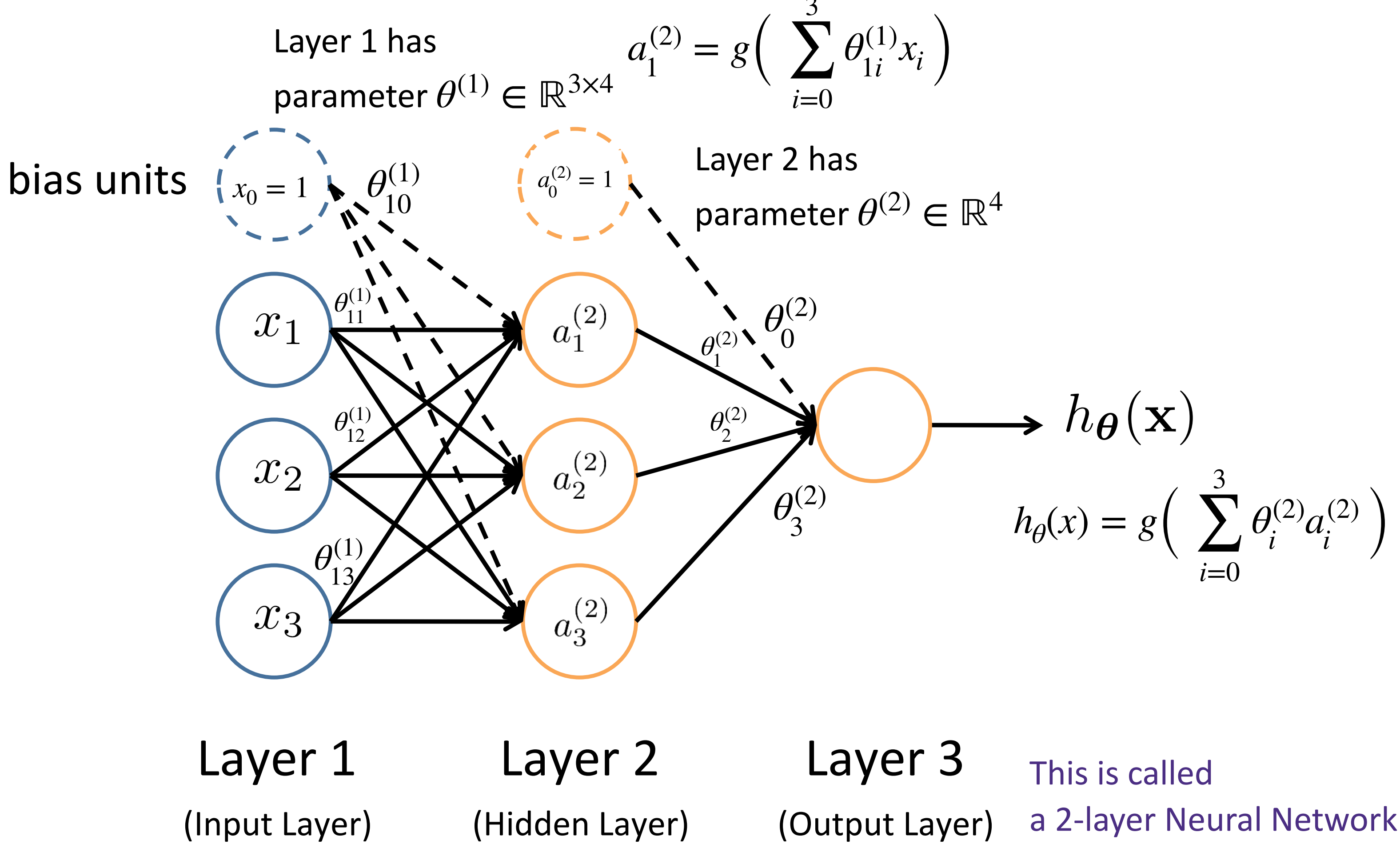
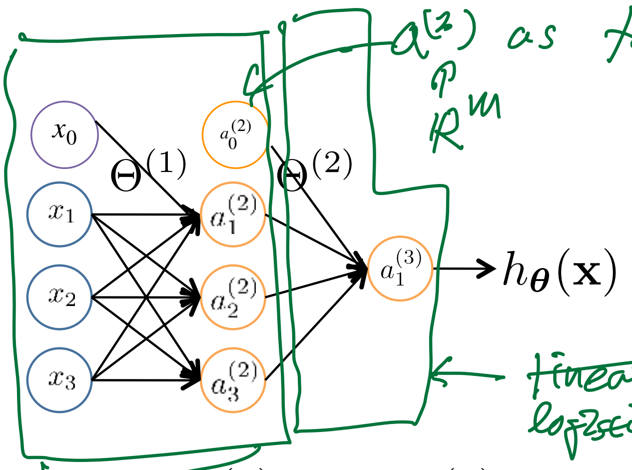
Lecture 19: Neural Networks (continued)

