

# FSAN/ELEG815: Statistical Learning Gonzalo R. Arce

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X: Neural Networks



### What is Deep Learning?

### Artificial Inteligence

Any technique that enables computers to mimic human behavior

### Machine Learning

Ability to learn without explicity being programed



### Deep Learning

Extract patterns from data using neural networks 3 ( 3 4 7 2 1 7 4 2 3 5



# Why Deep Learning?

# Hand engineered features are time consuming, brittle and not scalable in practice Can we learn the **underlying features** directly from data?



Line and Edges



Eyes, Nose and Ears



Facial Structure



# Why Now?

|      | $\sim$ |   |
|------|--------|---|
| 1952 |        | Stochastic Gradient<br>Descent                              |
| 1958 |        | Preceptron <ul> <li>Learnable Weights</li> </ul>            |
| 1986 |        | Backpropagation <ul> <li>Multi-layer Perceptron</li> </ul>  |
| 1995 |        | Deep Convolutional NN <ul> <li>Digit Recognition</li> </ul> |
|      |        |   |

Neural Networks date back decades, so why the resurgence?

- 1. Big Data
  - Large
     Datasets
  - Easier Collection and Storage
- IM ... GENET



### 2. Hardware

- Graphics
   Processing
   Units (GPUs)
- Massively Parallelizable



### 3. Software

- Improved Techniques
- New Models
- Toolboxes





















### **Activation Functions**

$$\hat{\mathbf{y}} = \mathbf{g} \left( \mathbf{w}_0 + \mathbf{X}^{\top} \mathbf{W} \right)$$

• Example: sigmoid function

$$g(\mathbf{Z}) = \sigma(\mathbf{Z}) = \tfrac{1}{1+e^{-\mathbf{Z}}}$$



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### **Common Activation Functions**



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### The Importance of Activation Functions

The purpose of the activation function is to **introduce non-linearities** into the network



What if we want to build a neural network to distinguish green vs red points?

### The Importance of Activation Functions

### The purpose of the activation function is to introduce non-linearities into







Linear activation functions produce linear decisions no matter the network size Non-linearities allow us to approximate arbitrarily complex functions



### The Perceptron: Example



We have 
$$\mathbf{w}_0 = 1$$
 and  $\mathbf{W} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$   
 $\hat{\mathbf{y}} = g(\mathbf{w}_0 + \mathbf{X}^\top \mathbf{W})$ 

$$\widehat{\mathbf{y}} = g\left(\mathbf{w}_0 + \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}^\top \begin{bmatrix} 3 \\ -2 \end{bmatrix}\right)$$

$$\hat{\mathbf{y}} = g(\underbrace{1+3\mathbf{x}_1-2\mathbf{x}_2})$$

This is just a line in 2D

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### The Perceptron: Example





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### The Perceptron: Example









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### Building Neural Network with Perceptron







# Building Neural Network with Perceptron



$$\mathsf{z} = \mathsf{w}_0 + \sum_{j=1}^m \mathsf{x}_j \mathsf{w}_j$$

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# **Combining Perceptrons**

Consider the target function in the figure which is a Boolean XOR function.

The perceptron cannot implement this classification.

Decompose the f into two perceptrons, corresponding to the lines in the figure.



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# **Combining Perceptrons**



$$f = \mathsf{g}_1 \overline{\mathsf{g}_2} + \overline{\mathsf{g}_1} \mathsf{g}_2$$

where AND is represented by multiplication, OR by addition and overbar for negation.



### **Combining Perceptrons**

OR and AND can be implemented by the perceptron:



Everything coming to a node is summed and then transformed by  $sign(\cdot)$  to get the final output



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# Creating Layers



(a) OR of the inputs  $z_1\overline{z_2}$  and  $\overline{z_1}z_2$  (b) The blue and red weights simulate the required ANDS ( $z_1\overline{z_2}$  and  $\overline{z_1}z_2$ ). Negative in te weights handle negations.



