

#### 10-301/10-601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

# **Neural Networks**

Matt Gormley Lecture 11 Oct. 4, 2023

### Reminders

- Homework 4: Logistic Regression
  - Out: Fri, Sep 29
  - Due: Mon, Oct 9 at 11:59pm
- Exam viewings
- Lecture on Friday

### A RECIPE FOR ML

### Background

## A Recipe for Machine Learning

Face

Face

1. Given training data: $\{m{x}_i,m{y}_i\}_{i=1}^N$ 

- 2. Choose each of these:
  - Decision function

 $\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$ 

Loss function

 $\ell(\hat{oldsymbol{y}},oldsymbol{y}_i)\in\mathbb{R}$ 

**Examples**: Linear regression, Logistic regression, Neural Network

Not a face

**Examples**: Mean-squared error, Cross Entropy

#### Background

## A Recipe for Machine Learning

1. Given training data: $\{m{x}_i,m{y}_i\}_{i=1}^N$ 

3. Define goal:  
$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

2. Choose each of these:

– Decision function

 $\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$ 

Loss function

 $\ell(\hat{\pmb{y}}, \pmb{y}_i) \in \mathbb{R}$ 

4. Train with SGD:(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

### Background

### A Recipe for

### Gradients

1. Given training dat **Backprop**  $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^{N}$ gradient!
And it's a

2. Choose each of t

– Decision function $\hat{m{y}}=f_{m{ heta}}(m{x}_i)$ 

– Loss function

 $\ell(\hat{oldsymbol{y}},oldsymbol{y}_i)\in\mathbb{R}$ 

Backpropagation can compute this gradient!

And it's a special case of a more general algorithm called reversemode automatic differentiation that can compute the gradient of any differentiable function efficiently!

opposite the gradient)

 $-\eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$ 

### A Recipe for

# Backgrou Goals for Today's Lecture

- Explore a new class of decision functions (Neural Networks)
  - 2. Consider variants of this recipe for training

#### 2. choose each or these

– Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

Loss function

 $\ell(\hat{\pmb{y}}, \pmb{y}_i) \in \mathbb{R}$ 

Train with SGD:
 ke small steps
 opposite the gradient)

 $oldsymbol{ heta}^{(t+1)} = oldsymbol{ heta}^{(t)} - \eta_t 
abla \ell(f_{oldsymbol{ heta}}(oldsymbol{x}_i), oldsymbol{y}_i)$ 





### Perceptron





### **COMPONENTS OF A NEURAL NETWORK**

## Neural Network



Suppose we already learned the weights of the neural network.

To make a new prediction, we take in some new features (aka. the input layer) and perform the feed-forward computation.

### Neural Network



 $.62 = \sigma(.50)$ .50 = 13(.1) + 2(.3) + 7(-.2)

The computation of each neural network unit resembles binary logistic regression.





## Neural Network



 $.57 = \sigma(.29)$ .29 = .62(-.7) + .80(.9)

 $.80 = \sigma(1.4)$ 1.4 = 13(-.4) + 2(.5) + 7(.8)

 $.62 = \sigma(.50)$ .50 = 13(.1) + 2(.3) + 7(-.2)

The computation of each neural network unit resembles binary logistic regression.

## Neural Network



target value for y at training We have to learn to create "useful" values of  $z_1$  and  $z_2$  in the hidden layer.

### From Biological to Artificial

The motivation for Artificial Neural Networks comes from biology...

#### **Biological "Model"**

- Neuron: an excitable cell
- **Synapse:** connection between neurons
- A neuron sends an electrochemical pulse along its synapses when a sufficient voltage change occurs
- **Biological Neural Network:** collection of neurons along some pathway through the brain

#### **Biological "Computation"**

- Neuron switching time : ~ 0.001 sec
- Number of neurons:  $\sim 10^{10}$
- Connections per neuron: ~ 10<sup>4-5</sup>
- Scene recognition time: ~ 0.1 sec

