Lecture 6: Neural Networks

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<https://shuaili8.github.io/Teaching/CS410/index.html>

Outline

- Perceptron
- Activation functions
- Multilayer perceptron networks
- Training: backpropagation
- Examples
- Overfitting
- Applications

Brief history of artificial neural nets

• The First wave

- 1943 McCulloch and Pitts proposed the McCulloch-Pitts neuron model
- 1958 Rosenblatt introduced the simple single layer networks now called Perceptrons
- 1969 Minsky and Papert's book *Perceptrons* demonstrated the limitation of single layer perceptrons, and almost the whole field went into hibernation

• The Second wave

- 1986 The Back-Propagation learning algorithm for Multi-Layer Perceptrons was rediscovered and the whole field took off again
- The Third wave
	- 2006 Deep (neural networks) Learning gains popularity
	- 2012 made significant break-through in many applications

Biological neuron structure

• The neuron receives signals from their dendrites, and send its own signal to the axon terminal

Biological neural communication

- Electrical potential across cell membrane exhibits spikes called action potentials
- Spike originates in cell body, travels down axon, and causes synaptic terminals to release neurotransmitters
- Chemical diffuses across synapse to dendrites of other neurons
- Neurotransmitters can be excitatory or inhibitory
- If net input of neuro transmitters to a neuron from other neurons is excitatory and exceeds some threshold, it fires an action potential

Perceptron

• Inspired by the biological neuron among humans and animals, researchers build a simple model called Perceptron

• It receives signals x_i 's, multiplies them with different weights w_i , and outputs the sum of the weighted signals after an activation function, step function

Neuron vs. Perceptron

Artificial neural networks

- Multilayer perceptron network
- Convolutional neural network
- Recurrent neural network

Perceptron

Training

- $W_i \leftarrow W_i \eta (o y) x_i$
	- y : the real label
	- \bullet o : the output for the perceptron
	- η : the learning rate

- Explanation
	- If the output is correct, do nothing
	- If the output is higher, lower the weight
	- If the output is lower, increase the weight

Properties

• Rosenblatt [1958] proved the training can converge if two classes are linearly separable and η is reasonably small

Limitation

- Minsky and Papert [1969] showed that some rather elementary computations, such as *XOR* problem, could not be done by Rosenblatt's one -layer perceptron
- However Rosenblatt believed the limitations could be overcome if more layers of units to be added, but no learning algorithm known to obtain the weights yet

Solution: Add hidden layers

An example of a Feed-forward Neural Network with one hidden layer (with 3 neurons)

• Two-layer feedforward neural network

Bias b_k

Activation Functions

Activation function values and derivatives

Sigmoid activation function

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• Sigmoid

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

- Its derivative $\sigma'(z) = \sigma(z)(1-\sigma(z))$
- Output range $(0,1)$
- Motivated by biological neurons and can be interpreted as the probability of an artificial neuron "firing" given its inputs
- However, saturated neurons make value vanished **(why?)**
	- $f(f(f(\cdots)))$
	- $f([0,1]) \subseteq [0.5, 0.732)$
	- $f([0.5, 0.732)) \subseteq (0.622, 0.676)$

Tanh activation function

• Tanh function $\tanh (z) =$ $sinh(z)$ $cosh(z)$ = $e^z - e^{-z}$

- Its derivative $tanh'(z) = 1 - tanh^2(z)$
- $e^z + e^{-z}$ Output range $(-1,1)$
	- Thus strongly negative inputs to the tanh will map to negative outputs
	- Only zero-valued inputs are mapped to near-zero outputs
	- These properties make the network less likely to get "stuck" during training

ReLU activation function

• ReLU (Rectified linear unity) function $ReLU(z) = max(0, z)$

• Its derivative

$$
ReLU'(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{if } z \le 0 \end{cases}
$$

- ReLU can be approximated by softplus function $f_{\text{Softplus}}(x) = \log(1 + e^x)$
- ReLU's gradient doesn't vanish as x increases
- Speed up training of neural networks
	- Since the gradient computation is very simple
	- The computational step is simple, no exponentials, no multiplication or division operations (compared to others)
- The gradient on positive portion is larger than sigmoid or tanh functions
	- Update more rapidly
	- 20 • The left "dead neuron" part can be ameliorated by Leaky ReLU

ReLU activation function (cont.)

