Neural Networks

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 10s: state-of-the-art techniques for many applications:
  - Computer Vision
  - Natural language processing
  - Speech recognition
  - Decision-making / control problems (AlphaGo, Dota, robots)
- Limited theory:
  - Non-convexity
  - Model are complex but generalization error is small

Neural Networks

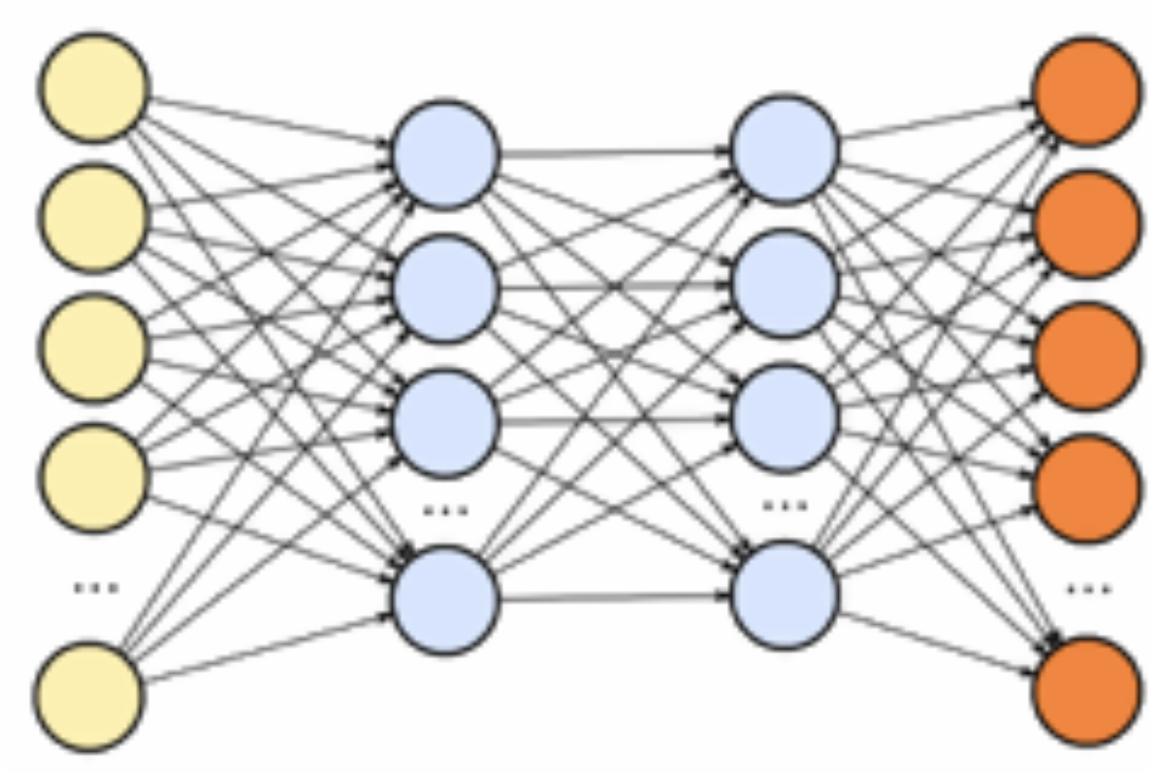
This week:

1. Definitions of neural networks

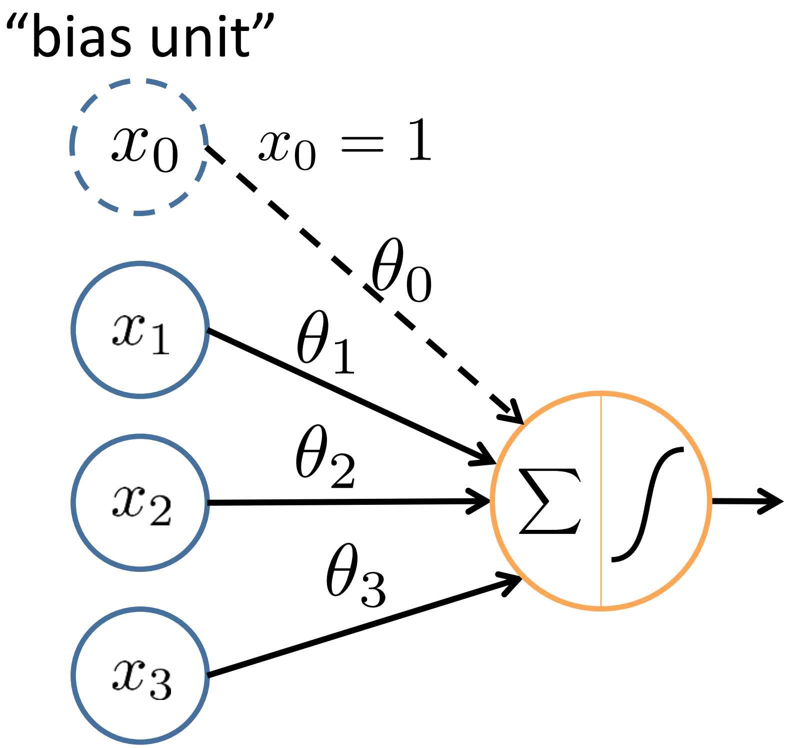
2. Training neural networks:
    1. Algorithm: back propagation
    2. Putting it to work

