Primer: introduction to Artificial Neural Networks

Lecture 8.1 by Marina Barsky An idea is inspired by the science of the brain

How computer works



Inputs

How brain works: neurons

Neuron is an electrically excitable cell that processes and transmits information by electrical and chemical signaling.



Mathematical model of a neuron (McCulloch and Pitt, 1943)



Input "neurons"



 An input vector x is the data given as one input to the processing "neuron" (corresponds to afferent neurons that transmit information to the brain).

How real neurons communicate

- The signal is transmitted to other neurons through *synapses*.
- The physical and neurochemical characteristics of each synapse determine the strength and polarity of the new input signal.
- This is where the brain is the most flexible: *neuroplasticity*.



Real neurons: signal summation

- **Dendrite(s)** receive an electric charge.
- The strengths of all the received charges are added together (spatial and temporal summation).
- The aggregate value is then passed to the soma (cell body) to axon hillock.



Real neurons: activation threshold

• If the aggregate input is greater than the axon hillock's threshold value, then the neuron *fires*, and an output signal is transmitted down the axon.



Real neurons: the output signal is constant

- The strength of the output is constant, regardless of whether the input was just above the threshold, or a hundred times as great.
- This uniformity is critical in an analogue device such as a brain where small errors can snowball, and where error correction is more difficult.

Modeling brain with networks

- The complicated biological phenomena may be modeled by a very simple model: nodes model neurons and edges model connections.
- The input nodes each have a weight that they contribute to the neuron, if the input is active. This corresponds to the strength of a synaptic connection.



Model: signal strength (weights)



 Weights w_i, are the weighted connections between input neurons and the processing neuron (these weights model the strength of synaptic connections in the brain).

Model: processing "neuron" - signal summation



• The summation function IN sums all the signals from the input vector multiplied by weights, and feeds the result into activation function g.

Model: output "neuron"

Weights vector (W)



- The output **y**, shows the resulting action of processing neuron: neuron fires(1) or not(0).
- We can write **y**(**x**, **W**) to remind that the output depends on the inputs to the algorithm and the current set of weights of the network.

Model: activation threshold



- The activation function $g(\cdot)$ is a mathematical function that describes the firing of the neuron as a response to the weighted inputs.
- As in real brain, this is a threshold function: neuron either fires, or not.

Simple threshold: sign



Model: the goal – predict y



- The model can be used to **predict a target variable y given input vector x**.
- Each input dimension (attribute) can be considered a separate input "neuron"
- Processing happens in the "axon" and based on the result the output neuron "fires" (or not)

Model: multiple predictions



- Conceptually there is no difference between input and output neurons
- So the same input vector can be used to activate multiple output "neurons", using a different set of weights

Let's build some neural networks

Networks that know the meaning of lights

Predicting smiles





Dataset

- We record people's reaction to lights into a table (dataset)
- Can we set up a single network which when presented with a combination of lights will correctly predict if a person will smile?
- Setting up the network means labeling the edges with correct weights

Bias node

- When we are presenting the network with combination [0, 0] then the weights do not matter: the data vector [0,0] is ignored by the network
- To prevent this information loss, we add to the input a special *bias node* which always has a constant value, and we assign to it weight *b*



red	ora	orange		е
\bigcirc	(\bigcirc	neg	
\bigcirc			pos	
	(\bigcirc	pos	
			pos	
	x ₁	x ₂	у	
	0	0	0	
	0	1	1	
	1	0	1	
	1	1	1	

Network that predicts smiles

Assigning sample weights







Network that predicts smiles

Checking correctness of predictions







Predicting two outputs







There is no conceptual difference between input and output nodes

Predicting both smiles and stops



orange

We already know that this prediction is correct: $y_1([0,0]) = -0.5(-)$ $y_1([0,1]) = 1 - 0.5 = 0.5(+)$ $y_1([1,0]) = 1 - 0.5 = 0.5(+)$ $y_1([1,1]) = 2 - 0.5 = 1.5(+)$



red	orange	stop
\bigcirc	\bigcirc	neg
\bigcirc		neg
	\bigcirc	neg
		pos

Predicting both smiles and stops



orange

We already know that this prediction is correct: $y_1([0,0]) = -0.5(-)$ $y_1([0,1]) = 1 - 0.5 = 0.5(+)$ $y_1([1,0]) = 1 - 0.5 = 0.5(+)$ $y_1([1,1]) = 2 - 0.5 = 1.5(+)$



