- Homework 3, due Friday, February 25,

Lecture 18:
Kernels (continued)

Recap: Kernel trick finds the optimal solution for linear models under a feature map $\phi(\cdot)$

- Once we have chosen a feature map $\phi(\cdot) \in \mathbb{R}^p$, what we want to solve is

$$\widehat{w} = \arg\min_{w \in \mathbb{R}^p} \sum_{i=1}^{n} \ell\left(y_i, w^T \phi(x_i)\right) \text{ for some convex loss } \ell(,)$$

- Kernel trick finds the optimal solution efficiently, by searching over the model that can be represented as $\widehat{w} = \sum_{i=1}^{n} \alpha_i \phi(x_i)$, which is equivalent to $\widehat{y}_{\text{new}} = \sum_{i=1}^{n} \alpha_i K(x_i, x_{\text{new}})$
- Gradient descent update (from initialization $w^{(0)} = 0$) that find the optimal solution is

$$w^{(t+1)} \leftarrow w^{(t)} - \eta \sum_{i=1}^{n} \underbrace{\ell'(y_i, w^T \phi(x_i))}_{\text{scalar}} \phi(x_i)$$

- One crucial observation is that all $w^{(t)}$'s (including the optimal solution $w^{(\infty)}$) lie on the subspace spanned by $\{\phi(x_1), \ldots, \phi(x_n)\}$, which is an n-dimensional subspace in $\mathbb{R}^p$
- Hence, it is sufficient to look for a solution that is represented as

$$\widehat{w} = \sum_{i=1}^{n} \alpha_i \phi(x_i) \text{ to find the optimal solution}$$

Fixed Feature V.S. Learned Feature

- Kernel method works well if we choose a good kernel such that the data is linearly separable in the corresponding (possibly infinite dimensional) feature space

- In practice, it is hard to choose a good kernel for a given problem

- Can we **learn** the feature mapping $\phi : \mathbb{R}^d \to \mathbb{R}^p$ from data also?

Bootstrap

- How to measure uncertainty in our predictions

Confidence interval

- suppose you have training data $\{(x_i, y_i)\}_{i=1}^n$ drawn i.i.d. from some true distribution $P_{x,y}$
- we train a kernel ridge regressor, with some choice of a kernel $K : \mathbb{R}^{d \times d} \to \mathbb{R}$

$$\text{minmize}_\alpha \; \|\mathbf{K}\alpha - \mathbf{y}\|_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

- the resulting predictor is

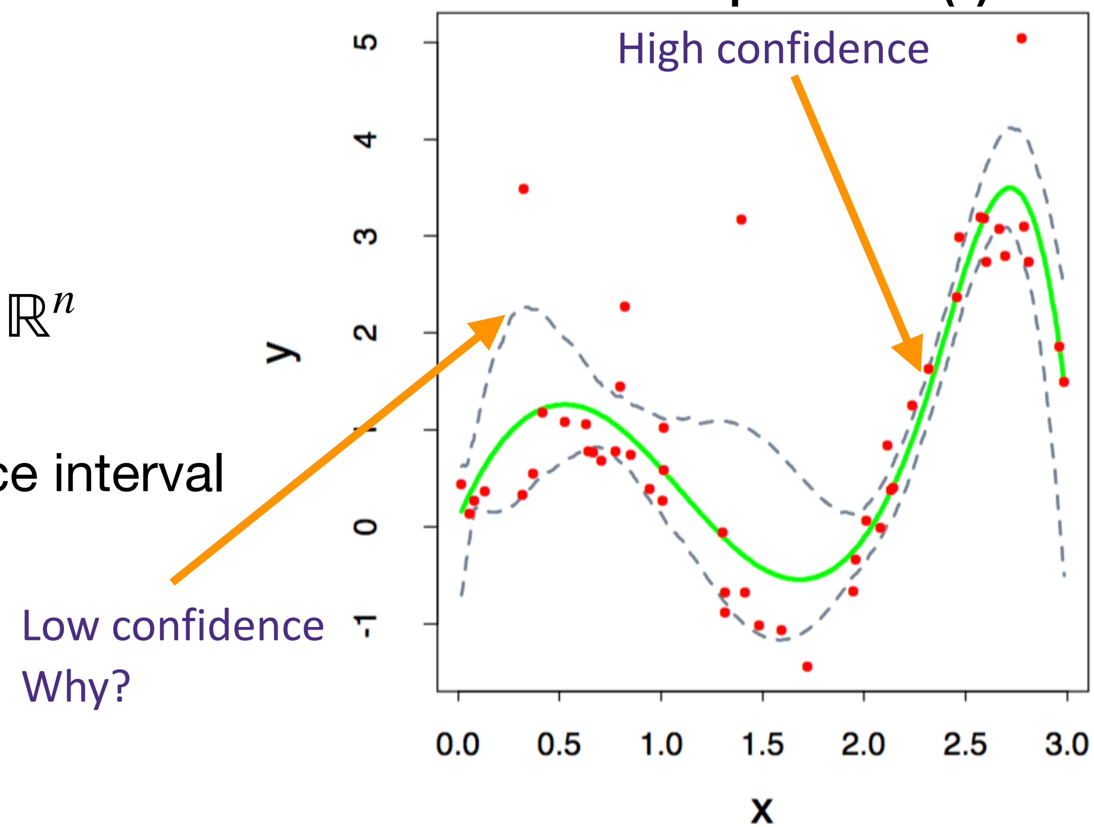
$$f(x) \;=\; \sum_{i=1}^{n} K(x_i, x)\hat{\alpha}_i,$$

where

$$\hat{\alpha} \;=\; (\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{y} \quad \in \mathbb{R}^n$$

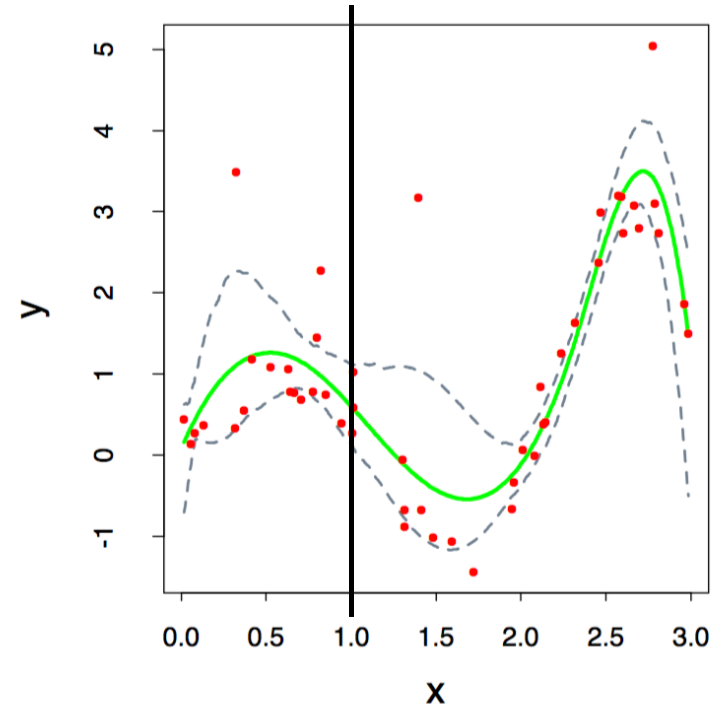
- we wish to build a confidence interval for our predictor $f(x)$, using 5% and 95% percentiles

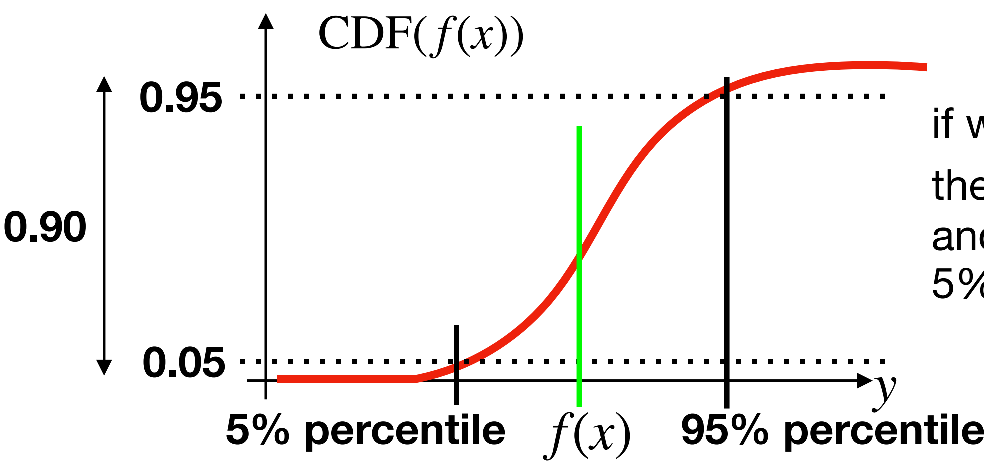
Example of 5% and 95% percentile curves for predictor f(x)



Confidence interval

- let's focus on a single $x \in \mathbb{R}^d$
- note that our predictor $f(x)$ is a random variable, whose randomness comes from the training data $S_{\text{train}} = \{(x_i, y_i)\}_{i=1}^n$
- if we know the statistics (in particular the CDF of the random variable $f(x)$) of the predictor, then the **confidence interval** with **confidence level 90%** is defined as





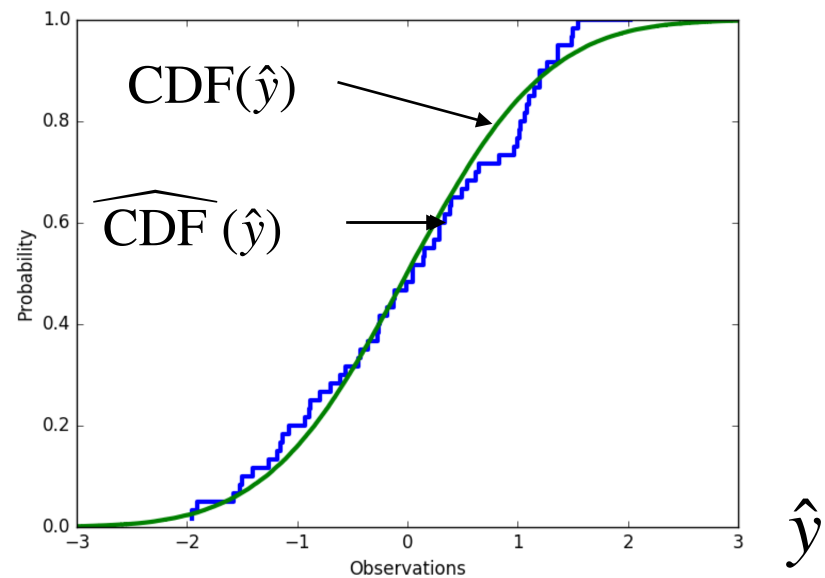
if we know the distribution of our predictor $f(x)$, the green line is the expectation $\mathbb{E}[f(x)]$ and the black dashed lines are the 5% and 95% percentiles in the figure above

- as we do not have the cumulative distribution function (CDF), we need to approximate them

Confidence interval

- hypothetically, if we can sample as many times as we want, then we can train $B \in \mathbb{Z}^+$ i.i.d. predictors, each trained on n fresh samples to get **empirical estimate of the CDF of** $\hat{y} = f(x)$

- for b=1,…,B
  - draw n fresh samples $\{(x_i^{(b)}, y_i^{(b)})\}_{i=1}^n$
  - train a regularized kernel regression $\alpha^{*(b)}$
  - Predict $\hat{y}^{(b)} = \sum_{i=1}^{n} K(x_i^{(b)}, x)\alpha_i^{*(b)}$



- let the empirical CDF of those B predictors $\{\hat{y}^{(b)}\}_{b=1}^B$ be $\widehat{\text{CDF}}(\hat{y})$, defined as

$$\widehat{\text{CDF}}(\hat{y}) = \frac{1}{B}\sum_{b=1}^{B} \mathbf{I}\{\, \hat{y}^{(b)} \le \hat{y} \,\} = \frac{1}{B}\sum_{b=1}^{B} \mathbf{I}\{\, (\alpha^{*(b)})^T h(x) \le \hat{y} \,\}$$

- compute the confidence interval using $\widehat{\text{CDF}}(\hat{y})$
- What is wrong?

