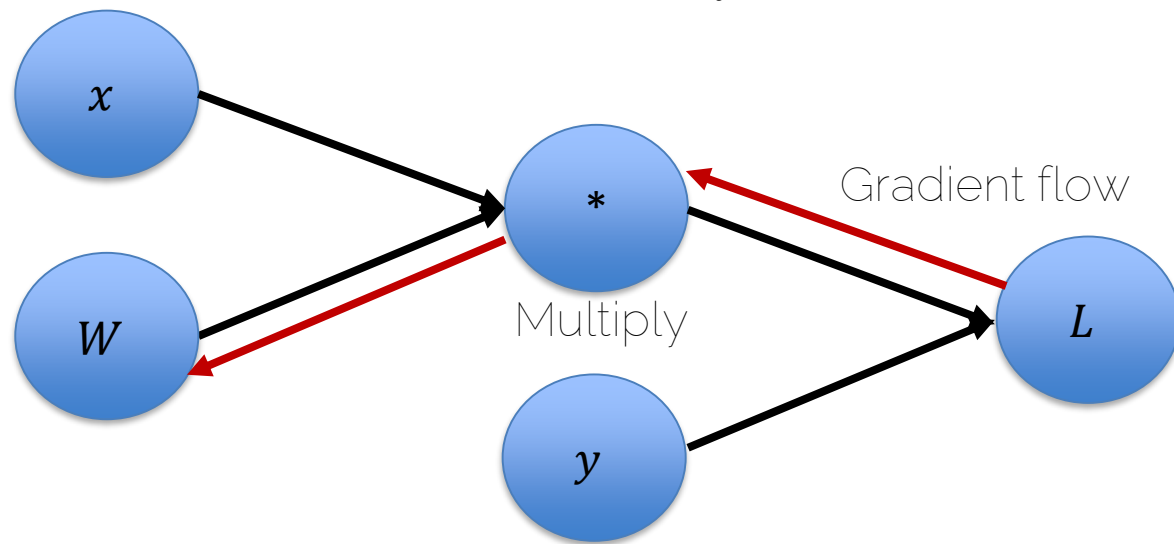
$$\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}) = \mathbf{W}\mathbf{x}, \quad \boldsymbol{\theta} = \mathbf{W}$$

Later  $\boldsymbol{\theta} = \{\mathbf{W}, \mathbf{b}\}$

- Given MSE Loss:  $L(\mathbf{y}, \hat{\mathbf{y}}; \boldsymbol{\theta}) = \frac{1}{n} \sum_i^n ||y_i - \hat{y}_i||_2^2$

# How to Find a Better NN?

- Given inputs  $\mathbf{x}$  and targets  $\mathbf{y}$
- Given one layer NN with no activation function
- Given MSE Loss:  $L(\mathbf{y}, \hat{\mathbf{y}}; \boldsymbol{\theta}) = \frac{1}{n} \sum_i^n ||y_i - \mathbf{W} \cdot x_i||_2^2$



# How to Find a Better NN?

- Given inputs  $\mathbf{x}$  and targets  $\mathbf{y}$
- Given one layer NN with no activation function

$$f_{\theta}(\mathbf{x}) = \mathbf{W}\mathbf{x}, \quad \theta = \mathbf{W}$$

- Given MSE Loss:  $L(\mathbf{y}, \hat{\mathbf{y}}; \theta) = \frac{1}{n} \sum_i^n ||\mathbf{W} \cdot \mathbf{x}_i - \mathbf{y}_i||_2^2$
- $\nabla_{\theta} L(\mathbf{y}, f_{\theta}(\mathbf{x})) = \frac{2}{n} \sum_i^n (\mathbf{W} \cdot \mathbf{x}_i - \mathbf{y}_i) \cdot \mathbf{x}_i^T$