# The Multilayer Perceptron

$$z_1(\mathbf{x}) = \mathbf{w}_1^\top \mathbf{x}$$
 and  $z_2(\mathbf{x}) = \mathbf{w}_2^\top \mathbf{x}$  are perceptrons:



### The Multilayer Perceptron

 $z_1(x) = w_1^\top x$  and  $z_2(x) = w_2^\top x$  are perceptrons:



3 layers compare to the perceptron (one) "Feedforward" No backward pointing arrows and no jumps to other layers

### A Powerful Model

Let's consider now a dis target function:



We can model more complex functions by adding more nodes (hidden unites) in the hidden layers (more perceptrons in the decomposition of f)

Because all inputs are densely connected to all outputs, these layers are called **Dense** layers:



$$\mathsf{z}_{\boldsymbol{i}} = \mathsf{w}_{0,\boldsymbol{i}} + \sum_{j=1}^{m} \mathsf{x}_{j} \mathsf{w}_{j,\boldsymbol{i}}$$



### Example with an image with 4 pixels, and 3 classes (cat/dog/ship)





### Example with an image with 4 pixels, and 3 classes (cat/dog/ship)



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### Interpreting a Linear Classifier: Visual Viewpoint

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### Interpreting a Linear Classifier: Geometric Viewpoint



f(x,W) = Wx + b



Array of **32x32x3** numbers (3072 numbers total)

Cat image by Nikita is licensed under CC-BY 2.0

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Plot created using Wolfram Cloud



# Linear Classifier: Three Viewpoints

Algebraic Viewpoint

f(x,W) = Wx



Visual Viewpoint

One template per class



Geometric Viewpoint

Hyperplanes cutting up space



### Multi-output Multi-layer perceptron



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# Multi-output Multi-layer perceptron



$$\begin{split} \mathsf{z}_3 &= \mathsf{w}_{0,3}^{(1)} + \sum_{j=1}^m \mathsf{x}_j \mathsf{w}_{j,3}^{(1)} \\ \mathsf{z}_3 &= \mathsf{w}_{0,3}^{(1)} + \mathsf{x}_1 \mathsf{w}_{1,3}^{(1)} + \mathsf{x}_2 \mathsf{w}_{2,3}^{(1)} + \mathsf{x}_3 \mathsf{w}_{3,3}^{(1)} \end{split}$$
 Generally

(1)

$$\mathbf{z} = \mathbf{W}^{(1)\top} \mathbf{x}^{(0)} + \mathbf{w}_0^{(1)}$$

m

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# Single Layer Neural Network



### Network with many layers - Example

Classify "1" vs "5". Decompose the two digits into basic components:

- $\blacktriangleright$  Every "1" should contain  $\phi_1,\,\phi_2$  and  $\phi_3$
- Every "5" should contain  $\phi_3$ ,  $\phi_4$ ,  $\phi_5$  and  $\phi_6$ , perhaps a little of  $\phi_1$



These shapes are *features* of the input. We want  $\phi_1$  to be large (close to 1) if the corresponding feature is in the input image and small (close to -1) if not.

### Network with many layers - Example

 $\phi_1$  is feature function which computes the presence (+1) and absence (-1) of the corresponding feature.



If we feed in "1",  $\phi_1$ ,  $\phi_2$  and  $\phi_3$  compute +1 and  $\phi_4$ ,  $\phi_5$  and  $\phi_6$  compute -1. Combining with the signs of the weights,  $z_1$  will be positive and  $z_2$  will be negative.

### Deep Neural Network



input **x** hidden layers  $1 \le l \le L$  output layer l = L

When f is not strictly decomposable into perceptrons, but the decision boundary is smooth ( $\theta$ ), then a multilayer perceptron can be close to implementing f.



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# Deep Neural Network




# **Combining Perceptrons**

Consider a simple perceptron  $z(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x}$ :

- θ(z) =sign(z) : Learning the weights is hard combinatorial problem (not smooth)
- θ(z) = tanh(z) : differentiable approximation to sign(·) that allows analytic methods for learning





## Example problem

Will I pass this class? Let's start with a simple two feature model:

- x<sub>1</sub> Number of lectures you attend
- ► x<sub>2</sub> Hours spent studying



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## Example problem: Will I pass this class?