Bootstrap

- as we cannot sample repeatedly (in typical cases), we use **bootstrap samples** instead
- bootstrap is a general tool for assessing statistical accuracy
- we learn it in the context of confidence interval for trained models

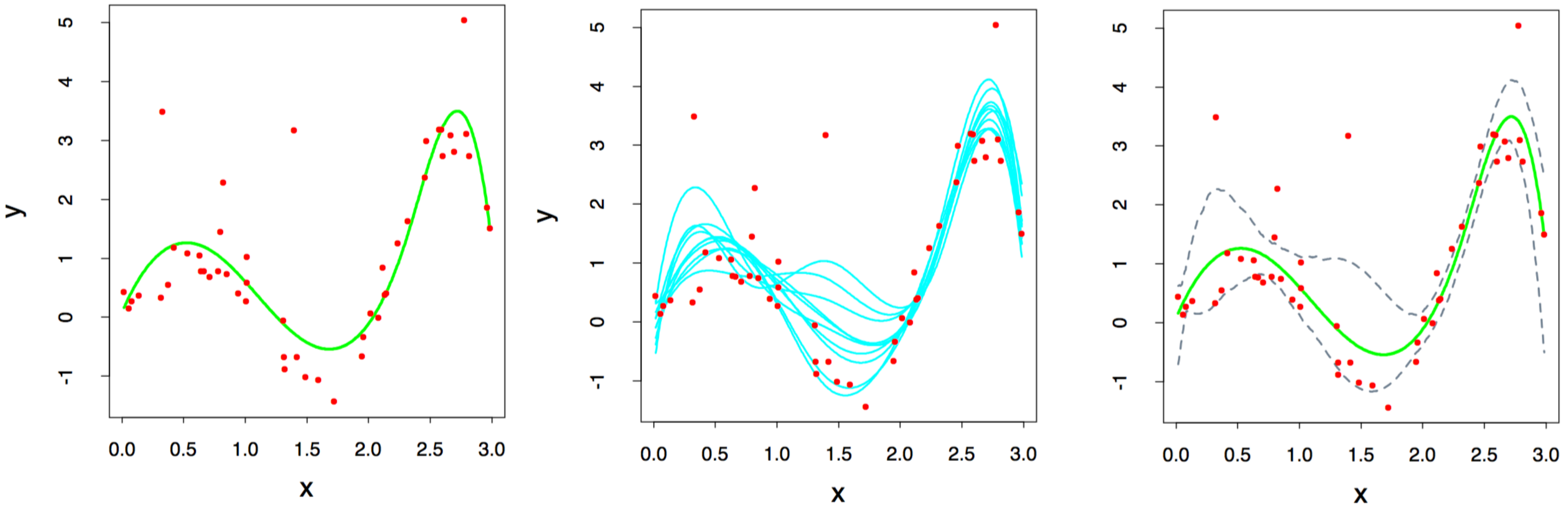
- a **bootstrap dataset** is created from the training dataset by taking n (the same size as the training data) examples uniformly at random **with replacement** from the training data $\{(x_i, y_i)\}_{i=1}^n$

- for b=1,…,B
  - create a bootstrap dataset $S^{(b)}_{\text{bootstrap}}$
  - train a regularized kernel regression $\alpha^{*(b)}$
  - predict $\hat{y}^{(b)} = \sum_{i=1}^{n} K(x_i^{(b)}, x)\alpha_i^{*(b)}$

- compute the empirical CDF from the bootstrap datasets, and compute the confidence interval

bootstrap

training a single predictor | **multiple bootstrapped predictors** | **90% confidence interval**



Figures from Hastie et al

Questions?

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 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:

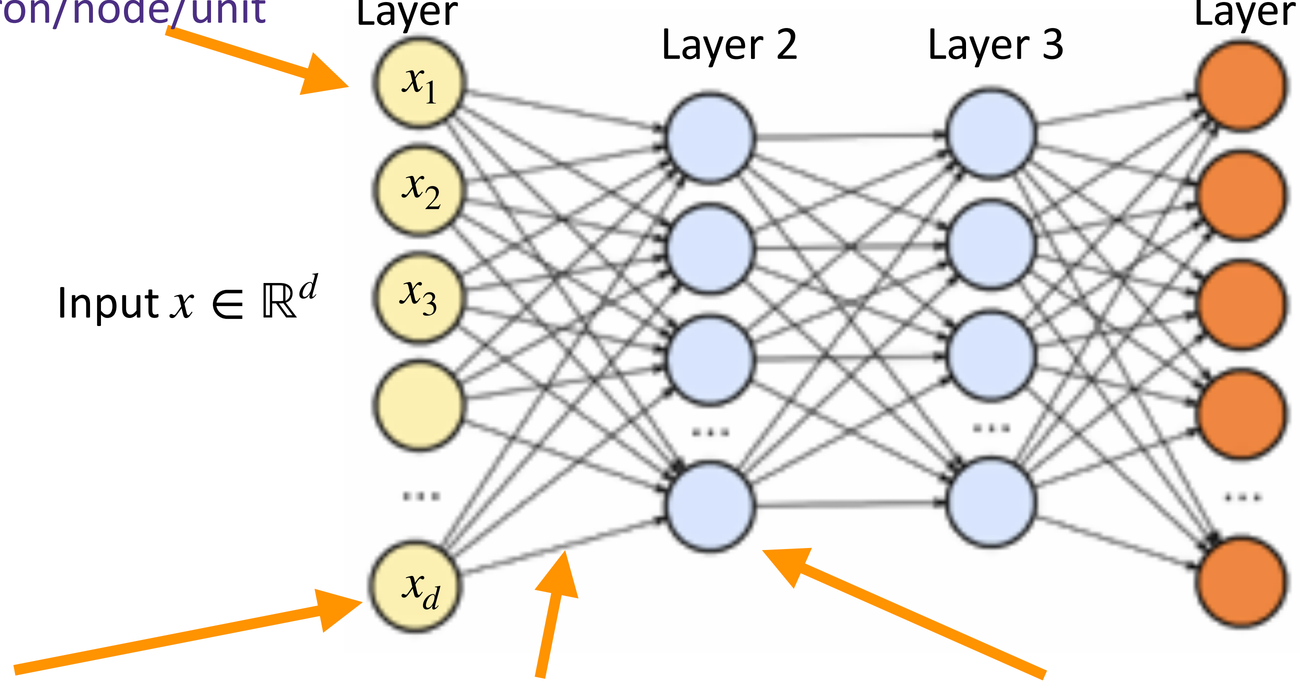
1. Definitions of neural networks

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



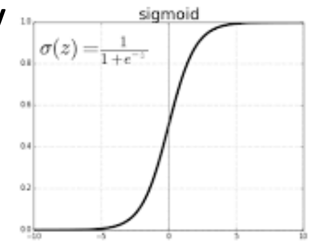
d nodes
each representing
a scalar value of
each coordinate of x

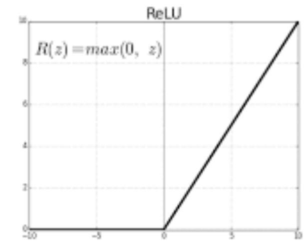
Link: maps output of
a neuron to input of
a neuron of the next layer,
each link has a scalar weight

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

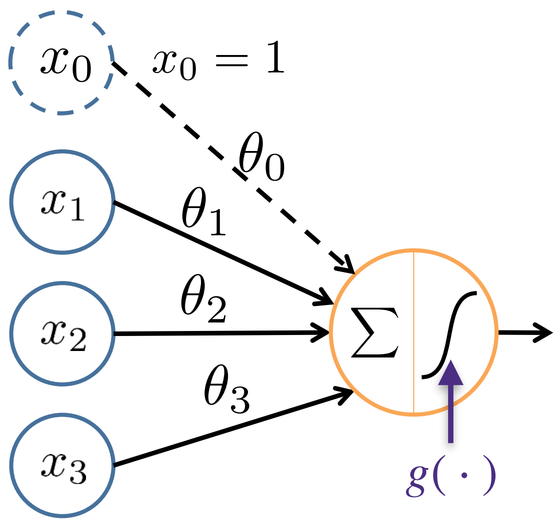
- For a single node with input $x \in \mathbb{R}^d$, the node is defined by
  - **Parameter** $\theta \in \mathbb{R}^{d+1}$ (including the intercept/bias)
  - **Activation function** $g : \mathbb{R} \rightarrow \mathbb{R}$
    - A common choice is sigmoid function: $g(z) = \dfrac{1}{1 + e^{-z}}$
   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





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

"bias unit"

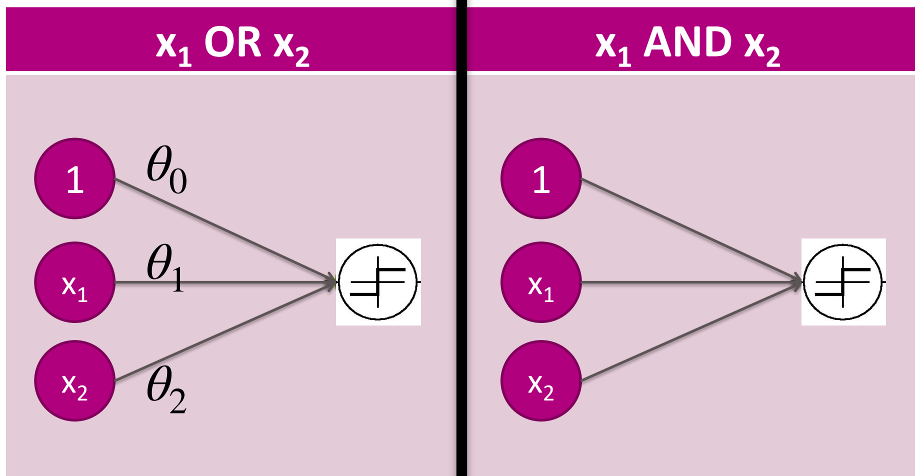


$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

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

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

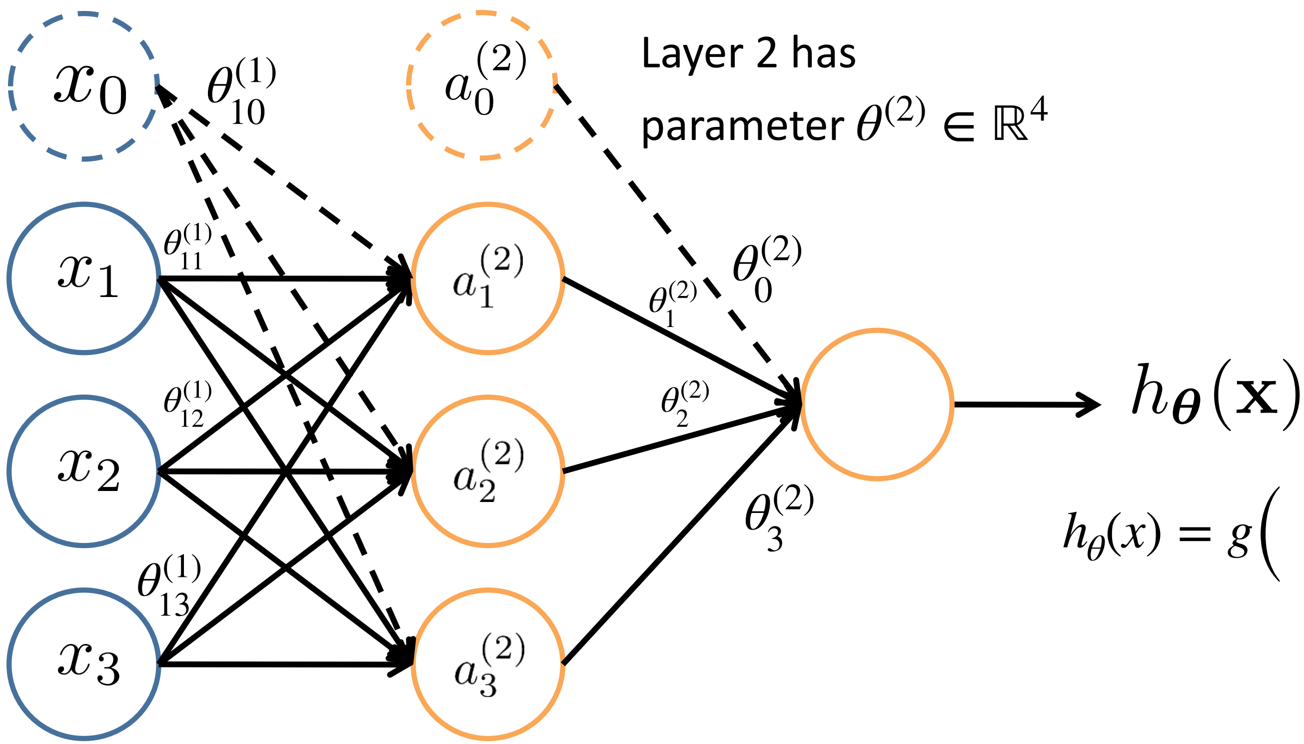
- Each layer performs simple operations
- Neural Network (with parameter $\theta = (\theta^{(1)}, \theta^{(2)})$) composes multiple layers of operations

Layer 1 has parameter $\theta^{(1)} \in \mathbb{R}^{3\times4}$

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

bias units

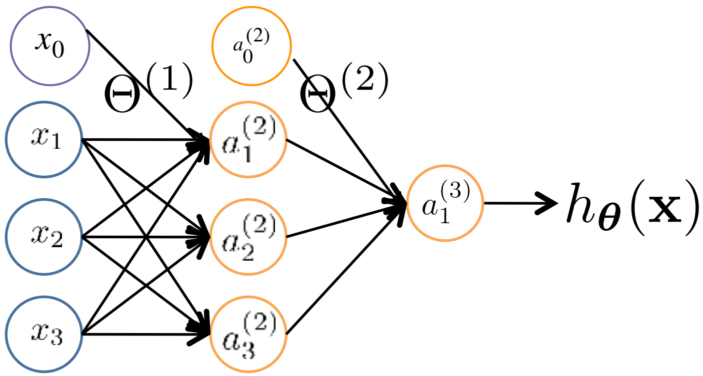
Layer 2 has parameter $\theta^{(2)} \in \mathbb{R}^{4}$



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

Layer 1 (Input Layer) | Layer 2 (Hidden Layer) | Layer 3 (Output Layer)

