# Neural Networks

# Applications of Neural Networks

Self-driving cars

Voice assistants


Machine translation

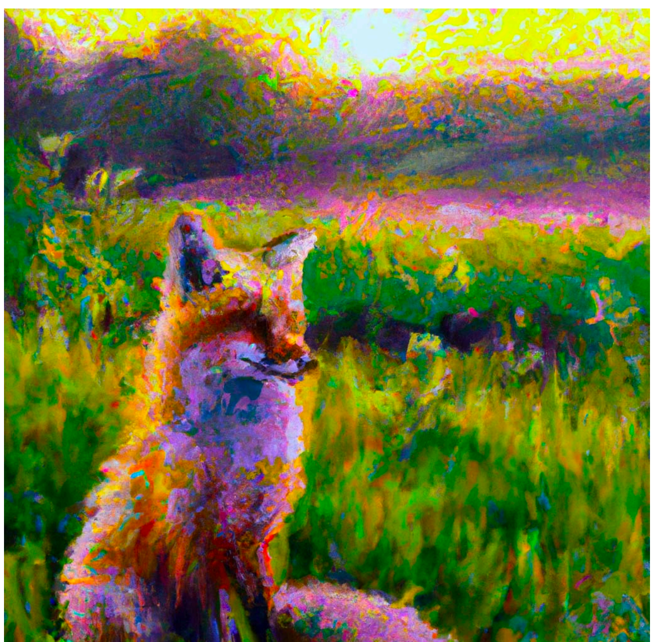


Image generation

*"a painting of a fox sitting in a field at sunrise in the style of Claude Monet"*

+ many more (images, text, audio)

**BUT:** Simple methods often still the best on tabular data.

# Neural Networks

- Origins: Algorithms that try to mimic the brain.
- Widely used in 80s and early 90s; popularity diminished in late 90s.
- Recent resurgence from 2010s: state-of-the-art techniques for many applications:
  - Computer Vision (AlexNet 2012)
  - Natural language processing
  - Speech recognition
  - Decision-making / control problems (AlphaGo, Games, robots)
- Limited theory:
  - Why do we find good minima with SGD for Non-convex loss?
  - Why do we not overfit when # of parameters $p$ is much larger than # of samples $n$?

# Neural Networks

Agenda:

1. Definitions of neural networks

2. Training neural networks:
    1. Algorithm: back propagation
    2. Putting it to work

3. Neural network architecture design:
    1. Convolutional neural network

# Neural Networks

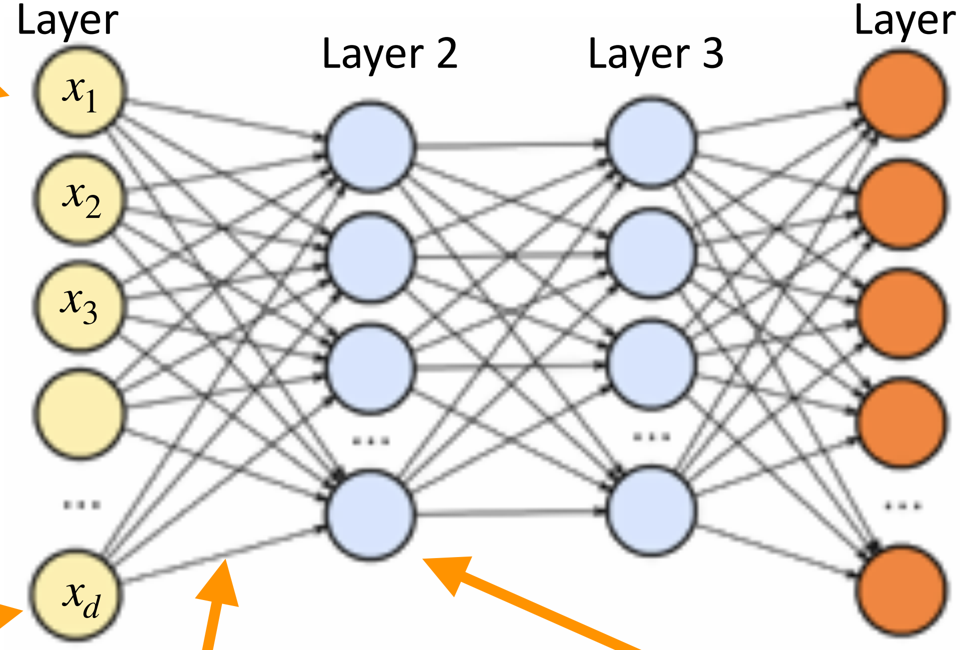
- **Neural Network** is a parametric family of functions from $x \in \mathbb{R}^d$ to $\hat{y} = h_\theta(x) \in \mathbb{R}^k$ with parameter $\theta \in \mathbb{R}^p$
- **Computation graph** illustrates the sequence of operations to be performed by a neural network

