Lecture 11: Neural Networks

Homework 2, due Wednesday, November 5 @ 11:59pm

Kernel Methods

Kernel ridge regression

- Ridge regression with feature map $\phi(\cdot) \in \mathbb{R}^p$

$$\widehat{w} = \arg\min_{w \in \mathbb{R}^p} \frac{1}{2}\|y - \phi(X)w\|_2^2 + \lambda \frac{1}{2}\|w\|_2^2$$

- $w = \sum_{i=1}^{n} \alpha_i \phi(x_i) = \phi(X)^T \alpha$
- Let $K \in \mathbb{R}^{n \times n}$ be the kernel matrix, where $K_{i,j} = \phi(x_i)^T \phi(x_j)$

$$\hat{\alpha} = \arg\min_{\alpha \in \mathbb{R}^n} \frac{1}{2}\|\mathbf{K}\alpha - \mathbf{y}\|_2^2 + \frac{1}{2}\lambda \alpha^T K \alpha$$

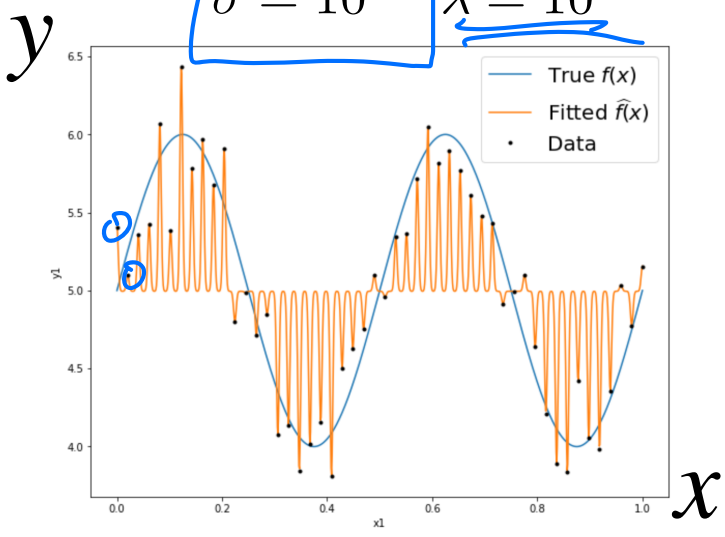
Thus, $\hat{\alpha}_{\text{kernel}} = (\mathbf{K} + \lambda \mathbf{I}_{n \times n})^{-1}\mathbf{y}$

- Prediction $\hat{y}_{\text{new}} = \hat{w}^T \phi(x_{\text{new}}) = \sum_{i=1}^{n} \alpha_i \phi(x_i)^T \phi(x_{\text{new}}) = \sum_{i=1}^{n} K(x_i, x_{\text{new}})\alpha_i$

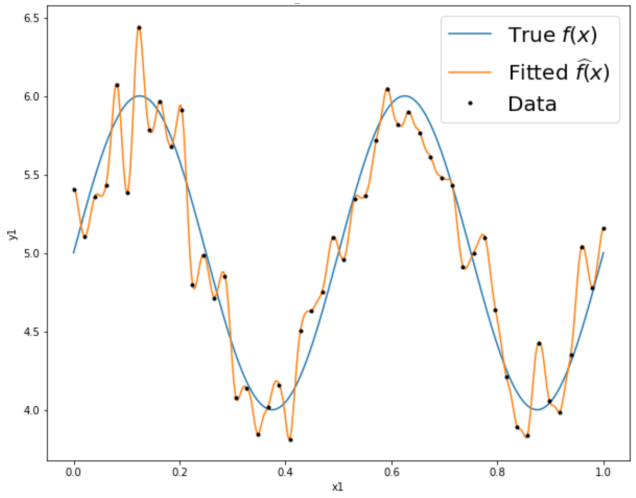
RBF kernel $k(x_i, x) = \exp\left\{ -\frac{\|x_i - x\|_2^2}{2\sigma^2} \right\}$

- $\mathcal{L}(\alpha) = \|\mathbf{K}\alpha - \mathbf{y}\|_2^2 + \lambda\|w\|_2^2$
- The bandwidth σ^2 of the kernel regularizes the predictor, and the regularization coefficient λ also regularizes the predictor

$\sigma = 10^{-3}$ $\lambda = 10^{-4}$



$\sigma = 10^{-2}$ $\lambda = 10^{-4}$

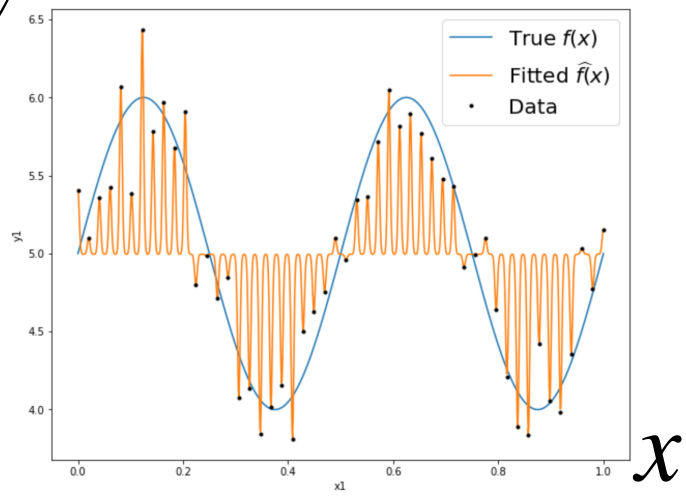


$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

RBF kernel $k(x_i, x) = \exp\left\{ -\frac{\|x_i - x\|_2^2}{2\sigma^2} \right\}$

- $\mathscr{L}(\alpha) = \|\mathbf{K}\alpha - \mathbf{y}\|_2^2 + \lambda\|w\|_2^2$
- The bandwidth σ^2 of the kernel regularizes the predictor, and the regularization coefficient λ also regularizes the predictor