This is called a 2-layer Neural Network



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

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

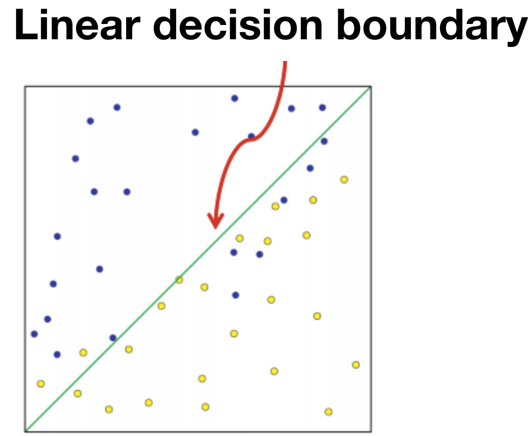
$$a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)}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

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

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

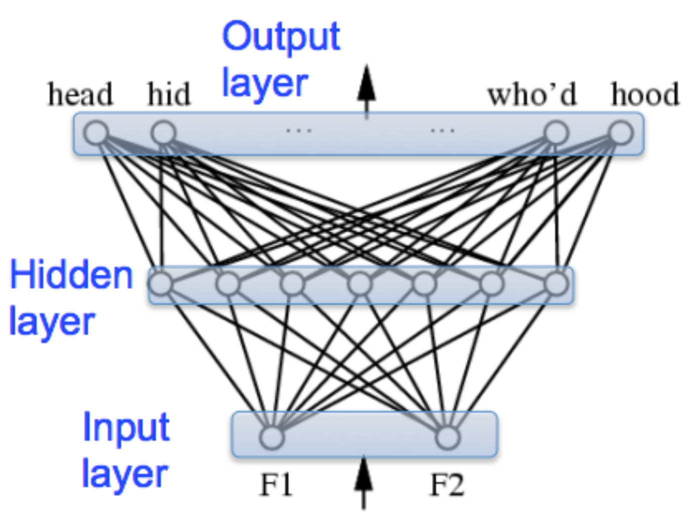
Example of 2-layer neural network in action

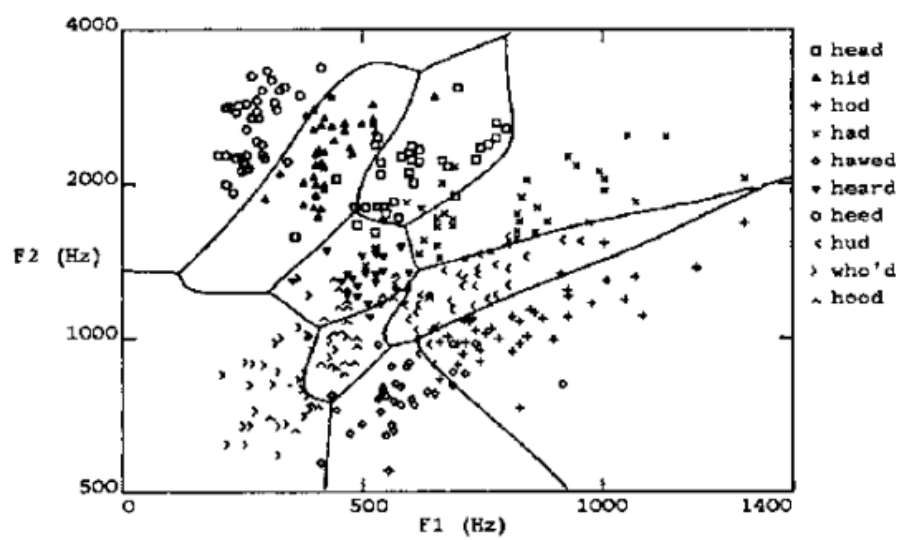
1-layer neural networks
only represents linear classifiers



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

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

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

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

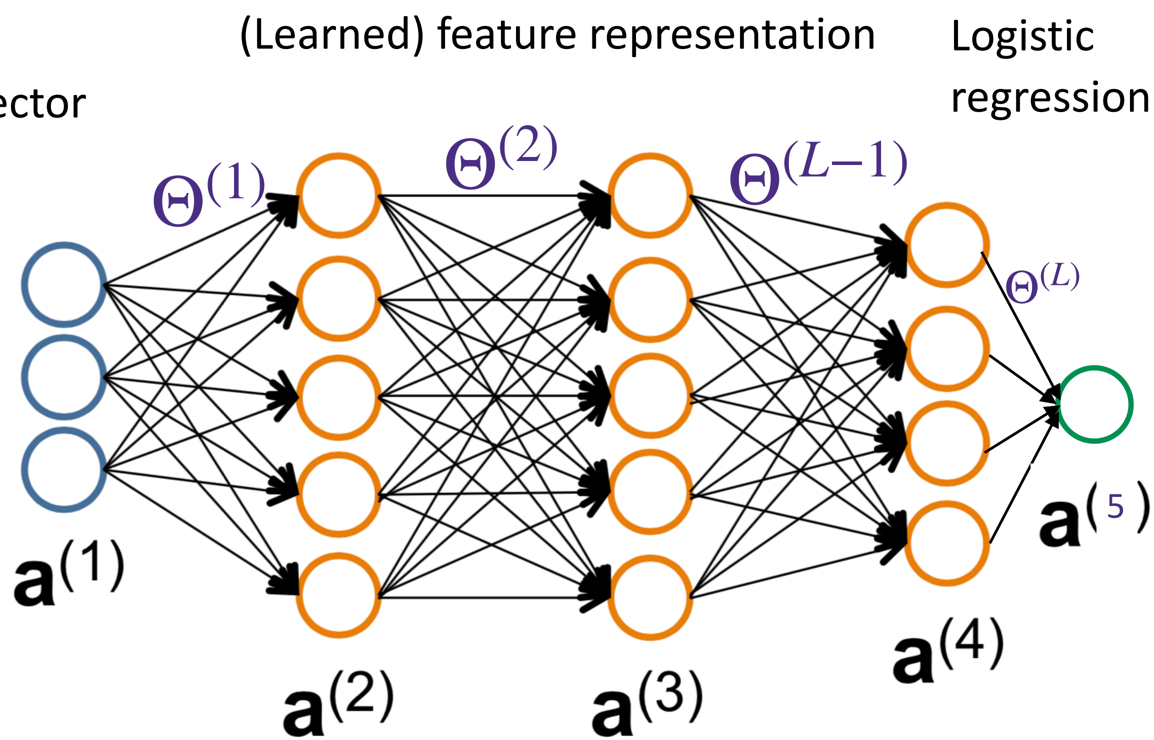
Scalar function g is applied coordinate-wise

⋮

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

⋮

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



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

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

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

Multi-layer Neural Network - Binary Classification

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

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

Sigmoid

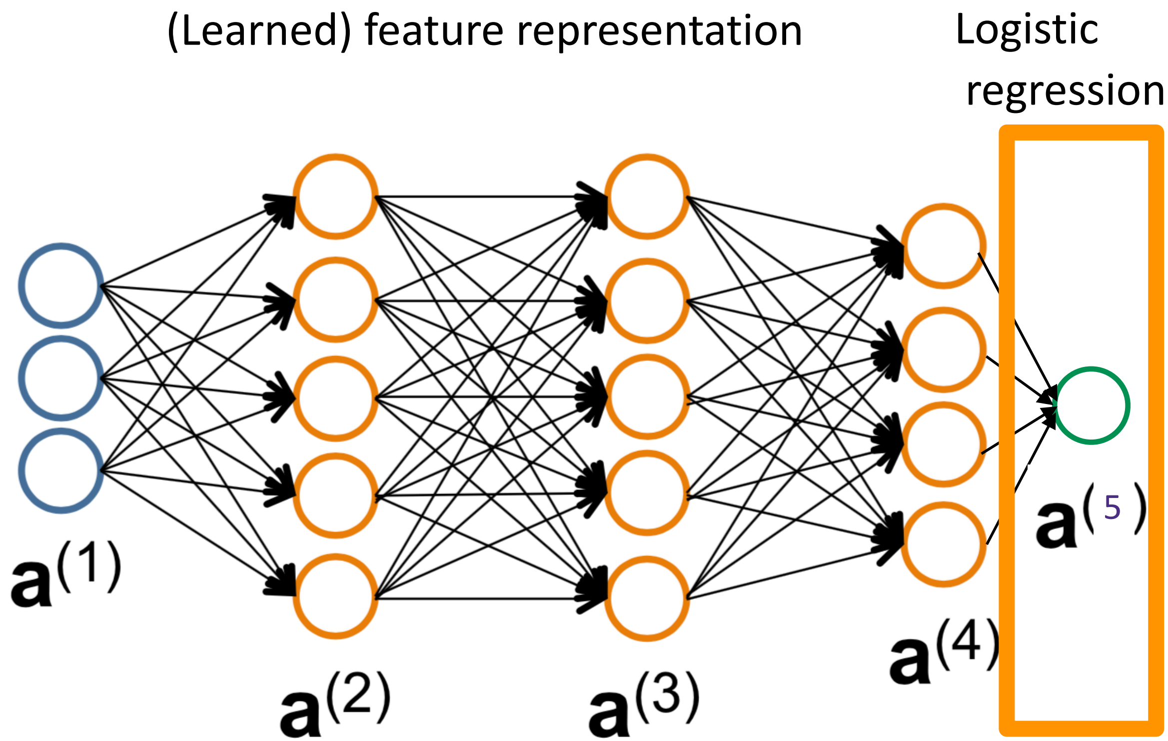
⋮

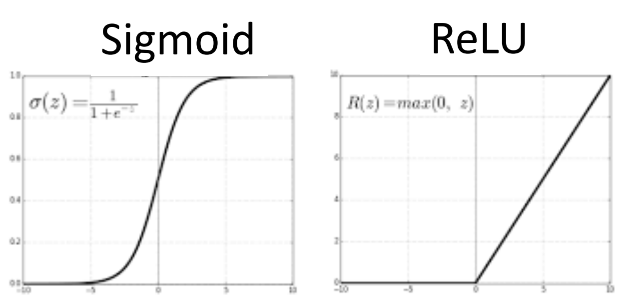
$$a^{(l+1)} = \sigma(\Theta^{(l)} a^{(l)})$$

⋮

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

ReLU





- Why is ReLU better than sigmoid?

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

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

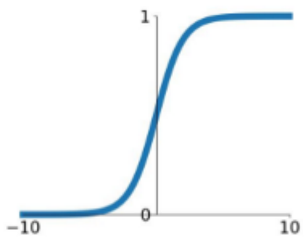
Binary Logistic Regression

Nonlinear activation function

- popular choices of activation function includes

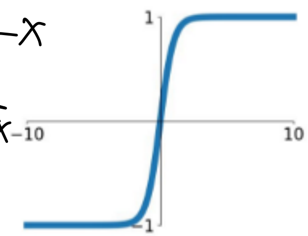
Sigmoid

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



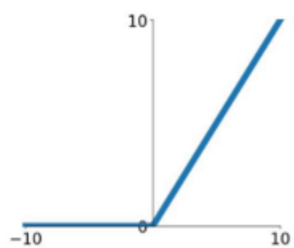
tanh

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



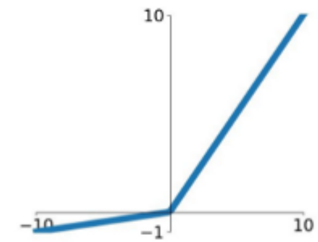
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

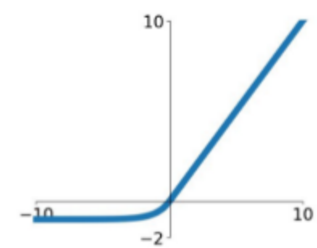


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

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?

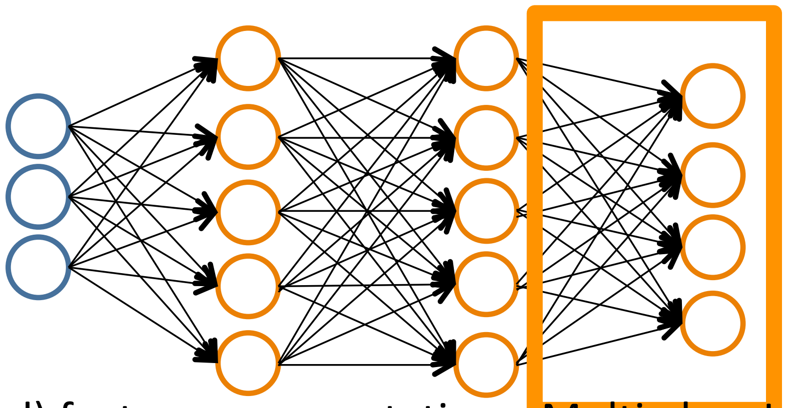
K-class Classification: multiple output units