red	orange	stop
\bigcirc	\bigcirc	neg
\bigcirc		neg
	\bigcirc	neg
		pos

Predicting both smiles and stops





red	orange	stop
\bigcirc	\bigcirc	neg
\bigcirc		neg
	\bigcirc	neg
		pos

We have built the system that recognizes OR and AND

Truth table for OR

Apply *sign* function to the output



Can we build a system that recognizes: x₁ AND NOT x₂?



Truth table for AND NOT

x ₁	x ₂	у
0	0	0
0	1	0
1	0	1
1	1	0

System that recognizes: $x_1 AND NOT x_2$



Truth table for AND NOT

x ₁	x ₂	у
0	0	0
0	1	0
1	0	1
1	1	0

System that recognizes: $x_1 AND NOT x_2$



y([0,0]) = sign(-0.5) = 0 y([0,1]) = sign(0 - 1 - 0.5) = 0 y([1,0]) = sign(1 + 0 - 0.5) = 1y([1,1]) = sign(1 - 1 - 0.5) = 0 Truth table for AND NOT



How about: NOT $(x_1 AND x_2)$



Truth table for NOT AND

x ₁	x ₂	у
0	0	1
0	1	1
1	0	1
1	1	0

System that recognizes: NOT $(x_1 AND x_2)$



y([0,0]) = sign(1.5) = 1y([0,1]) = sign(-1 + 1.5) = 1y([1,0]) = sign(-1 + 1.5) = 1y([1,1]) = sign(-2 + 1.5) = 0 Truth table for NOT AND

x ₁	x ₂	у
0	0	1
0	1	1
1	0	1
1	1	0

Our network is able to recognize linearly-separable binary classes



Why it works

- The network assumes that there is a linear correlation between the input vector x and the output y
- We just need to discover the equation of the separating line (hyperplane) y=wx +b, which expresses this linear correlation

Can machines learn the network parameters for a given problem automatically?

Yes, by looking at the labeled dataset (supervised learning)

Predict → **Compare** → **Learn** from errors
Neuron with learning capabilities: *Perceptron* (Rosenblatt, 1958)

- The network can learn its own weights
- It is presented with a set of inputs and known outputs
- Originally the predicted output is different from the actual output by some error
- We adjust the connection weights to produce a smaller error



Most basic Perceptron

Adjusting the weights with gradient descent: error



Objective error function - in this case:

$$E = \frac{1}{2} (y - t)^2$$

Cost

The error depends on weight

where y = w*x (predicted value), and t is the actual value of y, known from the labeled dataset

 $\partial E/\partial y = \frac{1}{2}*2(y - t) = y - t$

Adjusting the weights with gradient descent: derivative



$$E = \frac{1}{2} (y - t)^2$$

$$y = w^*x$$

$$\partial E/\partial y = y - t$$

To determine how to change weight w take derivative of E at point w dz = dz dy

$$\Delta = \partial E / \partial w = \partial E / \partial y^* \partial y / \partial w = (w^* x - t)^* x$$

$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}.$$

Chain rule!

If derivative is positive (function on the rise) we need to decrease the weight, if it is negative - we need to increase the weight



Adjusting the weights with gradient descent: delta rule



Delta rule: adjust weight w by Δ w = w - $\partial E/\partial w$ = w - Δ = w - (w*x - t)*x

More input dimensions - more weights to adjust

The network transforms input feature vector into target using two weights

The principle is the same:



 $E = \frac{1}{2} (w_1^* x_1 + w_2^* x_2 - t)^2$

Which weight contributed more to the error? Partial derivatives with respect to each weight: $\partial E/\partial w_1 = (w_1^*x_1 - t)^*x_1$

 $\partial E/\partial w_2 = (w_2^* x_2 - t)^* x_2$

Delta rules: update weights

$$w_1 = w_1 - \partial E / \partial w_1$$
$$w_2 = w_2 - \partial E / \partial w_2$$