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

Neural Networks



Single Node



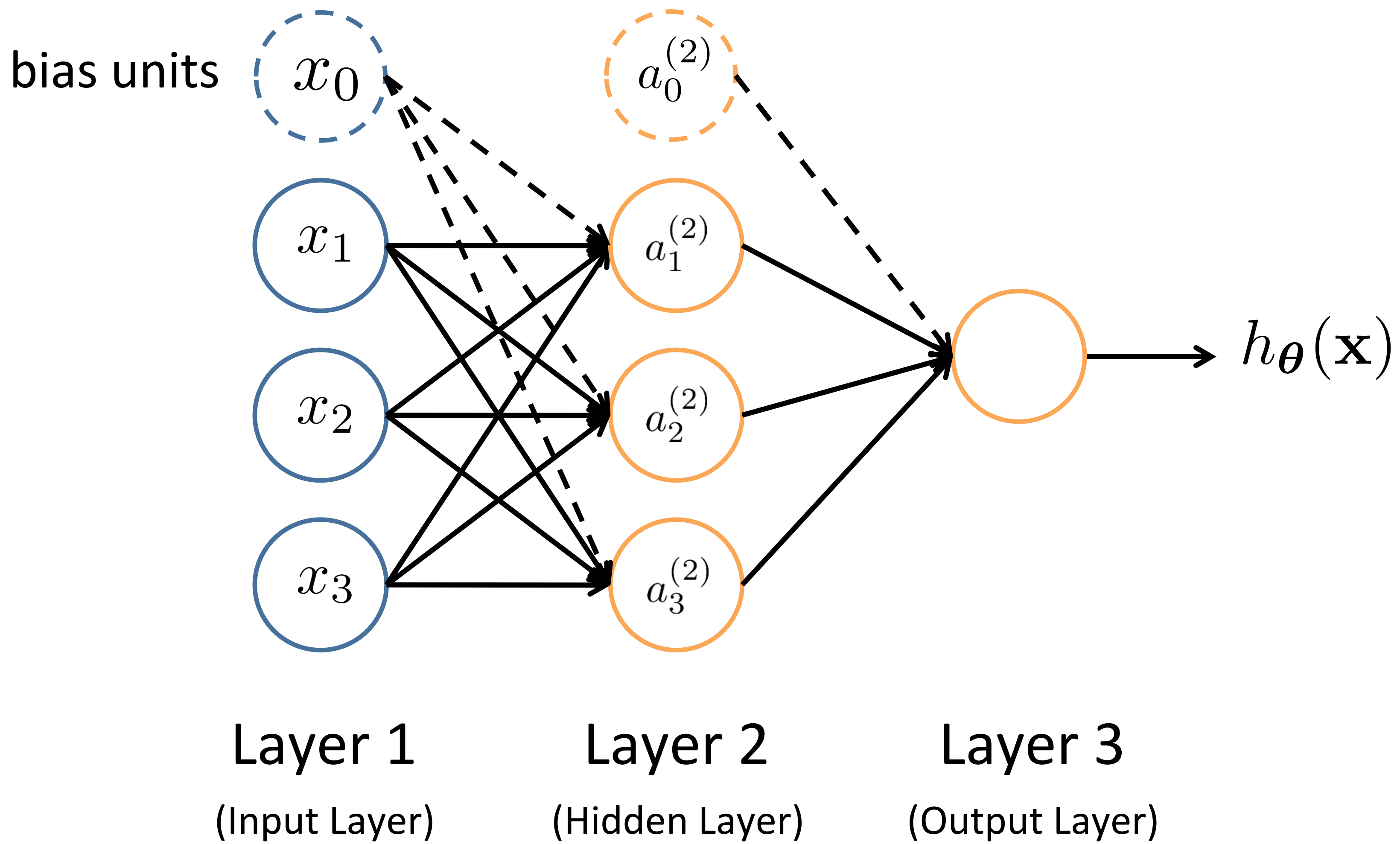
$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