• ReLU function $ReLU(z) = max(0, z)$

- The only non-linearity comes from the path selection with individual neurons being active or not
- It allows sparse representations:

• for a given input only a subset of neurons are active

Sparse propagation of activations and gradients

Multilayer Perceptron Networks

Neural networks

• Neural networks are built by connecting many perceptrons together, layer by layer

Hornik, Kurt, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators." *Neural networks* 2.5 (1989): 359-366

Increasing power of approximation

• With more neurons, its approximation power increases. The decision boundary covers more details

• Usually in applications, we use more layers with structures to approximate complex functions instead of one hidden layer with m any neurons 25

Common neuron network structures at a glance

Deep Learning Neural Network

Multilayer perceptron network

Single / Multiple layers of calculation

- Single layer function $f_{\theta}(x) = \sigma(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$
- Multiple layer function
	- $h_1(x) = \sigma(\theta_0^1 + \theta_1^1 x_1 + \theta_2^1 x_2)$
	- $h_2(x) = \sigma(\theta_0^2 + \theta_1^2 x_1 + \theta_2^2 x_2)$
	- $f_{\theta}(h) = \sigma(\theta_0 + \theta_1 h_1 + \theta_2 h_2)$

Training

Backpropagation

How to train?

- As previous models, we use gradient descent method to train the neural network
- Given the topology of the network (number of layers, number of neurons, their connections), find a set of **weights** to minimize the error function

Gradient interpretation

• Gradient is the vector (the red one) along which the value of the function increases most rapidly. Thus its opposite direction is where the value decreases most rapidly.

Gradient descent

- To find a (local) minimum of a function using gradient descent, one takes steps proportional to the negative of the gradient (or an approximation) of the function at the current point
- For a smooth function $f(x)$, ∂f ∂x is the direction that f increases most rapidly. So we apply

$$
x_{t+1} = x_t - \eta \frac{\partial f}{\partial x}(x_t)
$$

until x converges

Gradient descent

The chain rule

- The challenge in neural network model is that we only know the target of the output layer, but don't know the target for hidden and input layers, how can we update their connection weights using the gradient descent?
- The answer is the chain rule that you have learned in calculus

$$
y = f(g(x))
$$

\n
$$
\Rightarrow \frac{dy}{dx} = f'(g(x))g'(x)
$$

Feed forward vs. Backpropagation

Make a prediction

Two-layer feedforward neural network

Feed-forward prediction:

$$
h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_m w_{j,m}^{(1)} x_m) \quad y_k = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_j w_{k,j}^{(1)} h_j^{(1)})
$$
\n
$$
x = (x_1, \dots, x_m) \xrightarrow{\text{where}} h_j^{(1)} \xrightarrow{\text{where}} h_j^{(1)} \xrightarrow{\text{else}} net_k^{(2)} = \sum_j w_{k,j}^{(2)} h_j^{(1)}
$$
\n
$$
v_k^{(2)} = \sum_j w_{k,j}^{(2)} h_j^{(1)}
$$

Make a prediction (cont.)

Two-layer feedforward neural network

Feed-forward prediction:

$$
h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_m w_{j,m}^{(1)} x_m) \quad y_k = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_j w_{k,j}^{(1)} h_j^{(1)})
$$
\n
$$
x = (x_1, \dots, x_m) \xrightarrow{\text{where}} h_j^{(1)} = \sum_m w_{j,m}^{(1)} x_m \quad h_k^{(1)} = \sum_j w_{k,j}^{(2)} h_j^{(1)}
$$
\nwhere\n
$$
net_j^{(1)} = \sum_m w_{j,m}^{(1)} x_m
$$

Make a prediction (cont.)