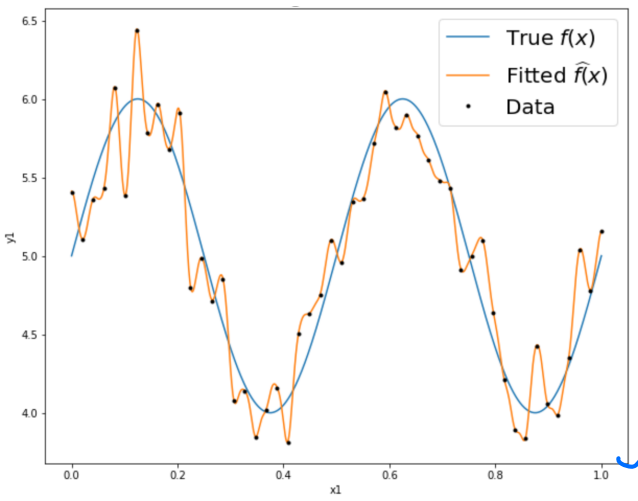
$\sigma = 10^{-3}$ $\lambda = 10^{-4}$



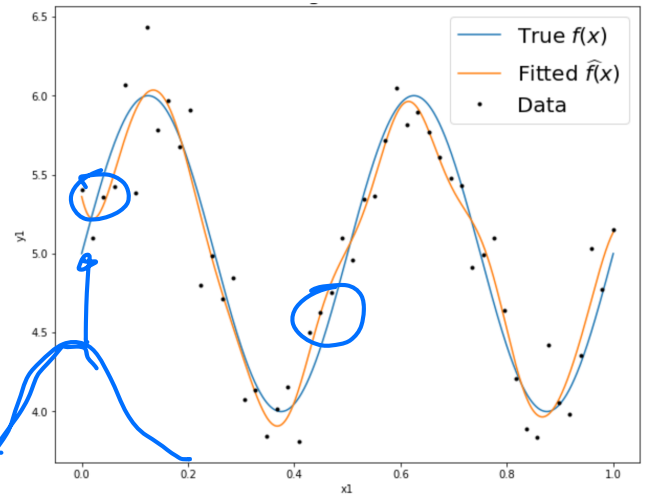
y

x

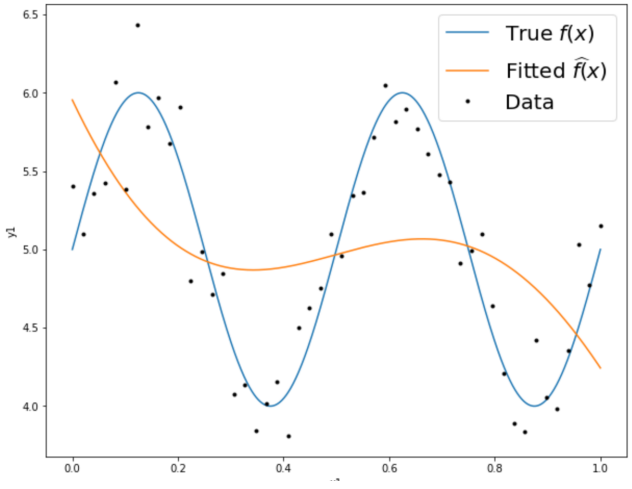
$\sigma = 10^{-2}$ $\lambda = 10^{-4}$



$\sigma = 10^{-1}$ $\lambda = 10^{-4}$



$\sigma = 10^{-0}$ $\lambda = 10^{-4}$



$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

Neural Networks

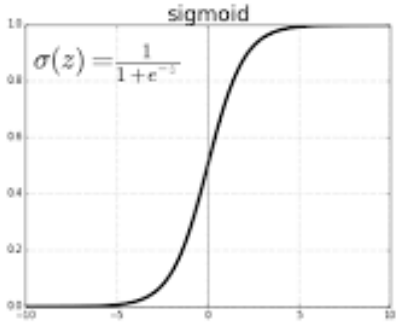
https://playground.tensorflow.org/

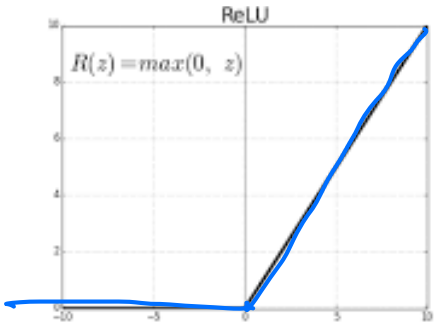
Single node of a neural network

- For a single node with input $x \in \mathbb{R}^d$, the node is defined by
  - **Parameter** $\theta \in \mathbb{R}^{d+1}$ (including the intercept/bias)

$$x = \begin{bmatrix} x_0 = 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}, \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}, \text{ such that } \theta^T x = \theta_0 + \theta_1 x_1 + \cdots + \theta_d x_d$$

  - **Activation function** g: $\mathbb{R} \to \mathbb{R}$
    - A common choice is sigmoid function: $g(z) = \dfrac{1}{1+e^{-z}}$
    - or Rectified Linear Unit (ReLU): $g(z) = \max\{0, z\}$



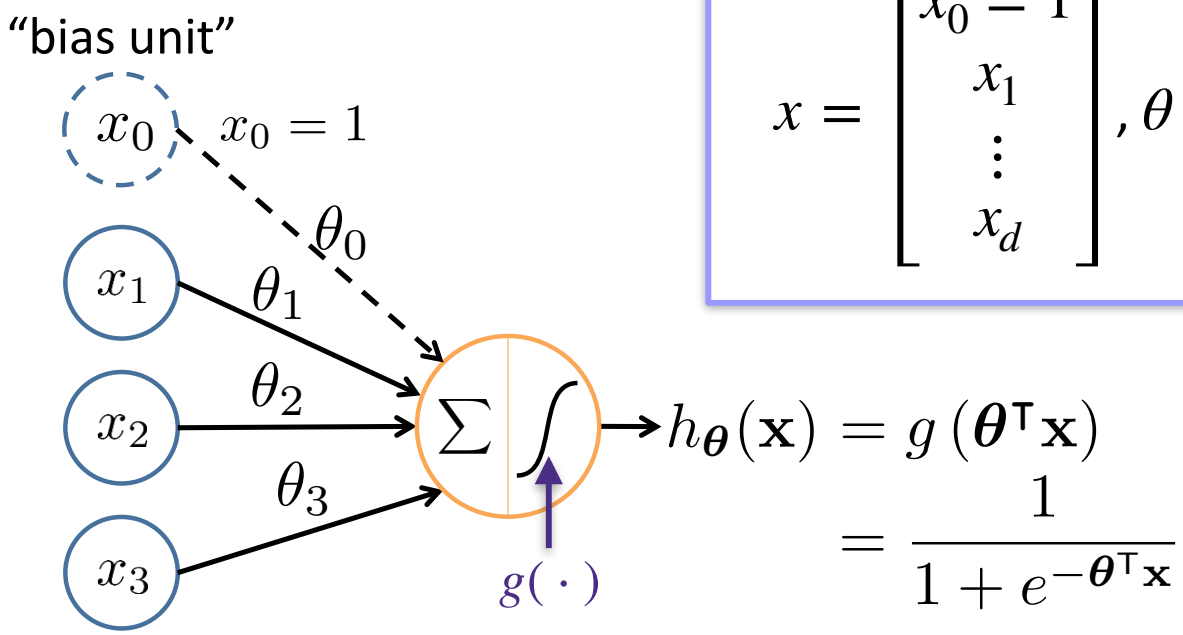


- The node performs $h_\theta(x) = g\left(\sum_{i=0}^{d} \theta_i x_i\right) = g(\theta^T x) = \dfrac{1}{1+e^{-\theta^T x}}$

