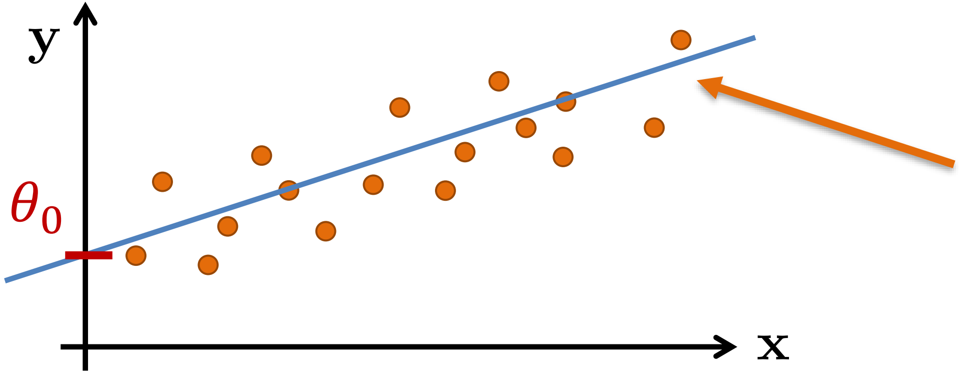
Introduction to Neural Networks

From Linear and Logitistic 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

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

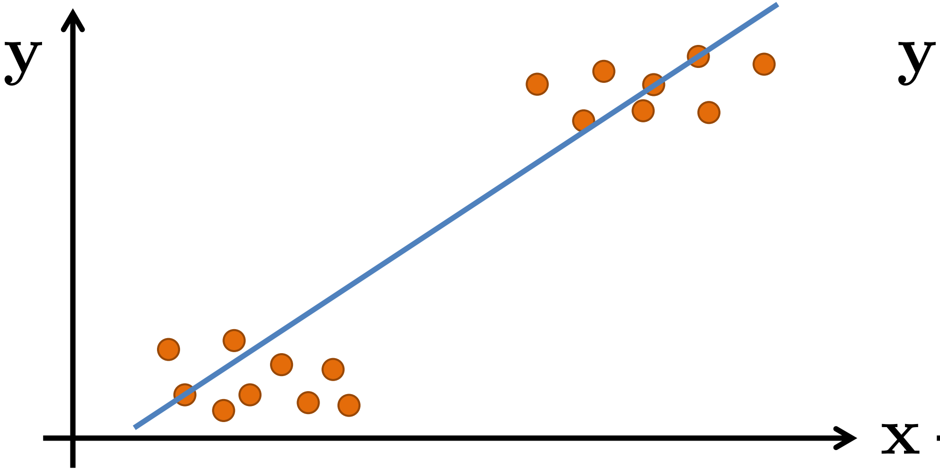
- Overall loss

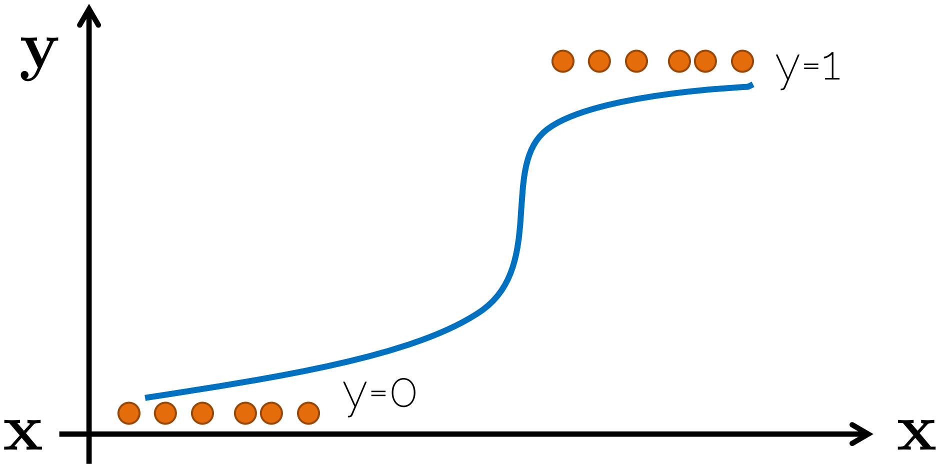
$$\mathcal{C}(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n}(y_i \cdot \log \hat{y}_i + (1 - y_i) \cdot \log[1 - \hat{y}_i])$$

Minimization

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

Linear vs Logistic Regression

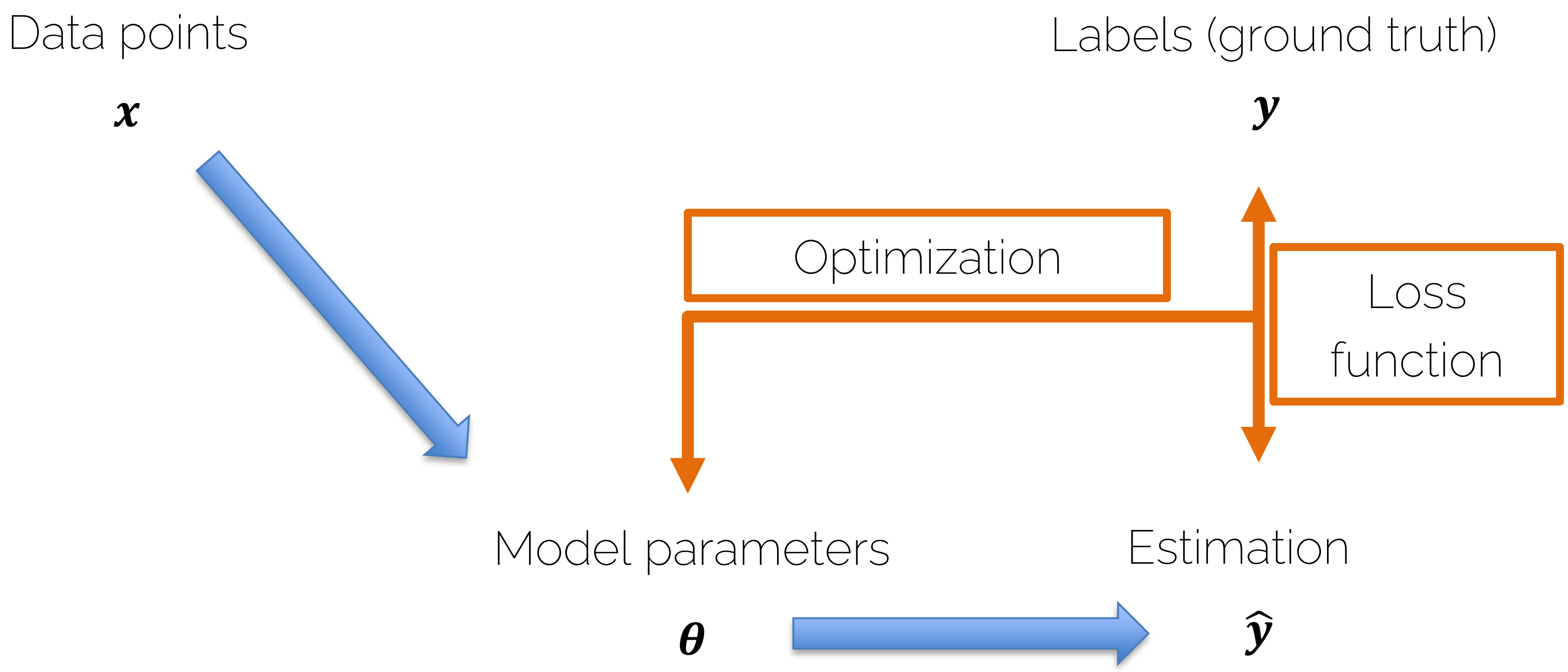




Predictions can exceed the range of the training samples
→ in the case of classification [0;1] this becomes a real issue

Predictions are guaranteed to be within [0;1]

How to obtain the Model?



Linear Score Functions

- Linear score function as seen in linear regression

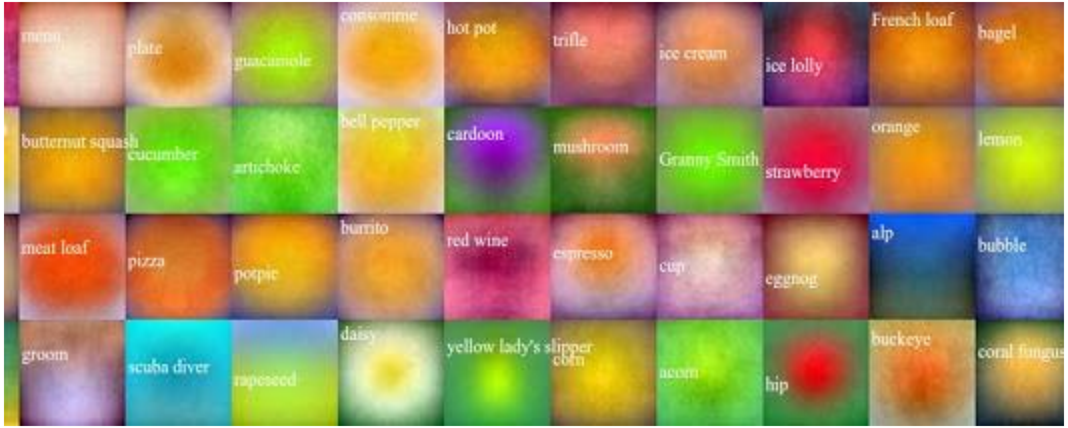
$$\boldsymbol{f_i} = \sum_{\boldsymbol{j}} w_{\boldsymbol{i,j}}\, x_{\boldsymbol{j}}$$

$$\boldsymbol{f} = \boldsymbol{W}\,\boldsymbol{x} \qquad \text{(Matrix Notation)}$$

Linear Score Functions on Images

- Linear score function $\boldsymbol{f} = \boldsymbol{W}\boldsymbol{x}$

On CIFAR-10

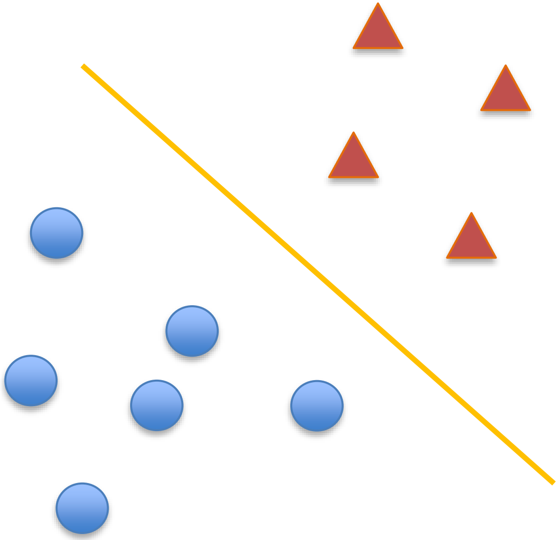


On ImageNet

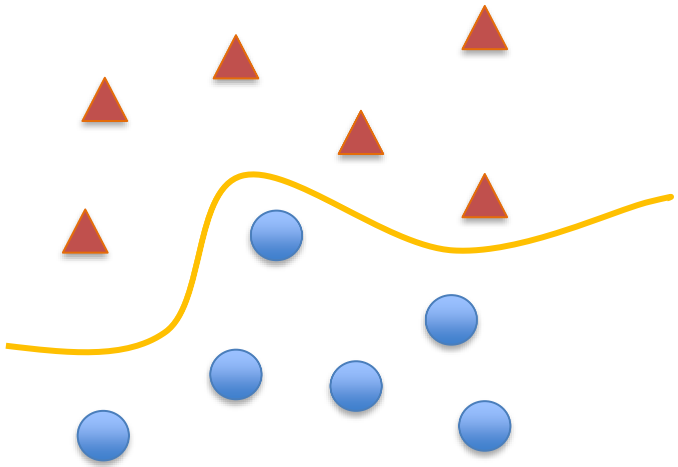
Source:: Li/Karpathy/Johnson

Linear Score Functions?