https://playground.tensorflow.org/

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

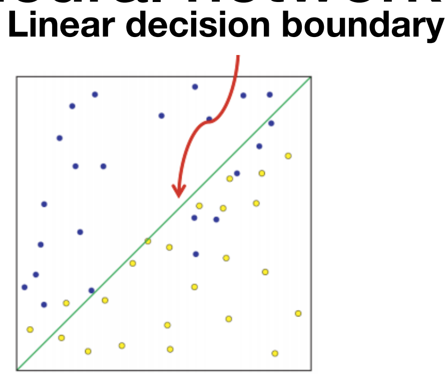
$\Theta^{(j)}$ = weight matrix stores parameters from layer j to layer $j + 1$

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

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

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

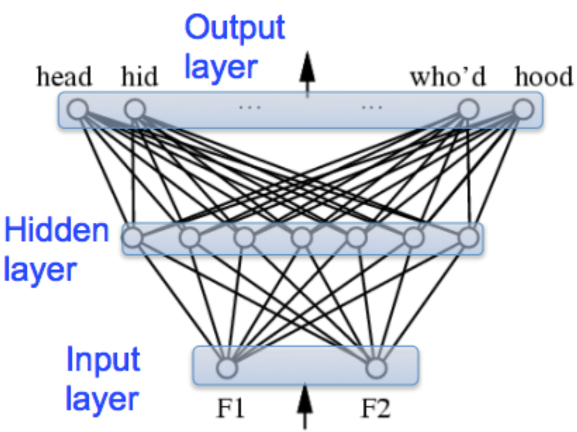
Example of 2-layer neural network in action

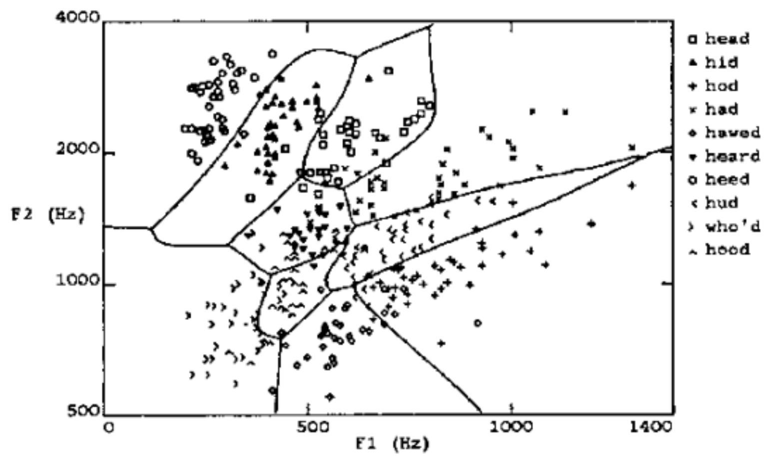


1-layer neural networks
only represents linear classifiers

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 $\{0,1\}$

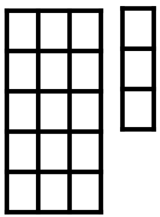
L-th layer plays the role of features, but trained instead of pre-determined