Sequence of operations performed at a single node

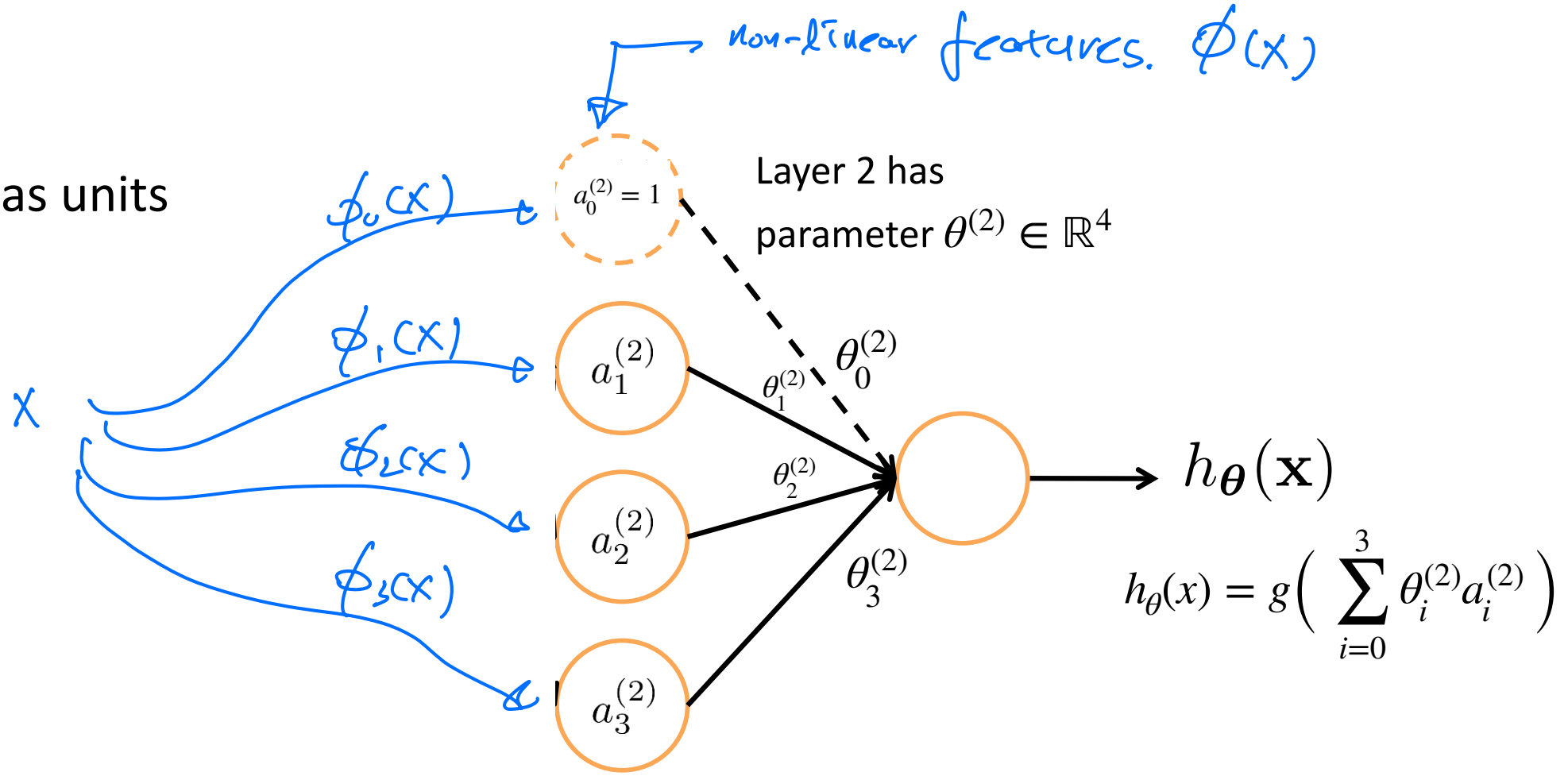
- For a single node with input $x \in \mathbb{R}^d$, the node is defined by
  - **Parameter** $\theta \in \mathbb{R}^{d+1}$ (including the intercept/bias)
  - **Activation function** $g : \mathbb{R} \to \mathbb{R}$
    - A common choice is sigmoid function: $g(z) = \dfrac{1}{1+e^{-z}}$
- The node performs $h_\theta(x) = g\left(\sum_{i=0}^{d} \theta_i x_i\right) = g(\theta^T x) = \dfrac{1}{1+e^{-\theta^T x}}$

$$x = \begin{bmatrix} x_0 = 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}, \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$



Neural Network composes simple functions to make complex functions

- Neural Network is a simple single node on features, in this example: $(a_0^{(2)}, a_1^{(2)}, a_3^{(2)}, a_3^{(2)})$ = input last layer
- These features are not manually chosen like polynomial features, but learned from data



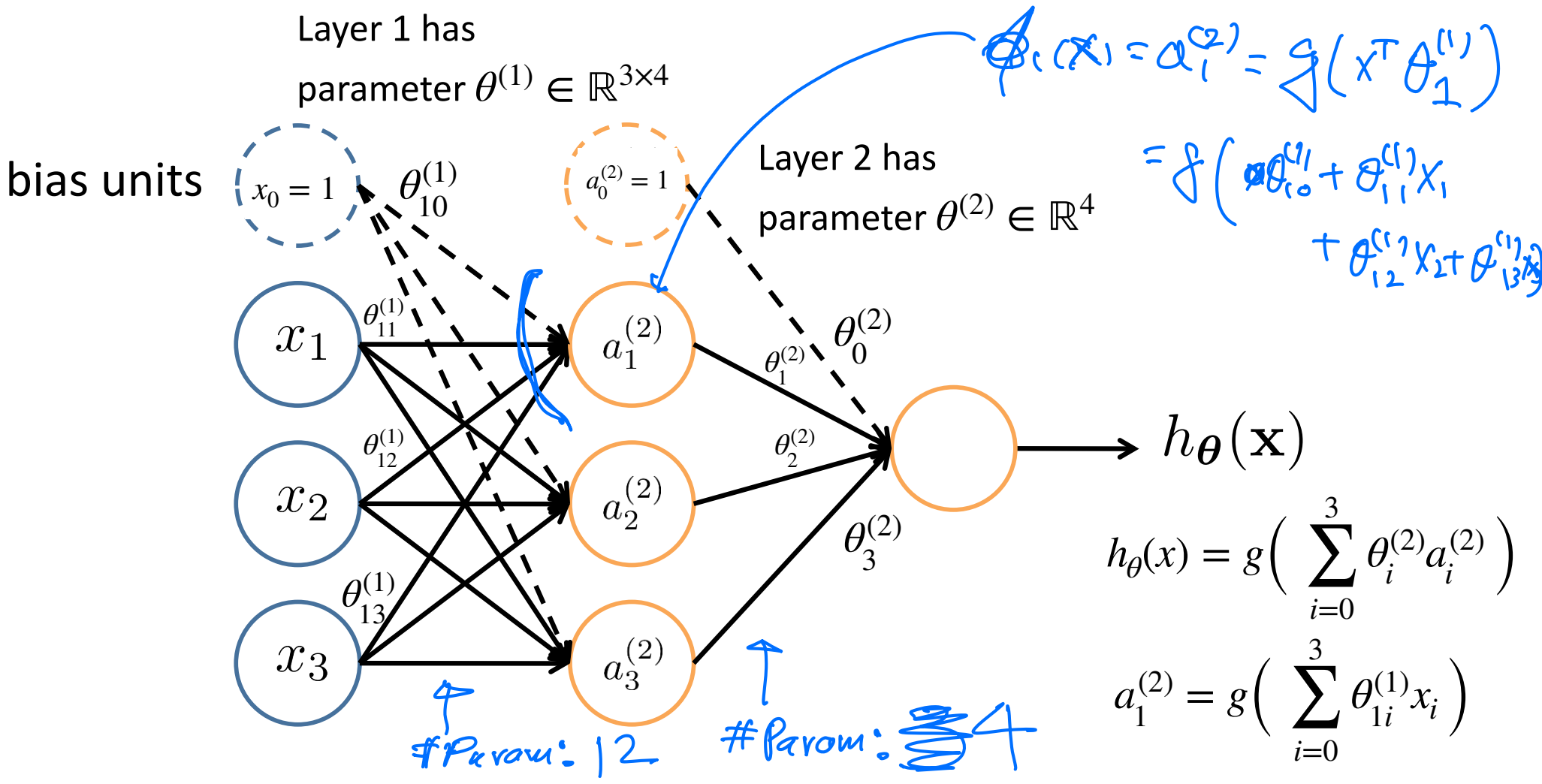
Layer 2 (Hidden Layer)