Feed-forward prediction:

$$
h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_m w_{j,m}^{(1)} x_m) \quad y_k = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_j w_{k,j}^{(1)} h_j^{(1)})
$$
\n
$$
x = (x_1, \dots, x_m) \xrightarrow{\text{where}} h_j^{(1)} = \sum_m w_{j,m}^{(1)} x_m \qquad \text{net}_k^{(2)} = \sum_j w_{k,j}^{(2)} h_j^{(1)}
$$
\nwhere\n
$$
net_j^{(1)} = \sum_m w_{j,m}^{(1)} x_m
$$

Backpropagation

Two-layer feedforward neural network

Feed-forward prediction:

$$
h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_m w_{j,m}^{(1)}) w_k = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_j w_{k,j}^{(1)}h_j^{(1)})
$$

\n
$$
x = (x_1, ..., x_m)
$$

\nwhere $net_j^{(1)} = \sum_m w_{j,m}^{(1)} x_m$
\n
$$
net_k^{(2)} = \sum_j w_{k,j}^{(2)}h_j^{(1)}
$$

\n
$$
net_k^{(2)} = \sum_j w_{k,j}^{(2)}h_j^{(1)}
$$

• Assume all the activation functions are sigmoid
\n• Error function
$$
E = \frac{1}{2} \sum_{k} (y_k - t_k)^2
$$

\n• $\frac{\partial E}{\partial y_k} = y_k - t_k$
\n• $\frac{\partial y_k}{\partial w_{k,j}^{(2)}} = f'_{(2)} \left(net_k^{(2)} \right) h_j^{(1)} = y_k (1 - y_k) h_j^{(1)}$
\n• $\Rightarrow \frac{\partial E}{\partial w_{k,j}^{(2)}} = -(t_k - y_k) y_k (1 - y_k) h_j^{(1)}$
\n• $\Rightarrow w_{k,j}^{(2)} \leftarrow w_{k,j}^{(2)} + \eta \delta_k^{(2)} h_j^{(1)}$
\n• Output of unit j

Backpropagation (cont.)

Feed-forward prediction:

• Error function
$$
E = \frac{1}{2} \sum_{k} (y_{k} - t_{k})^{2}
$$

\n• $\frac{\partial E}{\partial y_{k}} = y_{k} - t_{k}$
\n• $\delta_{k}^{(2)} = (t_{k} - y_{k}) y_{k} (1 - y_{k})$
\n• $\Rightarrow w_{k,j}^{(2)} \leftarrow w_{k,j}^{(2)} + \eta \delta_{k}^{(2)} h_{j}^{(1)}$
\n• $\frac{\partial y_{k}}{\partial h_{j}^{(1)}} = y_{k} (1 - y_{k}) w_{k,j}^{(2)}$
\n• $\frac{\partial h_{j}^{(1)}}{\partial w_{j,m}^{(1)}} = f'_{(1)} \left(net_{j}^{(1)} \right) x_{m} = h_{j}^{(1)} \left(1 - h_{j}^{(1)} \right) x_{m}$
\n• $\frac{\partial E}{\partial w_{j,m}^{(1)}} = -h_{j}^{(1)} \left(1 - h_{j}^{(1)} \right) \sum_{k} w_{k,j}^{(2)} (t_{k} - y_{k}) y_{k} (1 - y_{k}) x_{m}$
\n= $-h_{j}^{(1)} \left(1 - h_{j}^{(1)} \right) \sum_{k} w_{k,j}^{(2)} \delta_{k}^{(2)} x_{m}$
\n• $\Rightarrow w_{j,m}^{(1)} \leftarrow w_{j,m}^{(1)} + \eta \delta_{j}^{(1)} x_{m}$

$$
x = (x_1, \ldots, x_m) \xrightarrow{h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_{m} w_{j,m}^{(1)} x_m) \ y_k = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_{j} w_{k,j}^{(1)} h_j^{(1)})
$$
\nwhere\n
$$
net_j^{(1)} = \sum_{m} w_{j,m}^{(1)} x_m
$$
\n
$$
net_k^{(2)} = \sum_{j} w_{k,j}^{(2)} h_j^{(1)}
$$

Backpropagation algorithms

• Activation function: sigmoid

Initialize all weights to small random numbers Do until convergence

- For each training example:
	- 1. Input it to the network and compute the network output
	- 2. For each output unit k , o_k is the output of unit k

$$
\delta_k \leftarrow o_k (1 - o_k)(t_k - o_k)
$$

3. For each hidden unit j , o_j is the output of unit j

$$
\delta_j \leftarrow o_j(1 - o_j) \sum_{k \in next \ layer} w_{k,j} \delta_k
$$