Input Layer

Intermediate Layers

Output Layer

Neuron/node/unit




Input $x \in \mathbb{R}^d$

Output $\hat{y} \in \mathbb{R}^k$

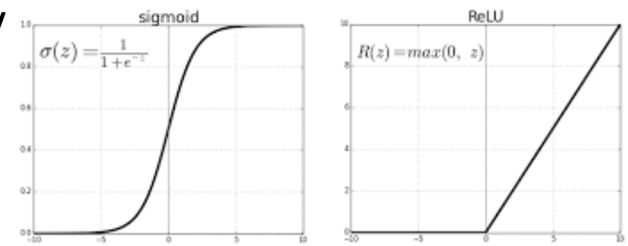
$d$ nodes each representing a scalar value of each coordinate of $x$

Link: maps output of a neuron to input of a neuron of the next layer, each link has a scalar weight

Neuron:
1. Input: weighted sum of previous layer
2. Apply scalar activation function
3. Output: links to the next layer

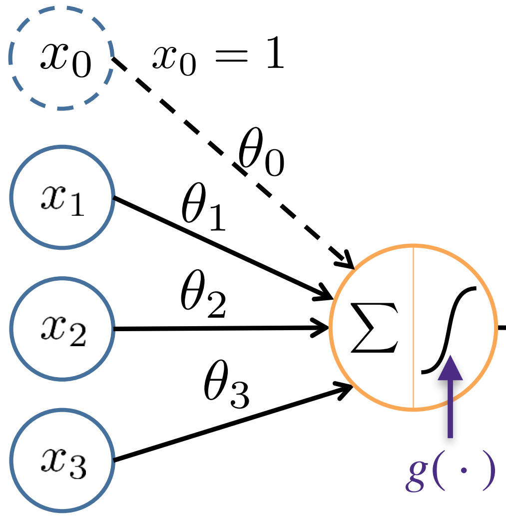
# Sequence of operations performed at a single node

- For a single node with input $x \in \mathbb{R}^d$, the node is defined by
  - **Parameters** $\theta \in \mathbb{R}^{d+1}$ (including the intercept/bias)
  - **Activation function** $g : \mathbb{R} \rightarrow \mathbb{R}$
    - A common choice is sigmoid function: $g(z) = \dfrac{1}{1 + e^{-z}}$
    - Another popular choice is Rectified Linear Unit (ReLU): $g(z) = \max\{0,z\}$




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

"bias unit"



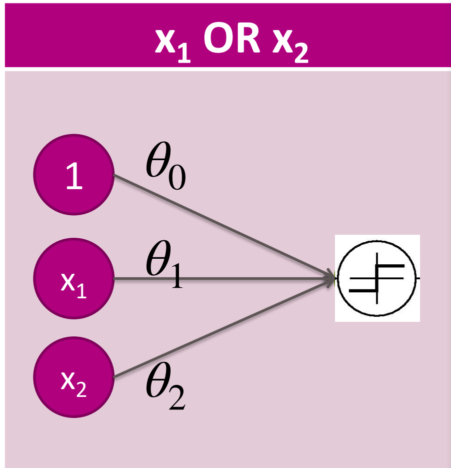

$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

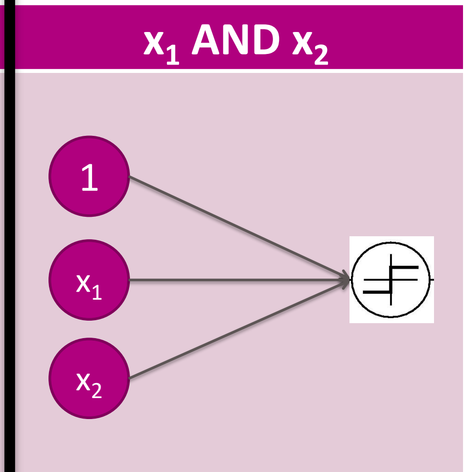
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}\right)$$

$$\left( = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}}} \quad \text{for sigmoid} \right)$$

## Toy example: What can be represented by a single node with $g(z) = \text{sign}(z)$?

| x[1] | x[2] | y |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 1 |




| x[1] | x[2] | y |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 0 |
| 1 | 0 | 0 |
| 1 | 1 | 1 |

