Neural Networks

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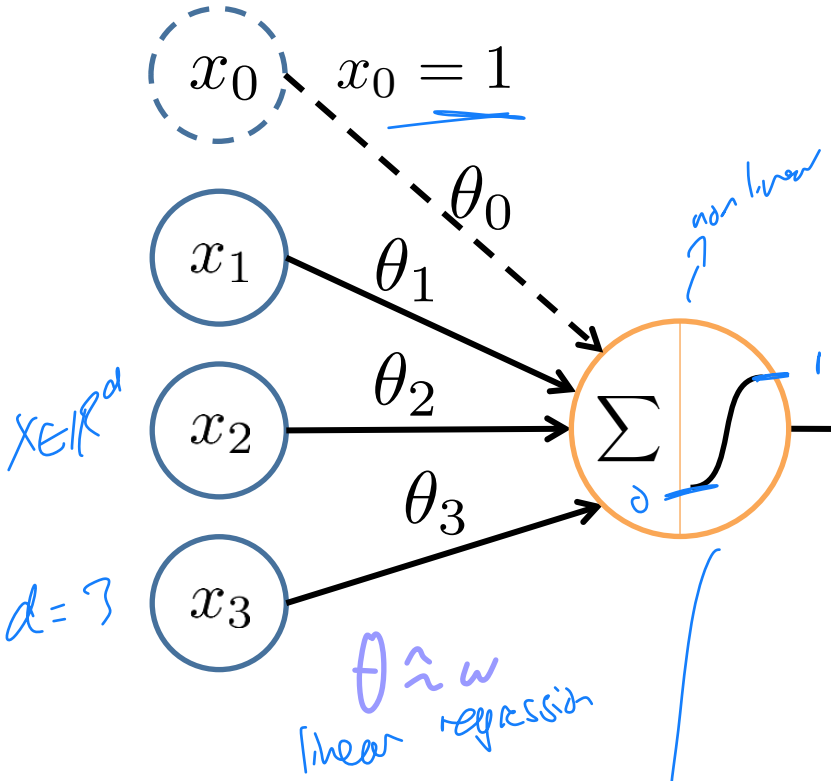
Single neuron/node = linear regression



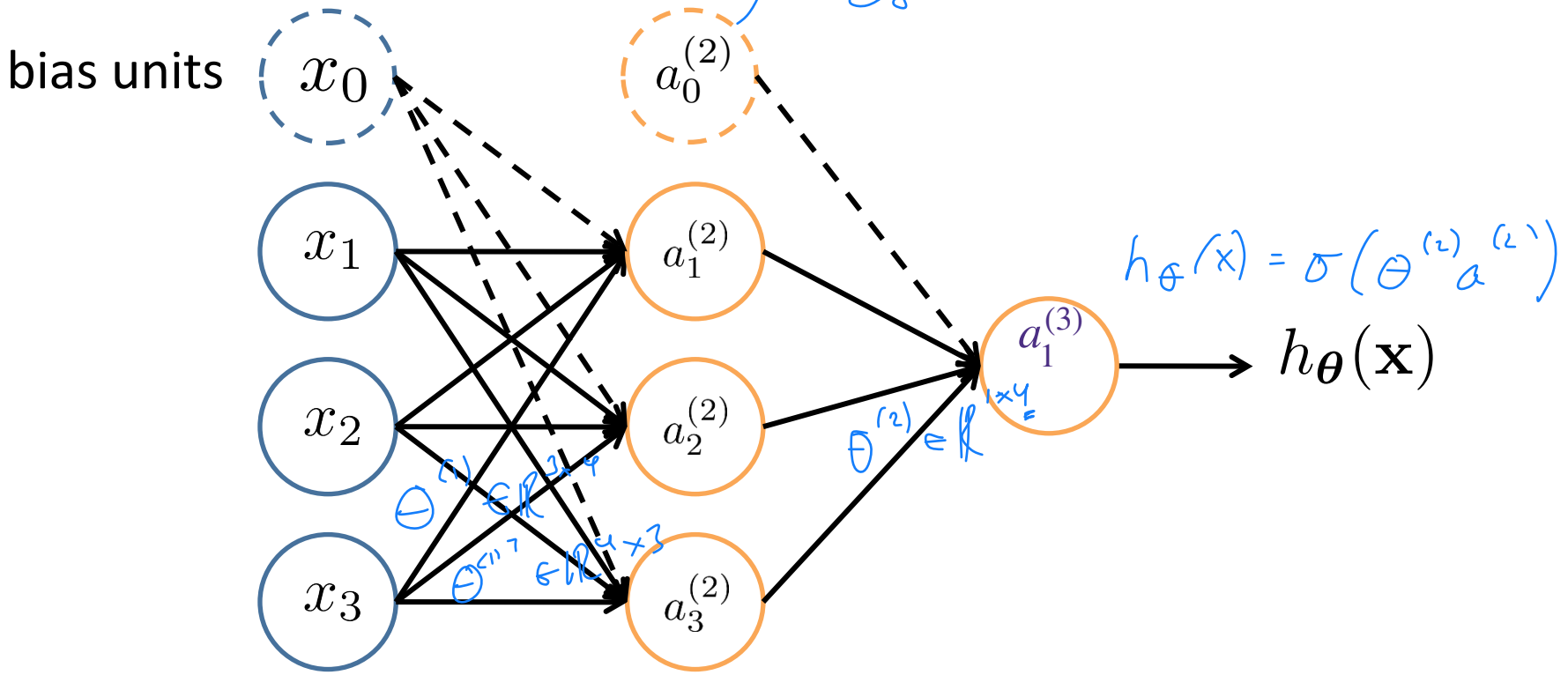
$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