$\Theta = (\theta^{(1)}, \theta^{(2)}, \theta^{(3)}, \theta^{(4)})$

This is a 5-dimensional vector

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

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



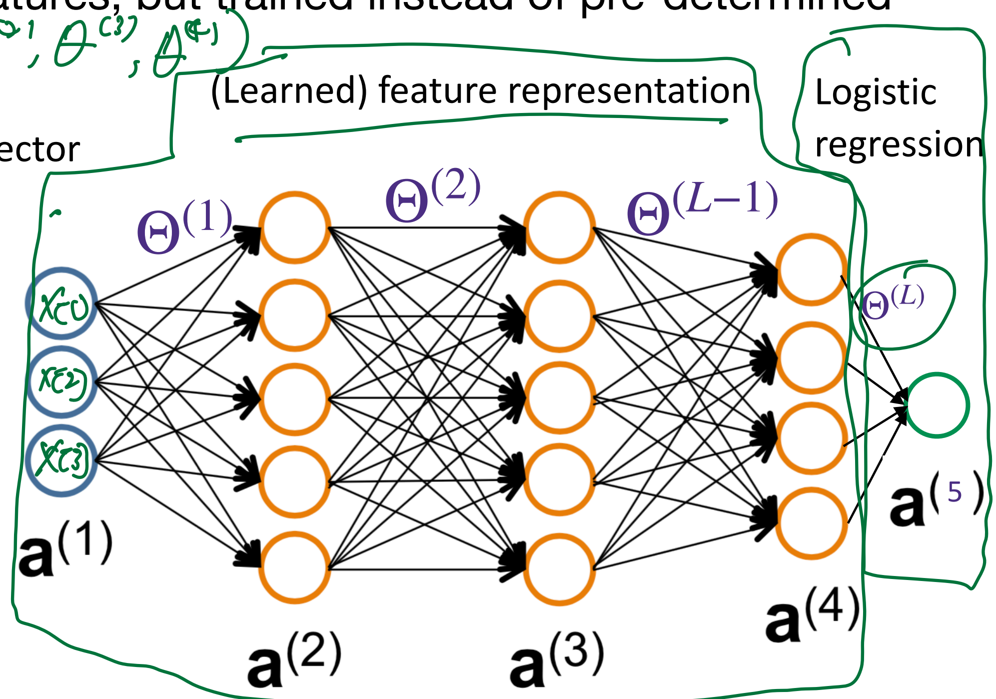
Scalar function g is applied coordinate-wise

⋮

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

⋮

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



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

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

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

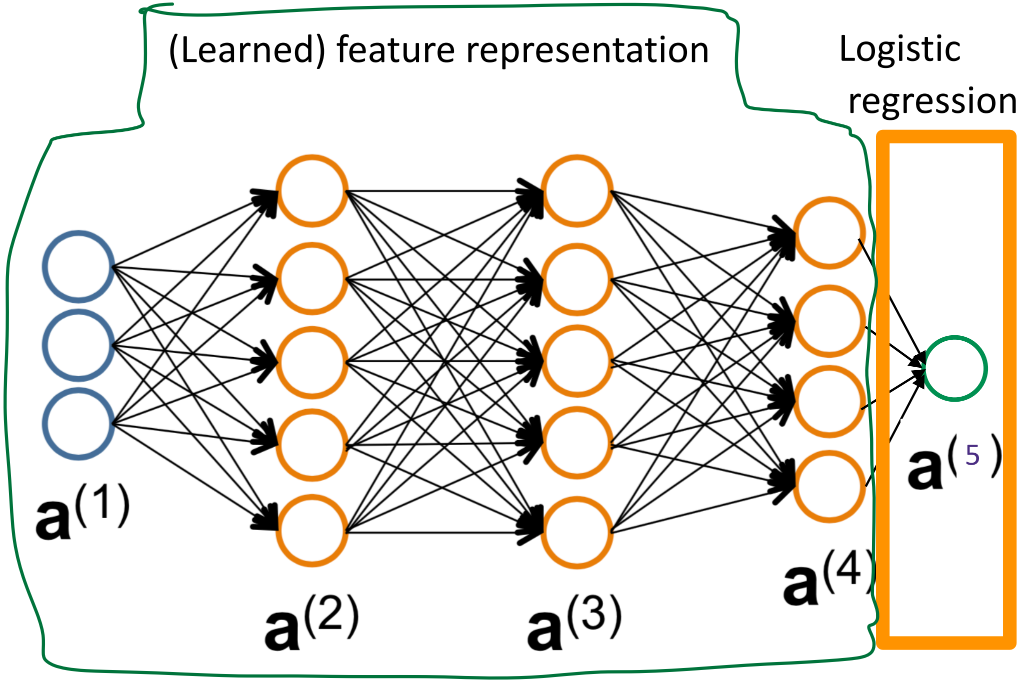
ReLU ~~Sigmoid~~

⋮

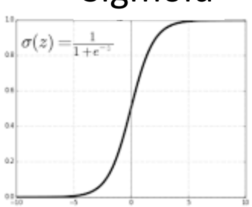
$$a^{(l+1)} = \sigma(\Theta^{(l)} a^{(l)})$$

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

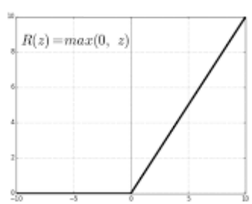
Sigmoid ~~ReLU~~



Sigmoid



ReLU



- Why is ReLU better than sigmoid?