Pedestrian

Car

Motorcycle

Truck



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

Multi-class Logistic Regression

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

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

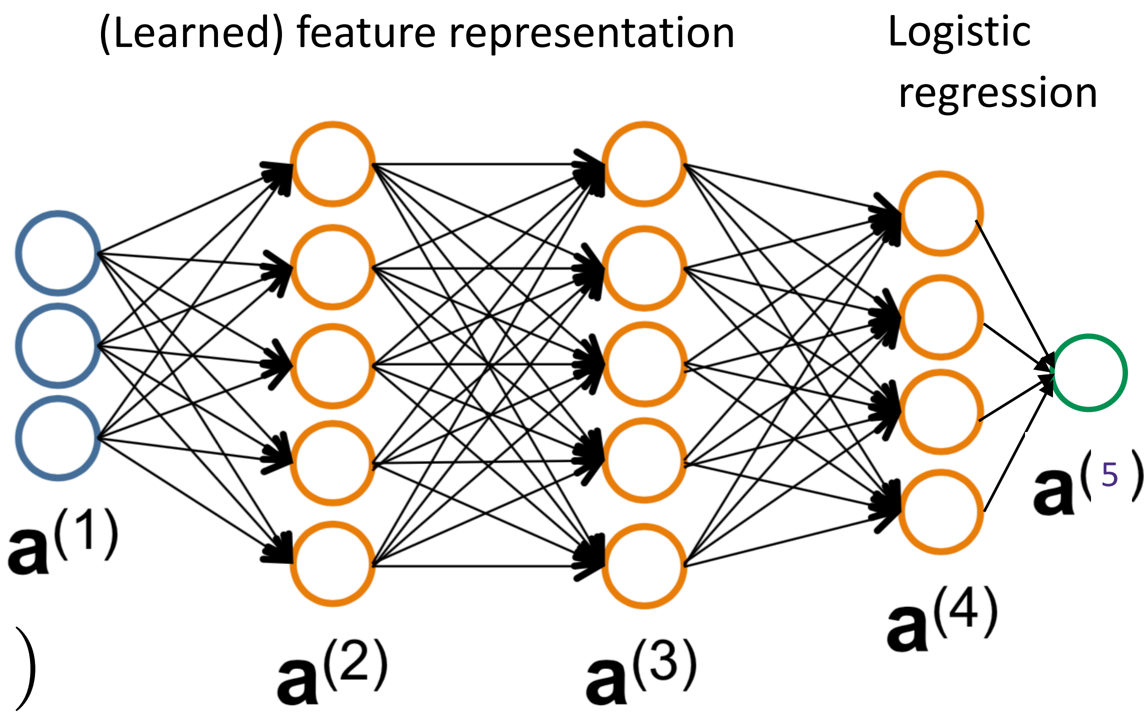
$$a^{(2)} = \sigma(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

