Neural Networks

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Morning Objectives

This morning's objectives are:

- Know the best use cases for neural networks
- Know the benefits and drawbacks of using a neural network
- Build a simple neural network for binary classification
- Train a neural network using backpropagation

Background

Neural Networks were introduced in the 1950's as a model which mimics the human brain.

- Biological neurons "fire" at a certain voltage threshold
- An artificial neuron will be modeled by an activation function like sign, the sigmoid function, or tanh
- Otherwise, not a good analogy
  - Don't think of neural networks as models for a brain

Why Neural Networks?

Pros:

- Works well with high dimensional data:
  - images
  - text
  - audio
- Can model *arbitrarily* complicated decision functions

Cons:

- Not interpretable
- Slow to train
- Easy to overfit
- Difficult to tune
  - Many parameters/choices when building the network

Example: Logistic Regression (1/3)

Recall logistic regression:

- Input $\mathbf{x}$
- Weights $\mathbf{w}$
- $\sigma(z) = \frac{1}{1+e^{-z}}$
- Classify $\mathbf{x}$ as positive if $\sigma(\mathbf{w}^T\mathbf{x}) > 0.5$
- Think of σ as an *activation function* which *activates* if the input is larger than 0

Example: Logistic Regression (2/3)

Draw logistic regression schematically as

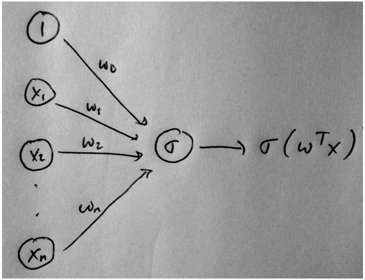


Figure 1:Logisitic Regression

Think of the diagram as having two *layers*

- Input layer: The nodes which hold the inputs $1, x_1, x_2, \dots, x_n$
- Output layer: The single node that holds the output value
- The weights $w_0, w_1, \dots, w_n$ transition between the two layers

Example: Logisitic Regression (3/3)

The hypothesis $h(\mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^T\mathbf{x})$ only models linear decision functions.

- The decision boundary is the set of points where $\mathbf{w}^T\mathbf{x} = 0$, a hyperplane
- What about more complicated behavior?

Example: Neural Network with Multiple Layers (1/2)

Consider the following network with 4 layers:

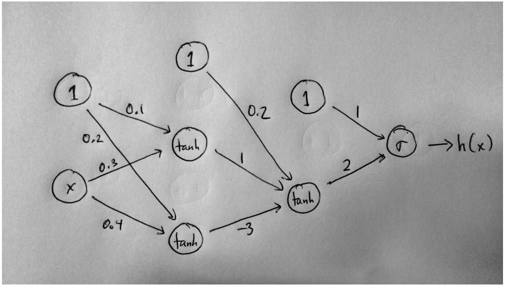


Figure 2:NN with Multiple Layers

- Input (layer 0): Contains the input value x and a bias term 1
- Two *hidden layers* (layers 1 and 2)
- Output (layer 3): Contains the output value (probability of positive classification)

Example: Neural Network with Multiple Layers (2/2)

Let's compute the output of the network for $x = 3$. We'll go layer by layer to keep things straight:

- Layer 1:
  - The first non-bias node is $\tanh((0.1)(1) + (0.3)(3)) = 0.76$
  - The second non-bias node is $\tanh((0.2)(1) + (0.4)(3)) = 0.89$
- Layer 2:
  - The non-bias node is $\tanh((0.2)(1) + (1)(0.76) + (-3)(0.89)) = -0.94$
- Output:
  - The value of the output layer is $\sigma((1)(1) + (2)(-0.94)) = 0.29$

So $h(3) = 0.29$ for this example.

Check for Mastery

Compute the output of the this neural network for $x = 1$.

Why tanh?

The hyperbolic tangent function is commonly used as an *activation function* in hidden layers:

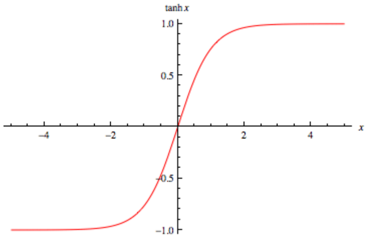


Figure 3:tanh

- Smooth (differentiable), unlike sign
- $\tanh(z) = 2\sigma(2z) - 1$
  - Same shape as the sigmoid function
  - Output values centered around 0
- $\tanh'(z) = 1 - \tanh^2(z)$

Check for Mastery

Why do you think the fact that the value of tanh being centered around 0 is important?