Layer 3 (Output Layer)

This is called a 2-layer Neural Network

Neural Network composes simple functions to make complex functions

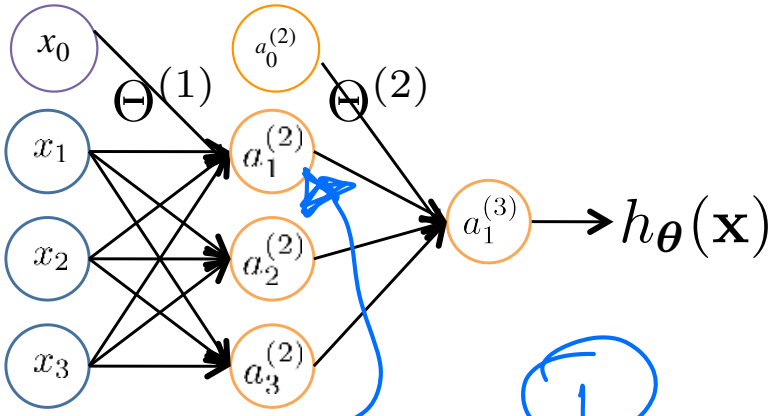
- Each layer performs simple operations
- Neural Network (with parameter $\theta = (\theta^{(1)}, \theta^{(2)})$) composes two layers



$$h_\theta(x) = g\left(\sum_{i=0}^{3} \theta_i^{(2)} a_i^{(2)}\right)$$

$$a_1^{(2)} = g\left(\sum_{i=0}^{3} \theta_{1i}^{(1)} x_i\right)$$

This is called
a 2-layer Neural Network



$\cdots g(\Theta^{(3)} \cdot g(\Theta^{(2)} \cdot g(\Theta^{(1)} \cdot x)))\cdots$

$a_i^{(j)}$ = "activation" of unit i in layer j

$\Theta^{(j)}$ = weight matrix stores parameters from layer j to layer $j+1$

1

$$\phi_1(x) = a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$

$$\phi_2(x) = a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$

$$\phi_3(x) = a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$

each layer

12 param.

2

$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

4 param

If network has s_j units in layer j *and* s_{j+1} units in layer j+1, then $\Theta^{(j)}$ has dimension $s_{j+1} \times (s_j+1)$

$$\Theta^{(1)} \in \mathbb{R}^{3\times 4} \qquad \Theta^{(2)} \in \mathbb{R}^{1\times 4}$$

coordinate-wise

$a^{(2)} = g(\Theta^{(1)} \cdot x)$

$= g(\begin{bmatrix} \\ \\ \\ \end{bmatrix} \begin{matrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{matrix})$

Multi-layer Neural Network - Binary Classification in $\{0,1\}$

L-th layer plays the role of features, but trained instead of pre-determined

This is a 5-dimensional vector

$$a^{(1)} = x$$

$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

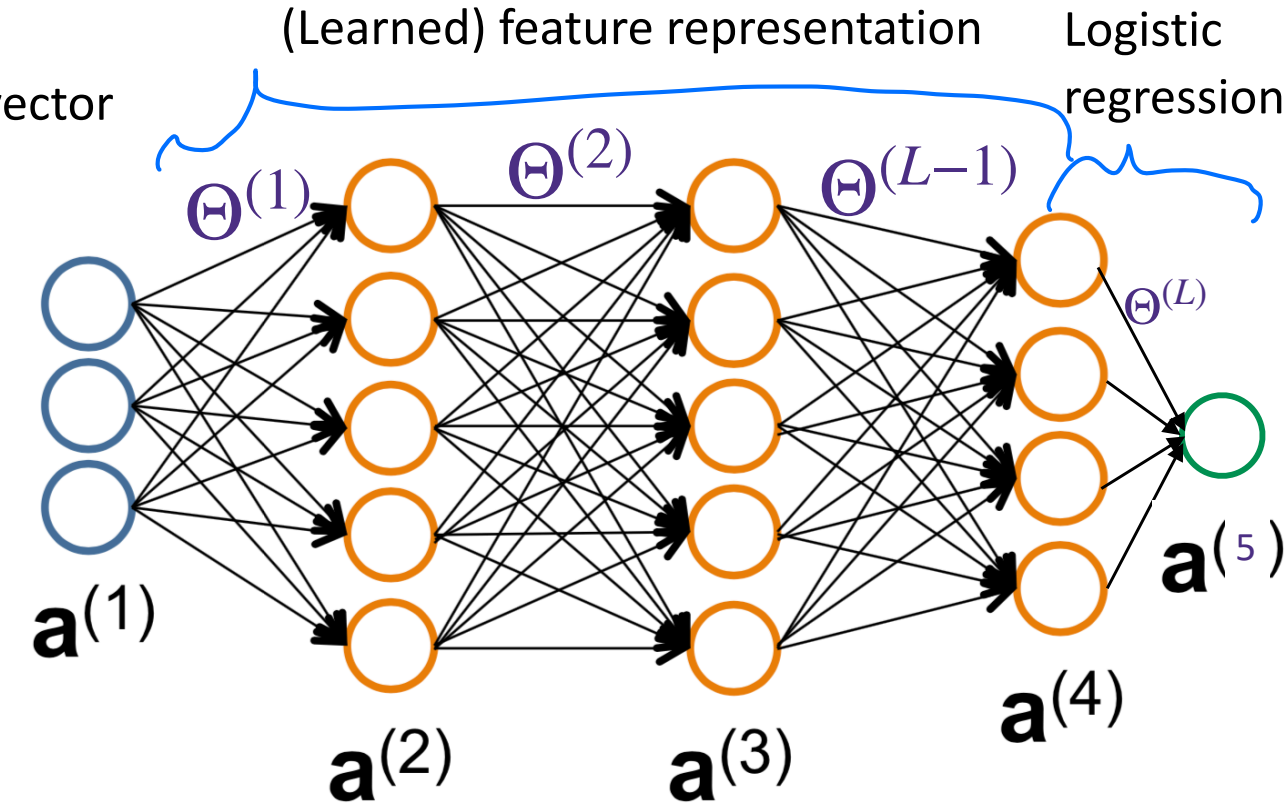
Scalar function g is applied coordinate-wise