**What should be the weights?**

$$f_\theta(x) = \text{sign}(\theta_0 + \theta_1 x[1] + \theta_2 x[2])$$

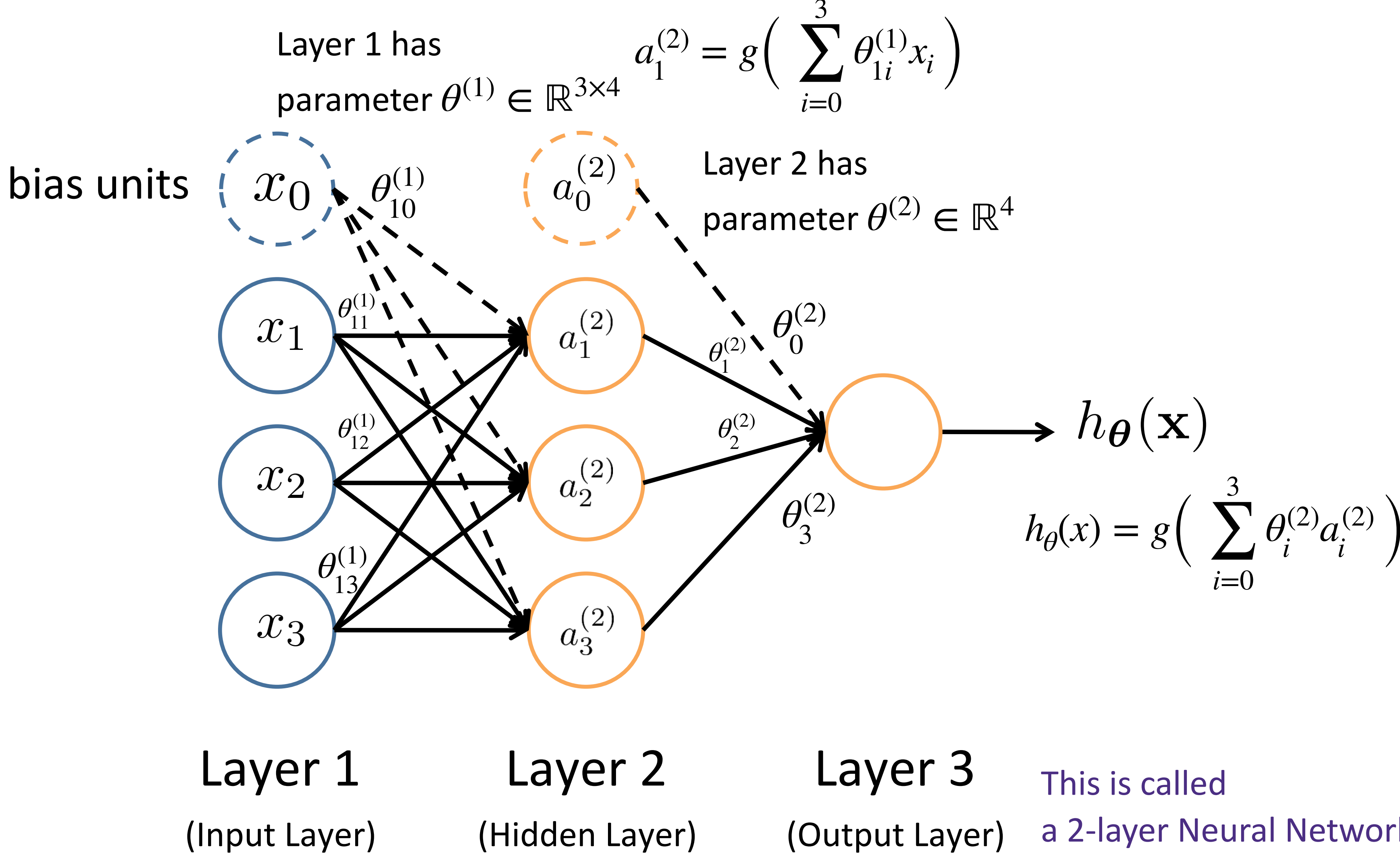
$$f_\theta(x) = \text{sign}(\theta_0 + \theta_1 x[1] + \theta_2 x[2])$$

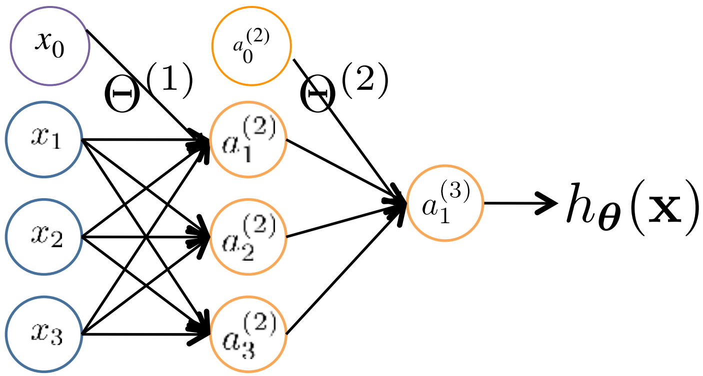
Note that there is a one-to-one correspondence between a **linear classifier** and a **neural network with a single node** of the above form