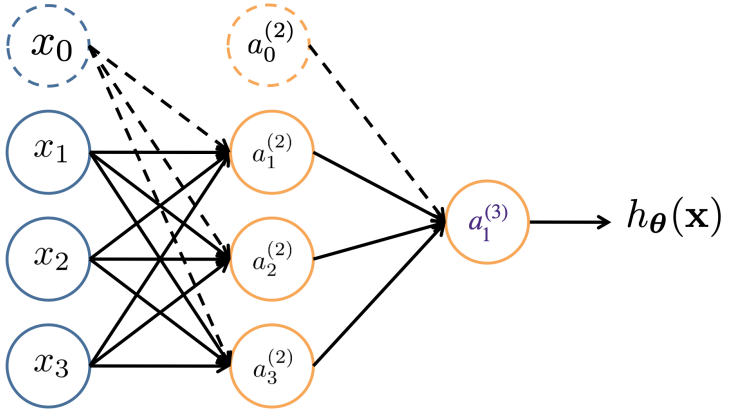
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \sigma(\boldsymbol{\theta}^\top \mathbf{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \mathbf{x}}}$$

Binary Logistic Regression

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

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

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

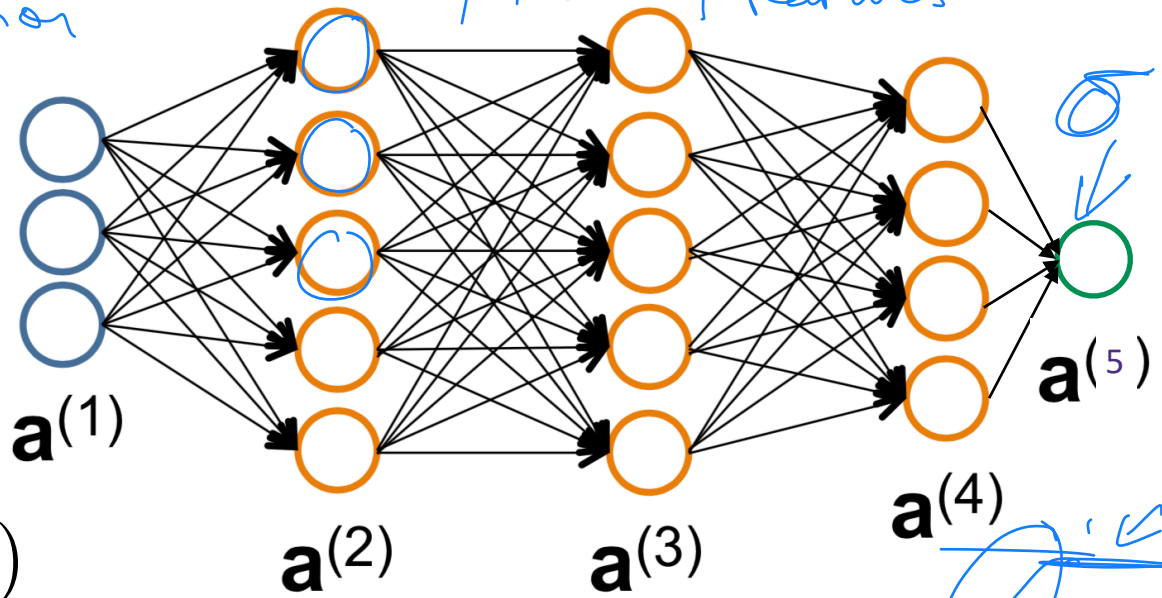
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

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



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

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

Binary Logistic Regression

Multi-layer Neural Network - Activation functions

Activation functions for nodes at intermediate layers include sigmoid, tanh, softplus, **ReLU**…

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

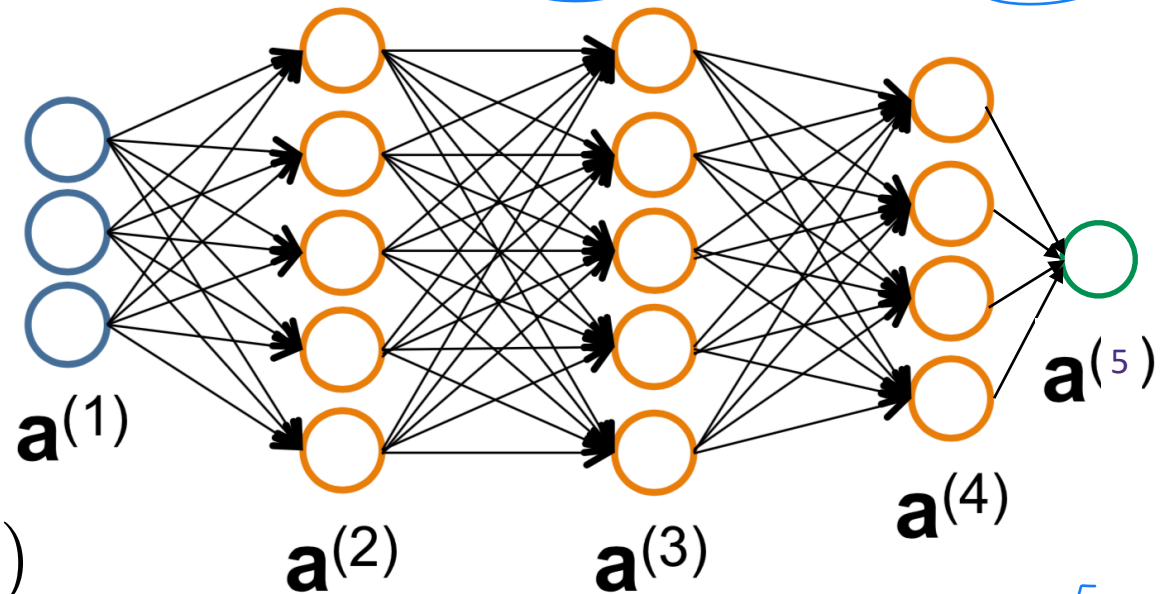
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