There is also a bias node, of course

Objective function: $E = \frac{1}{2} (w_1 * x_1 + w_2 * x_2 + b - t)^2$ $\partial E/\partial w_1 = (w_1 * x_1 - t) * x_1$ $\partial E/\partial w_2 = (w_2 x_2 - t) x_2$ constant - not depending on the current input vector $\partial E/\partial b = (b^*c - t)^*c$ С b W_1 **X**₁ Delta rule: W_2 X_2 $W_1 = W_1 - \partial E / \partial W_1$ $w_2 = w_2 - \partial E / \partial w_2$

 $b = b - \partial E / \partial b$

Incorporating learning rate η (eta)

 $w_{1} = w_{1} - \eta^{*} \partial E / \partial w_{1}$ $w_{2} = w_{2} - \eta^{*} \partial E / \partial w_{2}$ $b = b - \eta^{*} \partial E / \partial b$

where:

 $\frac{\partial E}{\partial w_1} = (w_1^* x_1 - t)^* x_1$ $\frac{\partial E}{\partial w_2} = (w_2^* x_2 - t)^* x_2$ $\frac{\partial E}{\partial b} = (cb - t)^* c$

Let's try to build a perceptron that recognizes XOR

 $\begin{array}{c|c} 1 & b \\ \hline \\ \hline \\ x_1 & \hline \\ w_2 \\ \hline \\ x_2 \\ \hline \end{array}$



Let's try to build a perceptron that recognizes XOR

Truth table for XOR



This failure caused a major delay in developing the idea of ANN in the 60s

Experiment with *basic perceptron* <u>here</u>

Idea: express XOR through known solutions

 $x_1 XOR x_2 = (x_1 OR x_2) AND (NOT(x_1 AND x_2))$



Add more layers!

 $x_1 XOR x_2 = (x_1 OR x_2) AND (NOT(x_1 AND x_2))$



h ₁ ([0,0]) = - 0.5 (-)	$\rightarrow 0$	h ₂ ([0,0]) = 1.5 (+)	\rightarrow 1	$y([0,0])=(-)\to 0$
$h_1([0,1]) = 1 - 0.5 = 0.5 (+)$	\rightarrow 1	$h_2([0,1]) = -1 + 1.5 = 0.5 (+)$	\rightarrow 1	$y([0,1])=(+)\to 1$
$h_1([1,0]) = 1 - 0.5 = 0.5 (+)$	\rightarrow 1	$h_2([1,0]) = -1 + 1.5 = 0.5 (+)$	\rightarrow 1	$y([1,0])=(+)\to 1$
$h_1([1,1]) = 2 - 0.5 = 1.5 (+)$	\rightarrow 1	$h_{2}([1,1]) = -2 + 1.5 = -0.5(-)$	$\rightarrow 0$	$y([1,1])=(-)\to 0$

Importance of nonlinearity!

$x_1 XOR x_2 = (x_1 OR x_2) AND (NOT(x_1 AND x_2))$



$h_1([0,0]) = -0.5(-) \rightarrow 0$	h ₂ ([0,0]) = 1.5 (+)	\rightarrow 1	$y([0,0])=(-)\to 0$
$h_1([0,1]) = 1 - 0.5 = 0.5 (+) \rightarrow 1$	$h_2([0,1]) = -1 + 1.5 = 0.5 (+)$	\rightarrow 1	$y([0,1])=(+)\to 1$
$h_1([1,0]) = 1 - 0.5 = 0.5 (+) \rightarrow 1$	$h_2([1,0]) = -1 + 1.5 = 0.5 (+)$	\rightarrow 1	$y([1,0])=(+)\to 1$
$h_1([1,1]) = 2 - 0.5 = 1.5 (+) \rightarrow 1$	$h_2([1,1]) = -2 + 1.5 = -0.5(-)$	\rightarrow 0	$y([1,1])=(-)\to 0$

Conclusion: neurons can be combined into multiple layers to create complex shapes from linear separation boundaries



Multi-layer Perceptron (MLP)

- Added: *hidden nodes*
- Organized nodes into layers. Edges are directed and carry weight
- No connections inside the layer!