Logistic Regression



Linear Separation Impossible!



Linear Score Functions?

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

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

- Operation remains linear:

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

- Solution → add non-linearity!!

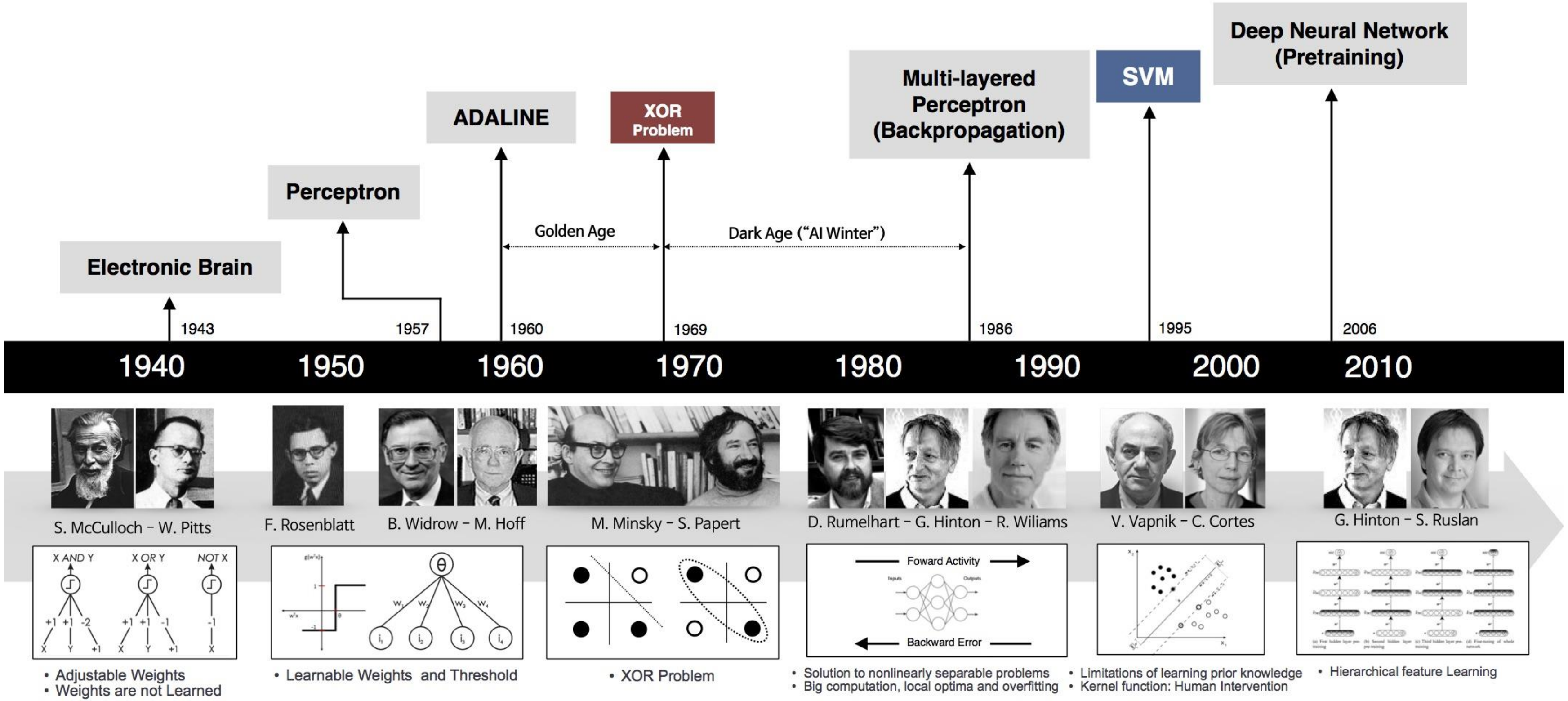
Neural Network

- Linear score function $\boldsymbol{f} = \boldsymbol{W}\boldsymbol{x}$

- Neural network is a nesting of 'functions'
  - 2-layers: $\boldsymbol{f} = \boldsymbol{W_2} \max(\boldsymbol{0}, \boldsymbol{W_1}\boldsymbol{x})$
  - 3-layers: $\boldsymbol{f} = \boldsymbol{W_3} \max(\boldsymbol{0}, \boldsymbol{W_2} \max(\boldsymbol{0}, \boldsymbol{W_1}\boldsymbol{x}))$
  - 4-layers: $\boldsymbol{f} = \boldsymbol{W_4} \tanh\,(\boldsymbol{W_3}, \max(\boldsymbol{0}, \boldsymbol{W_2} \max(\boldsymbol{0}, \boldsymbol{W_1}\boldsymbol{x})))$
  - 5-layers: $\boldsymbol{f} = \boldsymbol{W_5}\sigma(\boldsymbol{W_4} \tanh(\boldsymbol{W_3}, \max(\boldsymbol{0}, \boldsymbol{W_2} \max(\boldsymbol{0}, \boldsymbol{W_1}\boldsymbol{x}))))$
  - … up to hundreds of layers

Introduction to Neural Networks

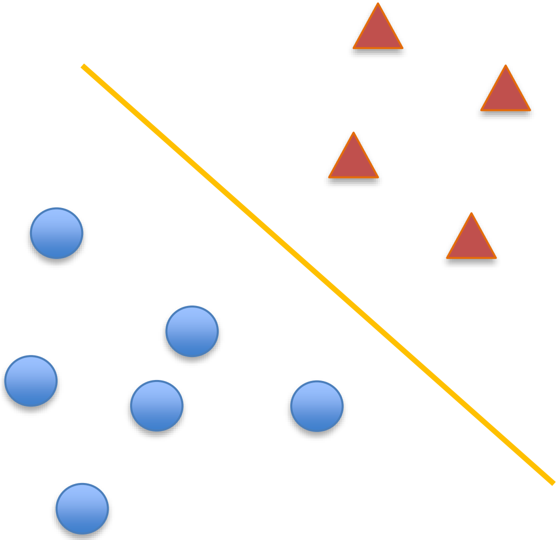
History of Neural Networks



Source: http://beamlab.org/deeplearning/2017/02/23/deep_learning_101_part1.html

Neural Network

Logistic Regression

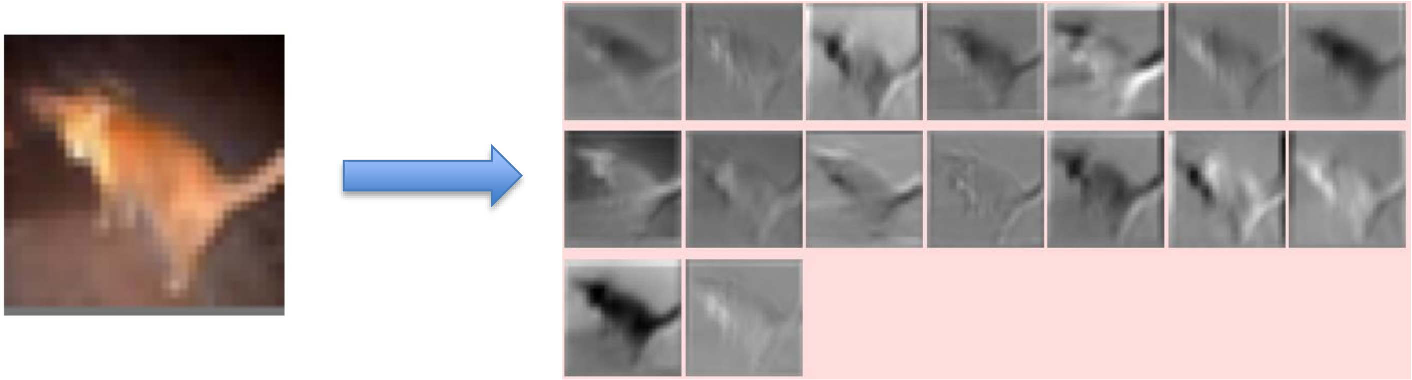


Neural Networks

Neural Network

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

On CIFAR-10



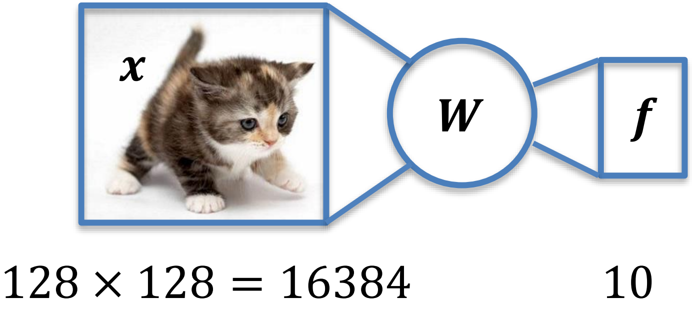
Visualizing activations of the first layer.

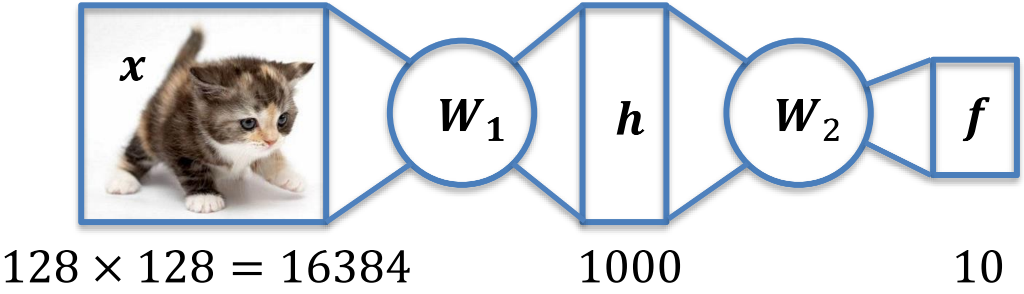
Source: ConvNetJS

Neural Network

1-layer network: $\boldsymbol{f} = \boldsymbol{W}\boldsymbol{x}$

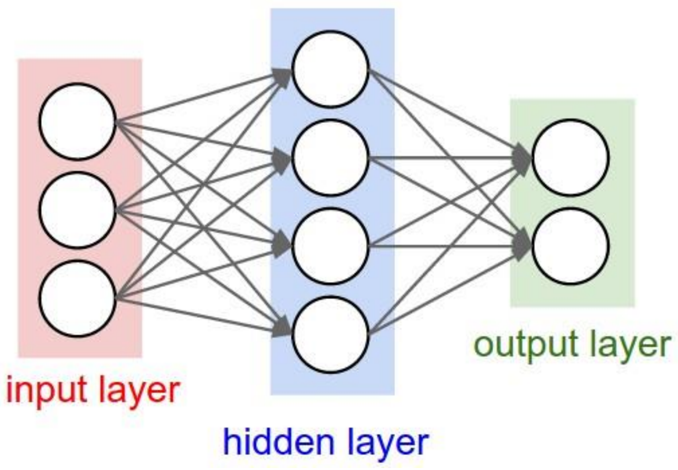
2-layer network: $\boldsymbol{f} = \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1\boldsymbol{x})$



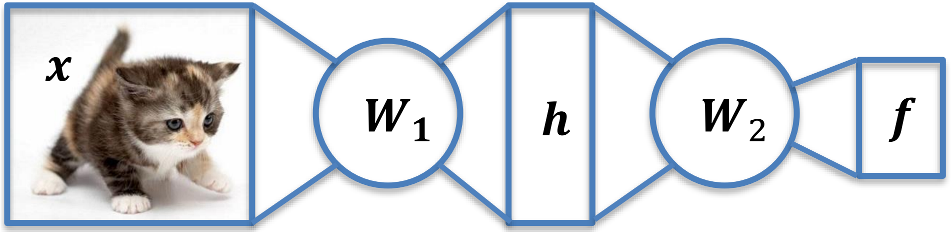


Why is this structure useful?