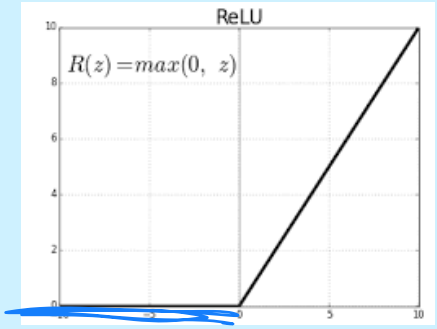
$$\vdots$$

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



ReLU (Rectified Linear Unit) is most common:

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



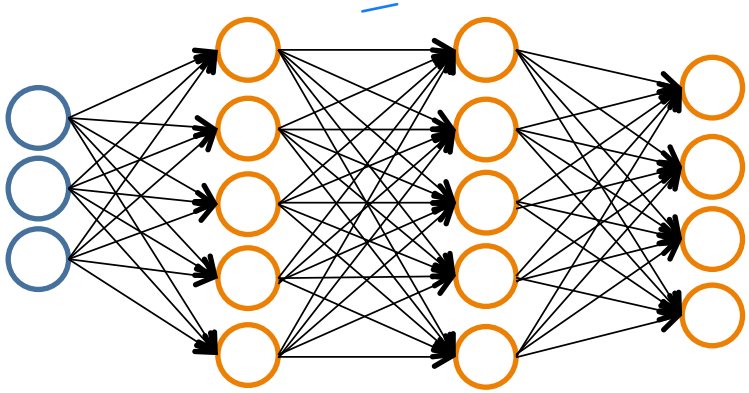
Multiple Output Units: One-vs-Rest

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

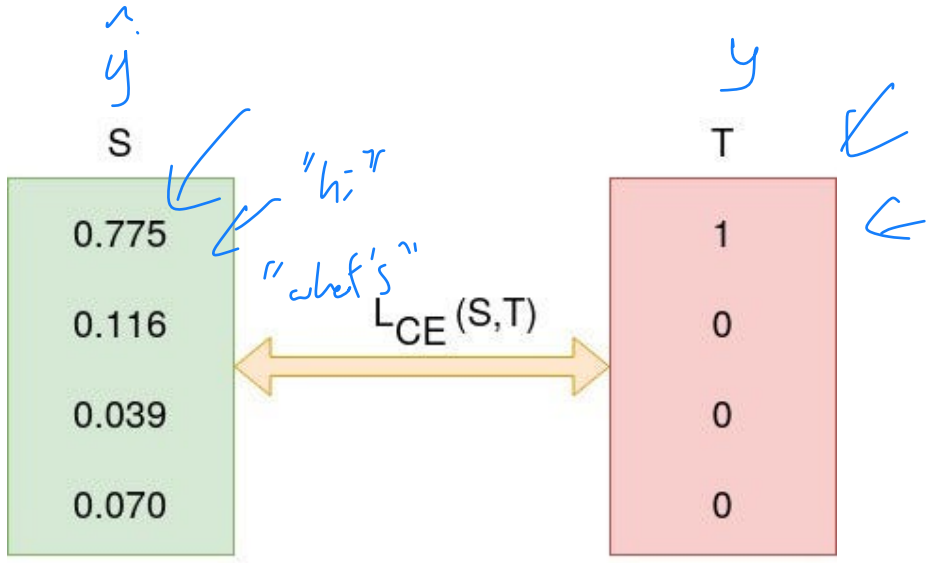
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$ when truck

Multi-class classification: Softmax + Binary Cross-Entropy

Recall: softmax function

$$P\left(y = c_j \middle| x\right) = \frac{e^{w_j^\top x}}{\sum_{j'} e^{w_{j'}^\top x}}$$

Network's final output layer is a **softmax layer**, applies softmax activation function