$$\vdots$$

$$a^{(l+1)} = g(\Theta^{(l)} a^{(l)})$$

$$\vdots$$

$$\widehat{y} = g(\Theta^{(L)} a^{(L)})$$



Multi-layer Neural Network - Binary Classification in $\{0,1\}$

L-th layer plays the role of features, but trained instead of pre-determined

This is a 5-dimensional vector

$$a^{(1)} = x$$

$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

Scalar function g is applied coordinate-wise

$$\vdots$$

$$a^{(l+1)} = g(\Theta^{(l)} a^{(l)})$$

$$\vdots$$

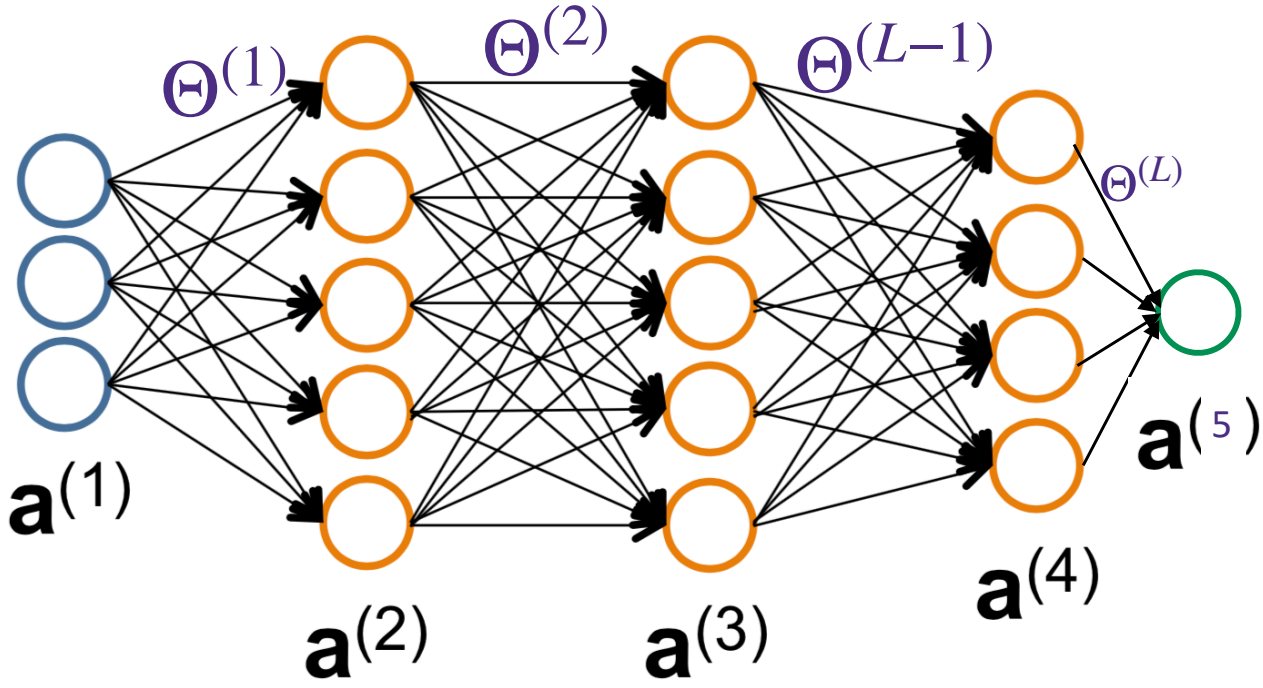
$$\hat{y} = g(\Theta^{(L)} a^{(L)})$$

$l_\theta(x,y)$

$\hat{Y} = f_\theta(x)$

(Learned) feature representation

Logistic regression



Cross entropy loss:

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

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

Binary Logistic Regression with learned feature $a^{(4)}$

Multi-layer Neural Network - Binary Classification

$$a^{(1)} = x$$

$$a^{(2)} = \sigma(\Theta^{(1)} a^{(1)})$$ ReLU

$$\vdots$$

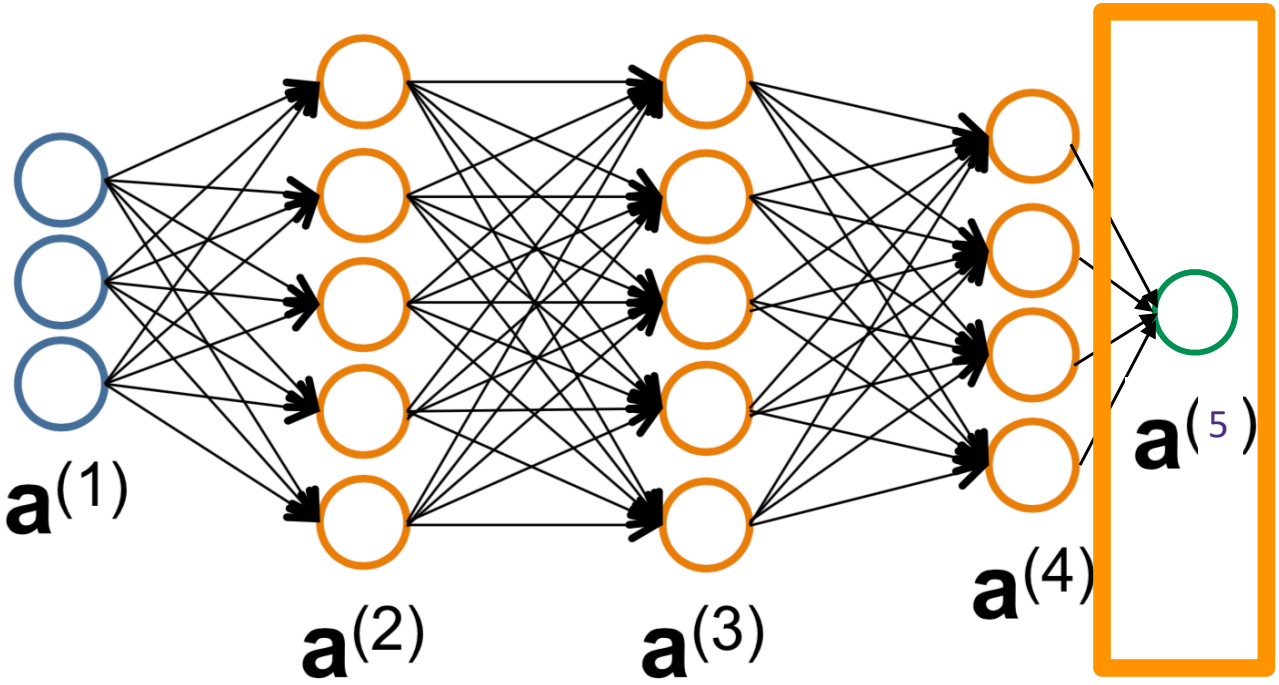
$$a^{(l+1)} = \sigma(\Theta^{(l)} a^{(l)})$$

$$\vdots$$

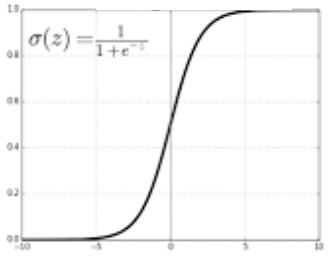
$$\hat{y} = g(\Theta^{(L)} a^{(L)})$$ Sigmoid