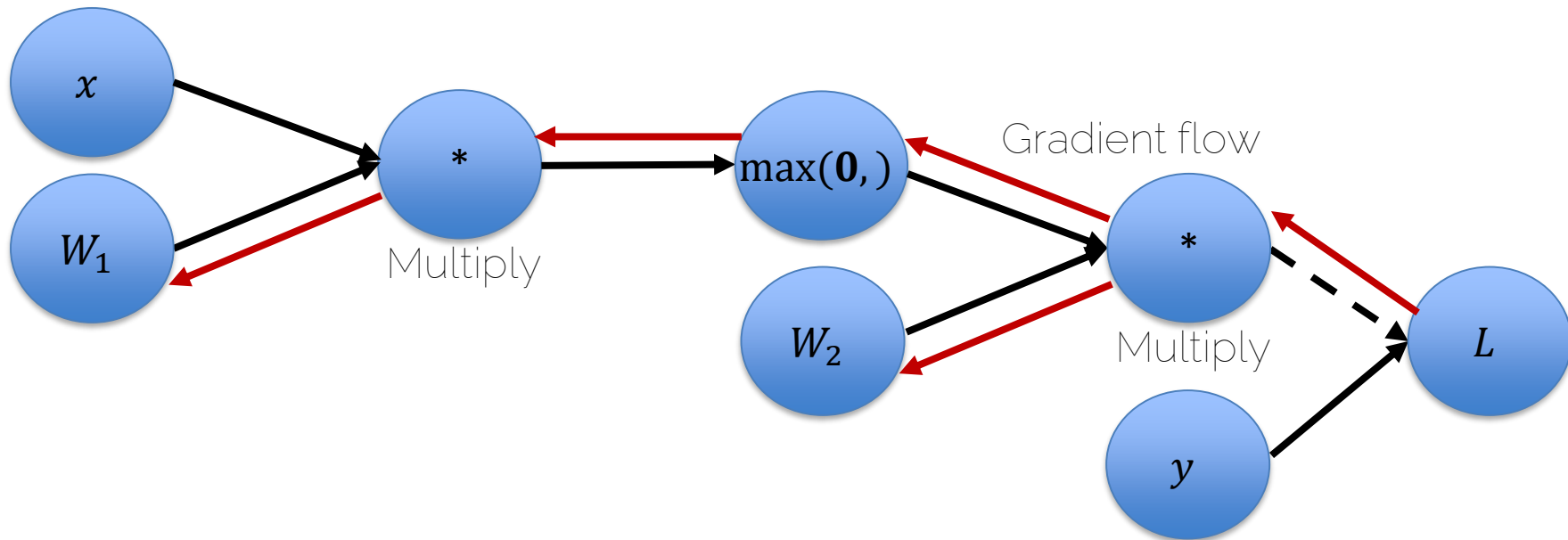


# How to Find a Better NN?

- Given inputs  $\mathbf{x}$  and targets  $\mathbf{y}$
- Given a multi-layer NN with many activations
$$\mathbf{f} = \mathbf{W}_5 \sigma(\mathbf{W}_4 \tanh(\mathbf{W}_3, \max(\mathbf{0}, \mathbf{W}_2 \max(\mathbf{0}, \mathbf{W}_1 \mathbf{x}))))$$
- Gradient descent for  $L(\mathbf{y}, \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}))$  w. r. t.  $\boldsymbol{\theta}$ 
  - Need to propagate gradients from end to first layer ( $\mathbf{W}_1$ ).

# How to Find a Better NN?

- Given inputs  $\mathbf{x}$  and targets  $\mathbf{y}$
- Given multi-layer NN with many activations



# How to Find a Better NN?

- Given inputs  $\mathbf{x}$  and targets  $\mathbf{y}$
- Given multilayer layer NN with many activations
$$\mathbf{f} = \mathbf{W}_5 \sigma(\mathbf{W}_4 \tanh(\mathbf{W}_3, \max(\mathbf{0}, \mathbf{W}_2 \max(\mathbf{0}, \mathbf{W}_1 \mathbf{x}))))$$
- Gradient descent solution for  $L(\mathbf{y}, f_{\boldsymbol{\theta}}(\mathbf{x}))$  w. r. t.  $\boldsymbol{\theta}$ 
  - Need to propagate gradients from end to first layer ( $\mathbf{W}_1$ )
- Backpropagation: Use chain rule to compute gradients
  - Compute graphs come in handy!

# How to Find a Better NN?

- Why gradient descent?
  - Easy to compute using compute graphs
- Other methods include
  - Newtons method
  - L-BFGS
  - Adaptive moments
  - Conjugate gradient

# Summary

- Neural Networks are computational graphs
- Goal: for a given train set, find optimal weights
- Optimization is done using gradient-based solvers
  - Many options (more in the next lectures)
- Gradients are computed via backpropagation
  - Nice because can easily modularize complex functions

# Next Lectures

- Next Lecture:
  - Backpropagation and optimization of Neural Networks
- Check for updates on website/piazza regarding exercises