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



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

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

Regression

Training Neural Networks

Intuition

https://playground.tensorflow.org/

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

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

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

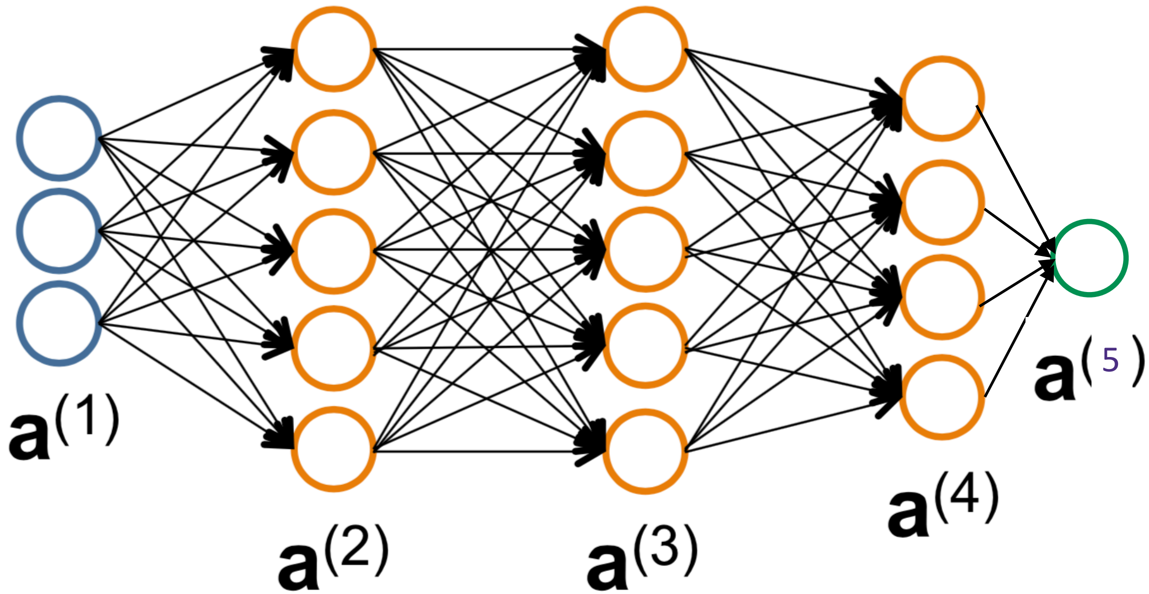
$$\vdots$$

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

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

$$\vdots$$

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



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

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

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

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

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

```
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**, **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

Back Propagation

Forward Propagation

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

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

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

$$\vdots$$

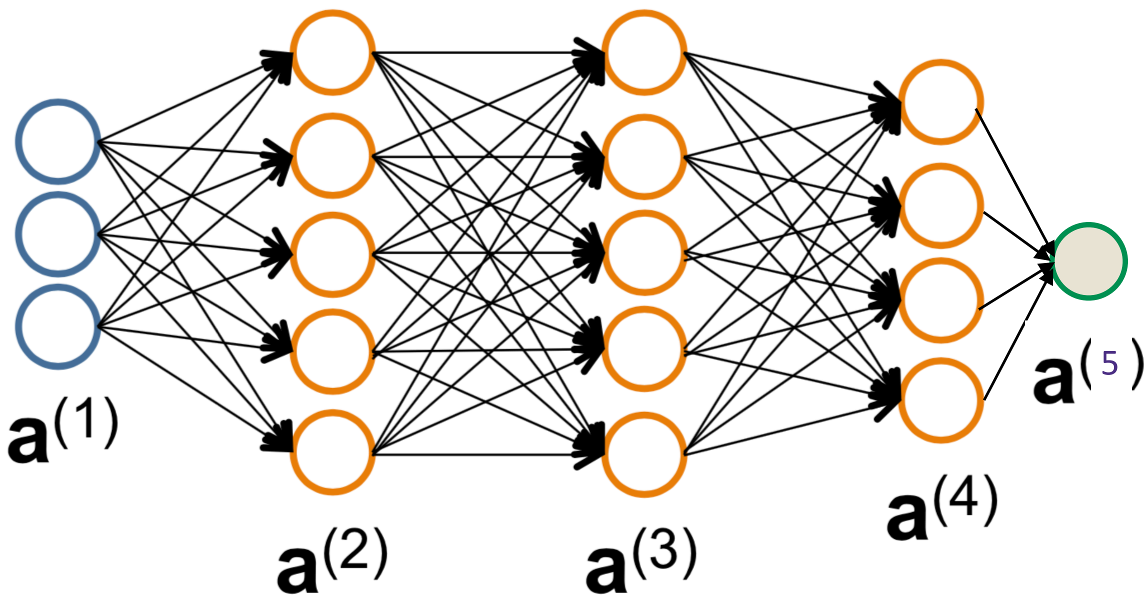
$$a^{(l)} = g(z^{(l)})$$

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

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

$$\vdots$$

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



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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

Train by Stochastic Gradient Descent:

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

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

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

Backprop

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

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

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

⋮

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

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

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

⋮

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

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

Train by Stochastic Gradient Descent:

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

Recursive Algorithm!

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

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

Backpropagation

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

For each training instance $(\mathbf{x}_i, y_i)$:

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

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

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

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

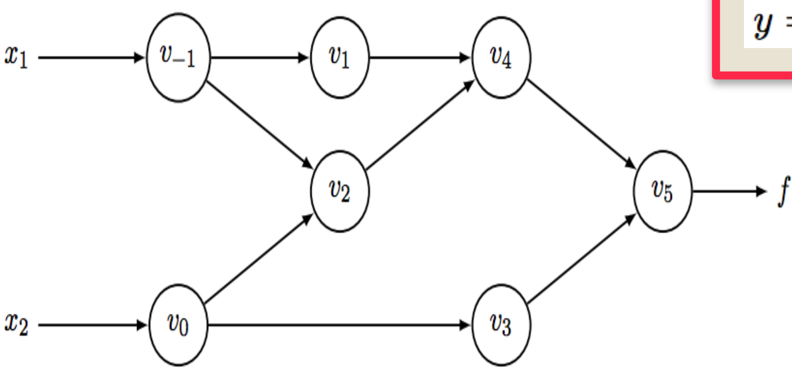
Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

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

Based on slide by Andrew Ng

Autodiff

Backprop for this simple network architecture is a special case of ***reverse-mode auto-differentiation:***



$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$

Forward Primal Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint (Derivative) Trace			
$\bar{x}_1$	$= \bar{v}_{-1}$		$= \mathbf{5.5}$
$\bar{x}_2$	$= \bar{v}_0$		$= \mathbf{1.716}$