Cross entropy loss:

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

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

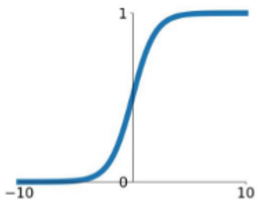
Binary Logistic Regression

Nonlinear activation function

- popular choices of activation function includes

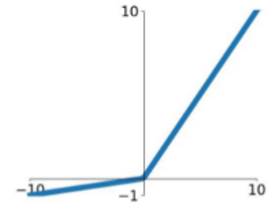
Sigmoid

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



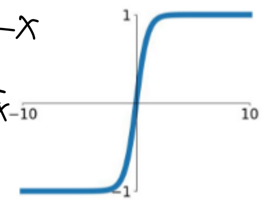
Leaky ReLU

$\max(0.1x, x)$



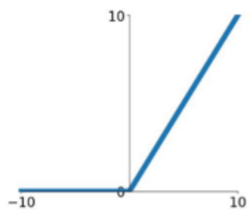
tanh

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



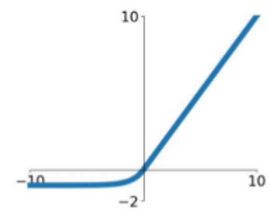
ReLU

$\max(0, x)$



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?

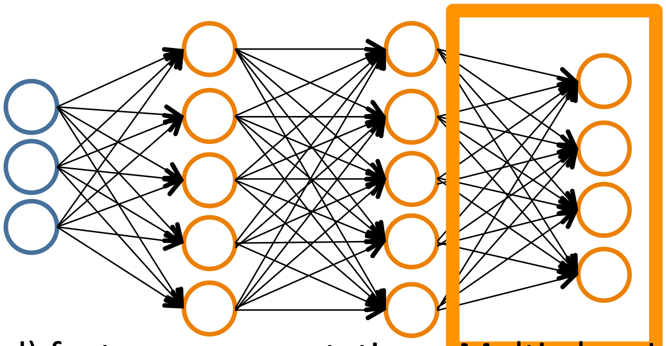
K-class Classification: multiple output units


Pedestrian


Car


Motorcycle


Truck



(Learned) feature representation   Multi-class Logistic regression

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

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

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

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

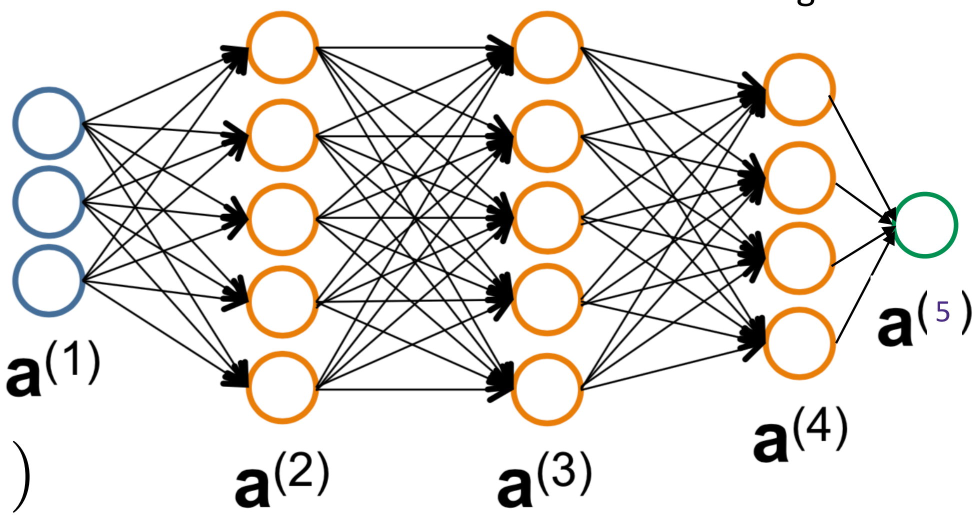
$$\vdots$$

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

$$\vdots$$

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

Linear model



Square loss:

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

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

Questions?