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

Ground truth label

Compare predicted values to ground truth using binary **cross-entropy**

$$H(y, \hat{y}) = -\sum_{j=1}^{K} y_j \log(\hat{y}_j)$$

Multi-layer Neural Network - Regression

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

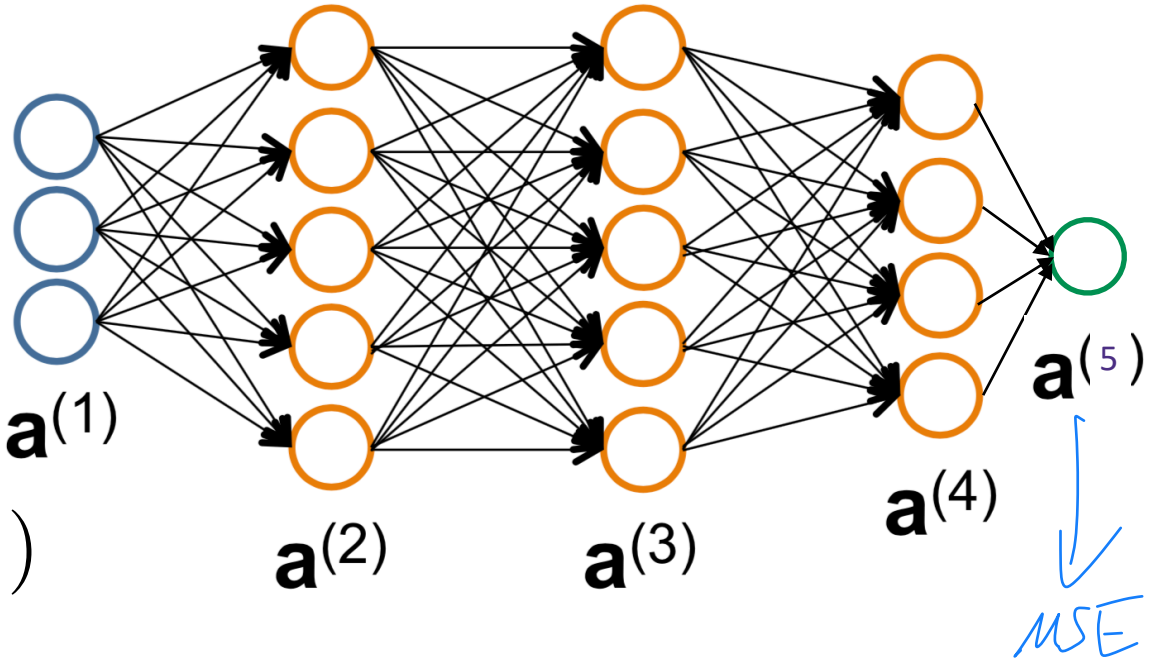
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

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



Regression: apply squared error loss to output

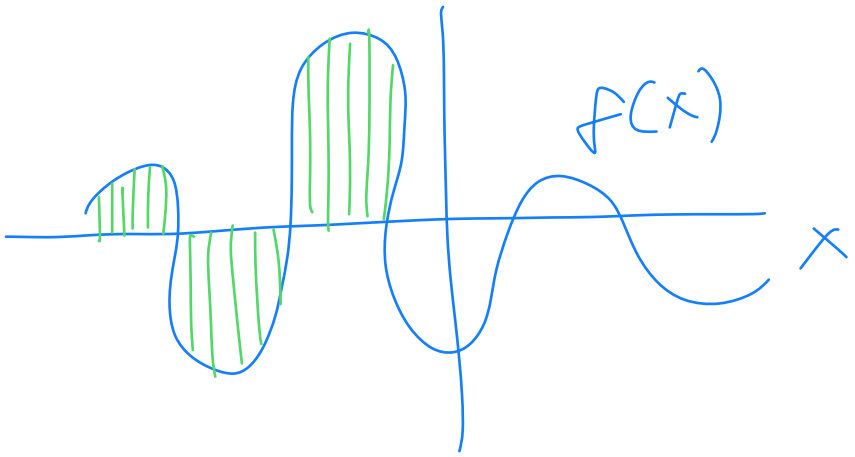
$$L(y, \widehat{y}) = (y - \widehat{y})^2$$

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

→ 1989

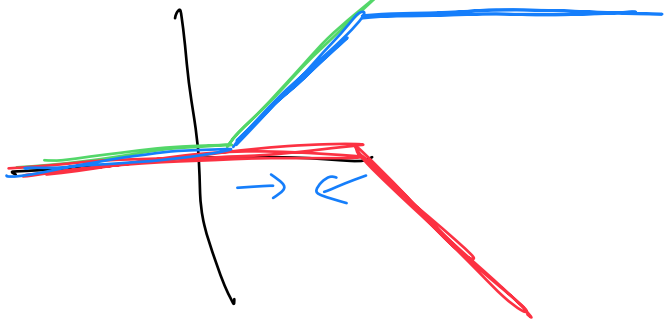
Cybenko, Hornik (theorem reproduced from CIML, Ch. 10)



How to construct a pulse with 4 ReLUs

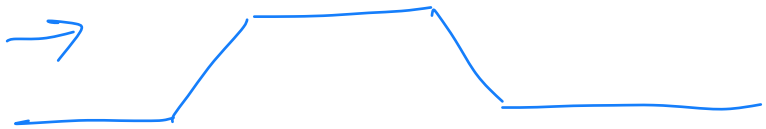
$g(x) = \max(0, x)$ // relu

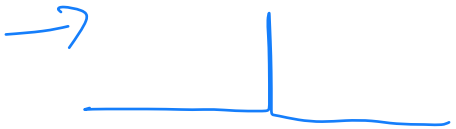
$a(x) = g(mx + b)$ // $\theta = \langle m, b \rangle$