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# Quantifying Loss

The loss of a network measures the cost incurred from incorrect predictions





### **Empirical Loss**

The empirical loss measures the total loss over the entire dataset





### Binary Cross Entropy Loss

**Cross entropy loss** can be used with models that output a probability between 0 and 1





### Mean Square Error Loss

**Mean square error loss** can be used with models that output a continuous real numbers





## Training Neural Networks: Loss Optimization

Find the network weights that achieve the lowest loss



$$\mathbf{W}^* = \operatorname*{arg\,min}_{\mathbf{W}} \frac{1}{n} \sum_{i=1}^n \mathcal{L}\left(f(\mathbf{x}_i; \mathbf{W}), \mathbf{y}_{(i)}\right)$$

$$\mathbf{W}^* = \operatorname*{arg\,min}_{\mathbf{W}} J(\mathbf{W})$$

Remember:

$$\mathbf{W} = \left\{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \ldots\right\}$$

The loss function is a function of the network weights



# Training Neural Networks: Loss Optimization



- 1. Randomly pick an initial  $(w_1, w_2)$
- 2. Compute the gradient:

 $\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$ 

- 3. Take a small step in the opposite direction of the gradient
- 4. Repeat until convergence



### Computing Gradients: Backpropagation





### Computing Gradients: Backpropagation







### Computing Gradients: Backpropagation







### How the network operates



input **x** hidden layers  $1 \le l \le L$  output layer l = L



# How the network operates

$$\mathbf{w}_{ij}^{(l)} = \begin{cases} 1 \leq l \leq L & \text{Layers} \\ 0 \leq i \leq d^{(l-1)} & \text{Layers} \\ 1 \leq j \leq d^{(l)} & \text{Layers} \end{cases}$$

$$\mathbf{x}_{j}^{(l)} = \theta(z_{j}^{(l)}) = \theta(\sum_{i=0}^{d^{(l-1)}} \mathbf{w}_{ij}^{l} \mathbf{x}_{i}^{(l-1)})$$

Apply **x** to 
$$\mathbf{x}_1^{(0)} \dots \mathbf{x}_{d^{(0)}}^{(0)} 
ightarrow \mathbf{x}_1^{(L)} = h(\mathbf{x})$$



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



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# Applying SGD

$$J(f(\mathbf{x}_n), y_n)) = J(\mathbf{w})$$

► To implement SGD, we need the gradient

$$\nabla \mathbf{J}(\mathbf{w}) = \frac{\partial J(\mathbf{w})}{\partial w_{ij}^{(l)}}, \quad \text{for all } i, j, l$$



# Compute $\nabla J(\mathbf{w})$

- We can evaluate  $\nabla \mathbf{J}(\mathbf{w}) = \frac{\partial J(\mathbf{w})}{\partial w_{ij}^{(l)}}$  one by one: analytically or numerically
- A trick for efficient computation:







## $\delta$ for the final layer

For the final layer l = L and j = 1:

$$\begin{split} \delta_1^{(L)} &= \frac{\partial J(\mathbf{w})}{\partial z_1^{(L)}} \\ J(\mathbf{w}) &= \left(x_1^{(L)} - y_n\right)^2 \\ x_1^{(L)} &= \theta\left(z_1^{(L)}\right) \\ \text{Since } \theta'(z) &= 1 - \theta^2(z) \quad \text{ for the tanh} \\ \frac{\partial J(\mathbf{w})}{\partial z_1^{(L)}} &= 2\left(\theta\left(z_1^{(L)}\right) - y_n\right)\left(1 - \theta^2(z_1^{(L)})\right) \\ \frac{\partial J(\mathbf{w})}{\partial z_1^{(L)}} &= 2\left(x_1^{(L)} - y_n\right)\left(1 - \left(x_1^{(L)}\right)^2\right) \end{split}$$

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# Backpropagation of $\delta$

$$\begin{split} \delta_i^{(l-1)} &= \frac{\partial J(\mathbf{w})}{\partial z_i^{(l-1)}} \\ &= \sum_{j=1}^{d^{(l)}} \frac{\partial J(\mathbf{w})}{\partial z_j^{(l)}} \times \frac{\partial z_j^{(l)}}{\partial x_i^{(l-1)}} \times \frac{\partial x_i^{(l-1)}}{\partial z_i^{(l-1)}} \\ &= \sum_{j=1}^{d^{(l)}} \delta_j^{(l)} \times w_{ij}^{(l)} \times \theta' \left( z_i^{(l-1)} \right) \\ \delta_j^{(l-1)} &= \left( 1 - \left( x_i^{(l-1)} \right)^2 \right) \sum_{j=1}^{d^{(l)}} w_{ij}^{(l)} \delta_j^{(l)} \end{split}$$



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# Backpropagation Algorithm

- linitialize all weights  $w_{ij}^{(l)}$  at small values chosen **at random**
- $\blacktriangleright$  Pick one sample  $n \in \{1,2,\cdots,N\}$  uniformly at random
- **Forward Part:** Compute all  $x_i^{(l)}$
- **•** Backward Part: Compute all  $\delta_i^{(l)}$
- Update the weights:

$$w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \eta \frac{\partial \mathbf{J}(\mathbf{w})}{\partial w_{ij}^{(l)}}$$
$$w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \eta x_i^{(l-1)} \delta_j^{(l)}$$

Iterate until it is time to stop.