Neural Network



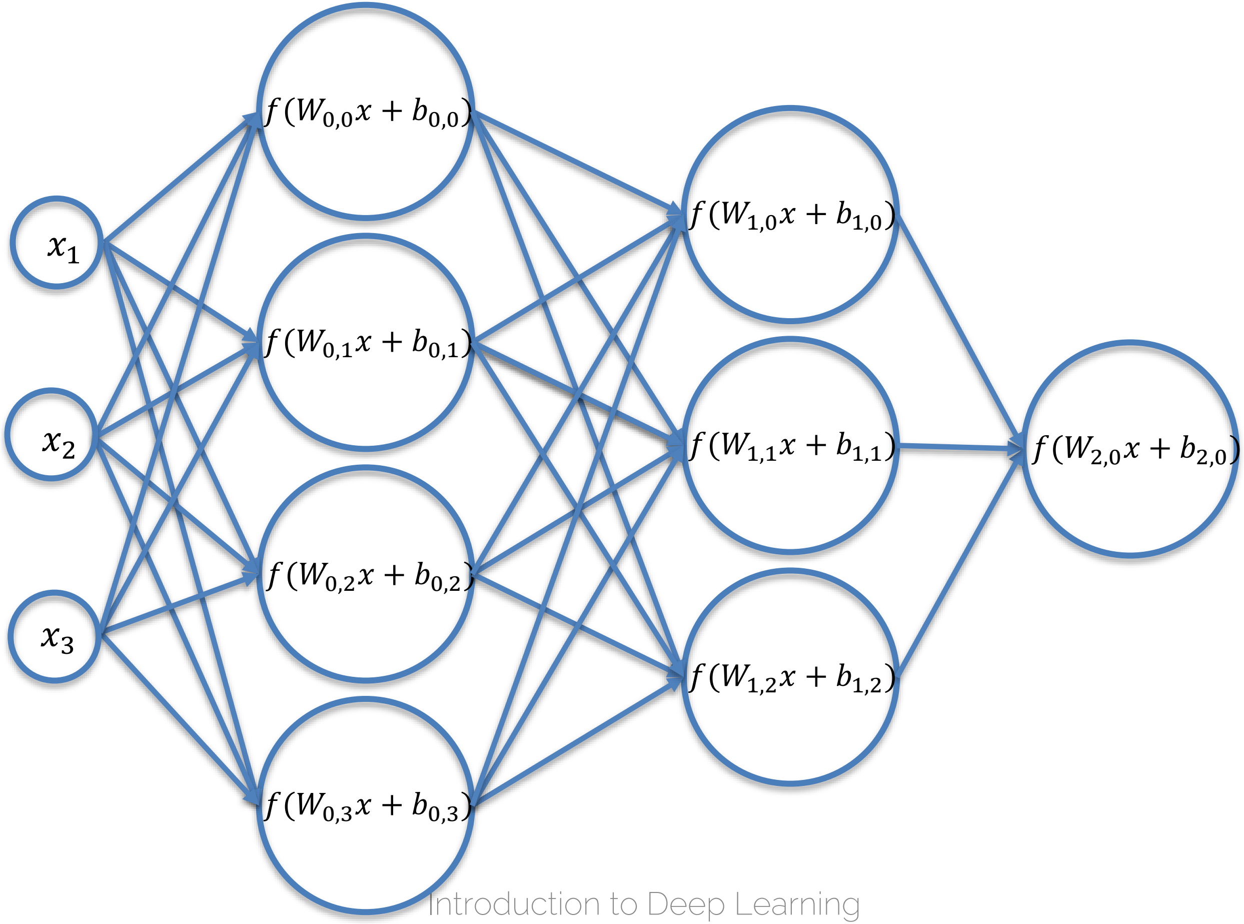
2-layer network: $\boldsymbol{f} = \boldsymbol{W_2} \max(\boldsymbol{0}, \boldsymbol{W_1 x})$



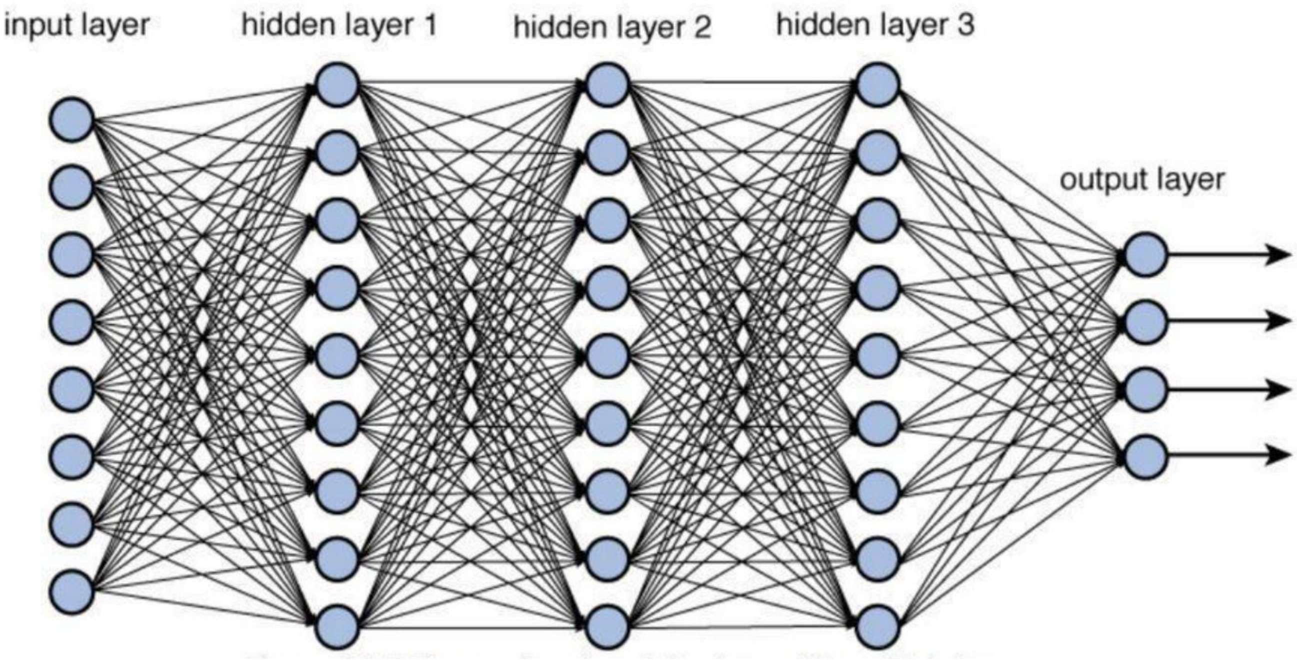
$128 \times 128 = 16384$ | 1000 | 10

Input Layer | Hidden Layer | Output Layer

Net of Artificial Neurons



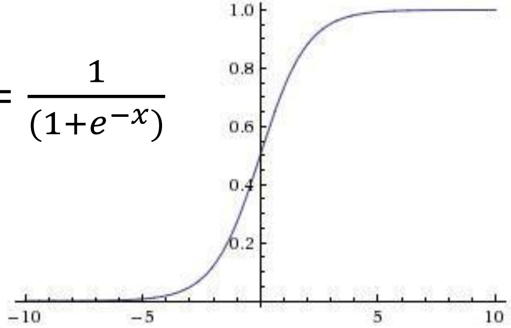
Neural Network



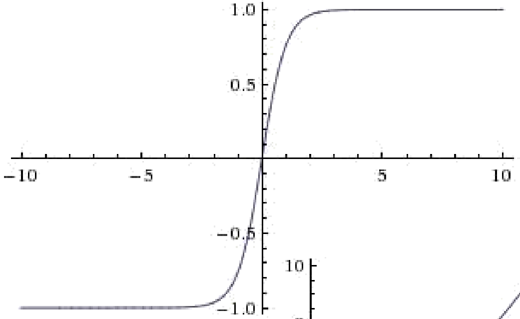
Source: https://towardsdatascience.com/training-deep-neural-networks-9fdb1964b964

Activation Functions

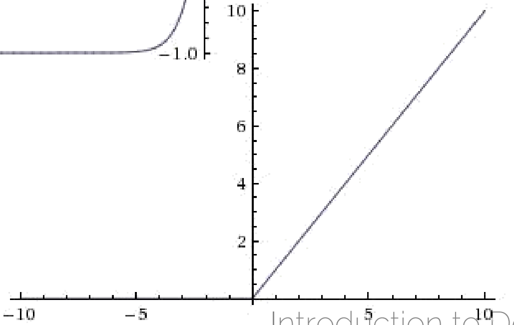
Sigmoid: $\sigma(x) = \frac{1}{(1+e^{-x})}$



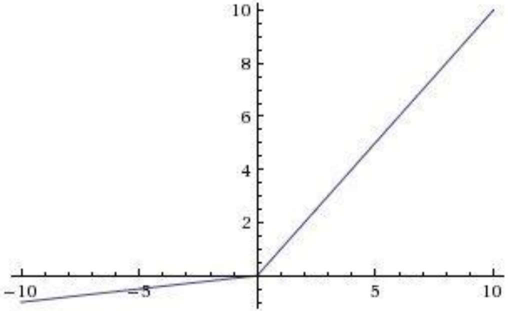
tanh: $\tanh(x)$



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

Neural Network

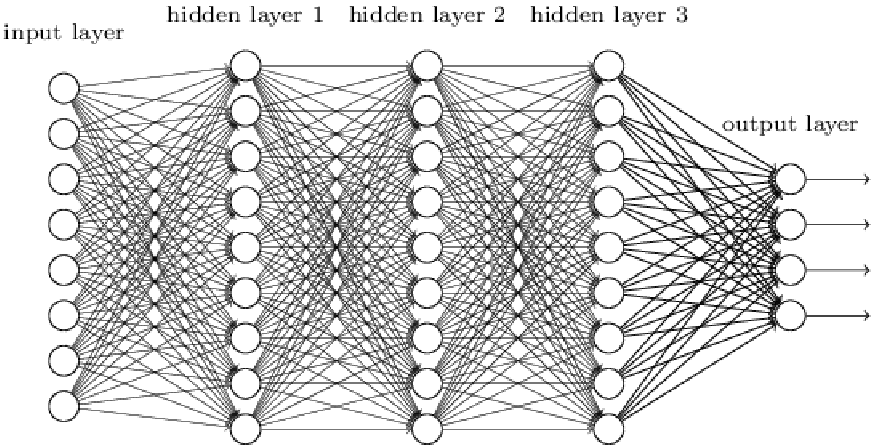
$$\boldsymbol{f} = \boldsymbol{W}_3 \cdot (\boldsymbol{W}_2 \cdot (\boldsymbol{W}_1 \cdot \boldsymbol{x}))$$

Why activation functions?