Training Neural Networks

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

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

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

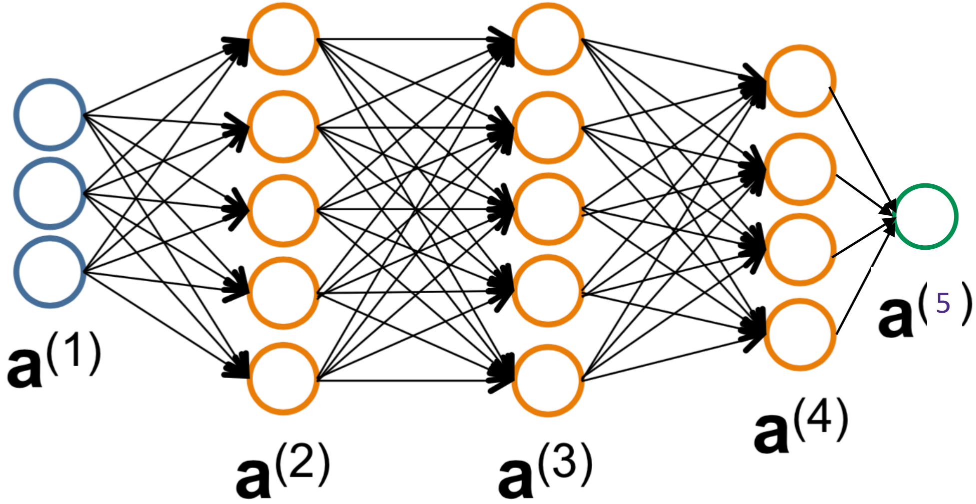
$$\vdots$$

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

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

$$\vdots$$

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



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

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

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

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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

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

Questions?

Back Propagation

Forward Propagation

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

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

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

$$\vdots$$

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

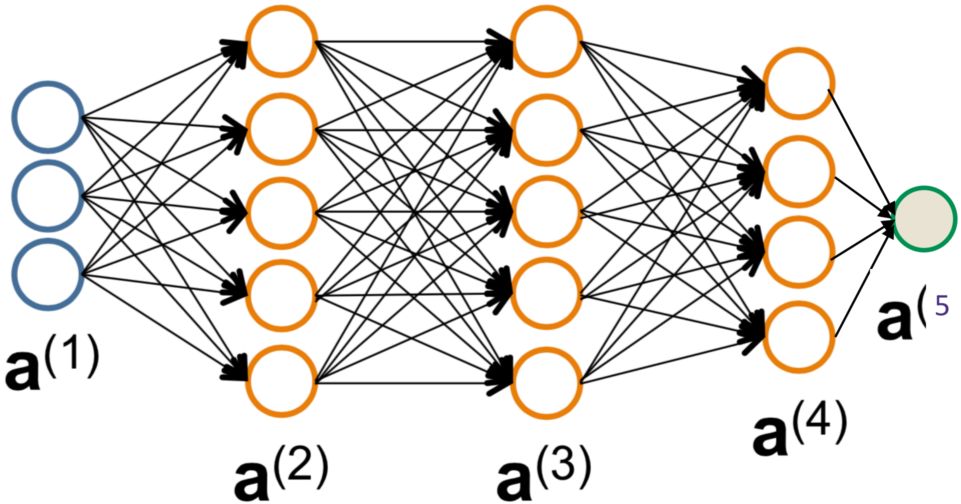
$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

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

$$\vdots$$

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

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



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

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

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

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

Train by Stochastic Gradient Descent:

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

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

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

Backprop

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

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

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

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

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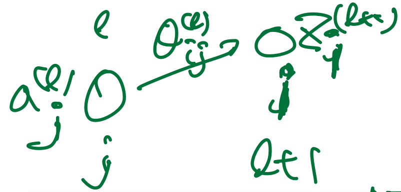
$$\hat{y} = a^{(L+1)}$$



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

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

*chain rule

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

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

$$z^{(\ell+1)} = \Theta^{(\ell)} \cdot g(z^{(\ell)})$$

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

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

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

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

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

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

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 + ℓ_2 regularizer

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

Questions?