4. Update each network weight, where x_i is the output for unit i

$$
w_{j,i} \leftarrow w_{j,i} + \eta \delta_j x_i
$$

• Error function
$$
E = \frac{1}{2} \sum_{k} (y_k - t_k)^2
$$

\n• $\delta_k^{(2)} = (t_k - y_k) y_k (1 - y_k)$
\n• $\Rightarrow w_{k,j}^{(2)} \leftarrow w_{k,j}^{(2)} + \eta \delta_k^{(2)} h_j^{(1)}$
\n• $\delta_j^{(1)} = h_j^{(1)} (1 - h_j^{(1)}) \sum_{k} w_{k,j}^{(2)} \delta_k^{(2)}$
\n• $\Rightarrow w_{j,m}^{(1)} \leftarrow w_{j,m}^{(1)} + \eta \delta_j^{(1)} x_m$

See the backpropagation demo

• [https://shuaili8.github.io/Teaching/VE445/L6%20backpropagation%20dem](https://shuaili8.github.io/Teaching/VE445/L6 backpropagation demo.html) o.html

Formula example for backpropagation

Formula example for backpropagation (cont.)

Calculation example

• Consider the simple network below:

- Assume that the neurons have sigmoid activation function and
	- Perform a forward pass on the network and find the predicted output
	- Perform a reverse pass (training) once (target = 0.5) with $\eta = 1$
	- Perform a further forward pass and comment on the result

Calculation example (cont.)

Answer:

 (i) Input to top neuron = $(0.35x0.1)+(0.9x0.8)=0.755$. Out = 0.68. Input to bottom neuron = $(0.9x0.6)+(0.35x0.4) = 0.68$. Out = 0.6637. Input to final neuron = $(0.3x0.68)+(0.9x0.6637) = 0.80133$. Out = 0.69.

 (ii)

Output error $\delta = (t - 0)(1 - 0) = (0.5 - 0.69)(1 - 0.69)0.69 = -0.0406$.

New weights for output layer $w1^+$ = w1+(δ x input) = 0.3 + (-0.0406x0.68) = 0.272392. $w2^+$ = w2+(δ x input) = 0.9 + (-0.0406x0.6637) = 0.87305.

Errors for hidden layers: δ 1 = δ x w1 = -0.0406 x 0.272392 x (1-o)o = -2.406x10⁻³ δ 2= δ x w2 = -0.0406 x 0.87305 x (1-o)o = -7.916x10⁻³

New hidden layer weights: $w3^+=0.1 + (-2.406 \times 10^{-3} \times 0.35) = 0.09916.$ $w4^+=0.8 + (-2.406 \times 10^{-3} \times 0.9) = 0.7978.$ $\text{w5}^+=0.4 + (-7.916 \times 10^{-3} \times 0.35) = 0.3972.$ $\text{w6}^+ = 0.6 + (-7.916 \times 10^{-3} \times 0.9) = 0.5928.$

 (iii) Old error was -0.19. New error is -0.18205. Therefore error has reduced. • For each output unit k , o_k is the output of unit k

$$
\delta_k \leftarrow o_k(1-o_k)(t_k-o_k)
$$

• For each hidden unit j , o_j is the output of unit *i*

$$
\delta_j \leftarrow o_j(1 - o_j) \sum_{k \in next \ layer} w_{k,j} \delta_k
$$

• Update each network weight, where x_i is the input for unit $$

$$
w_{j,i} \leftarrow w_{j,i} + \eta \delta_j x_i
$$

Calculation example (cont.)