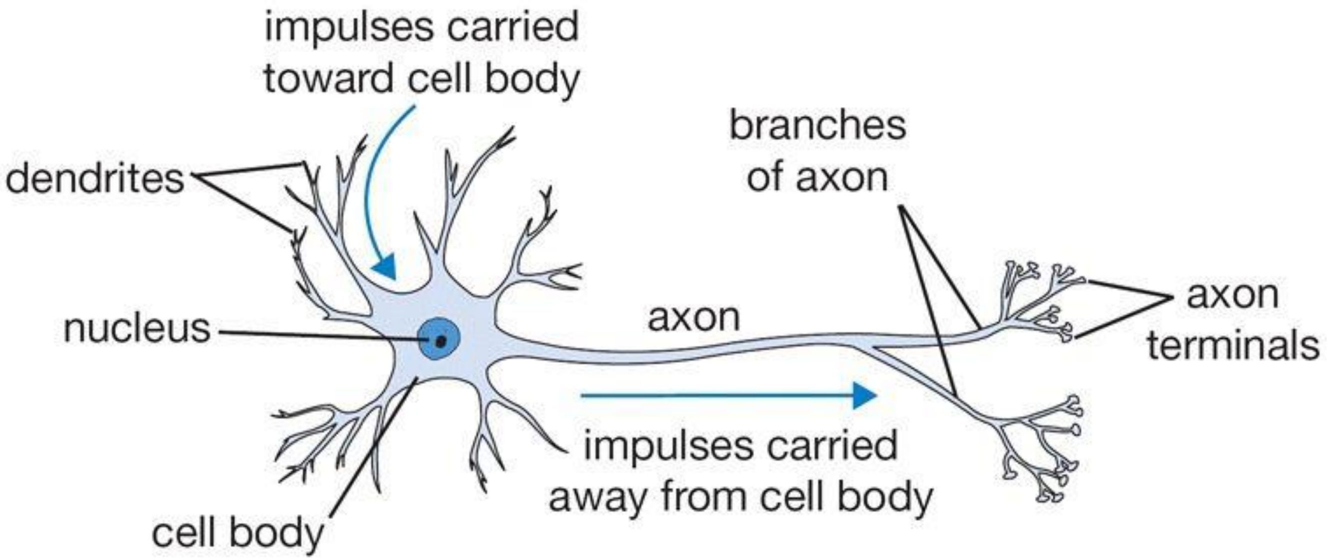
Simply concatenating linear layers would be so much cheaper...

Neural Network

Why organize a neural network into layers?

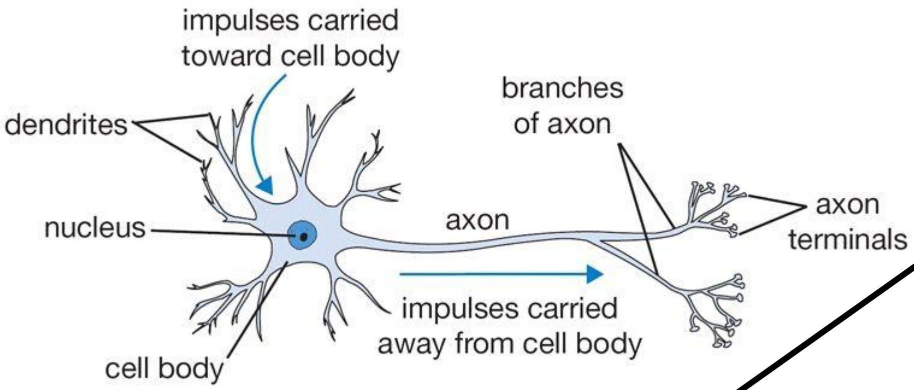


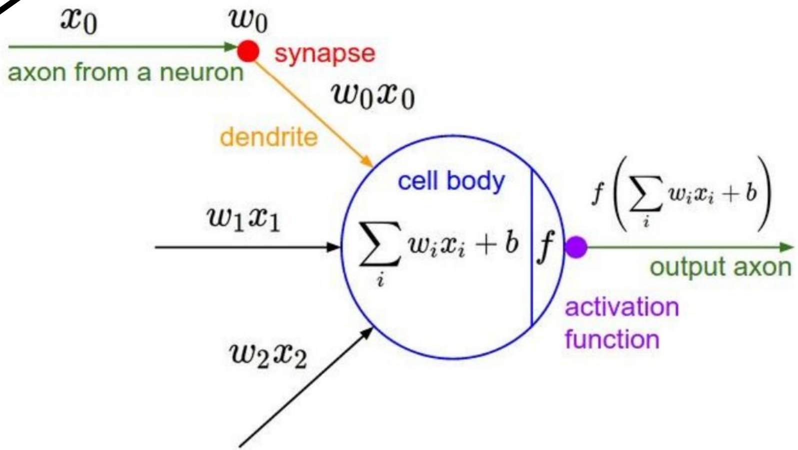
Biological Neurons



Credit: Stanford CS 231n

Biological Neurons



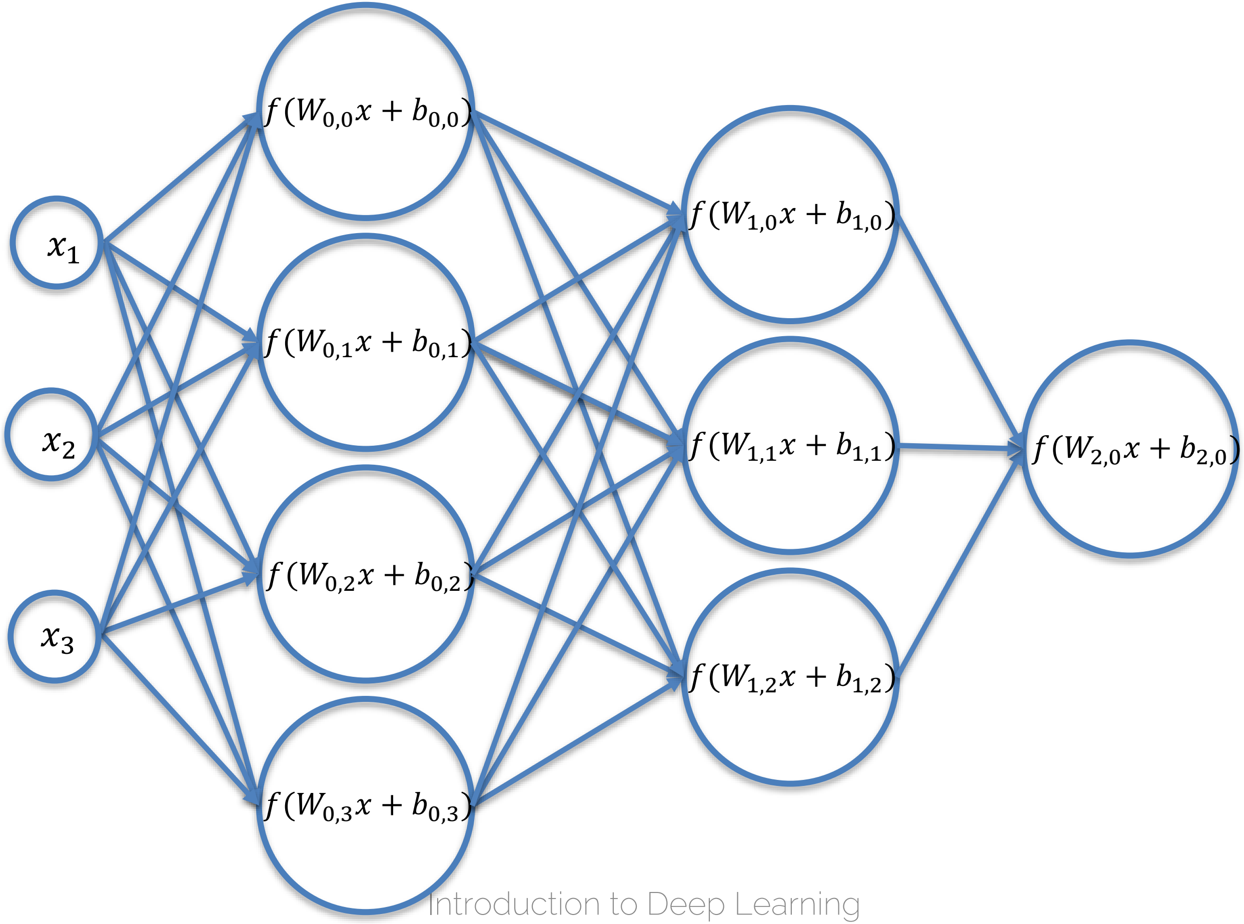


Credit: Stanford CS 231n

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 $\boldsymbol{W}$ 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

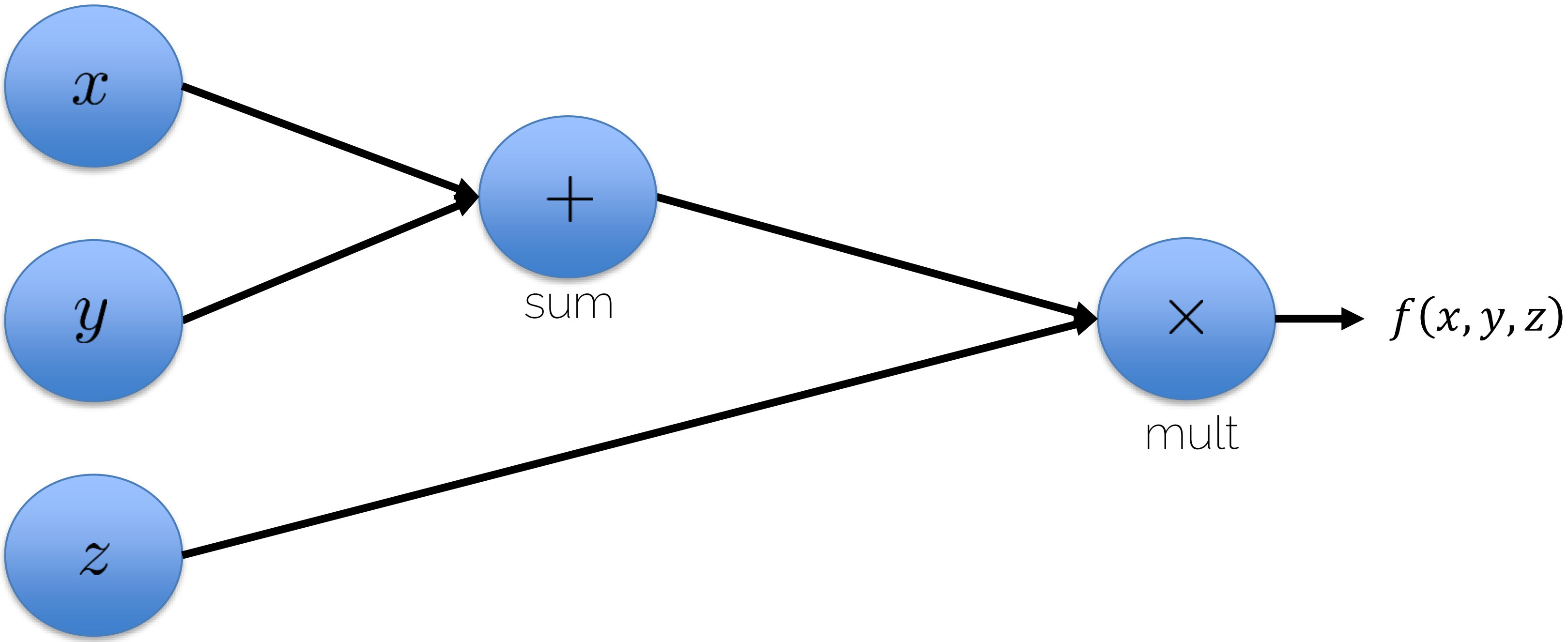
- Matrix operations are represented as compute nodes.