**What cannot be learned?**

# Neural Network composes simple functions to make complex functions

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






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

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

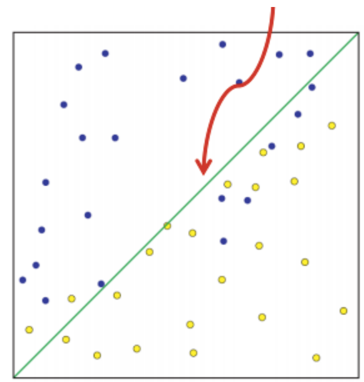
$$a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

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

$$\Theta^{(1)} \in \mathbb{R}^{3\times4} \qquad \Theta^{(2)} \in \mathbb{R}^{1\times4}$$

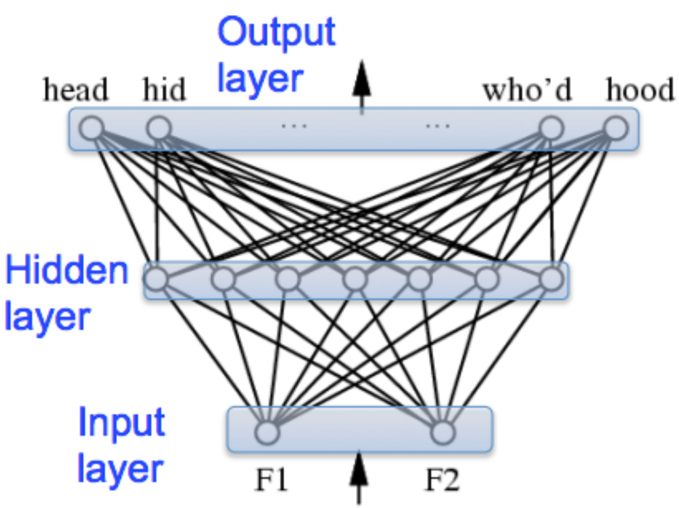
# Example of 2-layer neural network in action

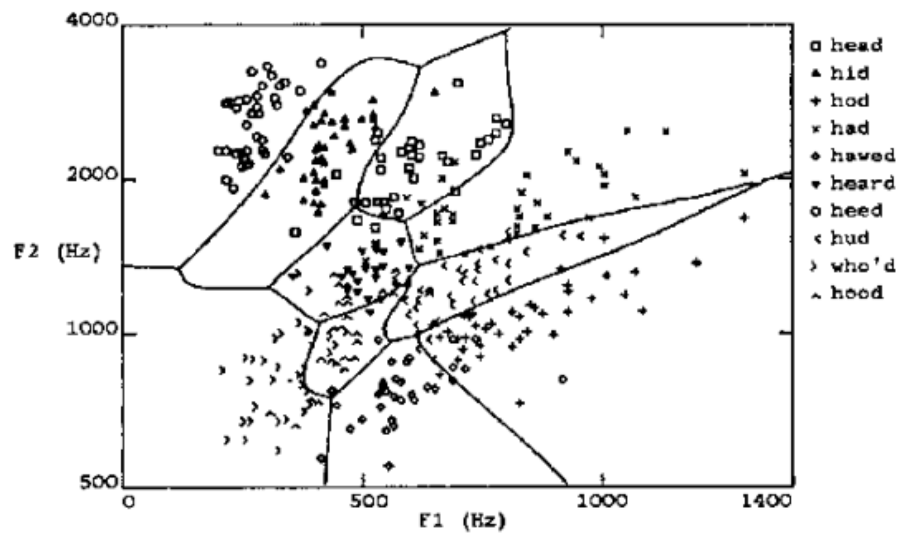
1-layer neural networks
only represents linear classifiers




Example: 2-layer neural network trained to distinguish vowel sounds using 2 formants (features)

A highly non-linear decision boundary can be learned from 2-layer neural networks



# Neural Networks are arbitrary function approximators

**Theorem 10** (Two-Layer Networks are Universal Function Approximators). *Let $F$ be a continuous function on a bounded subset of $D$-dimensional space. Then there exists a two-layer neural network $\hat{F}$ with a finite number of hidden units that approximate $F$ arbitrarily well. Namely, for all $\boldsymbol{x}$ in the domain of $F$, $|F(\boldsymbol{x}) - \hat{F}(\boldsymbol{x})| < \epsilon$.*

Cybenko, Hornik (theorem reproduced from CIML, Ch. 10)

But Deep Neural Networks have many powerful properties not yet understood theoretically.