↳ enables inverting and flipping the relu

↳ arbitrarily scale heights & slopes

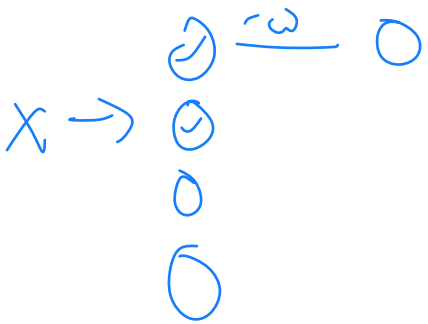


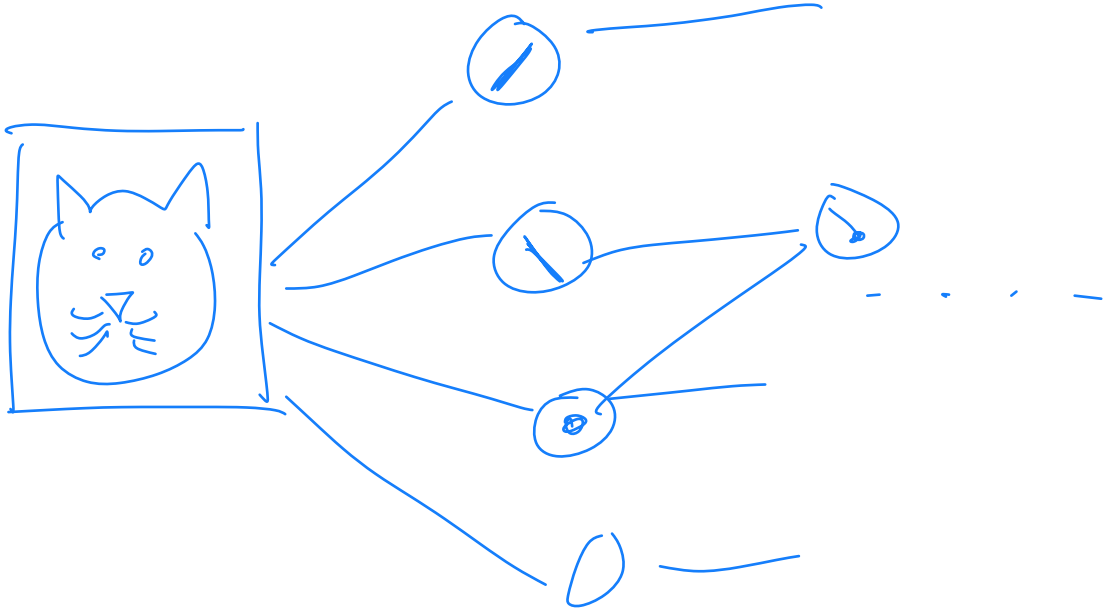


→ one pulse takes 4 relu neurons

Caveats

- how many neurons would we need? Don't know
- pulses are not what network might learn in practice
- pending optimization



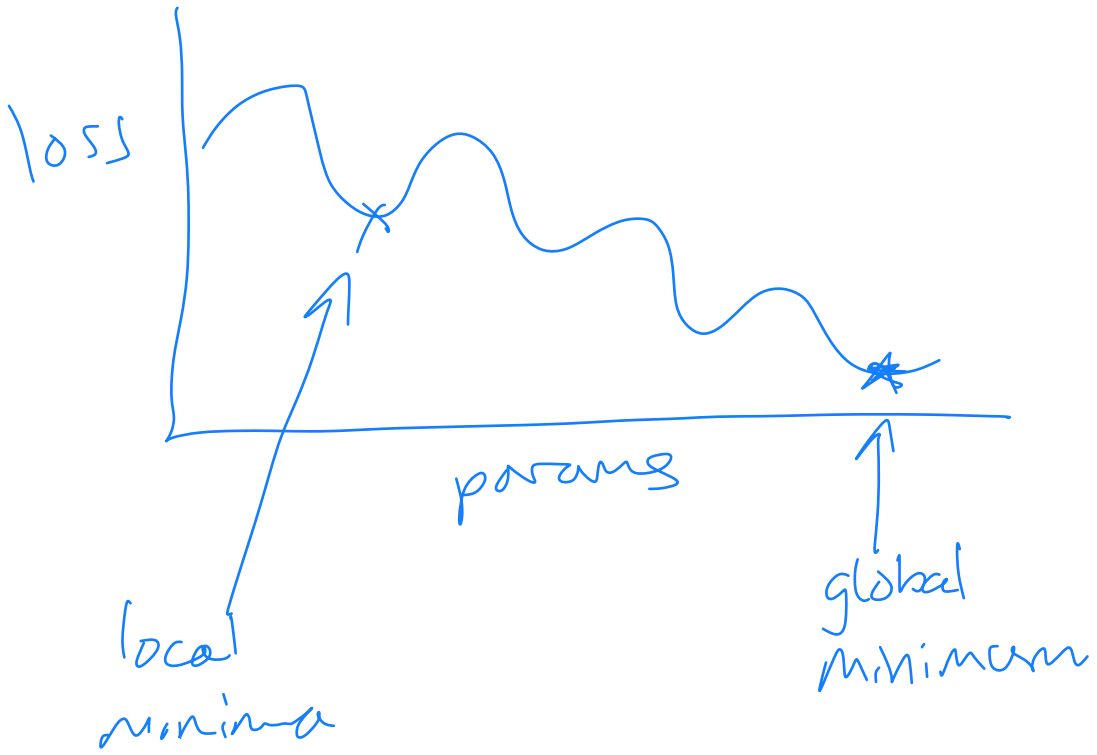


cat neuron google autoencoder youtube 2013?