- Vertex nodes are variables or operators like +, -, *, /, log(), exp() ...

- Directional edges show flow of inputs to vertices

Computational Graphs

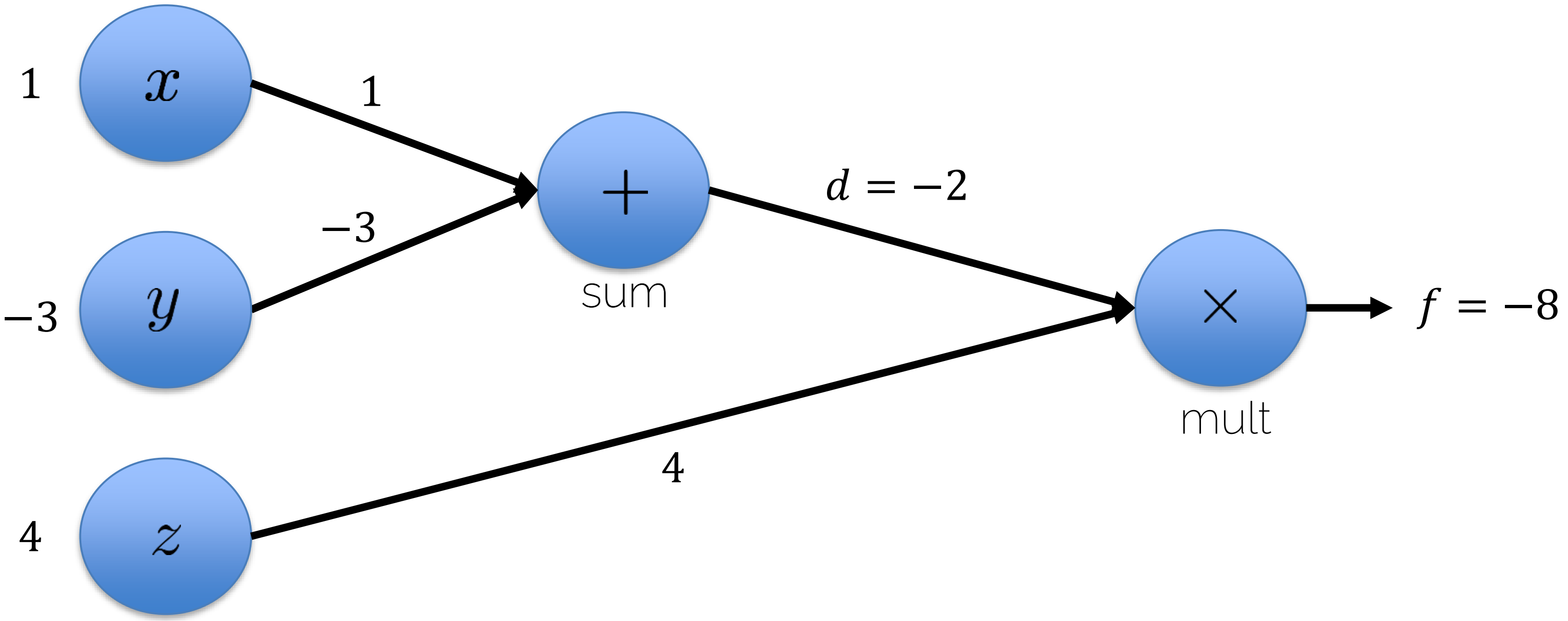
- $f(x, y, z) = (x + y) \cdot z$



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
$$\boldsymbol{f} = \boldsymbol{W}_5 \sigma(\boldsymbol{W}_4 \tanh(\boldsymbol{W}_3, \max(\boldsymbol{0}, \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1 \boldsymbol{x}))))$$

- Lot of matrix operations!

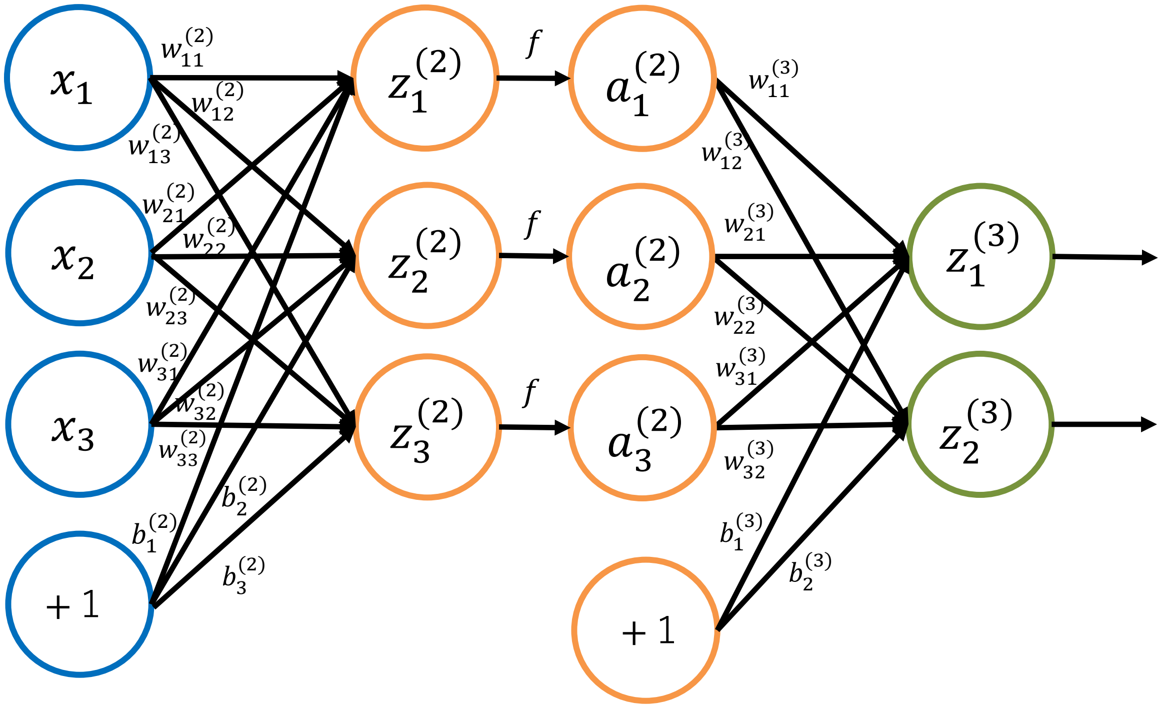
- Represent NN as computational graphs!

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



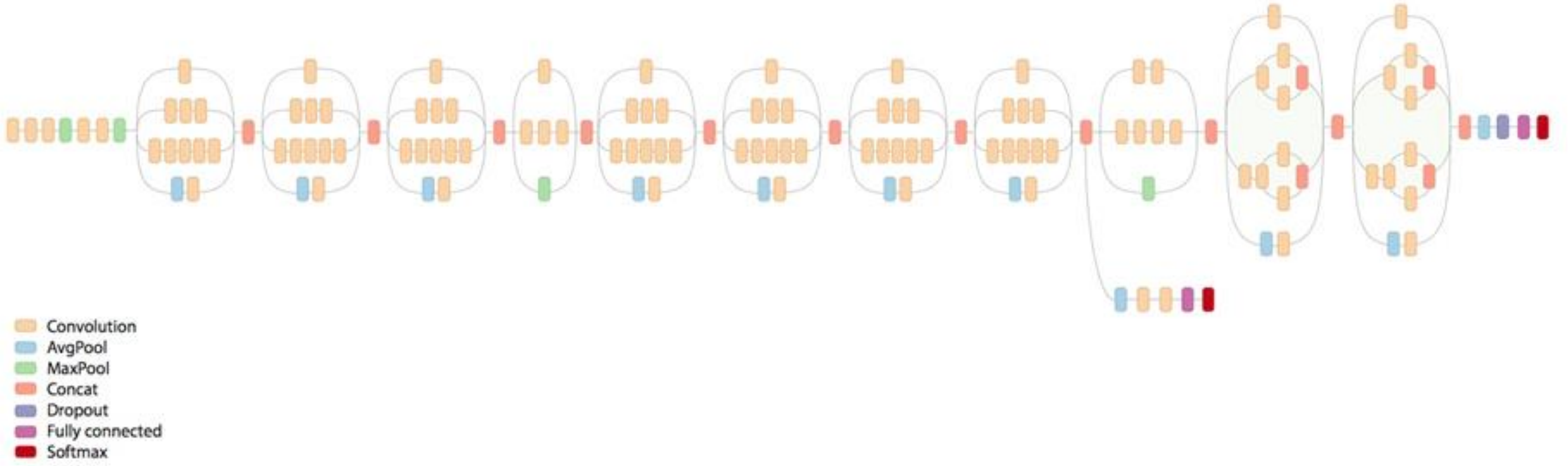
$$z_k^{(2)} = \sum_i x_i w_{ik}^{(2)} + b_k^{(2)}$$

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

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

Computational Graphs

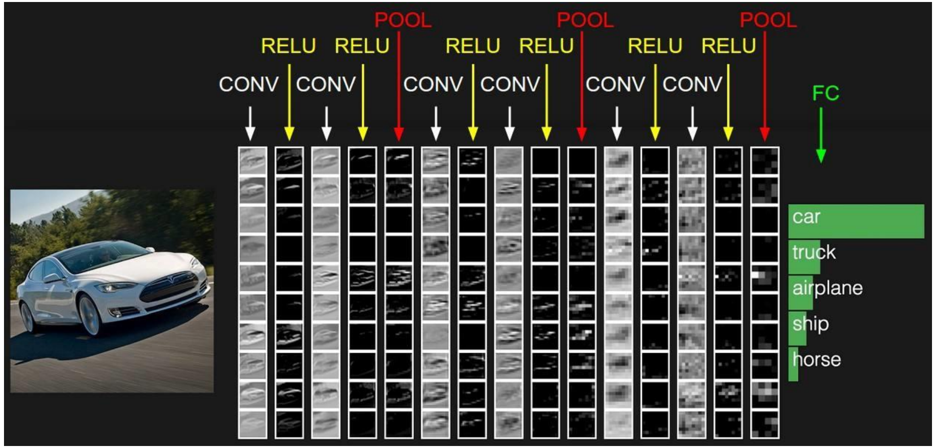
- From a set of neurons to a Structured Compute Pipeline