#### **Artificial Model**

- Neuron: node in a directed acyclic graph (DAG)
- Weight: multiplier on each edge
- Activation Function: nonlinear thresholding function, which allows a neuron to "fire" when the input value is sufficiently high

Synapse

Axon

• Artificial Neural Network: collection of neurons into a DAG, which define some differentiable function

#### **Artificial Computation**

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed processes



### DEFINING A 1-HIDDEN LAYER NEURAL NETWORK

### Example: Neural Network with One Hidden Layer



$$X in \in \mathbb{R}$$
  
 $Zm \in \mathbb{R}$  (general case)  
 $Zm \in (0,1)$  (for sigmoid act)

Let 
$$\sigma$$
 be an activation function  
If  $\sigma$  is signal:  $\sigma(q) = \frac{1}{2 + exp(-q)}$   
 $z_1 = \sigma(X_{11}X_1 + \alpha_{12}X_2 + \alpha_{10})$   
 $z_2 = \sigma(\alpha_{21}X_1 + \alpha_{22}X_2 + \alpha_{20})$   
 $\gamma = \sigma(\beta_1 z_1 + \beta_2 z_2 + \beta_0)$   
 $= \sigma(\beta_1 \sigma(\alpha_{11}X_1 + \alpha_{12}X_2 + \alpha_{10}) + \beta_2 \sigma(\alpha_{21}X_1 + \alpha_{12}X_2 + \alpha_{10}) + \beta_2 \sigma(\alpha_{11}X_1 + \alpha_{12}X_2 + \alpha_{11}X_1$ 



$$y = \sigma(eta_1 z_1 + eta_2 z_2)$$

$$z_2 = \sigma(\alpha_{21}x_1 + \alpha_{22}x_2 + \alpha_{23}x_3)$$
$$z_1 = \sigma(\alpha_{11}x_1 + \alpha_{12}x_2 + \alpha_{13}x_3)$$









### NONLINEAR DECISION BOUNDARIES AND NEURAL NETWORKS



## Logistic Regression







## Logistic Regression





### Neural Network Architectures

Even for a basic Neural Network, there are many design decisions to make:

- 1. # of hidden layers (depth)
- 2. # of units per hidden layer (width)
- 3. Type of activation function (nonlinearity)
- 4. Form of objective function
- 5. How to initialize the parameters

### **BUILDING WIDER NETWORKS**

# **D** = **M** Building a Neural Net

### Q: How many hidden units, D, should we use?


# D < M Building a Neural Net

#### Q: How many hidden units, D, should we use?



The hidden units could learn to be...

- a selection of the most useful features
- nonlinear combinations of the features
- a lower dimensional projection of the features
- a higher dimensional projection of the features
- a copy of the input features
- a mix of the above

# **D > M** Building a Neural Net

#### Q: How many hidden units, D, should we use?



The hidden units could learn to be...

- a selection of the most useful features
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# $D \ge M$ Building a Neural Net

In the following examples, we have two input features, M=2, and we vary the number of hidden units, D.



The hidden units could learn to be...

- a selection of the most useful features
- nonlinear combinations of the features
- a lower
  dimensional
  projection of
  the features
- a higher dimensional projection of the features
- a copy of the input features
- a mix of the above

Examples 1 and 2

#### **DECISION BOUNDARY EXAMPLES**



0.4

0.2

-0.8

-1.0

-1.0

#### Example #2: One Pocket



#### Example #4: Two Pockets







#### Example #1: Diagonal Band 2 1 -0 --1 --2 --3 -2 . О 1 1 -1 2 -3

LR1 for Tuned Neural Network (hidden=2, activation=logistic) 2 1 -Xz 0 - $Z_1 = f(\chi_1, \chi_2)$ -1 --2 -7 -3 -2 -10 2 -3 1 X





LR1 for Tuned Neural Network (hidden=2, activation=logistic)



LR2 for Tuned Neural Network (hidden=2, activation=logistic)



Tuned Neural Network (hidden=2, activation=logistic)









Tuned Neural Network (hidden=3, activation=logistic)