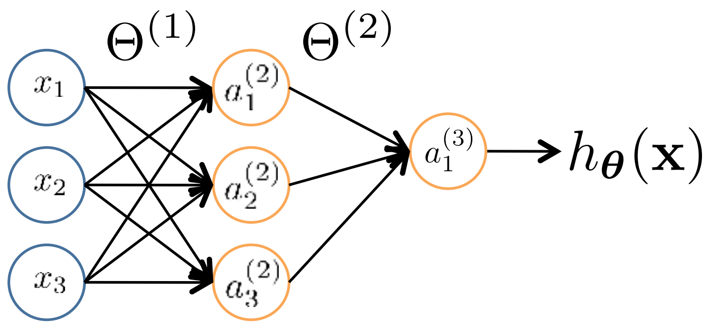
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^\intercal \mathbf{x}\right) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\intercal \mathbf{x}}}$$

Binary
Logistic
Regression

Sigmoid (logistic) activation function: $g(z) = \dfrac{1}{1 + e^{-z}}$

Neural Network





$a_i^{(j)}$ = "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 $s_{j+1} \times (s_j+1)$.

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

Multi-layer Neural Network - Binary Classification

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

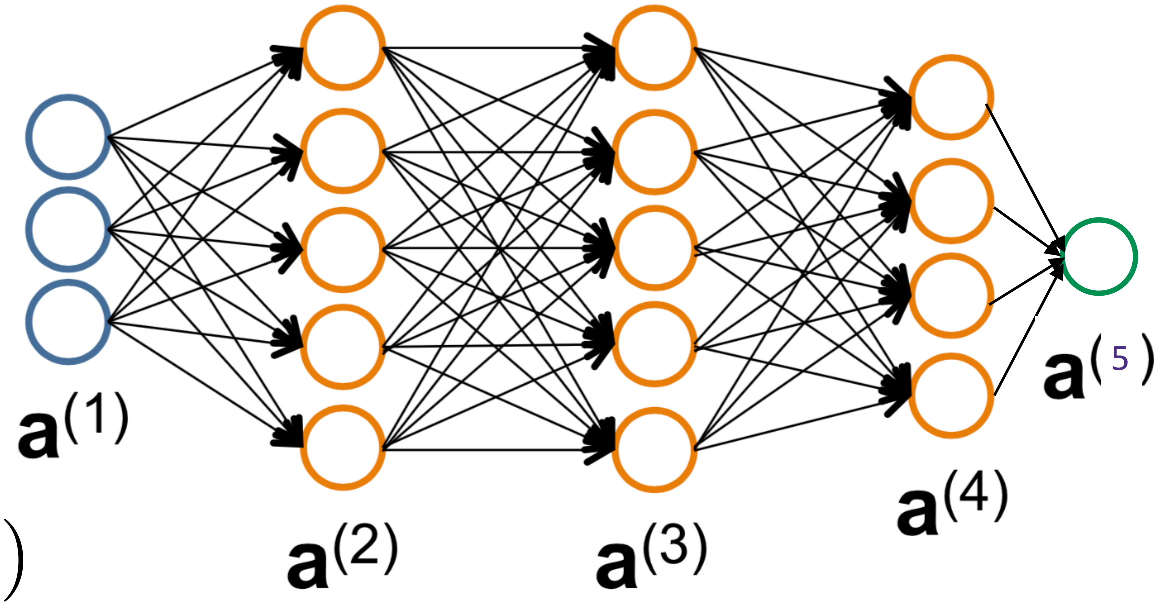
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