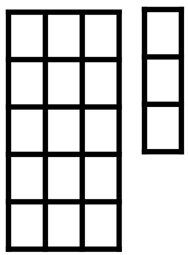
# Multi-layer Neural Network - Binary Classification in $\{0,1\}$

$L$-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

$$\vdots$$

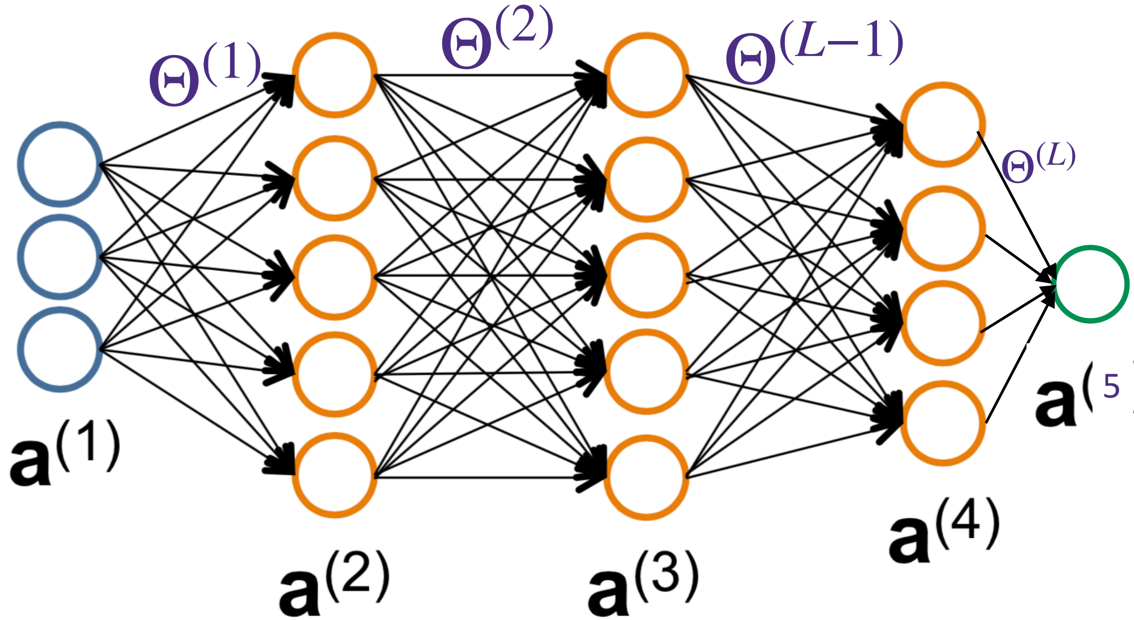
$$a^{(l+1)} = g(\Theta^{(l)} a^{(l)})$$

$$\vdots$$

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

(Learned) feature representation

Logistic regression




**Cross entropy loss:**

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

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

**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

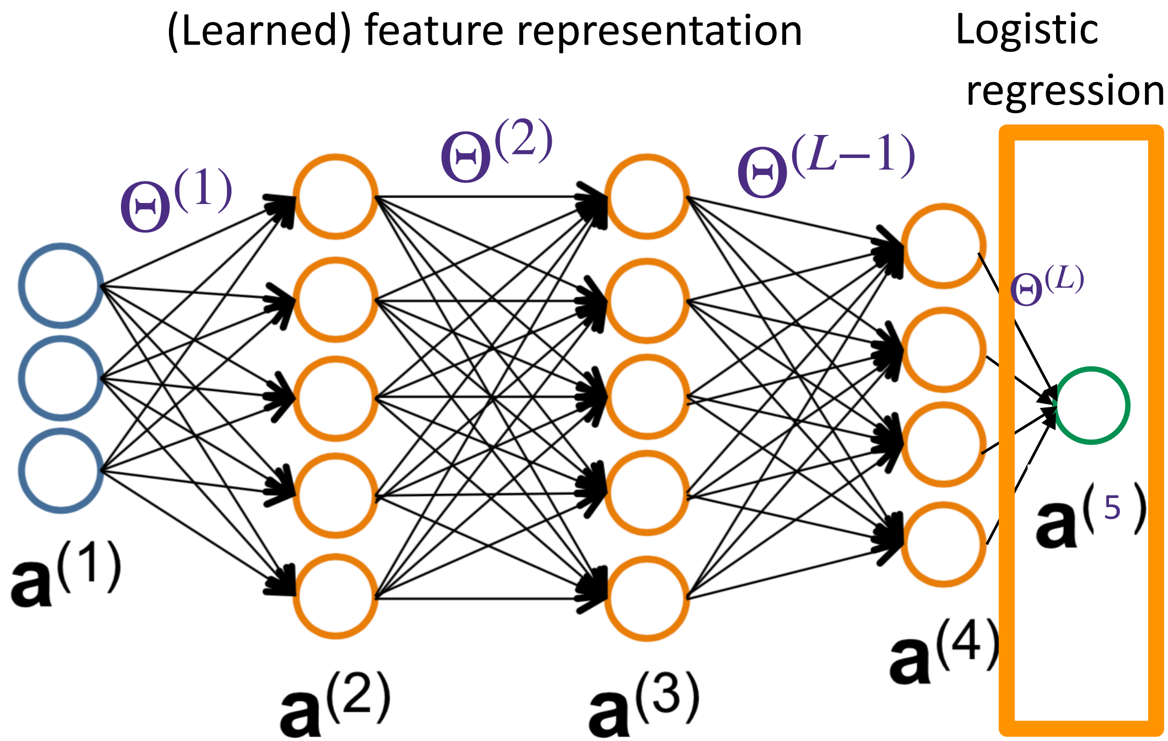
$\vdots$

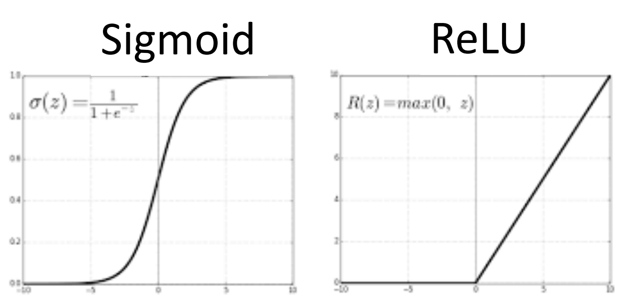
$$a^{(l+1)} = \sigma(\Theta^{(l)} a^{(l)})$$

$\vdots$

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

Sigmoid




- Why is ReLU better than sigmoid?