LR3 for Tuned Neural Network (hidden=3, activation=logistic) 2 -1 -0 -0.300  $^{-1}$ -2 --3 -2 ' 0  $\stackrel{\scriptscriptstyle |}{1}$ ' 2 -1-3





Examples 3 and 4

#### **DECISION BOUNDARY EXAMPLES**



0.4

0.2

-0.8

-1.0

-1.0























K-NN (k=5, metric=euclidean)



Tuned Neural Network (hidden=2, activation=logistic) 2 -1 -0 --1 --2 -2 ' 0  $\stackrel{\scriptscriptstyle{}}{1}$ ' 2 -1

Tuned Neural Network (hidden=3, activation=logistic) 2 -1 -0 --1 --2 -2 1 1 ' 2  $^{-1}$ 0

Tuned Neural Network (hidden=4, activation=logistic)



Tuned Neural Network (hidden=10, activation=logistic)


## **BUILDING DEEPER NETWORKS**

### Neural Network



Example: Neural Network with 2 Hidden Layers and 2 Hidden Units

$$z_{1}^{(1)} = \sigma(\alpha_{11}^{(1)}x_{1} + \alpha_{12}^{(1)}x_{2} + \alpha_{13}^{(1)}x_{3} + \alpha_{10}^{(1)})$$

$$z_{2}^{(1)} = \sigma(\alpha_{21}^{(1)}x_{1} + \alpha_{22}^{(1)}x_{2} + \alpha_{23}^{(1)}x_{3} + \alpha_{20}^{(1)})$$

$$z_{1}^{(2)} = \sigma(\alpha_{11}^{(2)}z_{1}^{(1)} + \alpha_{12}^{(2)}z_{2}^{(1)} + \alpha_{10}^{(2)})$$

$$z_{2}^{(2)} = \sigma(\alpha_{21}^{(2)}z_{1}^{(1)} + \alpha_{22}^{(2)}z_{2}^{(1)} + \alpha_{20}^{(2)})$$

$$y = \sigma(\beta_{1} z_{1}^{(2)} + \beta_{2} z_{2}^{(2)} + \beta_{0})$$



## Neural Network (Vector Form)

Neural Network with 1 Hidden Layers and 2 Hidden Units (Matrix Form)



#### Q: How many layers should we use?



#### Q: How many layers should we use?





#### Q: How many layers should we use?

- Theoretical answer:
  - A neural network with 1 hidden layer is a universal function approximator
  - Cybenko (1989): For any continuous function  $g(\mathbf{x})$ , there exists a 1-hidden-layer neural net  $h_{\theta}(\mathbf{x})$ s.t.  $|h_{\theta}(\mathbf{x}) - g(\mathbf{x})| < \epsilon$  for all  $\mathbf{x}$ , assuming sigmoid activation functions
- Empirical answer:
  - Before 2006: "Deep networks (e.g. 3 or more hidden layers) are too hard to train"
  - After 2006: "Deep networks are easier to train than shallow networks (e.g. 2 or fewer layers) for many problems"

Big caveat: You need to know and use the right tricks.

# Feature Learning



- Traditional feature engineering: build up levels of abstraction by hand
- **Deep networks** (e.g. convolution networks): learn the increasingly higher levels of abstraction from data
  - each layer is a learned feature representation
  - sophistication increases in higher layers

# Feature Learning



**Traditional feature engineering:** build up levels of abstraction by hand

**Deep networks** (e.g. convolution networks): learn the increasingly higher levels of abstraction from data

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# Feature Learning



 Traditional feature engineering: build up levels of abstraction by hand

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# Neural Network Errors

**Question X:** For which of the datasets below does there exist a one-hidden layer neural network that achieves zero *classification* error? **Select all that apply.** 

 $Q_2$ 

**Question Y:** For which of the datasets below does there exist a one-hidden layer neural network for *regression* that achieves *nearly* zero MSE? **Select all that apply.** 



## Neural Network Architectures

Even for a basic Neural Network, there are many design decisions to make:

- 1. # of hidden layers (depth)
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- 3. Type of activation function (nonlinearity)
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# **ACTIVATION FUNCTIONS**





So far, we've assumed that the activation function (nonlinearity) is always the sigmoid function...