compress

later features compose earlier features

Training Neural Networks


loss
params
local minima
global minimum

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

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

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

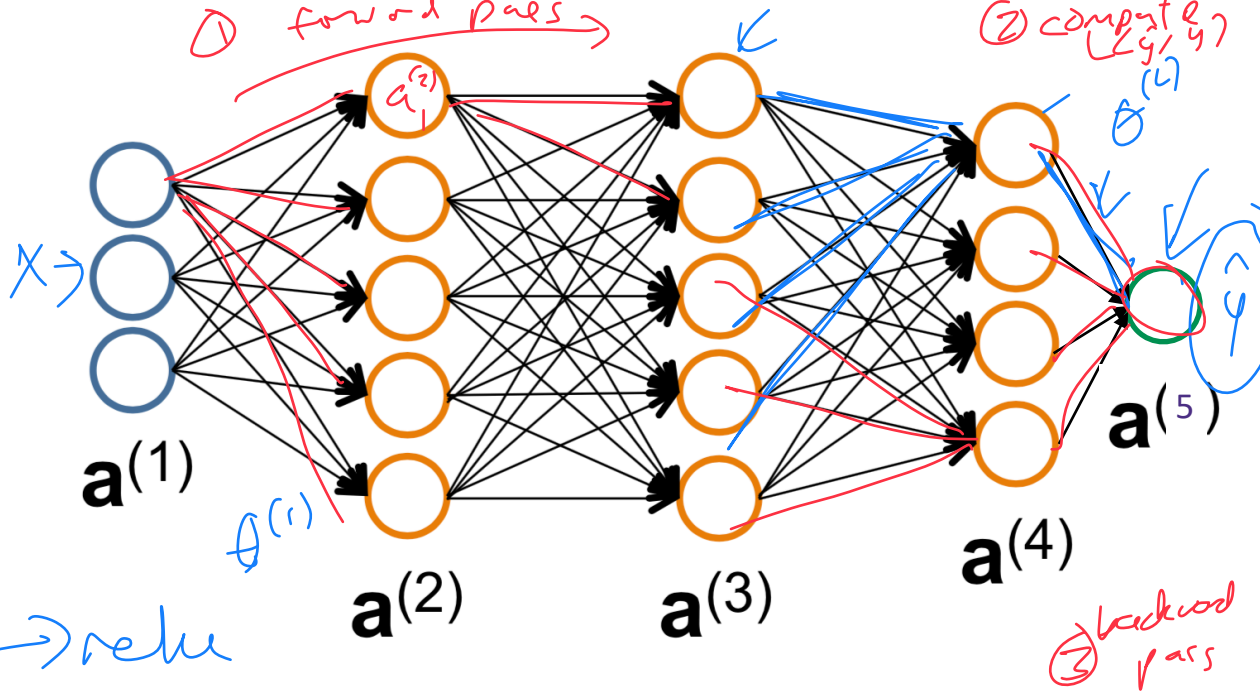
$$\vdots$$

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

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

$$\vdots$$

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



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

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

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

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Seems simple enough, why are packages like PyTorch, Jax, Tensorflow, Theano, Cafe, MxNet synonymous with deep learning?

1. Automatic differentiation

→ backprop
- chain rule
- bookkeeping → save redundant calc's efficient

→ for every func, know the derivative & how to compose w/ chain rule

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

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

1. Automatic differentiation

2. Convenient libraries

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
```

1000s of params in a few lines of code

MSE CE