**Cross entropy loss:**

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

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

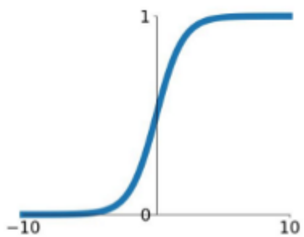
Binary Logistic Regression

# Nonlinear activation function

- popular choices of activation function includes

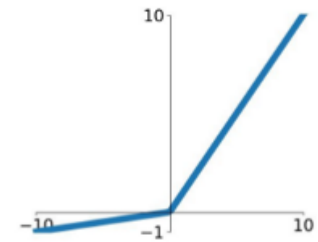
**Sigmoid**

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



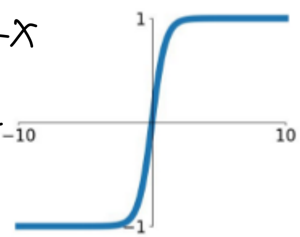

**Leaky ReLU**

$\max(0.1x, x)$



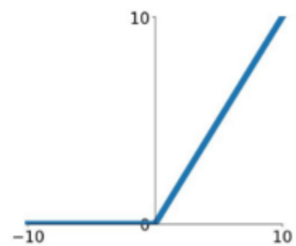

**tanh**

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



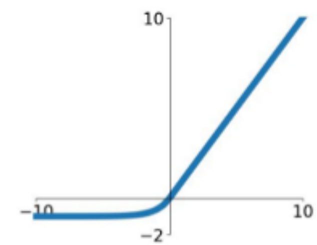

**ReLU**

$\max(0, x)$




**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?

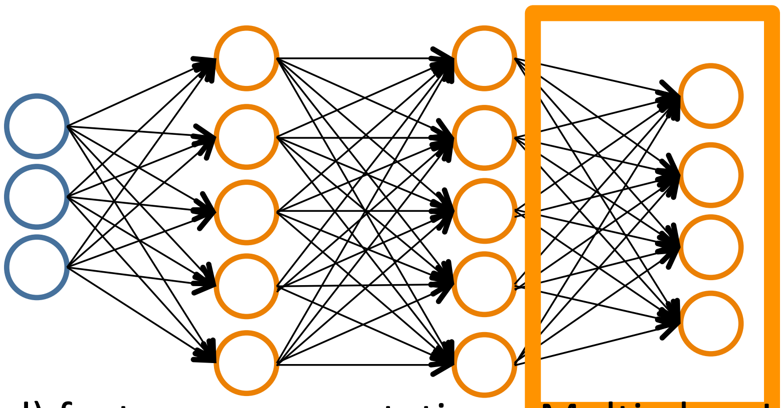
# $K$-class Classification: multiple output units

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:

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

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

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

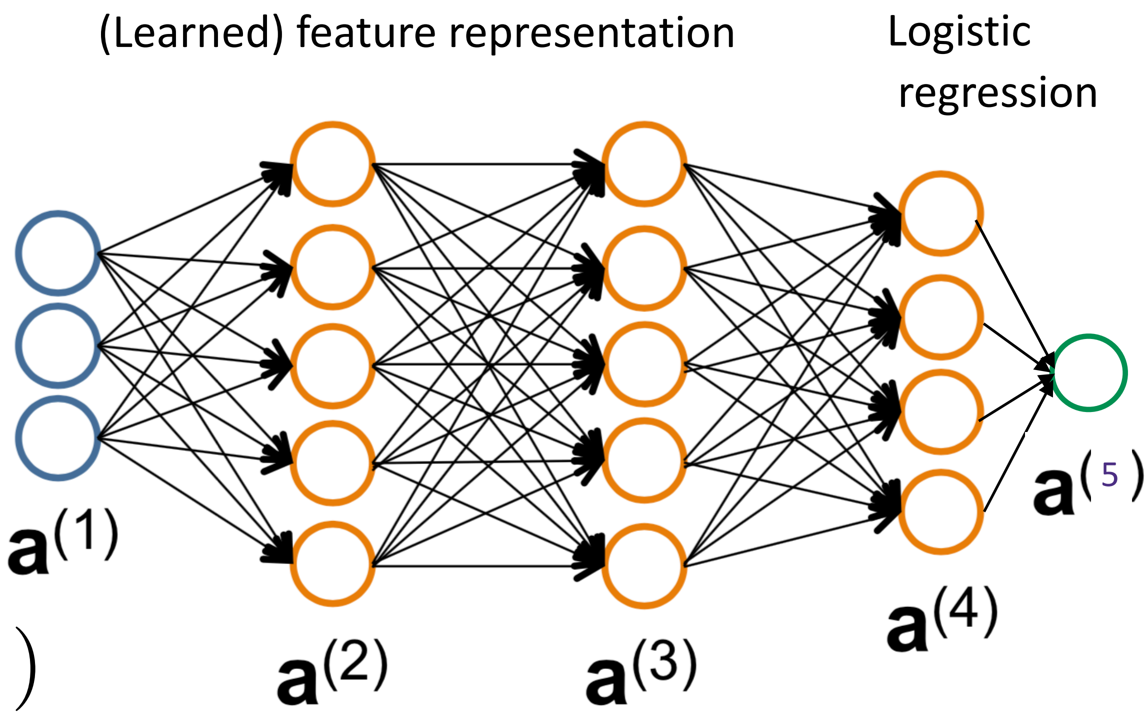
$$\vdots$$

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

$$\vdots$$

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

Linear model




Square loss:

$$L(y, \widehat{y}) = (y - \widehat{y})^2$$

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

# Training Neural Networks

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

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

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

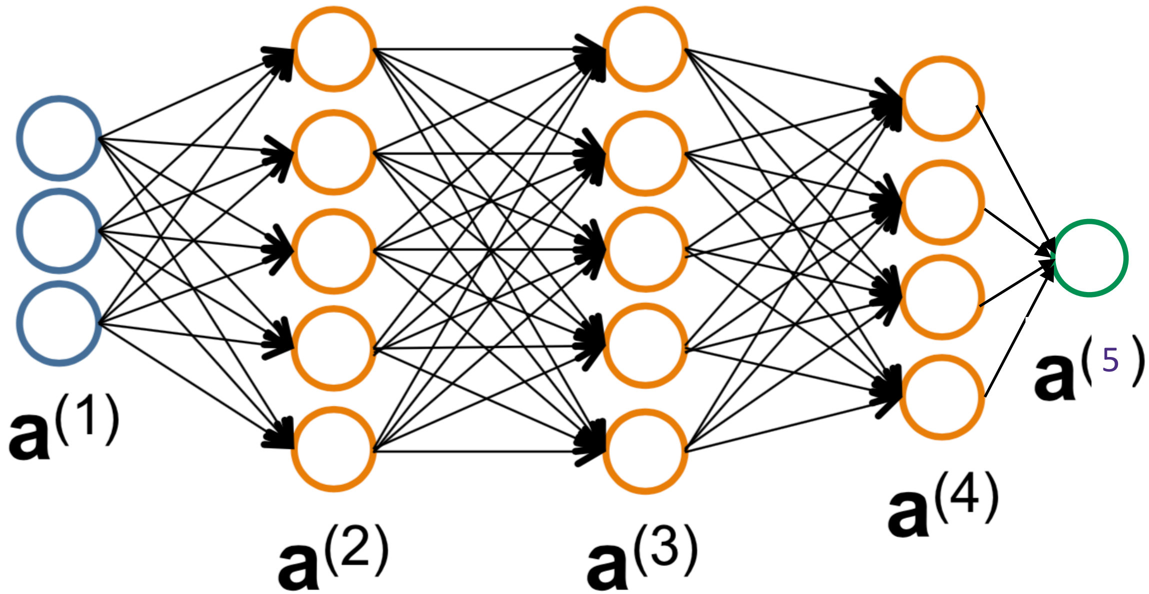
$$\vdots$$

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

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

$$\vdots$$

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




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

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

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

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

Seems simple enough - what do packages like PyTorch, Tensorflow, Jax, Theano, Caffe, 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

Gradient Descent:

Seems simple enough, Theano, Cafe, MxNet s

1. Automatic differ

2. Convenient libra

```
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        # 1 input image channel, 6 output channels, 3x3 square convolution
        # kernel
        self.conv1 = nn.Conv2d(1, 6, 3)
        self.conv2 = nn.Conv2d(6, 16, 3)
        # an affine operation: y = Wx + b
        self.fc1 = nn.Linear(16 * 6 * 6, 120)  # 6*6 from image dimension
        self.fc2 = nn.Linear(120, 84)
        self.fc3 = nn.Linear(84, 10)

    def forward(self, x):
        # Max pooling over a (2, 2) window
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))
        # If the size is a square you can only specify a single number
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(-1, self.num_flat_features(x))
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