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

Computational Graphs

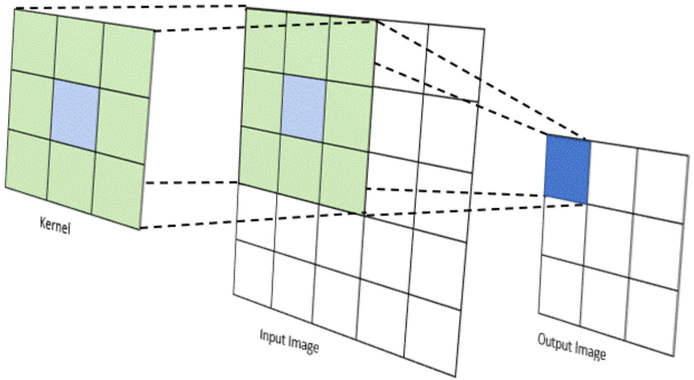
- The computation of Neural Network has further meanings:
  - The multiplication of $\boldsymbol{W}$ and $\boldsymbol{x}$: encode input information
  - The activation function: select the key features



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

Computational Graphs

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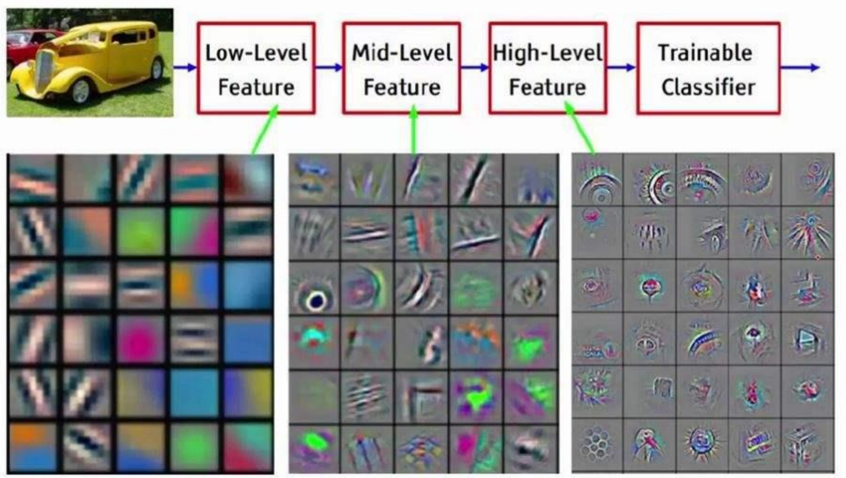
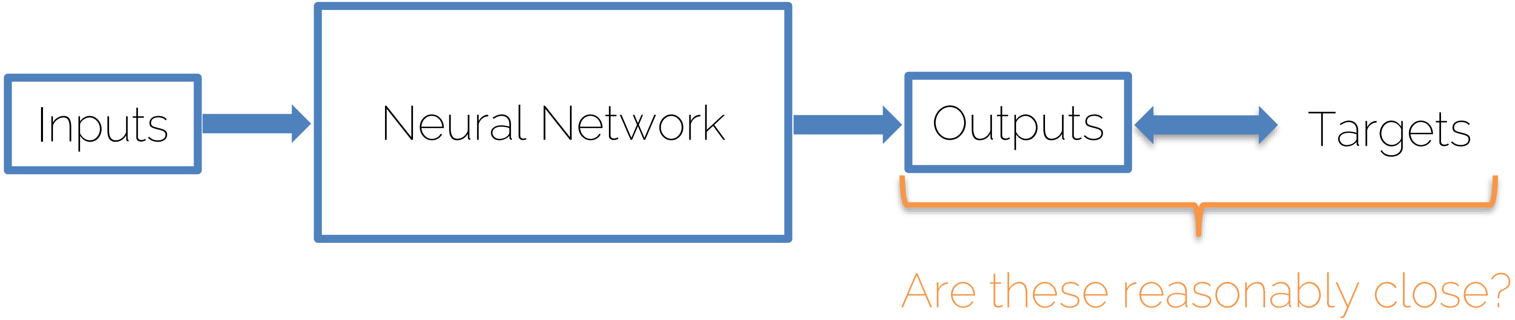


Source: https://www.zybuluo.com/liuhui0803/note/981434

Loss Functions

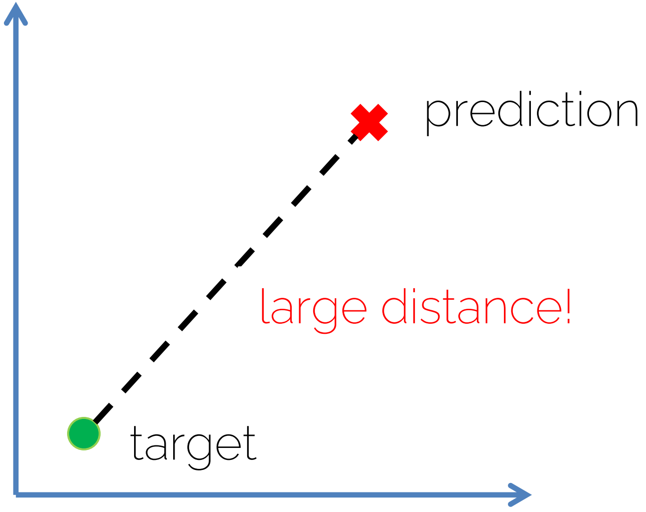
What's Next?



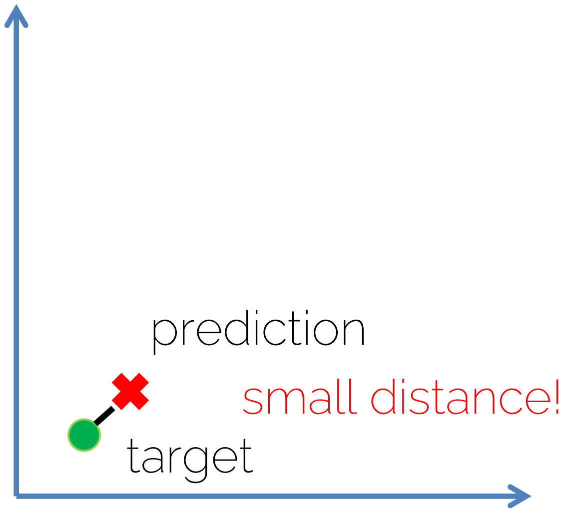
We need a way to describe how close the network's outputs (= predictions) are to the targets!

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 ($\rightarrow$ 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:

$$L(\boldsymbol{y}, \widehat{\boldsymbol{y}};\ \boldsymbol{\theta}) = \frac{1}{n}\sum_{i}^{n} ||y_i - \widehat{y}_i||_1$$

- MSE Loss:

$$L(\boldsymbol{y}, \widehat{\boldsymbol{y}};\ \boldsymbol{\theta}) = \frac{1}{n}\sum_{i}^{n} ||y_i - \widehat{y}_i||_2^2$$

Binary Cross Entropy

- Loss function for binary (yes/no) classification

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

Yes! (0.8)

No! (0.2)

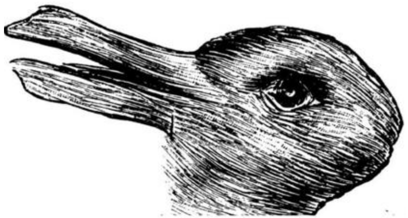
The network predicts the probability of the input belonging to the "yes" class!

Cross Entropy

Generalizes to multi-class classification:

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

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



dog (0.1)

rabbit (0.2)

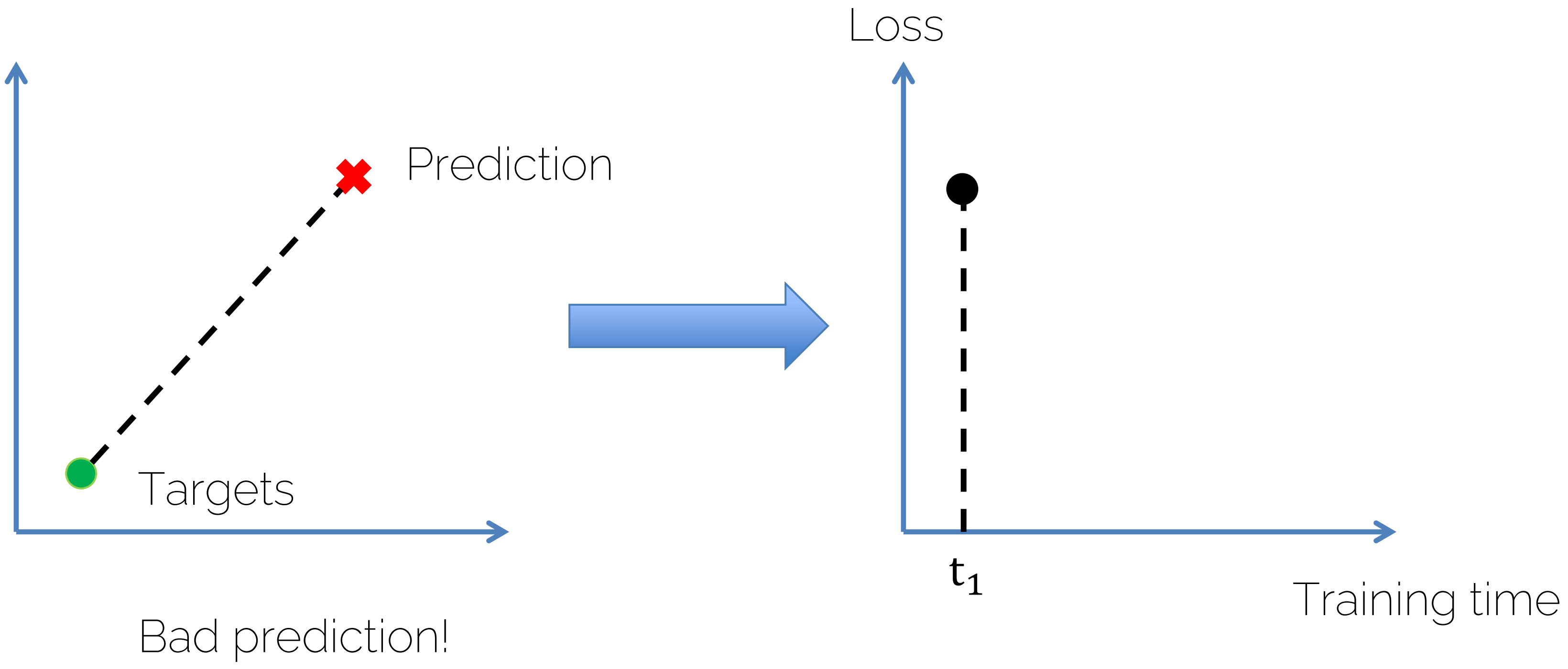
duck (0.7)

...