When is the best time to stop?



# Training Neural Networks



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Li, H. et al. Visualizing the loss landscape of neural nets (2017).



### Loss Functions Can Be Difficult to Optimize

#### Remember: Optimization through gradient descent:

$$\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$$

 $\eta \rightarrow$  How can we set the learning rate?





### Training Neural Networks: Loss Optimization

- Small learning rate converges slowly and gets stuck in false local minima
- Large learning rates overshoot, become unstable and diverge
- Stable learning rates converge smoothly and avoid local minima



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### How to select the learning rate

### Idea 1:

Try a lots of different learning rates and see what works "just right"

### Idea 2:

#### Do something smarter!

Design an adaptive learning rate that "adapts" to the landspace



## Adaptive Learning Rates

#### Learning Rates are not longer fixed

- Can be made larger or smaller depending on:
  - how large the gradient is
  - how fast learning is happening
  - size of particular weights
  - etc...

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### Neural Networks in Practice: Mini-batches

### Gradient Descent:

Compute:

 $\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}} \rightarrow \text{ Can be very computational intensive to compute!}$ 

### Stochastic Gradient Descent:

Pick a single point i and compute:

 $\frac{\partial J_i(\mathbf{W})}{\partial \mathbf{W}} \rightarrow \mathsf{Easy \ to \ compute \ but \ very \ noisy \ (stochastic)!}$ 



### Neural Networks in Practice: Mini-batches

### Mini-batches:

Pick B pints and compute:

$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}} = \frac{1}{B} \sum_{k=1}^{B} \frac{\partial J_k(\mathbf{W})}{\partial \mathbf{W}}$$

- More accurate estimation of the gradient
  - Smoother convergence
  - Allows for large learning rates
- Lead to fast training
  - Can parallelize
  - Achieve significant speed increases on GPU's



# Neural Networks in Practice: Overfitting

#### The overfitting problem:





### What is it?

Technique that constrains our optimization problem to discourage complex models

#### Why we need it?

Improve generalization of our models on unseen data



### Dropout:

During training, at each iteration, randomly set some activations to 0





### Dropout:

During training, at each iteration, randomly set some activations to 0



#### Dropout:

During training, at each iteration, randomly set some activations to 0

- ▶ Typically "drop" 50% of activations in layer
- Forces network to not rely on any node





### **Early Stopping**

Stop training before we have a chance to overfit





### Working with Real Data Sets: The Iris Data set

 ${\bf x}$  is a  $150\times 4 \rightarrow$  it has 4 features and we have 150 samples





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### Image Features

- Width
   ▶ Petal
   ▶ Sepal
- 2. Length
  - Petal
  - Sepal





# Approach



Generate fully connected layers with multiple activation functions to solve a multi feature classification problem.

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## An efficient coding method: Keras





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## Solutions

### Accurate boundary lines for Classification





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# Code

```
input = keras.layers.Input(4,name="Input")
hidden = keras.layers.Dense(4,activation='sigmoid',name="Hidden")(input)
output = keras.layers.Dense(3,activation='sigmoid', name="Output")(hidden)
modelIRIS = keras.Model(input,output)
modelIRIS.layers[1].set_weights([w1,b1])
modelIRIS.layers[2].set_weights([w2,b2])
keras.utils.plot_model(modelIRIS,show_shapes=True)
# print(modeLIRIS.predict(np.array([0,1,1,2],ndmin=2)))
```

```
X,y = datasets.make_blobs(centers = 4,random_state=2,n_samples = 500)
plt.scatter(X[:,0],X[:,1],c=y)
plt.title("Hand-made Example")
plt.show()
```



# Acknowledgement

Alexander Amini and Ava Soleimanym, MIT 6.S191: Introduction to Deep Learning, IntroToDeepLearning.com