```
# create your optimizer
optimizer = optim.SGD(net.parameters(), lr=0.01)

# in your training loop:
optimizer.zero_grad()   # zero the gradient buffers
output = net(input)
loss = criterion(output, target)
loss.backward()
optimizer.step()    # Does the update
```

# Common training issues

## Neural networks are **non-convex**

- For large networks, **gradients** can **blow up** or **go to zero**. This can be helped by **batchnorm** 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

-Overfitting is common and not undesirable: typical to achieve 100% training accuracy even if test accuracy is just 80%

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

- Start from a code that someone else has tried and tested

# Common training issues

## Training is too slow:

- Use larger step sizes, develop step size reduction schedule
- Use GPU resources
- Change batch size
- Use momentum and more advanced optimizers (e.g., Adam)
- Apply batch normalization
- Make network larger or smaller (# layers, # filters per layer, etc.)

## Test accuracy is low

- Try modifying all of the above, plus changing other hyperparameters

# 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 $\{a^{(2)}, \ldots, a^{(L)}\}$

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

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

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

$$\vdots$$

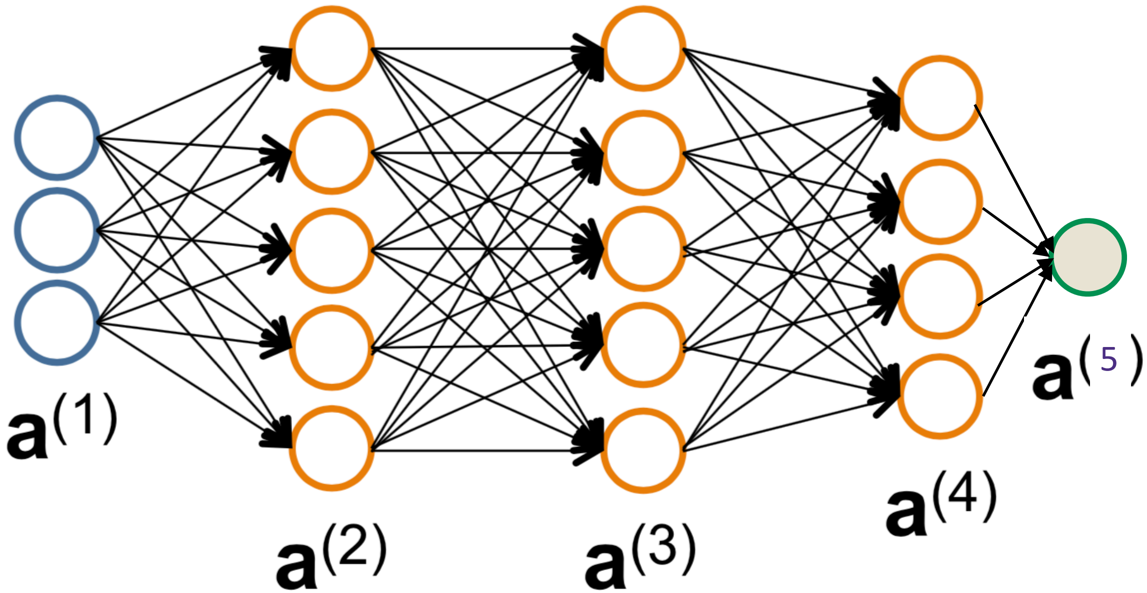
$$a^{(l)} = g(z^{(l)})$$

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

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

$$\vdots$$

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




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

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

# Backprop

- Parameters: $\Theta^{(1)} \in \mathbb{R}^{m \times d}, \Theta^{(2)}, \cdots \Theta^{(L-1)} \in \mathbb{R}^{m \times m}$
- 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

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

**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 $z_i^{(\ell+1)} = \Theta_{i,j}^{(\ell)} a_j^{(\ell)}$

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

**Train by Stochastic Gradient Descent:**

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

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

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

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

# Backprop

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

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

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

$\vdots$

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

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

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

$\vdots$

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

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

$$\delta_i^{(l)} = \frac{\partial L(y, \hat{y})}{\partial z_i^{(l)}} = \sum_k \underbrace{\frac{\partial L(y, \hat{y})}{\partial z_k^{(l+1)}}}_{\delta_k^{(\ell+1)}} \cdot \underbrace{\frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}}}_{\Theta_{k,i}^{(l)}\, g'(z_i^{(l)})}$$

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

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

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

# Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

Computed in the forward pass

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

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

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

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

# Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

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

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

# Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

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

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

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

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

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

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

# Backprop

Recursive Algorithm!

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

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

# Backpropagation

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

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

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

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 + $\ell_2$ regularizer

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