Sigmoid (aka. logistic) function

... but the sigmoid is not widely used in modern neural networks



- sigmoid,  $\sigma(x)$ 
  - output in range(0,1)
  - good for
     probabilistic
     outputs
- hyperbolic tangent, tanh(x)
  - similar shape to sigmoid, but output in range (- 1,+1)

Sigmoid (aka. logistic) function



Hyperbolic tangent function



#### Understanding the difficulty of training deep feedforward neural networks



Figure from Glorot & Bentio (2010)

- Rectified Linear Unit (ReLU)
  - avoids the vanishing gradient problem
  - derivative is fast to compute

 $\operatorname{ReLU}(x) = max(0, x)$ 



- Rectified Linear Unit (ReLU)
  - avoids the vanishing gradient problem
  - derivative is fast to compute

 $\operatorname{ReLU}(x) = max(0, x)$ 

- Exponential Linear Unit (ELU)
  - same as ReLU on positive inputs
  - unlike ReLU, allows negative outputs and smoothly transitions for x < 0</li>

$$\mathsf{ELU}(x) = \begin{cases} x, & \text{if } x > 0\\ \alpha(\exp(x) - 1), & \text{if } x \le 0 \end{cases}$$







- 1. Training loss converges fastest with ELU
- 2. ELU(x) yields lower test error than ReLU(x) on CIFAR-10

Figure from Clevert et al. (2016)

## **LOSS FUNCTIONS & OUTPUT LAYERS**

#### Neural Network for Classification



#### Neural Network for Regression



### **Objective Functions for NNs**

- 1. Quadratic Loss:
  - the same objective as Linear Regression
  - i.e. mean squared error

$$J = \ell_Q(y, y^{(i)}) = \frac{1}{2}(y - y^{(i)})^2$$
$$\frac{dJ}{dy} = y - y^{(i)}$$

- 2. Binary Cross-Entropy:
  - the same objective as Binary Logistic Regression
  - i.e. negative log likelihood
  - This requires our output y to be a probability in [0,1]

$$J = \ell_{CE}(y, y^{(i)}) = -(y^{(i)} \log(y) + (1 - y^{(i)}) \log(1 - y))$$
$$\frac{dJ}{dy} = -\left(y^{(i)} \frac{1}{y} + (1 - y^{(i)}) \frac{1}{y - 1}\right)$$

## **Objective Functions for NNs**

**Cross-entropy vs. Quadratic loss** 



Figure 5: Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers,  $W_1$  respectively on the first layer and  $W_2$  on the second, output layer.

Figure from Glorot & Bentio (2010)

## Multiclass Output



#### **Multiclass Output**



## Objective Functions for NNs

- 3. Cross-Entropy for Multiclass Outputs:
  - i.e. negative log likelihood for multiclass outputs
  - Suppose output is a random variable Y that takes one of K values
  - Let  $\mathbf{y}^{(i)}$  represent our true label as a one-hot vector:

$$\mathbf{y}^{(i)} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & \dots & 0 \\ 1 & 2 & 3 & 4 & 5 & 6 & \dots & K \end{bmatrix}$$

– Assume our model outputs a length K vector of probabilities:

$$y = softmax(f_{scores}(x, \theta))$$

Then we can write the log-likelihood of a single training example (x<sup>(i)</sup>, y<sup>(i)</sup>) as:

$$J = \ell_{CE}(\mathbf{y}, \mathbf{y}^{(i)}) = -\sum_{k=1}^{K} y_k^{(i)} \log(y_k)$$

# Neural Networks Objectives

You should be able to...

- Explain the biological motivations for a neural network
- Combine simpler models (e.g. linear regression, binary logistic regression, multinomial logistic regression) as components to build up feed-forward neural network architectures
- Explain the reasons why a neural network can model nonlinear decision boundaries for classification
- Compare and contrast feature engineering with learning features
- Identify (some of) the options available when designing the architecture of a neural network
- Implement a feed-forward neural network