$\bar{v}_{-1}$	$= \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$	$= \bar{v}_{-1} + \bar{v}_1 / v_{-1}$	$= 5.5$
$\bar{v}_0$	$= \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1}$	$= \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

This is the special sauce in Tensorflow, PyTorch, Theano, …

Convolutional Neural Network

Multi-layer Neural Network

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

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

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

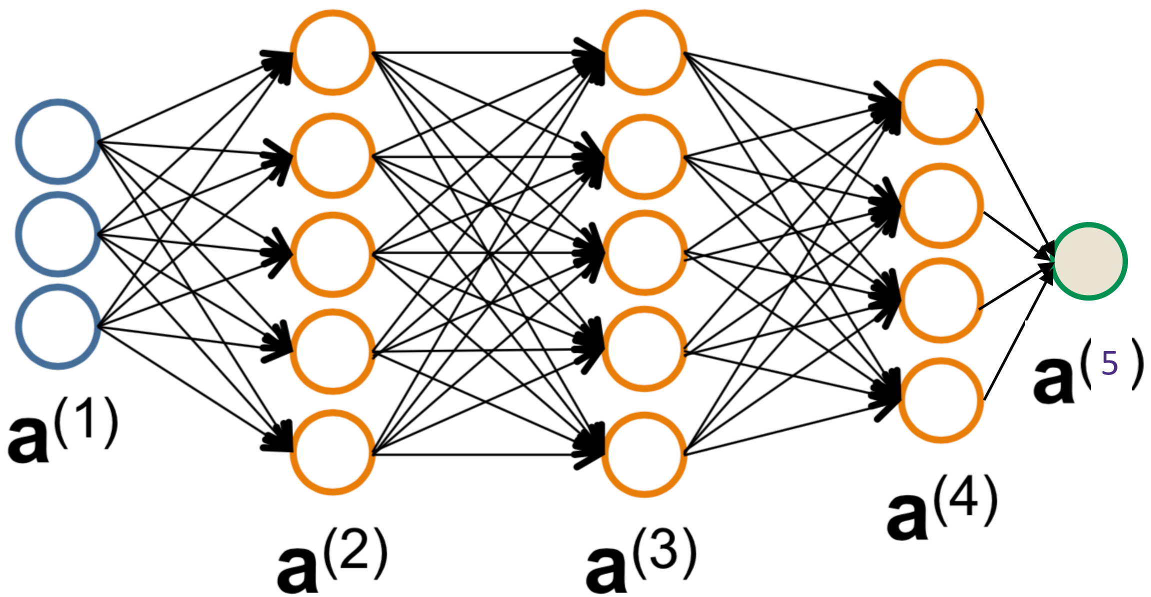
$$\vdots$$

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

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

$$\vdots$$

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



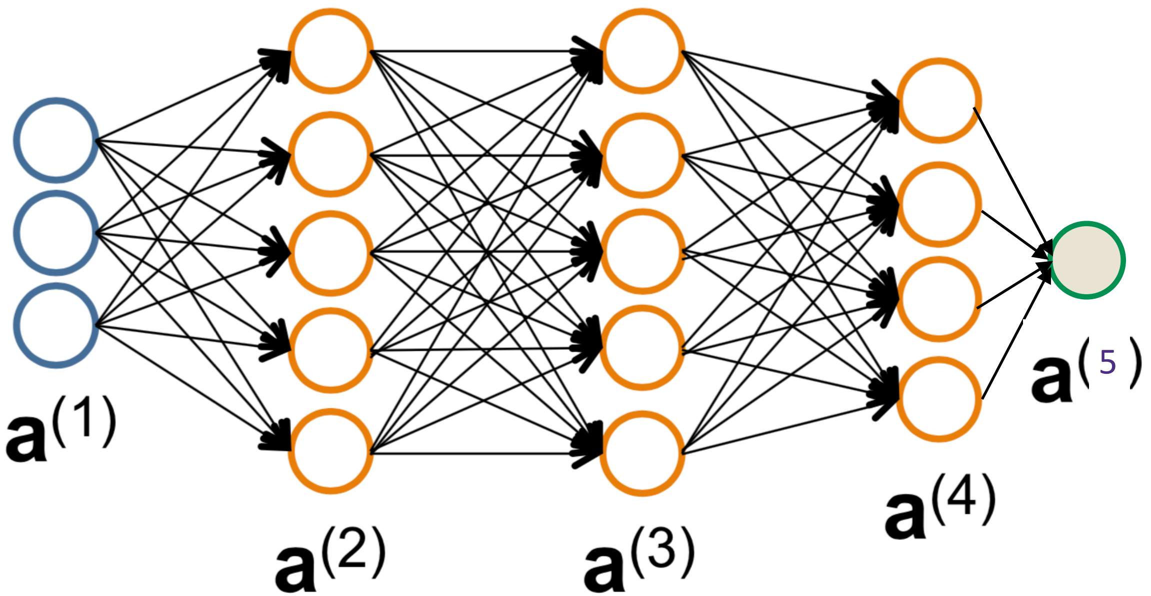
$$L(y, \hat{y}) = y \log(\hat{y}) + (1 - y)\log(1 - \hat{y})$$

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

Binary Logistic Regression

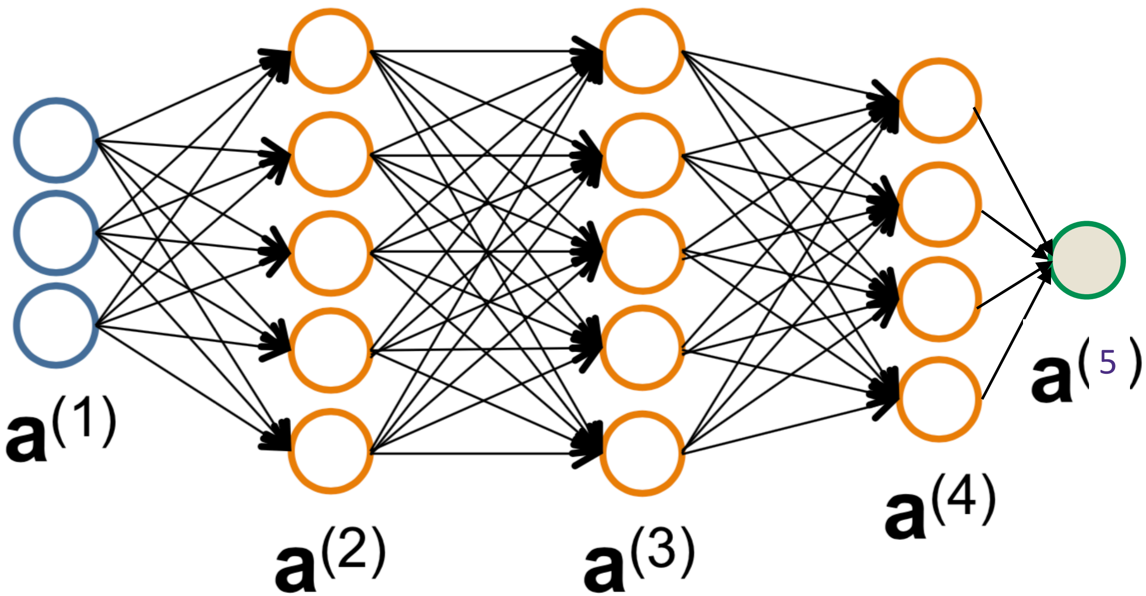
Neural Network Architecture

The neural network architecture is defined by the number of layers, and the number of nodes in each layer, but also by **allowable edges**.



Neural Network Architecture

The neural network architecture is defined by the number of layers, and the number of nodes in each layer, but also by **allowable edges**.



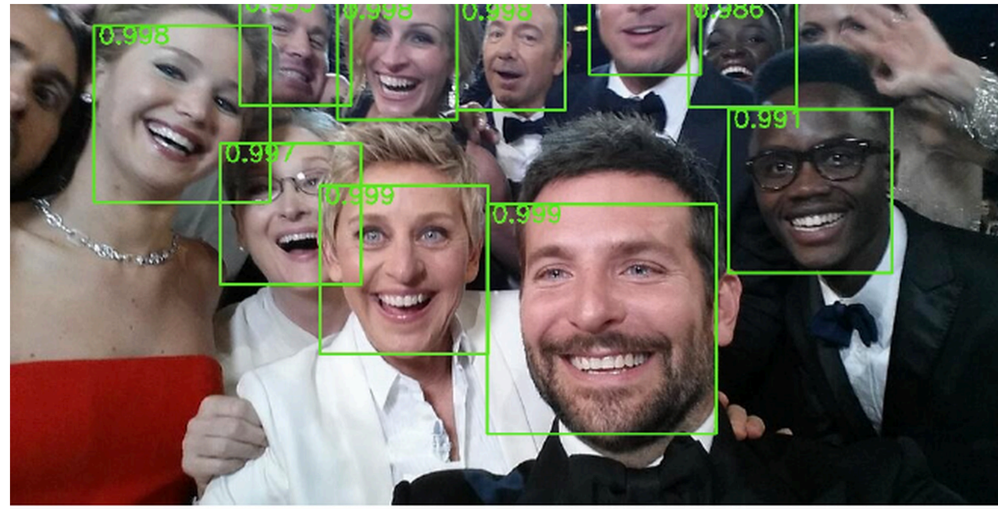
We say a layer is **Fully Connected (FC)** if all linear mappings from the current layer to the next layer are permissible.

$$\mathbf{a}^{(k+1)} = g(\Theta \mathbf{a}^{(k)}) \quad \text{for any } \Theta \in \mathbb{R}^{n_{k+1} \times n_k}$$

A lot of parameters!! $n_1 n_2 + n_2 n_3 + \cdots + n_L n_{L+1}$

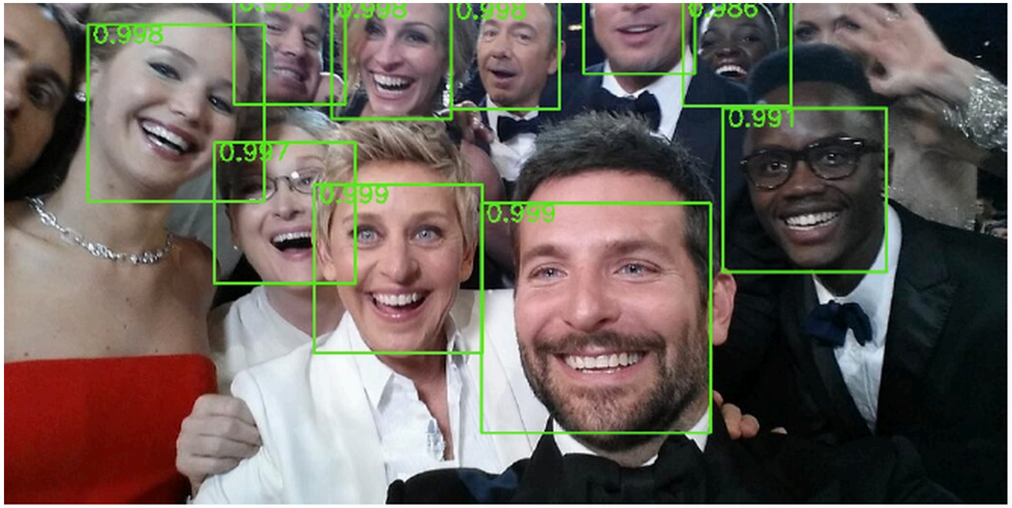
Neural Network Architecture

Objects are often **localized in space** so to find the faces in an image, not every pixel is important for classification—makes sense to drag a window across an image.

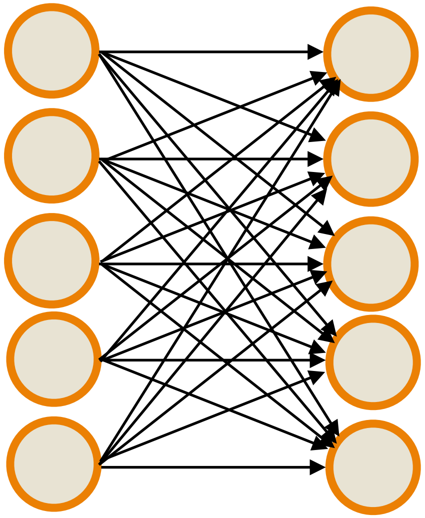


Neural Network Architecture

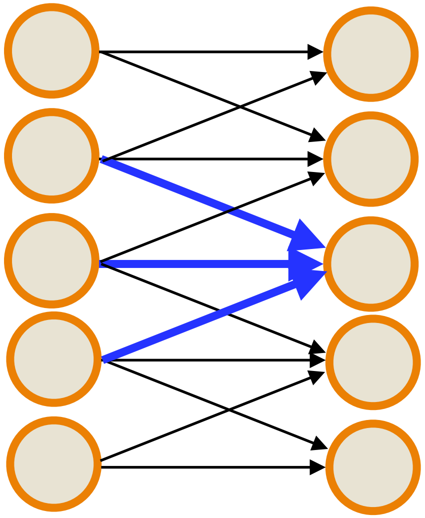
Objects are often **localized in space** so to find the faces in an image, not every pixel is important for classification—makes sense to drag a window across an image.



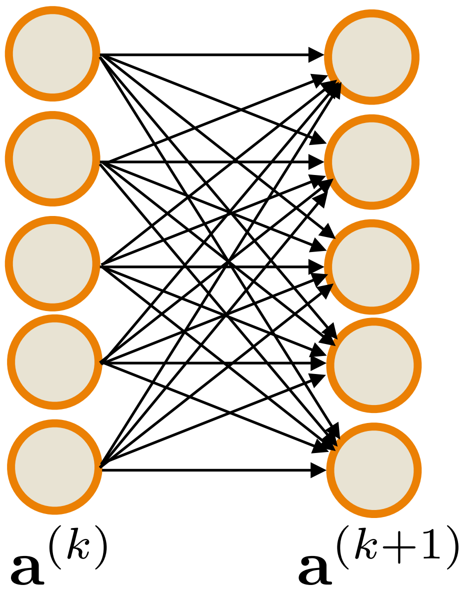
Similarly, to identify edges or other local structure, it makes sense to only look at **local information**



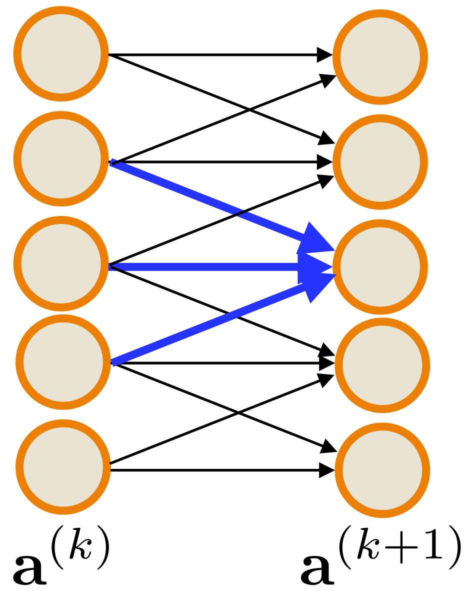
vs.



Neural Network Architecture



vs.

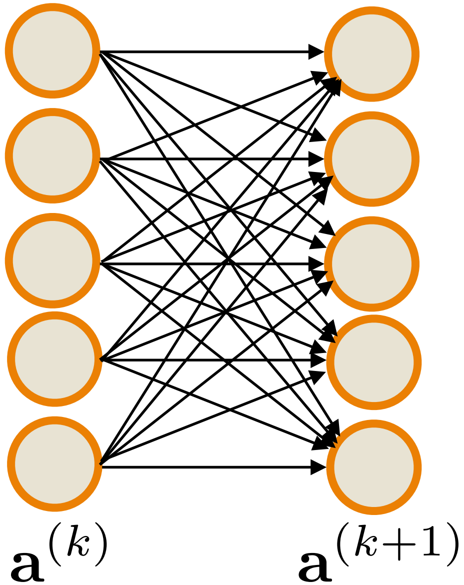


$$\begin{bmatrix} \Theta_{0,0} & \Theta_{0,1} & \Theta_{0,2} & \Theta_{0,3} & \Theta_{0,4} \\ \Theta_{1,0} & \Theta_{1,1} & \Theta_{1,2} & \Theta_{1,3} & \Theta_{1,4} \\ \Theta_{2,0} & \Theta_{2,1} & \Theta_{2,2} & \Theta_{2,3} & \Theta_{2,4} \\ \Theta_{3,0} & \Theta_{3,1} & \Theta_{3,2} & \Theta_{3,3} & \Theta_{3,4} \\ \Theta_{4,0} & \Theta_{4,1} & \Theta_{4,2} & \Theta_{4,3} & \Theta_{4,4} \end{bmatrix} \qquad \begin{bmatrix} \Theta_{0,0} & \Theta_{0,1} & 0 & 0 & 0 \\ \Theta_{1,0} & \Theta_{1,1} & \Theta_{1,2} & 0 & 0 \\ 0 & \Theta_{2,1} & \Theta_{2,2} & \Theta_{2,3} & 0 \\ 0 & 0 & \Theta_{3,2} & \Theta_{3,3} & \Theta_{3,4} \\ 0 & 0 & 0 & \Theta_{4,3} & \Theta_{4,4} \end{bmatrix}$$

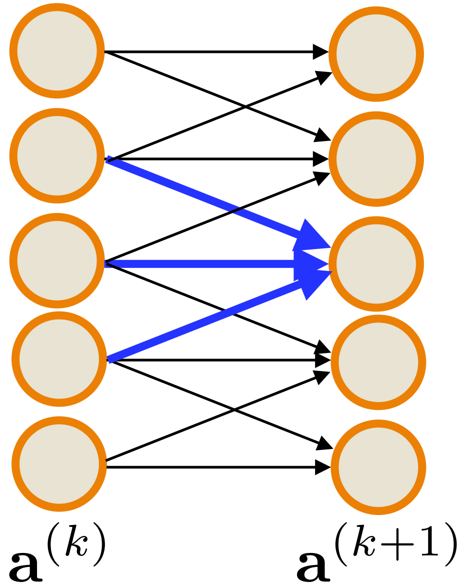
Parameters: n^2 $3n-2$

$$\mathbf{a}_i^{(k+1)} = g\left(\sum_{j=0}^{n-1} \Theta_{i,j}\mathbf{a}_j^{(k)}\right)$$

Neural Network Architecture



vs.



Mirror/share local weights everywhere (e.g., structure equally likely to be anywhere in image)