Multi-layer Perceptron: learning

Objective of learning - did not change: determine the optimal values of weights to separate all labeled instances by a hyperplane



MLP: learning optimal weights



Because we need derivatives: instead of *sign* - use more complex nonlinear functions: **sigmoidal** functions

MLP: learning optimal weights



Because we need derivatives: instead of *sign* - use more complex nonlinear functions: **sigmoidal** functions

Non-linear activation functions

Logistic function (sigmoid)

 $g(h)=rac{1}{1+e^{-2eta h}},$

where β is a positive constant (we generally use $2\beta = 1$ obtaining a standard logistic function)



Sigmoid gives a value in range from 0 to 1. Note: when IN = 0, f = 0.5 We consider all values >0 as positive predictions

Alternatively can use tanh:

 $\tanh x = \frac{\sinh x}{\cosh x} = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{e^{2x} - 1}{e^{2x} + 1}$ which has the same shape as sigmoid but in range -1 to 1.

More recently - *rectified linear units* (**ReLU**): $f(x) = x^+ = \max(0, x)$ This function is 0 for negative argument values, and some units will yield activations 0, making networks sparse. Moreover, the gradient is particularly simple—either 0 or 1.

MLP learning algorithm

Training the MLP consists of **two parts**:

- Working out what the outputs are for the given inputs and the current weights – Forward phase
- Updating the weights according to the error, which is a function of the difference between the outputs and the targets – Backward phase

Forward: prediction



Forward phase: 1. input-to-hidden layer: summation



 $h_{1} = w_{1}^{*}x_{1} + w_{2}^{*}x_{2} + b_{1}$ $h_{2} = w_{3}^{*}x_{1} + w_{4}^{*}x_{2} + b_{2}$

Forward phase: 2. input-to-hidden layer: activation



 $h_{1} = w_{1}^{*}x_{1} + w_{2}^{*}x_{2} + b_{1}$ $h_{2} = w_{3}^{*}x_{1} + w_{4}^{*}x_{2} + b_{2}$ $g_{1} = \sigma(h_{1})$ $g_{2} = \sigma(h_{2})$

Forward phase: 3. hidden-to-output layer: prediction



 $h_{1} = w_{1}^{*}x_{1} + w_{2}^{*}x_{2} + b_{1}$ $h_{2} = w_{3}^{*}x_{1} + w_{4}^{*}x_{2} + b_{2}$ $g_{1} = \sigma(h_{1})$ $g_{2} = \sigma(h_{2})$ $y = g_{1}^{*}w_{5} + g_{2}^{*}w_{6} + b_{3}$

Step-by-step example initialize weights at random



The input vector **x** = **[1, 4]**, and the actual output **t** = **0.1**

Step-by-step example 1. input to hidden layer: summation



 $h_1 = w_1^* x_1 + w_2^* x_2 + b_1 = 0.5 + 0.1^* 1 + 0.2^* 4 = 1.4$ $h_2 = w_3^* x_1 + w_4^* x_2 + b_2 = 0.5 + 0.3^* 1 + 0.4^* 4 = 2.4$

Step-by-step example 2. input to hidden layer: activation



 $h_{1} = 1.4$ $h_{2} = 2.4$ $g_{1} = \sigma(h_{1}) = 0.8021838885585817481543 \approx 0.80$ $g_{2} = \sigma(h_{2}) = 0.9168273035060776293371 \approx 0.92$ https://keisan.casio.com/exec/system/15157249643325

Step-by-step example 3. hidden-to-output layer: prediction



Step-by-step example compute error



 $h_1 = 1.4$

- $h_2 = 2.4$
- $g_1 = 0.80$
- $g_2 = 0.91$
- y = 1.45

 $E = \frac{1}{2} (1.45 - 0.1)^2 = 0.845$

Error **directly** depends on the weights w_5 , w_6 , and b_3

$$E = \frac{1}{2}(0.80 * w_5 + 0.92w_6 + b_3 - 0.1)^2$$

We try to make it smaller by simultaneously adjusting w_5 , w_6 , and b_3

Backward phase: 4. output-to-hidden weight updates



 $c = y_2(y - t)^2$ $y = g_1^* W_5 + g_2^* W_6 + b_3$ To find how to update w_5 , w_6 , and b_3 Partial derivatives:

 $\partial E/\partial w_5 = \partial E/\partial y^* \partial y/\partial w_5 = (y - t)^* g_1$ $\partial E/\partial w_6 = (y - t)^* g_2$ $\partial E/\partial b_3 = (y - t)^* 1$