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



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

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

Binary Logistic Regression

Multi-layer Neural Network - Binary Classification

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

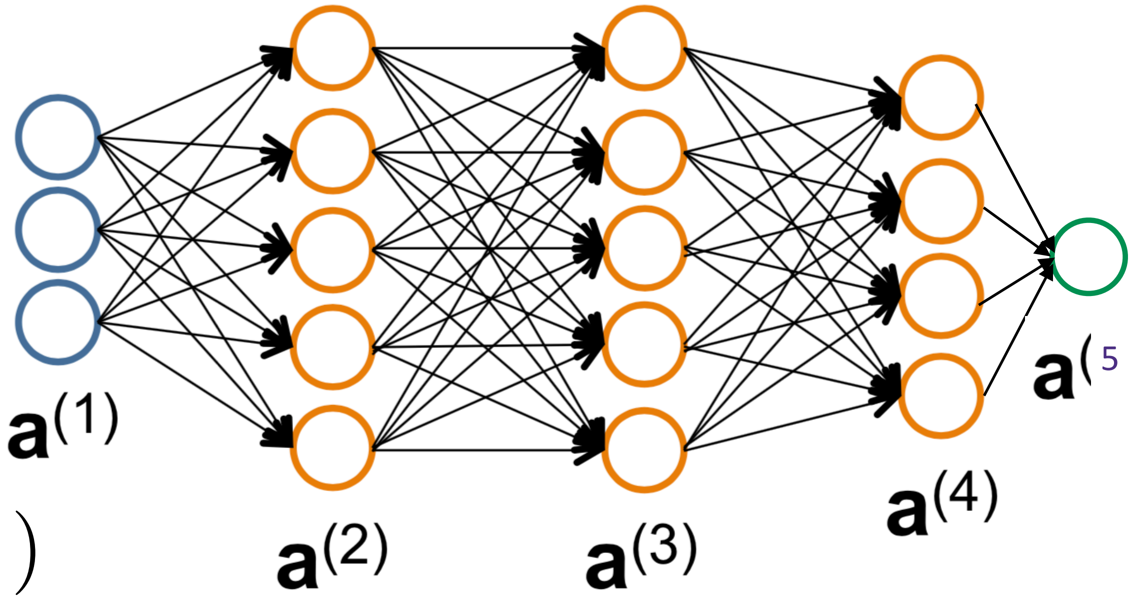
$$a^{(2)} = \sigma(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