$$\begin{bmatrix} \Theta_{0,0} & \Theta_{0,1} & \Theta_{0,2} & \Theta_{0,3} & \Theta_{0,4} \\ \Theta_{1,0} & \Theta_{1,1} & \Theta_{1,2} & \Theta_{1,3} & \Theta_{1,4} \\ \Theta_{2,0} & \Theta_{2,1} & \Theta_{2,2} & \Theta_{2,3} & \Theta_{2,4} \\ \Theta_{3,0} & \Theta_{3,1} & \Theta_{3,2} & \Theta_{3,3} & \Theta_{3,4} \\ \Theta_{4,0} & \Theta_{4,1} & \Theta_{4,2} & \Theta_{4,3} & \Theta_{4,4} \end{bmatrix} \quad \begin{bmatrix} \Theta_{0,0} & \Theta_{0,1} & 0 & 0 & 0 \\ \Theta_{1,0} & \Theta_{1,1} & \Theta_{1,2} & 0 & 0 \\ 0 & \Theta_{2,1} & \Theta_{2,2} & \Theta_{2,3} & 0 \\ 0 & 0 & \Theta_{3,2} & \Theta_{3,3} & \Theta_{3,4} \\ 0 & 0 & 0 & \Theta_{4,3} & \Theta_{4,4} \end{bmatrix} \quad \begin{bmatrix} \theta_1 & \theta_2 & 0 & 0 & 0 \\ \theta_0 & \theta_1 & \theta_2 & 0 & 0 \\ 0 & \theta_0 & \theta_1 & \theta_2 & 0 \\ 0 & 0 & \theta_0 & \theta_1 & \theta_2 \\ 0 & 0 & 0 & \theta_0 & \theta_1 \end{bmatrix}$$

Parameters: n^2 $\quad$ $3n-2$ $\quad$ 3

$$\mathbf{a}_i^{(k+1)} = g\left(\sum_{j=0}^{n-1} \Theta_{i,j}\mathbf{a}_j^{(k)}\right)$$

$$\mathbf{a}_i^{(k+1)} = g\left(\sum_{j=0}^{m-1} \theta_j \mathbf{a}_{i+j}^{(k)}\right)$$

Neural Network Architecture

Fully Connected (FC) Layer

$$\begin{bmatrix} \Theta_{0,0} & \Theta_{0,1} & \Theta_{0,2} & \Theta_{0,3} & \Theta_{0,4} \\ \Theta_{1,0} & \Theta_{1,1} & \Theta_{1,2} & \Theta_{1,3} & \Theta_{1,4} \\ \Theta_{2,0} & \Theta_{2,1} & \Theta_{2,2} & \Theta_{2,3} & \Theta_{2,4} \\ \Theta_{3,0} & \Theta_{3,1} & \Theta_{3,2} & \Theta_{3,3} & \Theta_{3,4} \\ \Theta_{4,0} & \Theta_{4,1} & \Theta_{4,2} & \Theta_{4,3} & \Theta_{4,4} \end{bmatrix}$$

$$\mathbf{a}_i^{(k+1)} = g\left(\sum_{j=0}^{n-1} \Theta_{i,j}\mathbf{a}_j^{(k)}\right)$$

Convolutional (CONV) Layer (1 filter)

$$\begin{bmatrix} \theta_1 & \theta_2 & 0 & 0 & 0 \\ \theta_0 & \theta_1 & \theta_2 & 0 & 0 \\ 0 & \theta_0 & \theta_1 & \theta_2 & 0 \\ 0 & 0 & \theta_0 & \theta_1 & \theta_2 \\ 0 & 0 & 0 & \theta_0 & \theta_1 \end{bmatrix}$$

m=3

$$\mathbf{a}_i^{(k+1)} = g\left(\sum_{j=0}^{m-1} \theta_j \mathbf{a}_{i+j}^{(k)}\right) = g([\theta * \mathbf{a}^{(k)}]_i)$$

Convolution*

$\theta = (\theta_0, \ldots, \theta_{m-1}) \in \mathbb{R}^m$ is referred to as a "filter"

Example (1d convolution)

$$(\theta * x)_i = \sum_{j=0}^{m-1} \theta_j x_{i+j}$$

1	1	1	0	0

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

1	0	1

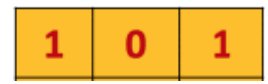
Filter $\theta \in \mathbb{R}^m$

Output $\theta * x$

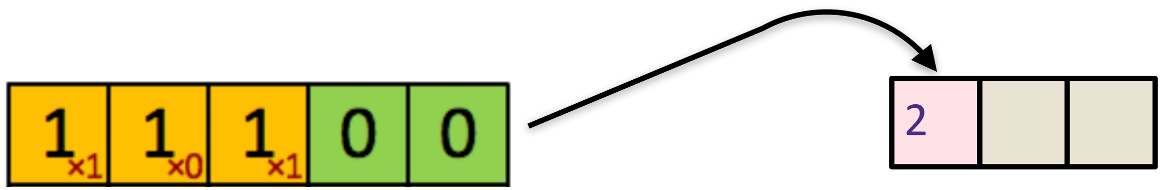
Example (1d convolution)

$$(\theta * x)_i = \sum_{j=0}^{m-1} \theta_j x_{i+j}$$

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



Filter $\theta \in \mathbb{R}^m$

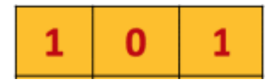


Output $\theta * x$

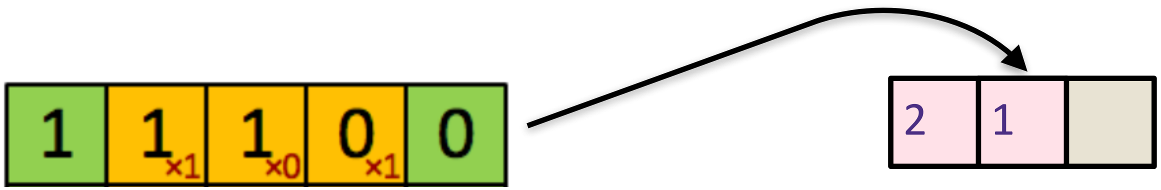
Example (1d convolution)

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

$$(\theta * x)_i = \sum_{j=0}^{m-1} \theta_j x_{i+j}$$



Filter $\theta \in \mathbb{R}^m$



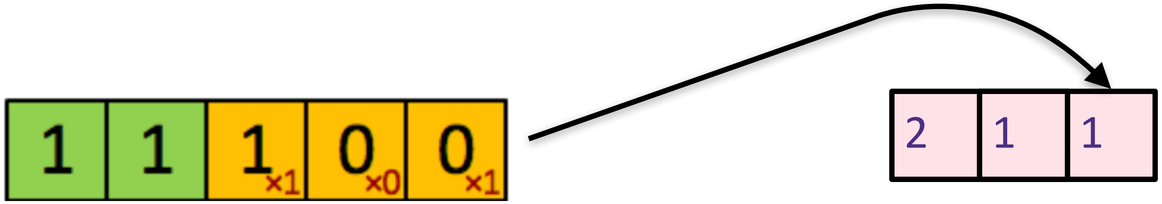
Output $\theta * x$

Example (1d convolution)

$$(\theta * x)_i = \sum_{j=0}^{m-1} \theta_j x_{i+j}$$

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

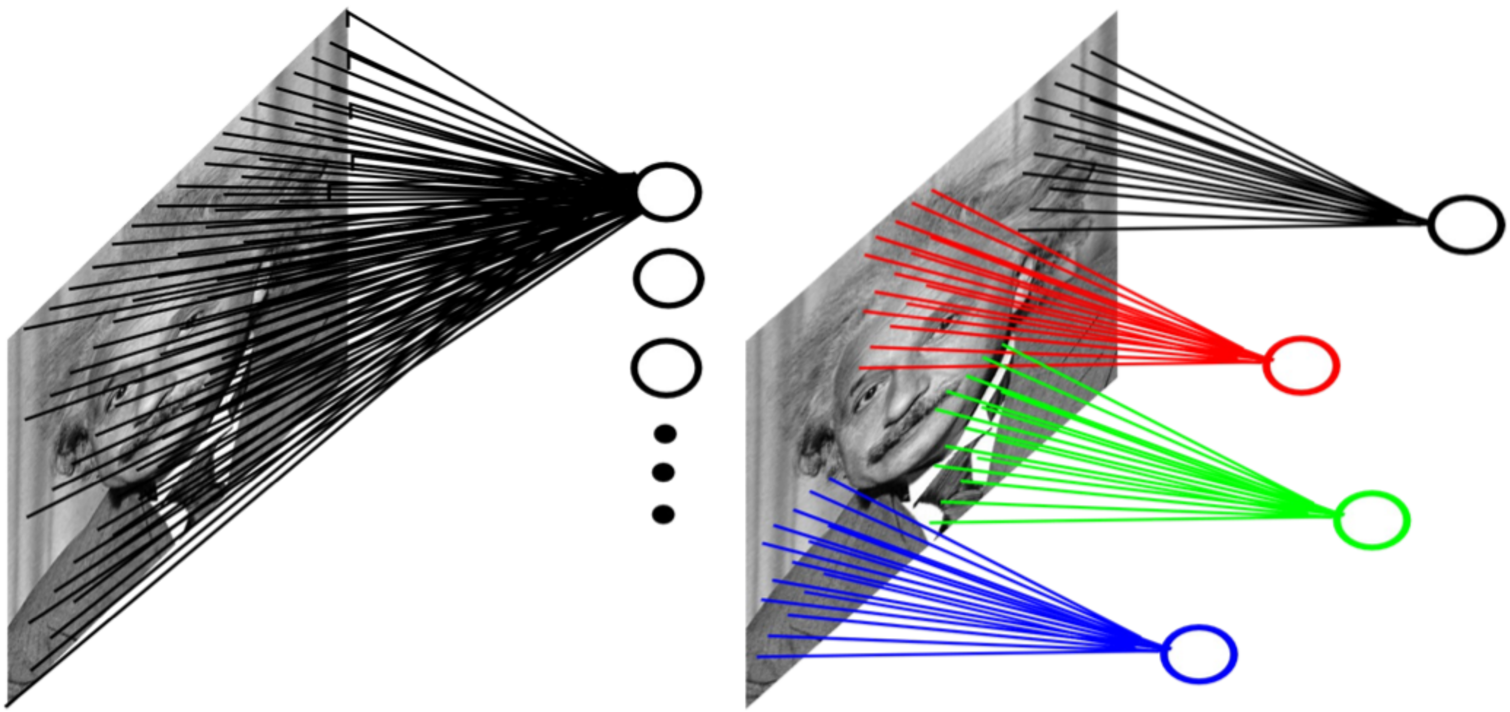
Filter $\theta \in \mathbb{R}^m$



Output $\theta * x$

2d Convolution Layer

- **Example: 200x200 image**
  - Fully-connected, 400,000 hidden units = 16 billion parameters