```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
```

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

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

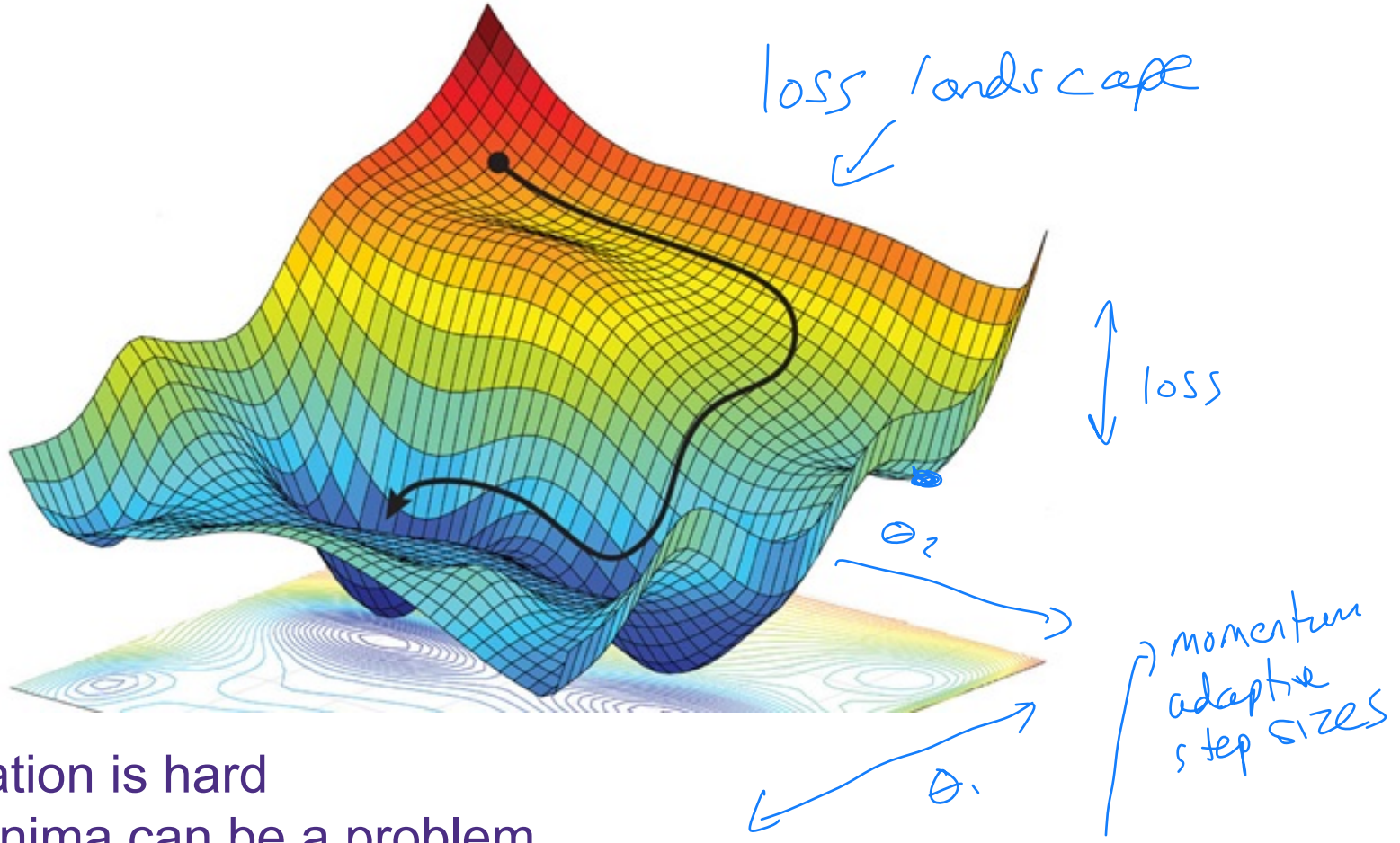
1. Automatic differentiation

2. Convenient libraries

3. GPU support

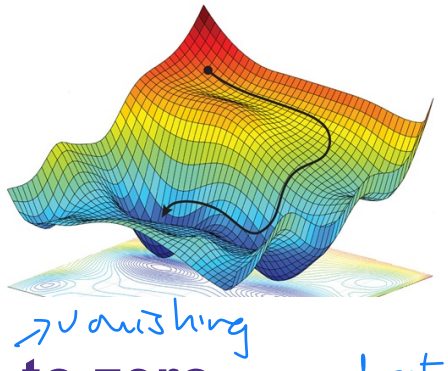
Common training issues

Neural networks are **non-convex**



- Optimization is hard
- Local minima can be a problem
- Rich history of work on getting these things to train effectively

Common training issues



Neural networks are **non-convex**

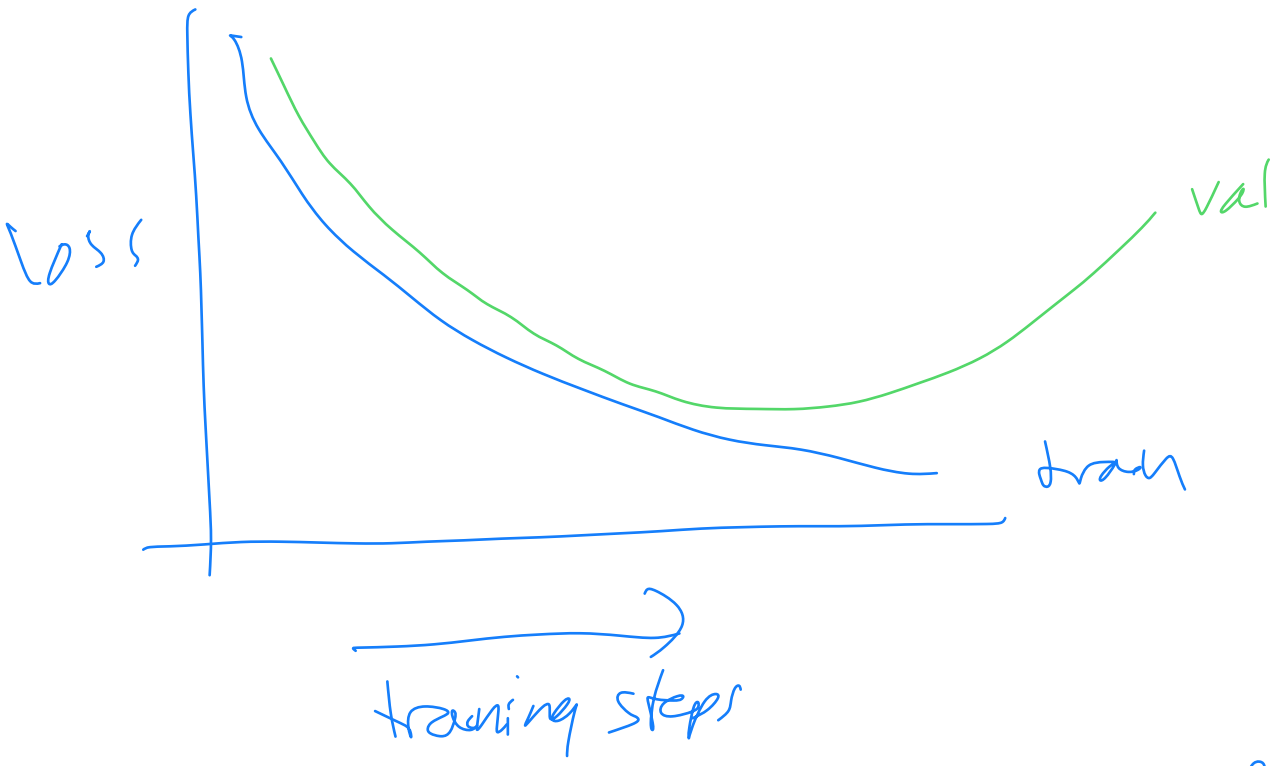
- For large networks, **gradients** can **blow up** or **go to zero**. This can be helped by **batchnorm** or ResNet architecture

- **Hyperparameters** like **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%

- **Overparameterization:** Making the network *bigger* may make training *faster* and it might generalize *better!*



each step = forward & backward pass of GD

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

Common training issues

https://playground.tensorflow.org/

Backprop

Backprop

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

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

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

$$\vdots$$

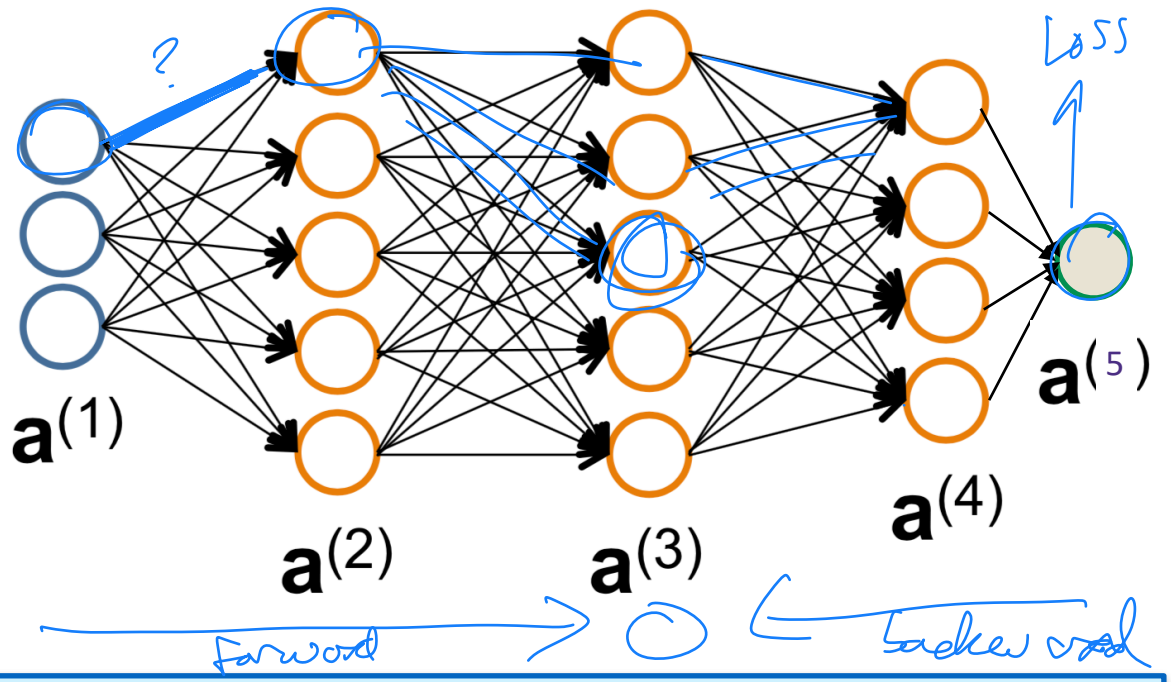
$$a^{(l)} = g\left(z^{(l)}\right)$$

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

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

$$\vdots$$

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



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

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

Backprop

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Train by Stochastic Gradient Descent:

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

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

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

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

Backprop

Chain rule

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

forward pass = activations before this node
backward pass = gradients ahead of this node

$$a^{(1)} = x$$
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$$a^{(2)} = g\left(z^{(2)}\right)$$