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



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

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

Binary Logistic Regression

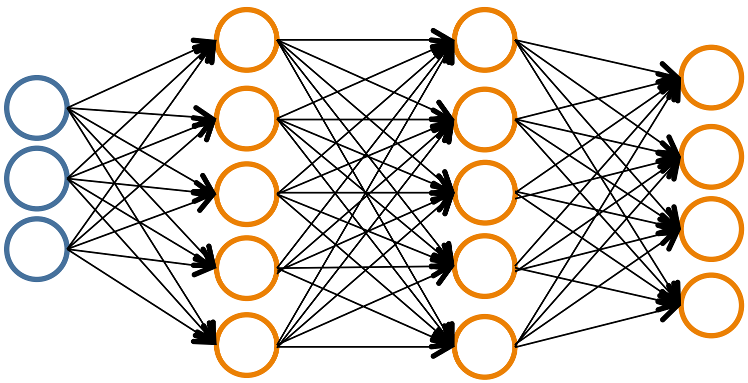
Multiple Output Units: One-vs-Rest

Pedestrian

Car

Motorcycle

Truck



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

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

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

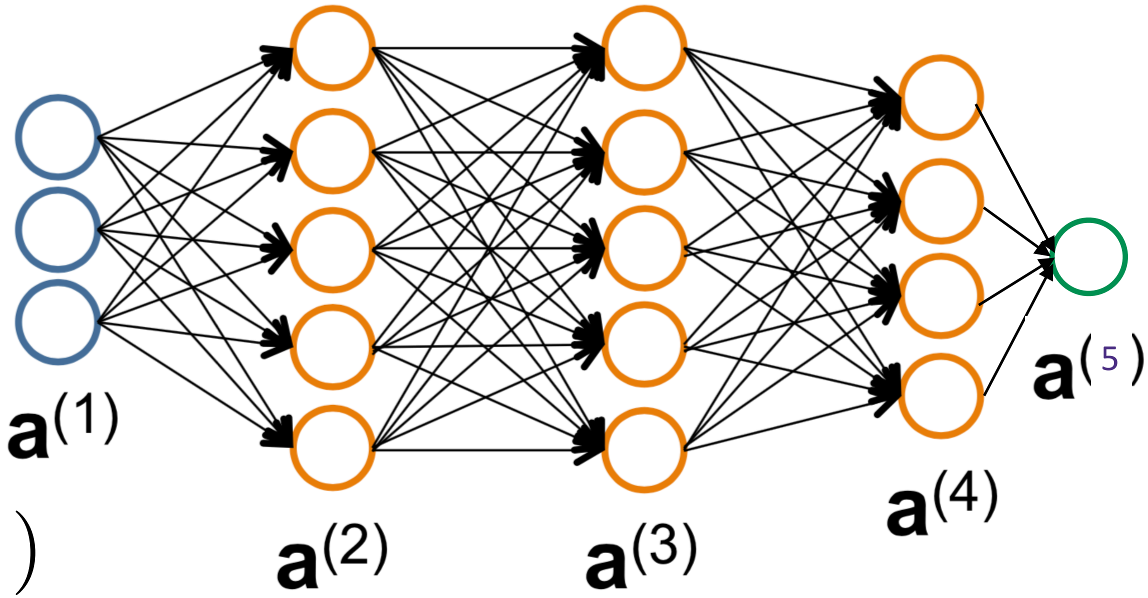
$$a^{(2)} = \sigma(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

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



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

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

Regression

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, $\left|F(\boldsymbol{x}) - \hat{F}(\boldsymbol{x})\right| < \epsilon$.*

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

Training Neural Networks

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

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

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

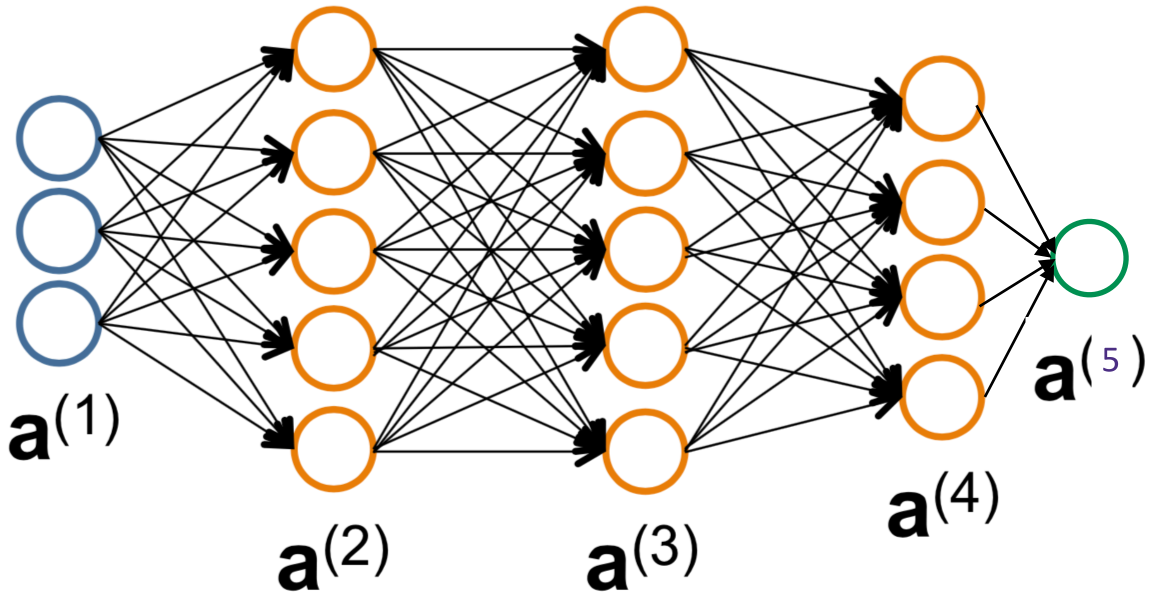
$$\vdots$$

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

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

$$\vdots$$

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



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

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

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, why are packages like PyTorch, Tensorflow, Theano, Cafe, MxNet synonymous with deep learning?

1. Automatic differentiation

2. Convenient libraries

3. GPU support

Gradient Descent:

Seems simple enough,
Theano, Cafe, MxNet s

1. Automatic differ

2. Convenient libra

```python
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
```

```python
# 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**, **batchsize**, **momentum** all 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!*

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 exotic 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

Intuition

https://playground.tensorflow.org/