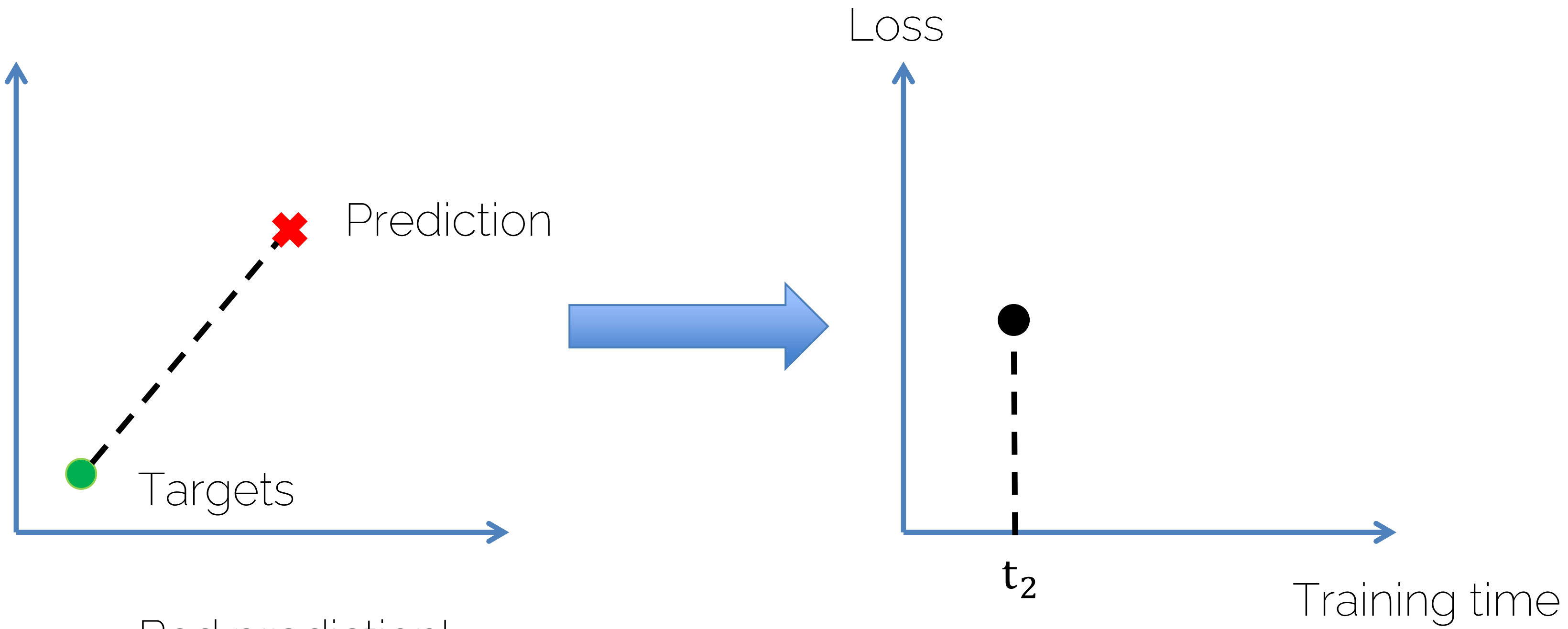
More General Case

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

Initially

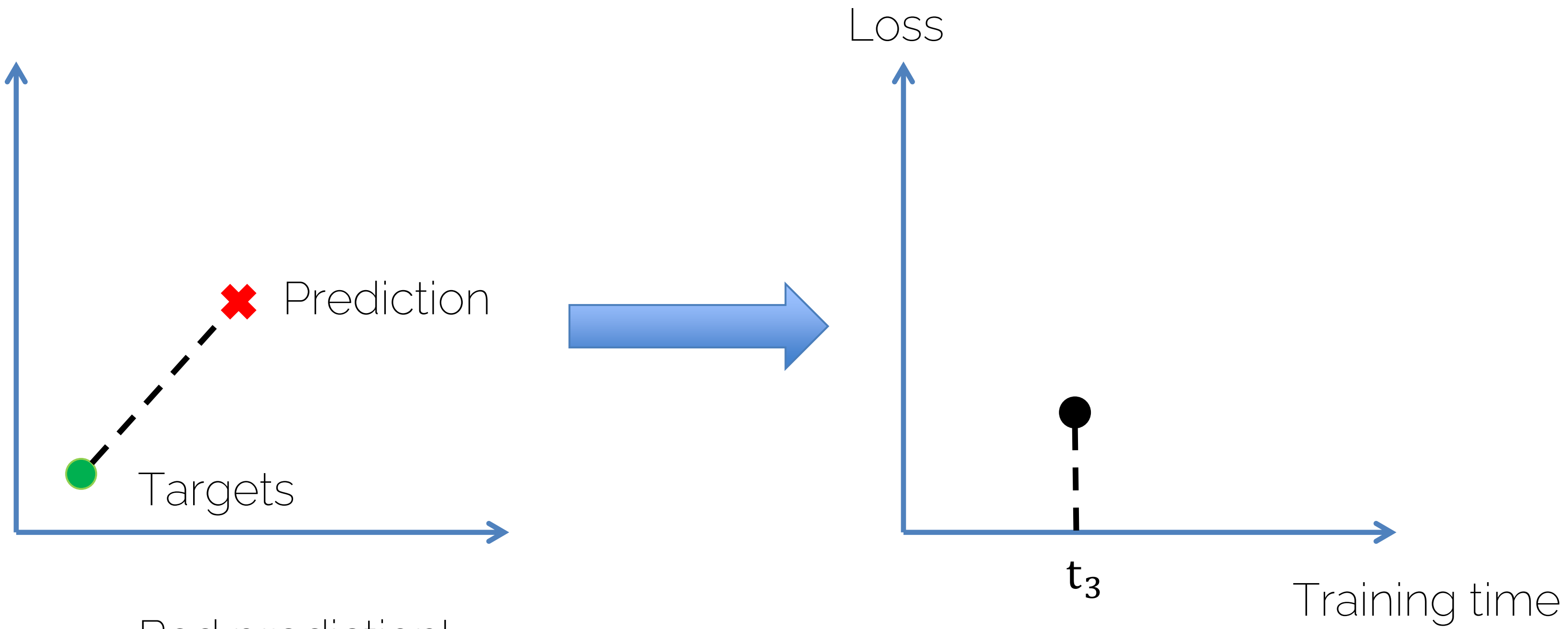


During Training…



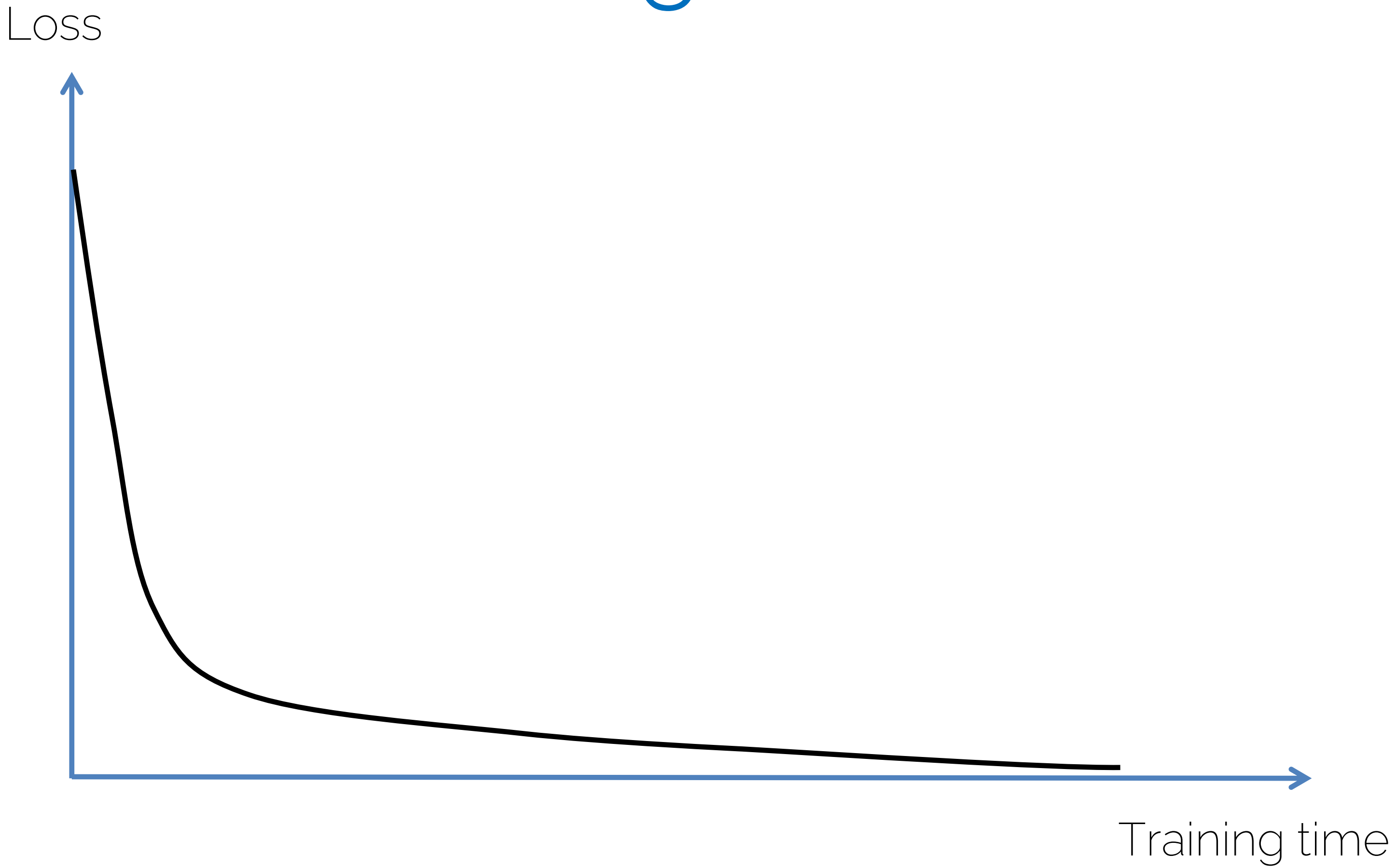
Bad prediction!