  - Locally-connected, 400,000 hidden units 10x10 fields = 40 million params
  - Local connections capture local dependencies



Convolution of images (2d convolution)

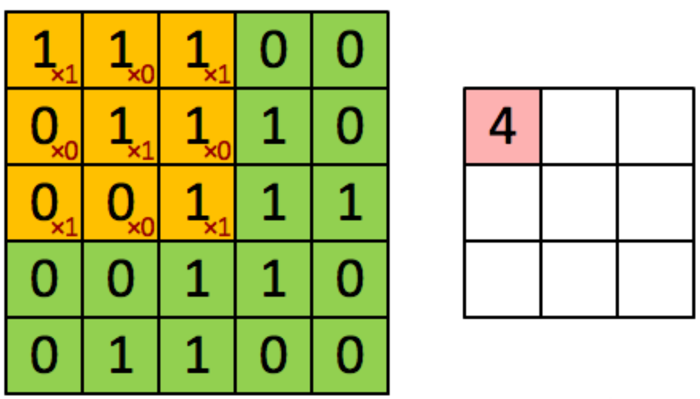
$$(I * K)(i,j) = \sum_{m} \sum_{n} I(i+m, j+n) K(m,n)$$

1	1	1	0	0
0	1	1	1	0
0	0	1	1	1
0	0	1	1	0
0	1	1	0	0

Image I

1	0	1
0	1	0
1	0	1

Filter K



Image

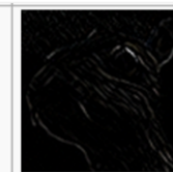
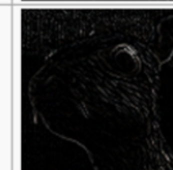
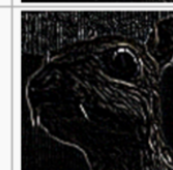
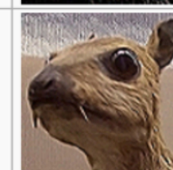
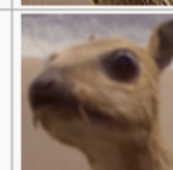
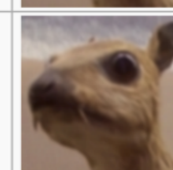
Convolved Feature

$I * K$

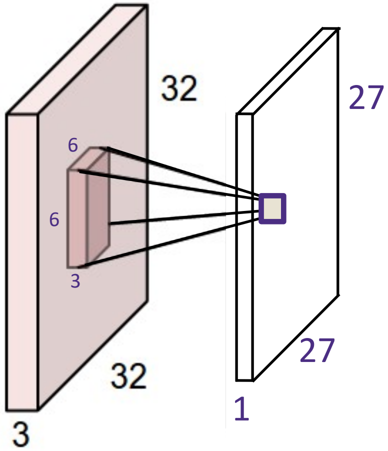
Convolution of images

$$(I * K)(i,j) = \sum_m \sum_n I(i+m, j+n)K(m,n)$$

Image I

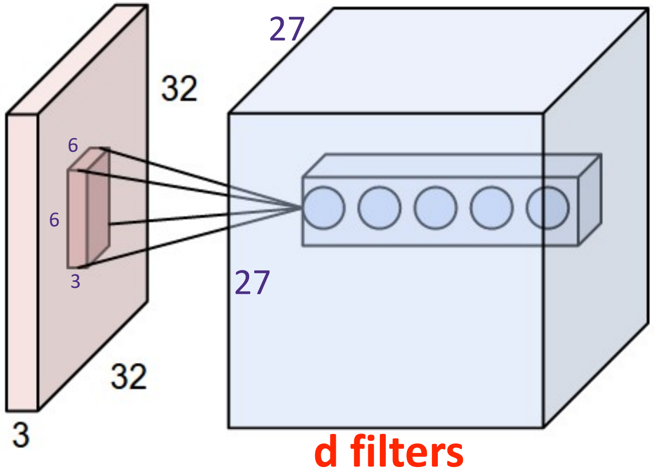
Operation	Filter K	Convolved Image $I * K$
Edge detection	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Box blur (normalized)	$\frac{1}{9}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	
Gaussian blur (approximation)	$\frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	

Stacking convolved images



$$x \in \mathbb{R}^{n \times n \times r}$$

Stacking convolved images

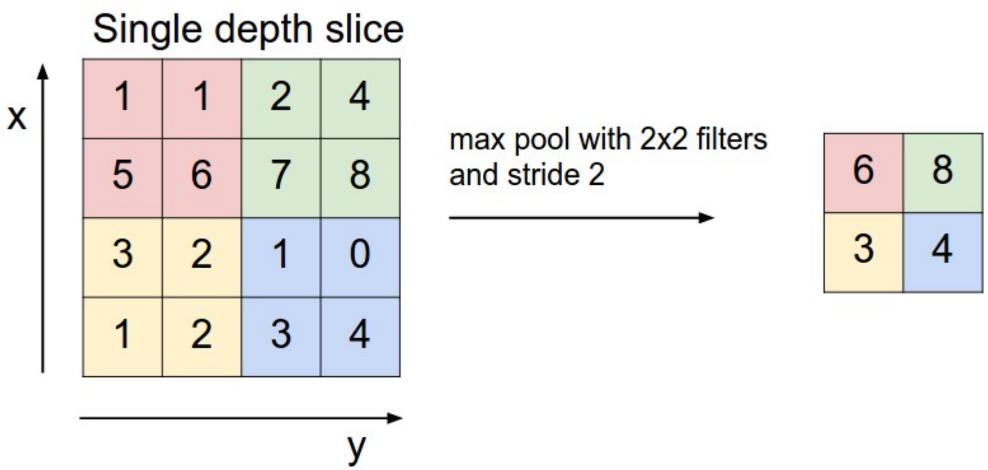


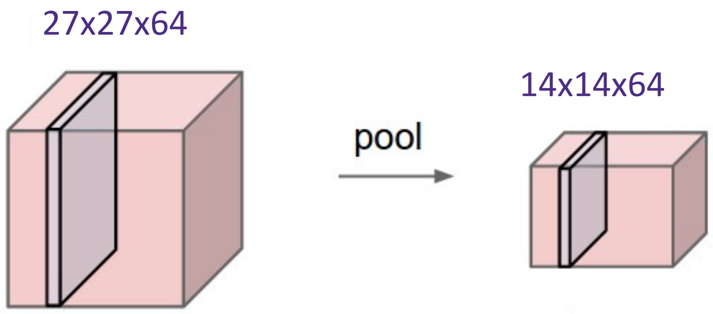
d filters

Repeat with d filters!

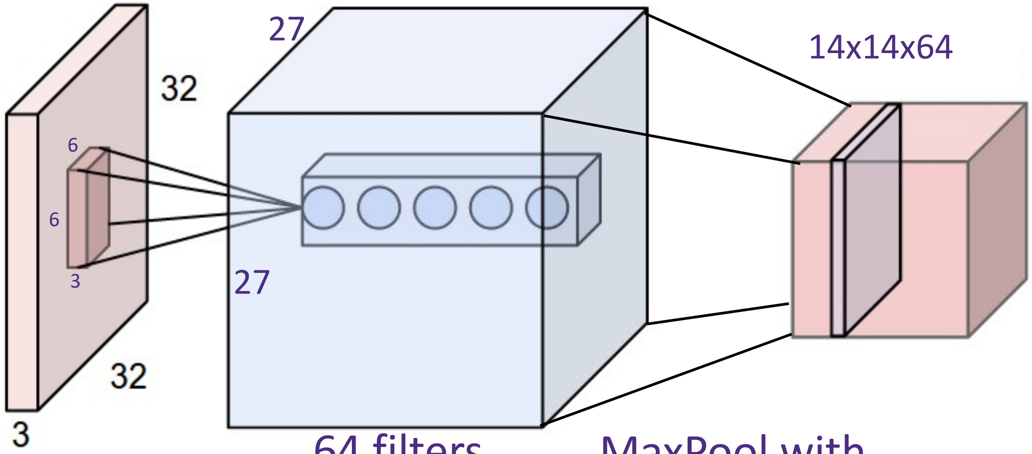
Pooling

Pooling reduces the dimension and can be interpreted as "This filter had a high response in this general region"





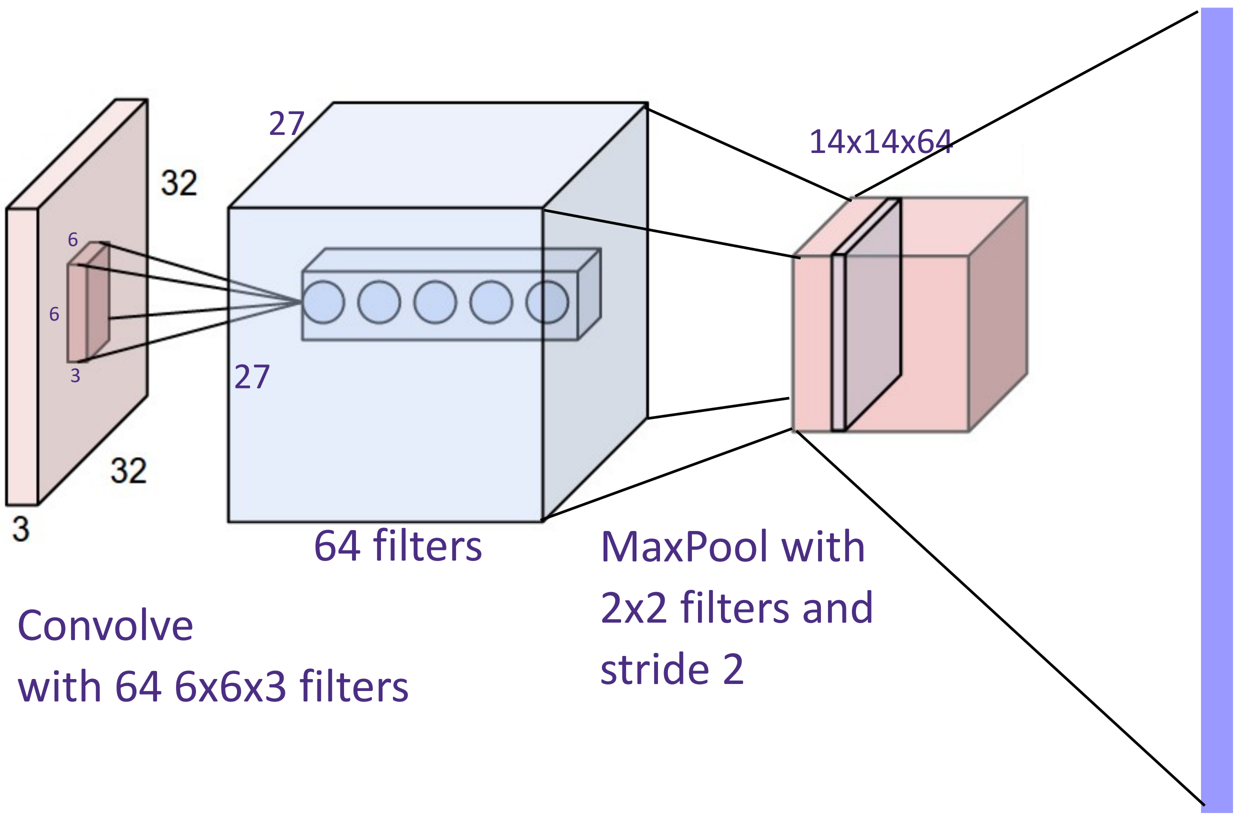
Pooling Convolution layer



MaxPool with
2x2 filters and
stride 2

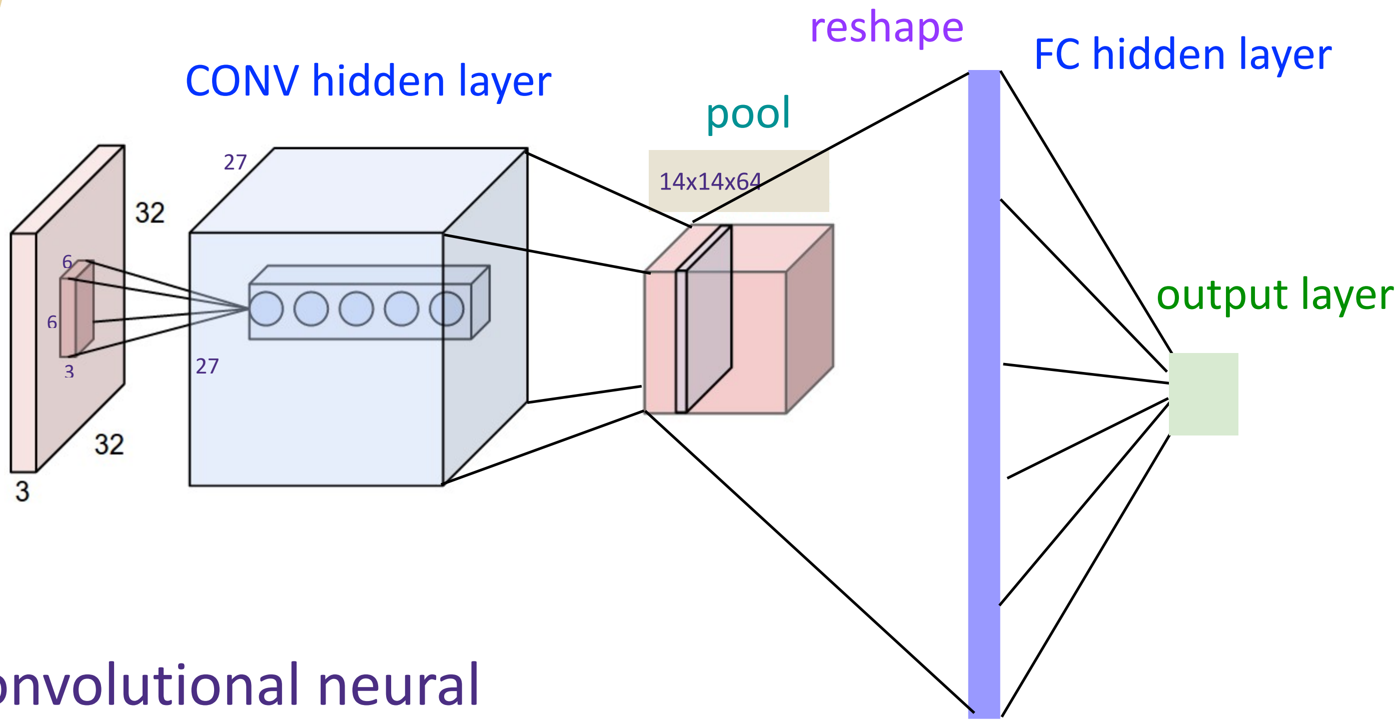
Convolve
with 64 6x6x3 filters

Flattening



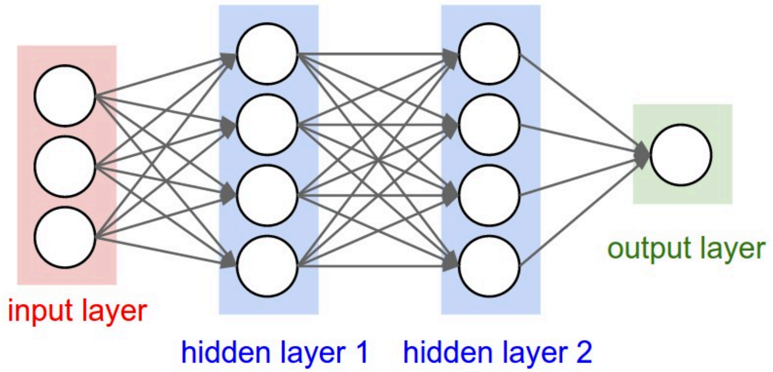
Flatten into a single vector of size 14*14*64=12544

Training Convolutional Networks

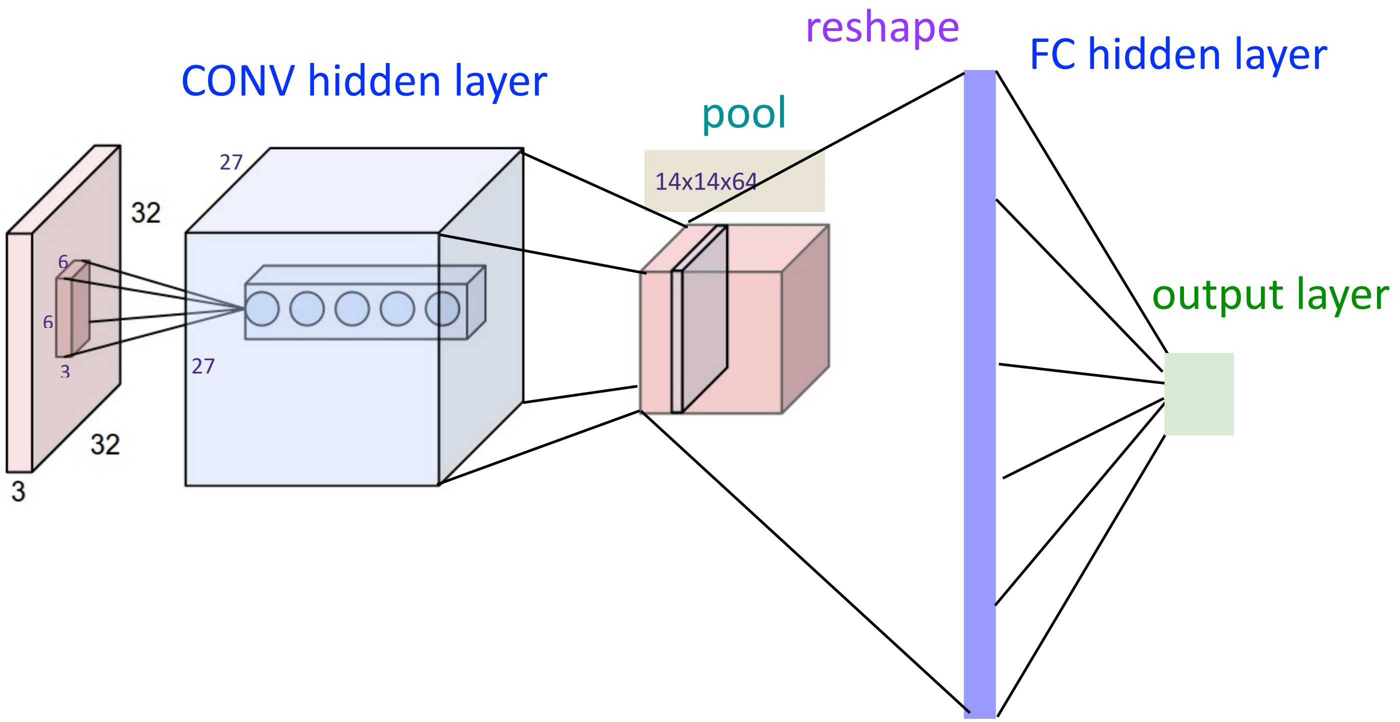


Recall: Convolutional neural networks (CNN) are just regular fully connected (FC) neural networks with some connections removed.

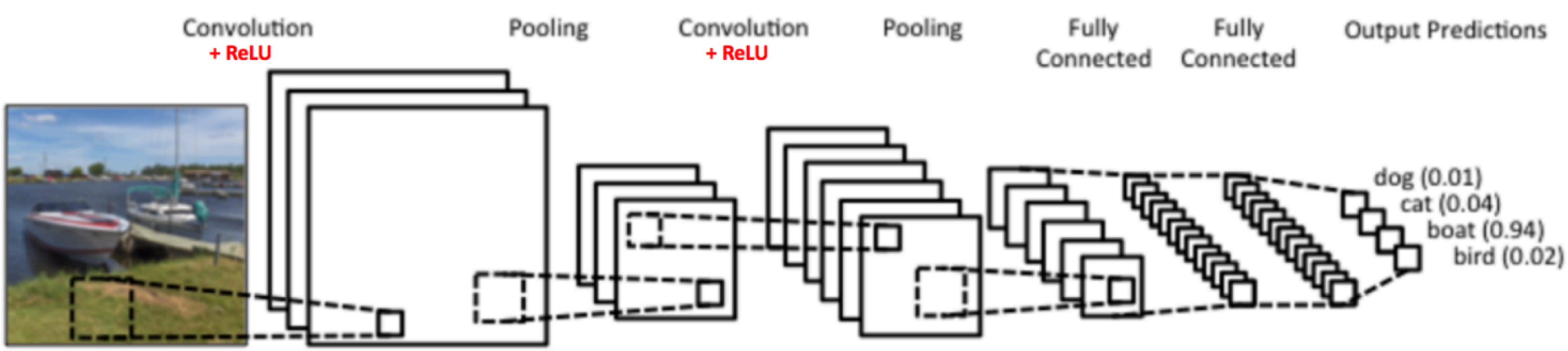
Train with SGD!

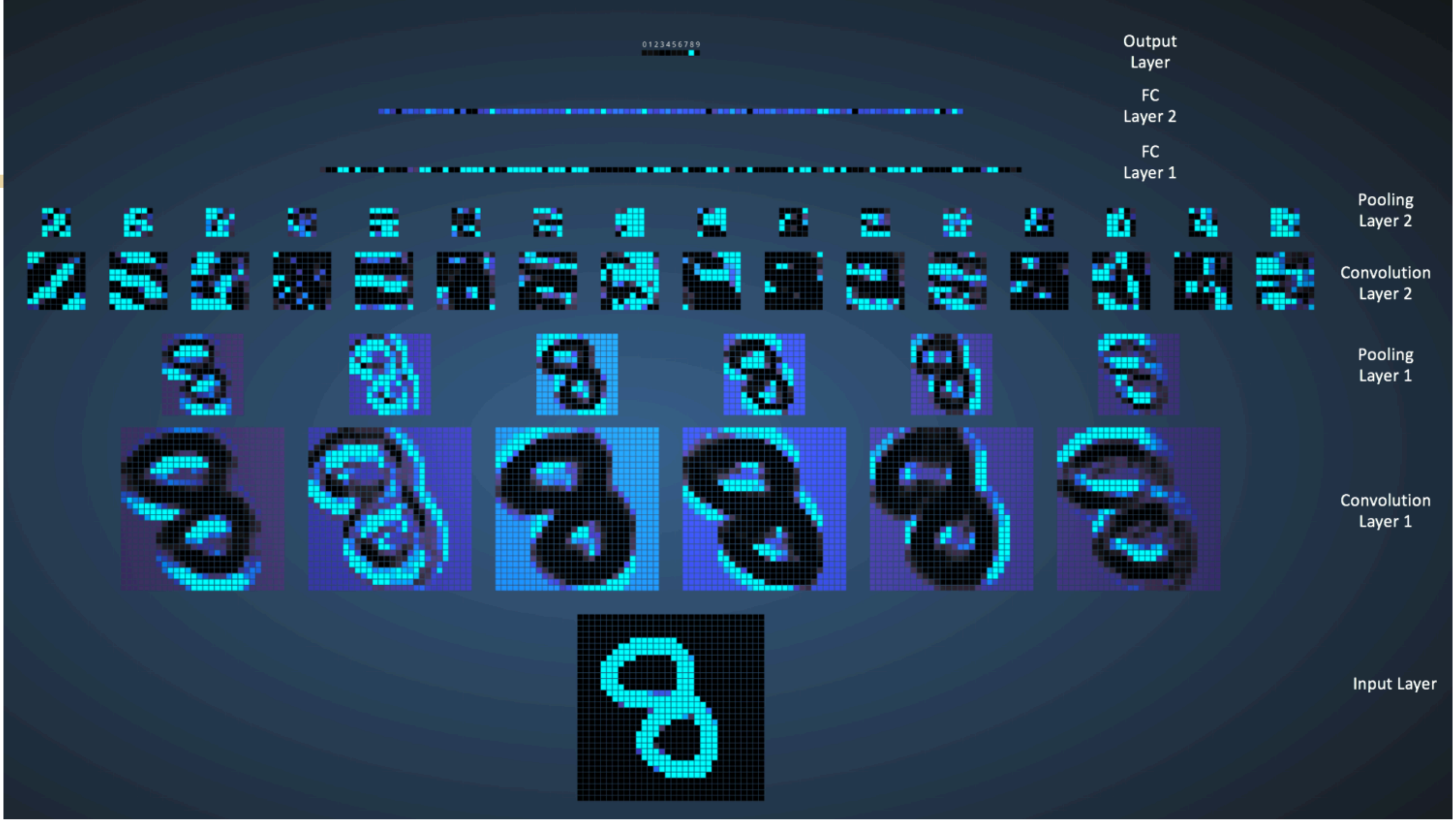


Training Convolutional Networks

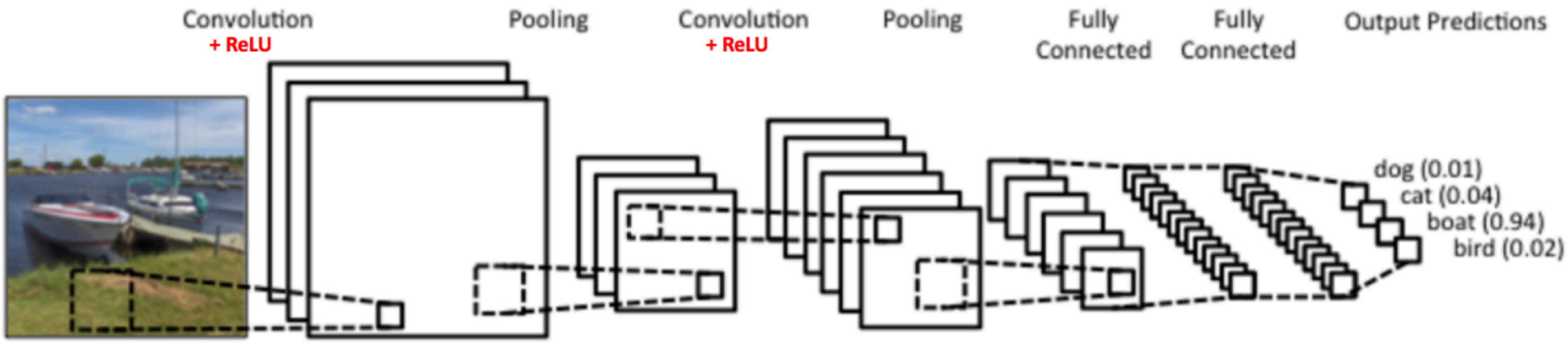


Real example network: LeNet





Real example network: LeNet



Remarks

- Convolution is a fundamental operation in signal processing. Instead of hand-engineering the filters (e.g., Fourier, Wavelets, etc.) **Deep Learning *learns* the filters and CONV layers with back-propagation**, replacing fully connected (FC) layers with convolutional (CONV) layers
- **Pooling** is a dimensionality reduction operation that summarizes the output of convolving the input with a filter

- Typically the last few layers are **Fully Connected (FC)**, with the interpretation that the CONV layers are feature extractors, preparing input for the final FC layers. Can replace last layers and retrain on different dataset+task.

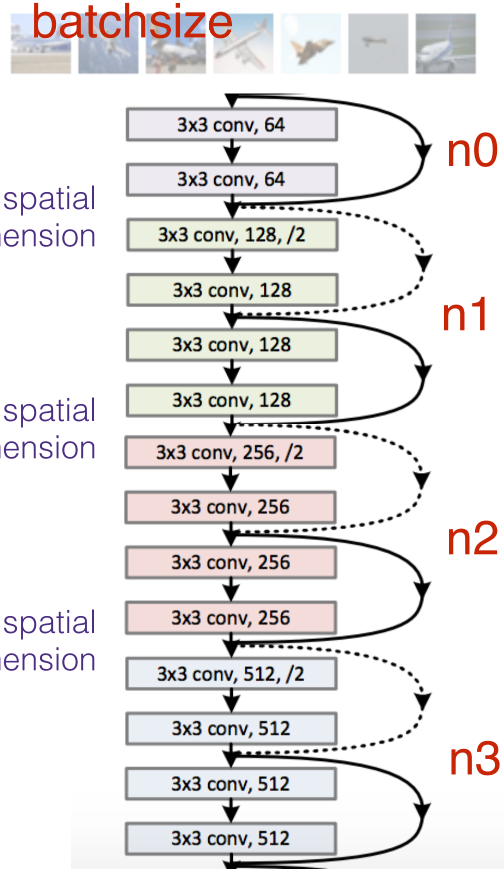
- Just as hard to train as regular neural networks.
- More exotic network architectures for specific tasks

Real networks

Residual Network of [HeZhangRenSun'15]

Modern networks have dozens of parameters to tune.

batchsize



n0 layers of f0 filters

Reduce spatial dimension

n1 layers of f1 filters

Reduce spatial dimension

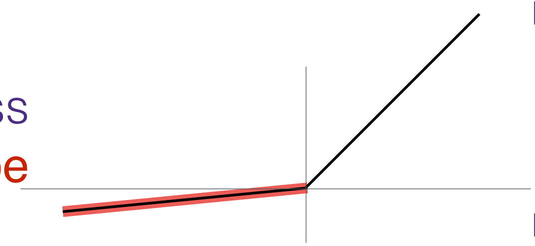
n2 layers of f2 filters

Reduce spatial dimension

n3 layers of f3 filters

Data augmentation?
Batch norm?

RELU leakiness
slope



Learning rate schedule