Step-by-step example 4. output-to-hidden weight updates



Step-by-step example 4. output-to-hidden weight updates



Step-by-step example 4. output-to-hidden weight updates



Backward phase: 5. hidden-to-output weight updates



Error function E **indirectly** depends on w_1 , w_2 , w_3 , w_4 , b_1 , b_2 To find the contribution of each variable: partial derivatives For example:

$$\partial E/\partial w_1 = \partial E/\partial y^* \partial y/\partial g_1^* \partial g_1/\partial w_1$$

$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}.$$
Chain rule!

Backward phase: 5. hidden-to-output weight updates



Computing delta for w₁ $\partial E/\partial w_1 = \partial E/\partial y^* \partial y/\partial g_1^* \partial g_1/\partial w_1$ $E(y) = \frac{1}{2}(y-t)^2 \rightarrow \qquad \partial E/\partial y = y-t$ $y(g_1) = g_1^* w_5 + g_2^* w_6 + b_3 \rightarrow \qquad \partial y/\partial g_1 = w_5$ $g_1(w_1) = \sigma(h_1) = \sigma(w_1^* x_1 + w_2^* x_2 + b_1) \rightarrow \qquad \partial g_1/\partial w_1 = g_1^* (1 - g_1)^* x_1$

Backward phase: 5. hidden-to-output weight updates



Computing delta for w_1

 $\frac{\partial E}{\partial w_1} = \frac{\partial E}{\partial y^* \partial y} \frac{\partial g_1^* \partial g_1}{\partial w_1}$ $\Delta = \frac{\partial E}{\partial w_1} = (y - t)^* w_5^* g_1^* (1 - g_1)^* x_1$

 $w_1 = w_1 - \eta \Delta$
Step-by-step example 5. hidden-to-output weight update for w₁



Role of nonlinearity



- Somewhere inside the hidden layer we <u>must</u> have a mechanism which will ignore some correlations
- Otherwise the network will serve as a basic linear separator and be no better than a single-layer perceptron

Experiment with *multi-layer-perceptron* <u>here</u>

Multi-layer perceptron: vanilla (basic) neural networks



What do we gain from the extra layers



1st layer draws linear boundaries



2nd layer combines the boundaries



3rd layer can generate arbitrarily complex boundaries

Very powerful model

- With sigmoidal activation function we can show that a 3layer net can approximate any function to arbitrary accuracy: property of Universal Approximation
- Proof by thinking of superposition of sigmoids
- Not practically useful as we might need arbitrarily large number of neurons more of an existence proof
- Same is true for a 2-layer net providing function is continuous and from one finite dimensional space to another

Universal Approximation Theorem

For any given constant ε and continuous function $h(x_1, \dots, x_m)$, there exists a three-layer ANN with the property that

$$|h(x_{1},...,x_{m}) - H(x_{1},...,x_{m})| < \varepsilon$$

where $H(x_1, ..., x_m) = \sum_{i=1}^{k} a_i f(\sum_{j=1}^{m} w_{ij}x_j + b_i)$

Applications of ANNs

- Credit card frauds
- Kinect gesture recognition
- Facial recognition
- Self-driving cars
- ...

Example: breast cancer diagnosis

• Dataset:

https://archive.ics.uci.edu/ml/data sets/Breast+Cancer+Wisconsin+(Di agnostic)

- Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass
- Diagnosing breast cancer from mammograms is a very hard nontrivial task



Run and see how MLP learns to diagnose breast cancer

Make computers as capable as humans?

Brain is a highly complex, non-linear, massively-parallel system

- Response of integrated response circuit: 1 nanosecond = 10⁻⁹sec
- Response of neuron:
 - 1 millisecond = 10^{-3} sec

The only advantage of the brain: massively parallel – 10 billion neurons with 60 trillions of connections working together

Artificial neural network is an abstract idea – media-independent

- To simulate the brain we could theoretically construct thousands of circuits working in parallel
- We can simulate them using a program that is executed on a conventional serial processor
- The solutions are *theoretically* equivalent
- We can simulate the neural behavior by a virtual machine which is functionally identical to a real machine that currently is prohibitively complex and expensive to build