$$\vdots$$
$$a^{(l)} = g\left(z^{(l)}\right)$$
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Train by Stochastic Gradient Descent:

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

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

Backprop

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

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

$$z_k^{(l+1)} = \Theta_{k,:}^{(l)\top} a^{(l)} = \left[\Theta_{k,:}^{(l)}\right]^\top g\left(z^{(l)}\right)$$

$$\frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}} = \Theta_{ki}^{(l)} g'\left(z_i^{(l)}\right)$$

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

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

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

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

sigmoid deriv

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

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

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

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

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

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

final layer

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

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

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

→ real #

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

CE

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

Backprop

forward pass

backward pass

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

Recursive Algorithm! → pytorch does it for you

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

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

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 $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_i$ // deriv at last layer using loss

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

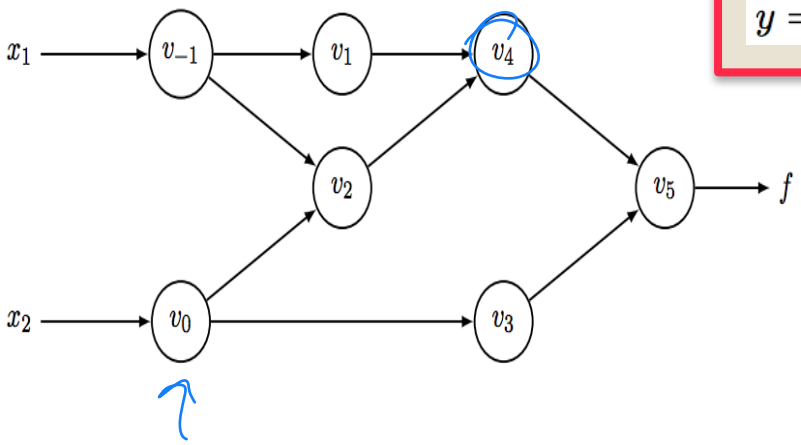
Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

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

$D^{(l)}$ is the matrix of partial derivatives of $J(\Theta)$

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, …