(Learned) feature representation

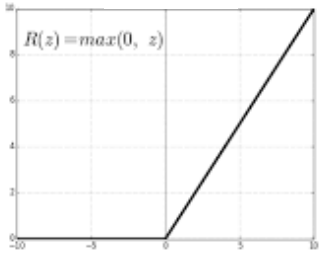
Logistic regression



Sigmoid



ReLU



Cross entropy loss:

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

$$\sigma(z) = \max\{0, z\} \quad g(z) = \frac{1}{1+e^{-z}}$$ Binary Logistic Regression

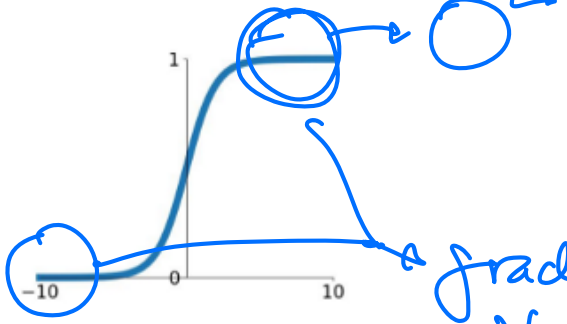
Nonlinear activation function

$$\sum_{i=1}^{n} l_\theta(x_i, y_i) + \lambda \|w\|_1$$

- popular choices of activation function includes

Sigmoid

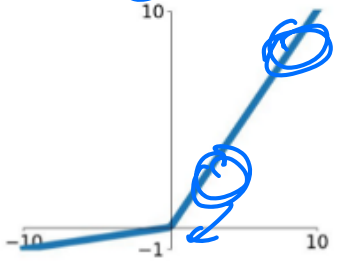
$$\sigma(x) = \frac{1}{1+e^{-x}}$$



gradient Very small

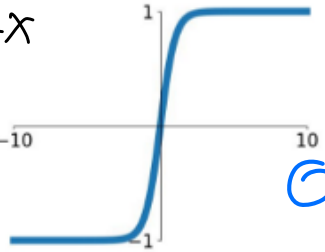
Leaky ReLU

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



tanh

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

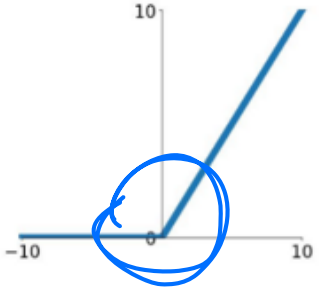


Optimize: Convex: non-convex

Smoothness: non-smooth

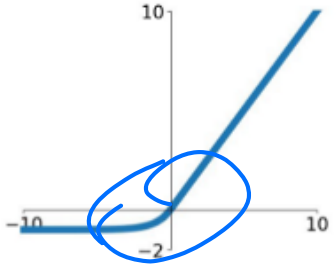
ReLU

$$\max(0, x)$$

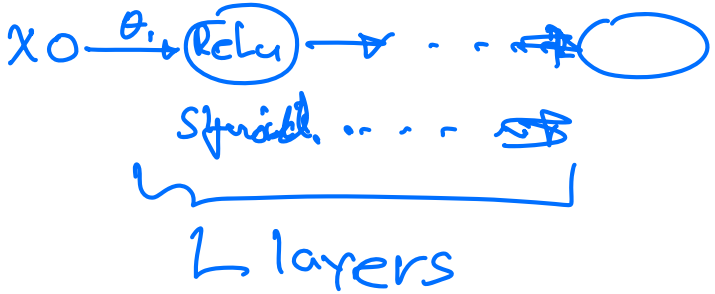


ELU

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



- Why is ReLU better than Sigmoid?
- Why is ELU better than ReLU?



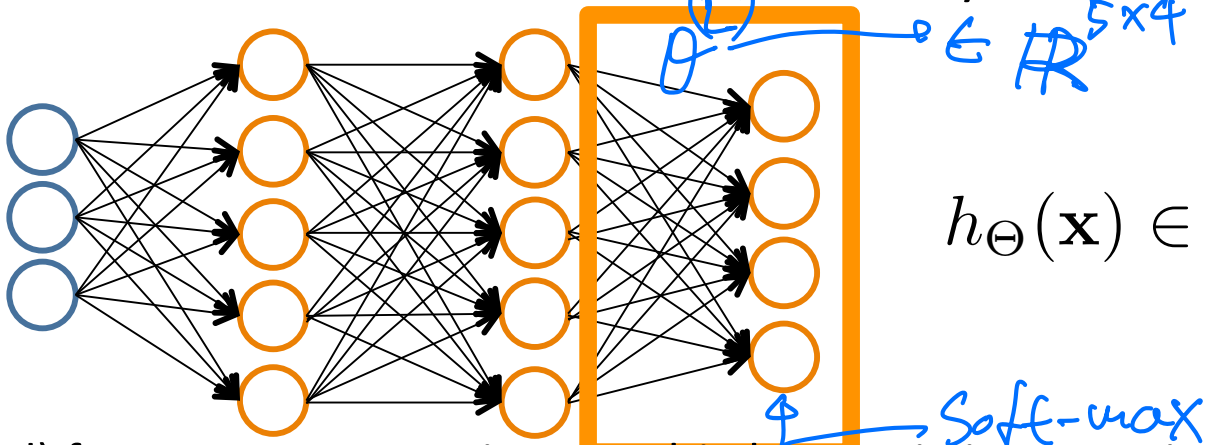
K-class Classification: multiple output units

Pedestrian

Car

Motorcycle

Truck



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

Multi-class Logistic Regression

(Learned) feature representation

Multi-class Logistic regression

We want:

y_i : one-hot encoding

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

when pedestrian

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

when car

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

when motorcycle

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

when truck

Multi-layer Neural Network - Regression

$$a^{(1)} = x$$

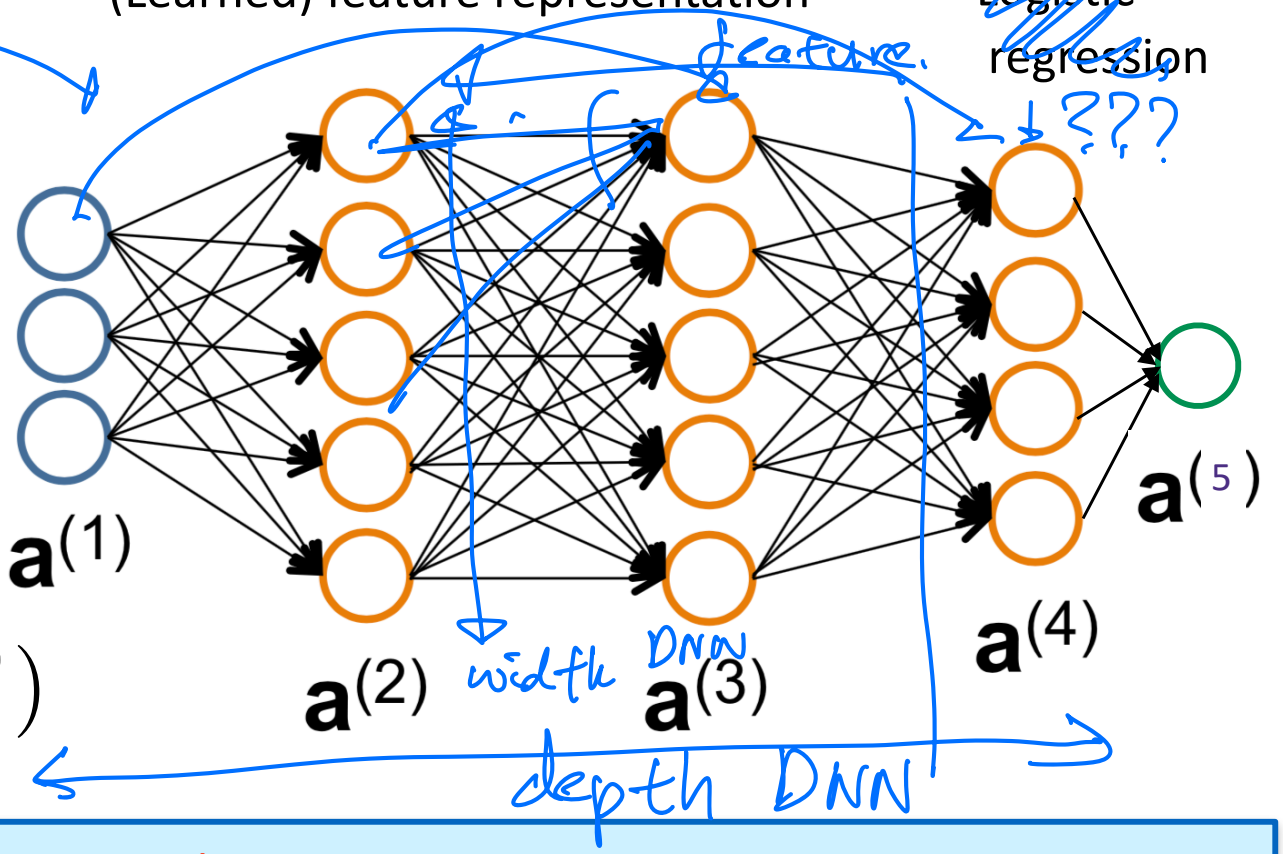
$$a^{(2)} = \sigma(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

$$a^{(l+1)} = \sigma(\Theta^{(l)} a^{(l)})$$

(Learned) feature representation

Logistic regression



no activation.

$$\hat{y} = \Theta^{(L)} a^{(L)}$$

Linear model

Square loss:

$$L(y, \hat{y}) = (y_i - \hat{y}_i)^2 + \lambda \|\theta\|_2$$

weight decay

$$\sigma(z) = \max\{0, z\}$$

Training Neural Networks

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

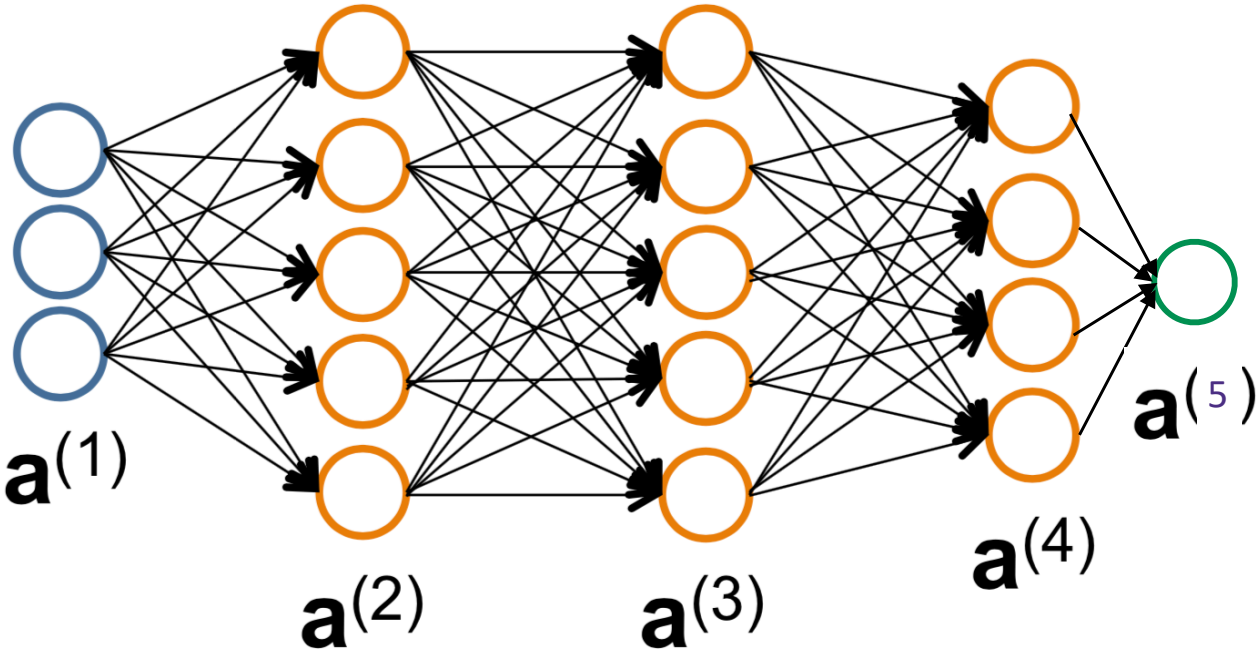
$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = g(\Theta^{(L)} a^{(L)})$$



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

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

Gradient Descent: $\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \hat{y}) \qquad \forall l$

Gradient Descent: $\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \hat{y}) \qquad \forall l$

Seems simple enough, what do packages like PyTorch, Tensorflow, Theano, Cafe, MxNet provide?

1. Automatic differentiation
    1. Given a NN, compute the gradient automatically
    2. Compute the gradient efficiently
2. Convenient libraries
    1. Set-up NN
    2. Choose algorithms (SGD,Adam,etc.) for Training
    3. Hyper-parameter Tuning
3. GPU support
    1. Linear algebraic operations

Common training issues

Neural networks are **non-convex**

- For large networks, **gradients** can **blow up** or **go to zero**. This can be helped by **batch-norm** or **ResNet** architecture

- **Stepsize** and **batchsize** have large impact on optimizing the training error *and* generalization performance

- Fancier alternatives to SGD (Adagrad, Adam, LAMB, etc.) can significantly improve training

- Making the network *bigger* may make training *faster!*

Back Propagation

Forward Propagation

- We are not writing the intercept at each layer for simplicity
- To compute gradients, we first run forward pass to get the intermediate representations $\{a^{(2)}, \ldots, a^{(L)}\}$