- Answer (i)
	- Input to top neuron = $0.35 \times 0.1 + 0.9 \times 0.8 = 0.755$. Out=0.68
	- Input to bottom neuron = $0.35 \times 0.4 + 0.9 \times 0.6 = 0.68$. Out= 0.6637
	- Input to final neuron = $0.3 \times 0.68 + 0.9 \times 0.6637 = 0.80133$. Out= 0.69
- (ii) It is both OK to use new or old weights when computing δ_j for hidden units
	- Output error $\delta = (t \rho)\rho(1 \rho) = (0.5 0.69) \times 0.69 \times (1 0.69) = -0.0406$
	- Error for top hidden neuron $\delta_1 = 0.68 \times (1 0.68) \times 0.3 \times (-0.0406) = -0.00265$
	- Error for top hidden neuron $\delta_2 = 0.6637 \times (1 0.6637) \times 0.9 \times (-0.0406) = -0.008156$
	- New weights for the output layer
	- $W_{01} = 0.3 0.0406 \times 0.68 = 0.272392$
	- $W_{0.2} = 0.9 0.0406 \times 0.6637 = 0.87305$
	- New weights for the hidden layer
	- $W_{1A} = 0.1 0.00265 \times 0.35 = 0.0991$
	- $W_{1B} = 0.8 0.00265 \times 0.9 = 0.7976$
	- $W_{2A} = 0.4 0.008156 \times 0.35 = 0.3971$
	- $W_{2B} = 0.6 0.008156 \times 0.9 = 0.5927$

- Input to top neuron = $0.35 \times 0.0991 + 0.9 \times 0.7976 = 0.7525$. Out=0.6797
- Input to bottom neuron = $0.35 \times 0.3971 + 0.9 \times 0.5927 = 0.6724$. Out= 0.662
- Input to final neuron = $0.272392 \times 0.6797 + 0.87305 \times 0.662 = 0.7631$. Out= 0.682
- New error is -0.182 , which is reduced compared to old error -0.19

• For each output unit k , o_k is the output of unit k

$$
\delta_k \leftarrow o_k(1-o_k)(t_k-o_k)
$$

• For each hidden unit j , o_j is the output of unit *i*

$$
\delta_j \leftarrow o_j(1 - o_j) \sum_{k \in next \ layer} w_{k,j} \delta_k
$$

• Update each network weight, where x_i is the input for unit $$

 $w_{i,i} \leftarrow w_{i,i} + \eta \delta_i x_i$

 \bullet (iii)

More on backpropagations

- It is gradient descent over entire network weight vectors
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
	- In practice, often work well (can run multiple times)
- Often include weight momentum α $\Delta w_{i,i}(n) \leftarrow \eta \delta_i x_i + \alpha \Delta w_{i,i}(n-1)$
- Minimizes error over *training* examples
	- Will it generalize well to unseen examples?
- Training can take thousands of iterations, slow!
- Using network after training is very fast

An Training Example

Network structure

- What happens when we train a network?
- Example:

Input and output

• A target function:

• Can this be learned?

Learned hidden layer

Convergence of sum of squared errors

Hidden unit encoding for 01000000

Convergence of first layer weights

Convergence of backpropagation

- Gradient descent to some local minimum
	- Perhaps not global minimum
	- Add momentum
	- Stochastic gradient descent
	- Train multiple nets with different initial weights
- Nature of convergence
	- Initialize weights near zero
	- Therefore, initial networks near-linear
	- Increasingly approximate non-linear functions as training progresses

Expressiveness of neural nets

- Boolean functions:
	- Every Boolean function can be represented by network with single hidden layer
	- But might require exponential (in number of inputs) hidden units
- Continuous functions:
	- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer
	- Any function can be approximated to arbitrary accuracy by network with two hidden layers

Tensorflow playground

• <http://playground.tensorflow.org/>

Overfitting

Two examples of overfitting

Avoid overfitting

- $E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{kd} o_{kd})^2 + \left| \gamma \sum_{i,j} w_{ji}^2 \right|$ • Penalize large weights:
- Train on target slopes as well as values:

$$
E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} \left[(t_{kd} - o_{kd})^2 + \mu \sum_{j \in inputs} \left(\frac{\partial t_{kd}}{\partial x_d^j} - \frac{\partial o_{kd}}{\partial x_d^j} \right)^2 \right]
$$

- Weight sharing
	- Reduce total number of weights
	- Using structures, like convolutional neural networks
- Early stopping
- Dropout **61**

Applications

Autonomous self-driving cars

• Use neural network to summarize observation information and learn path planning

Autonomous self-driving cars (cont.)

A recipe for training neural networks

- By Andrej Karpathy
- <https://karpathy.github.io/2019/04/25/recipe/>