During Training…



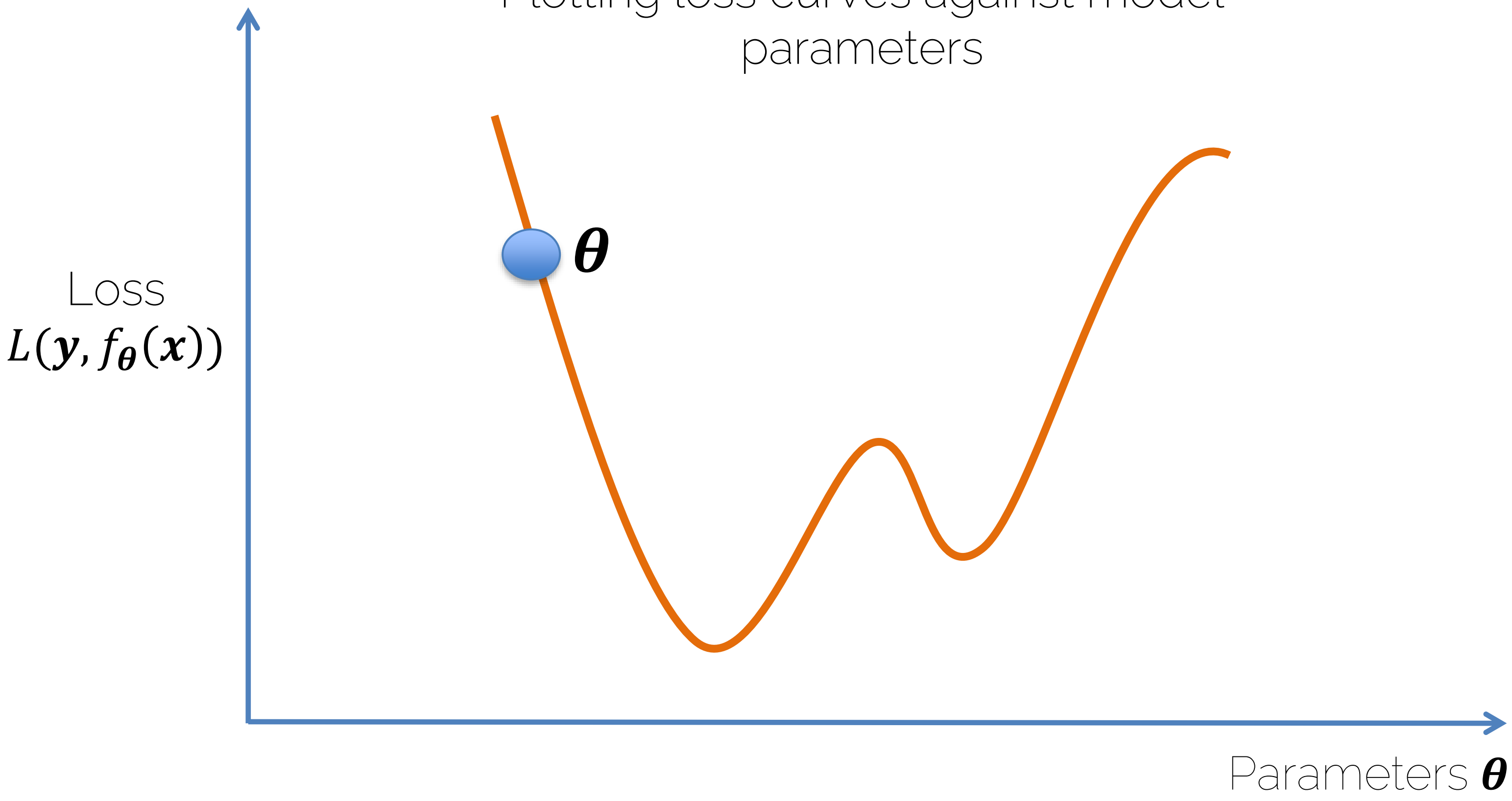
Bad prediction!

Training Curve



How to Find a Better NN?

Plotting loss curves against model parameters



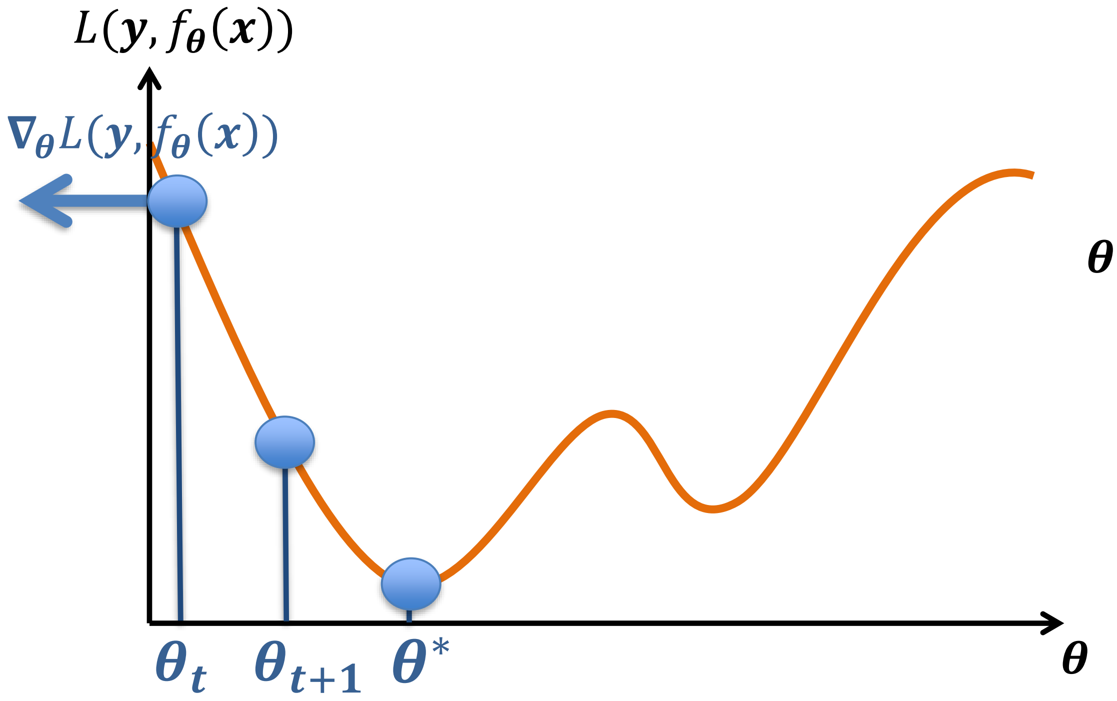
How to Find a Better NN?

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

→ Optimization! We train compute graphs with some optimization techniques!

Gradient Descent

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



step size / learning rate

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

$t \to \infty$

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

How to Find a Better NN?

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

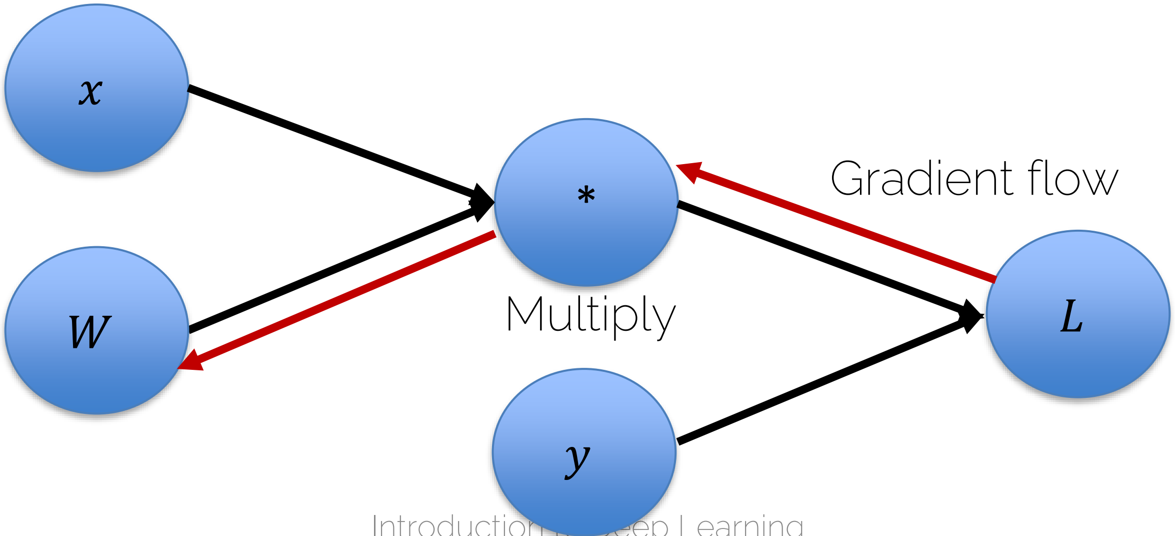
$$\boldsymbol{f_\theta}(\boldsymbol{x}) = \boldsymbol{W}\boldsymbol{x}\,, \qquad \boldsymbol{\theta} = \boldsymbol{W}$$

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

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

How to Find a Better NN?

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



How to Find a Better NN?

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

$$f_\theta(\boldsymbol{x}) = \boldsymbol{W}\boldsymbol{x}, \qquad \boldsymbol{\theta} = \boldsymbol{W}$$

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

How to Find a Better NN?

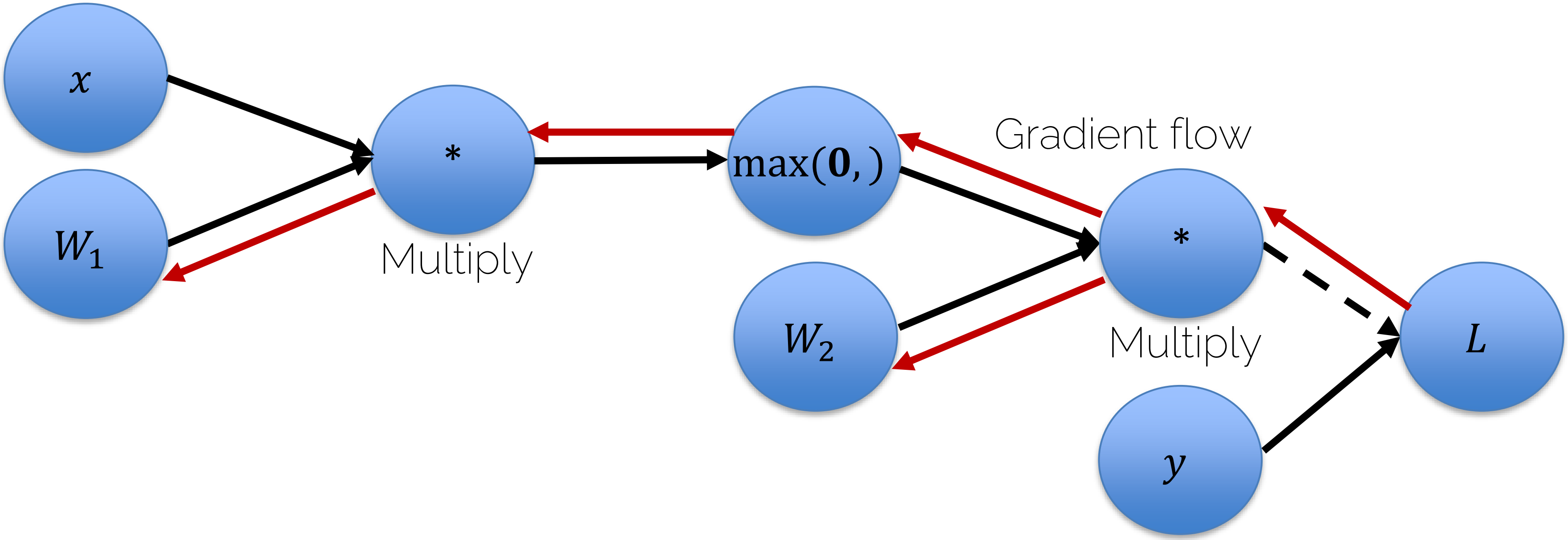
- Given inputs $\boldsymbol{x}$ and targets $\boldsymbol{y}$
- Given a multi-layer NN with many activations

$$\boldsymbol{f} = \boldsymbol{W}_5 \sigma(\boldsymbol{W}_4 \tanh(\boldsymbol{W}_3, \max(\boldsymbol{0}, \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1 \boldsymbol{x}))))$$

- Gradient descent for $\boldsymbol{L}\left(\boldsymbol{y}, \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{x})\right)$ w. r. t. $\boldsymbol{\theta}$
  – Need to propagate gradients from end to first layer ($\boldsymbol{W}_1$).

How to Find a Better NN?

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



How to Find a Better NN?

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

  $\boldsymbol{f} = \boldsymbol{W}_5 \sigma(\boldsymbol{W}_4 \tanh(\boldsymbol{W}_3, \max(\boldsymbol{0}, \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1 \boldsymbol{x}))))$
- Gradient descent solution for $L\big(\boldsymbol{y}, f_{\boldsymbol{\theta}}(\boldsymbol{x})\big)$ w. r. t. $\boldsymbol{\theta}$
  - Need to propagate gradients from end to first layer ($\boldsymbol{W}_1$)
- 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