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

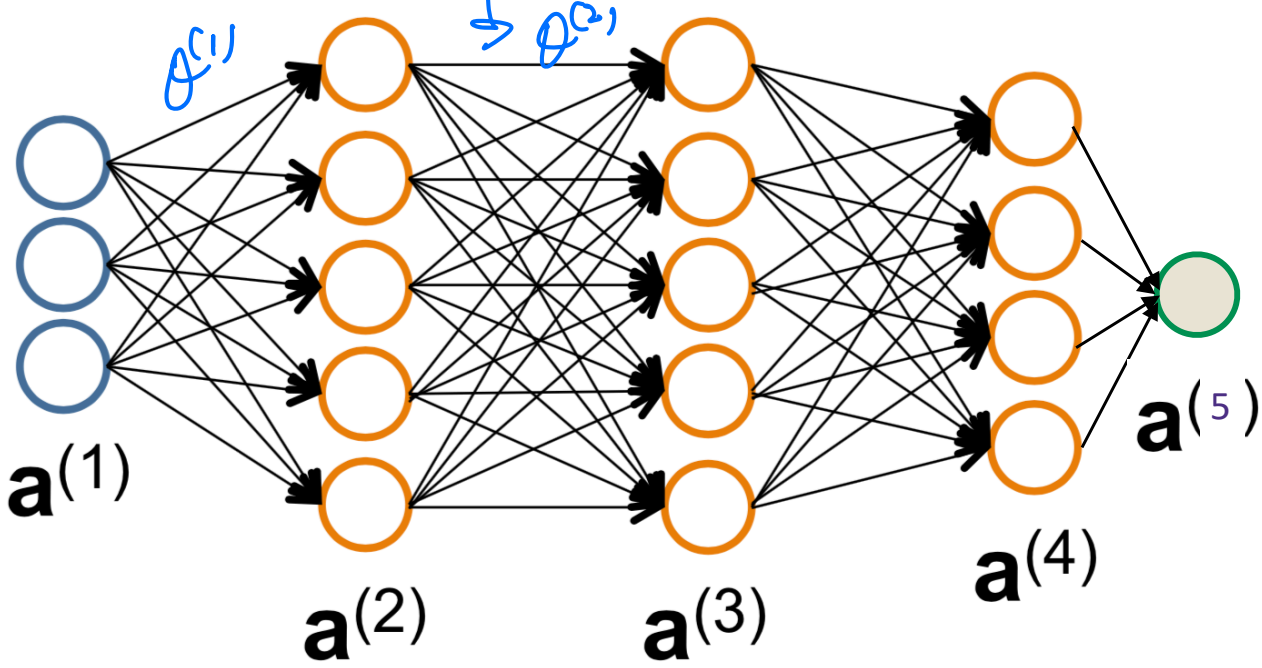
$$a^{(l)} = g\left(z^{(l)}\right)$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$



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

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

Backprop

- Parameters: $\Theta^{(1)} \in \mathbb{R}^{m \times d}, \Theta^{(2)}, \ldots \Theta^{(L-1)} \in \mathbb{R}^{m \times m}$
- Naive implementation takes $O(L^2)$ time, as each layer requires a full forward pass (with $O(L)$ operations) and some backward pass
- Backprop requires only $O(L)$ operations

backprop $L \approx 100$

Dynamic Programming

$$a^{(1)} = x \in \mathbb{R}^d$$

$$z^{(2)} = \Theta^{(1)} a^{(1)} \in \mathbb{R}^m$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g\left(z^{(l)}\right)$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

Train by Stochastic Gradient Descent:

$$\Theta_{i,j}^{(l)} \leftarrow \Theta_{i,j}^{(l)} - \eta \frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}}$$

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

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

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g\left(z^{(l)}\right)$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

Recursively computed in one backward pass

Computed in the forward pass

- Chain rule with $z_i^{(\ell+1)} = \Theta_{i,j}^{(\ell)} a_j^{(\ell)}$

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} = \delta_i^{(l+1)} \cdot a_j^{(l)}$$

output – input

Train by Stochastic Gradient Descent:

$$\Theta_{i,j}^{(l)} \leftarrow \Theta_{i,j}^{(l)} - \eta \frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}}$$

Forward pass

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

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

$$\delta_i^{(l+1)} \triangleq \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

Chain Rule

$$\delta_i^{(l)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l)}} = \sum_k \frac{\partial L(y, \hat{y})}{\partial z_k^{(l+1)}} \cdot \frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}}$$

next layer

$$\delta_k^{(\ell+1)} \cdot \Theta_{k,i}^{(l)} g'(z_i^{(l)})$$

$$z_k^{(\ell+1)} = \sum_{i=1}^{m} \Theta_{k,i}^{(l)} g(z_i^{(l)})$$

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

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

$$\delta_i^{(l+1)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g\left(z^{(l)}\right)$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

$g(z) = \frac{1}{1+e^{-z}}$: sigmoid.

$$\frac{\partial L(y,\hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l)}} = \sum_k \frac{\partial L(y,\hat{y})}{\partial z_k^{(l+1)}} \cdot \frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}}$$

$$= \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)} \, g'(z_i^{(l)})$$

Pre-computed in the forward pass.

Computed in the forward pass

$$= a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)}$$

$g'(z) = g(z)(1-g(z))$

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

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

$$\delta_i^{(l+1)} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l+1)}}$$

$$g'(z) = g(z)(1-g(z))$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g\left(z^{(l)}\right)$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

2L compute ⇒ all the gradients

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)}$$

forward pass

parameter

- We can recursively compute all $\delta^{(\ell)}$'s in a single backward pass
- And compute all gradients via

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

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

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g\left(z^{(l)}\right)$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$a^{(L+1)} = g(z^{(L+1)})$$

$$\hat{y} = a^{(L+1)}$$

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)}$$

$$\delta_i^{(L+1)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(L+1)}} = \frac{\partial}{\partial z_i^{(L+1)}} \left[-y \log(g(z^{(L+1)})) - (1 - y)\log(1 - g(z^{(L+1)}))\right]$$

$$= -\frac{y}{g(z^{(L+1)})} g'(z^{(L+1)}) + \frac{1 - y}{1 - g(z^{(L+1)})} g'(z^{(L+1)})$$

$$= g(z^{(L+1)}) - y = a^{(L+1)} - y$$

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

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

$$\delta_i^{(l+1)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}}$$

$$g'(z) = g(z)(1 - g(z))$$

Backprop

Recursive Algorithm!

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$a^{(l)} = g\left(z^{(l)}\right)$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

$$\delta^{(L+1)} = a^{(L+1)} - y$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}^{(l)}$$

$$\frac{\partial L(y, \hat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

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

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l+1)}}$$

Backpropagation

SGD

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)

For each training instance (x_k, y_k) :

Set $\mathbf{a}^{(1)} = x_k$

Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation : O(L)

Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_i$

Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \ldots, \boldsymbol{\delta}^{(2)}\}$: backward propagation : O(L)

Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Compute avg regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

Intercept do not have regularizer

Average loss + ℓ_2 regularizer

$$\frac{1}{n}\sum_{k=1}^{n} L(y_k, \hat{y}) + \lambda \|\Theta\|_2^2$$

We give data.

Questions?

[Homework 3 Problem B1 on Perceptron]
[Homework 3 Problem A4 on PyTorch on simple NNs]
[Homework 3 Problem A5 on Simple NN with MNIST]
[Homework 4 Problem A3 on CNN and CIFAR]