Let's Keep it Simple For Now

Since this is some heavy-duty stuff, let's keep things as simple as possible while still trying to grasp the general picture:

- Stick to networks for binary classification (a single output node)
- The output node will use the sigmoid activation function σ
- Hidden layers will use the tanh activation function
- θ will always represent an activation function (like sign, tanh, σ, or something else like a rectifier)

Notation (1/2)

We need a way to write down the network mathematically to do anything with it. As a warning, this can get quite messy:

- Layers are given by indices $0, 1, 2, \ldots, L$ where 0 is the input layer, and L is the output layer
- For each layer ℓ:
  - $\mathbf{s}^{(\ell)}$ is the $d^{(\ell)}$-dimensional input vector
  - $\mathbf{x}^{(\ell)}$ is the $d^{(\ell)} + 1$-dimensional output vector
  - $W^{(\ell)}$ is the $d^{(\ell-1)} + 1 \times d^{(\ell)}$ matrix of input weights. $W_{ij}^{(\ell)}$ is the weight of the edge from the i-th node in layer $\ell - 1$ to the j-th node in ℓ

Notation (2/2)

If we zoom in to a single node in a single layer, the picture looks like:

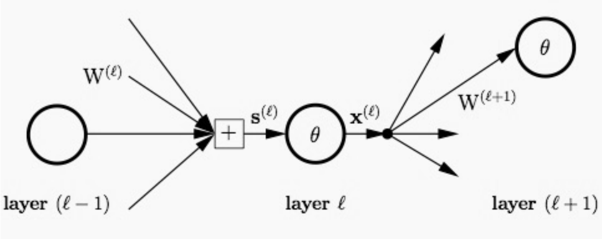


Figure 4:Artificial Neuron Schematic

Schematic

In general, neural networks look something like

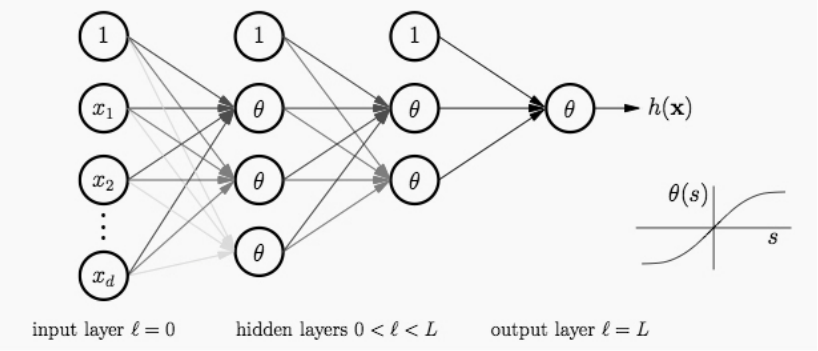


Figure 5:Neural Network

Example: Notation in Toy Network from Before (1/2)

Let's go back to our earlier example to clear up as much confusion as possible:

- $\mathbf{x}^{(0)}$ is $\begin{bmatrix} 1 \\ 3 \end{bmatrix}$
- $\mathbf{s}^{(1)}$ is the result of applying the weights on the edges between layer 0 and 1:

$$\begin{bmatrix} (0.1)(1) + (0.3)(3) \\ (0.2)(1) + (0.4)(3) \end{bmatrix} = \begin{bmatrix} 1 \\ 1.4 \end{bmatrix}$$

- $W^{(1)} = \begin{bmatrix} 0.1 & 0.2 \\ 0.3 & 0.4 \end{bmatrix}$
- $\mathbf{x}^{(1)}$ is the output of layer 1 after applying tanh and adding a bias node:

$$\begin{bmatrix} 1 \\ \tanh(1) \\ \tanh(1.4) \end{bmatrix} = \begin{bmatrix} 1 \\ 0.76 \\ 0.89 \end{bmatrix}$$

Example: Notation in Toy Network from Before (2/2)

Continuing:

- $\mathbf{s}^{(2)} = \begin{bmatrix}(0.2)(1) + (1)(0.76) + (-3)(0.89)\end{bmatrix} = \begin{bmatrix}-1.71\end{bmatrix}$
- $W^{(2)} = \begin{bmatrix}0.2 \\ 1 \\ -3\end{bmatrix}$
- $\mathbf{x}^{(2)} = \begin{bmatrix}1 \\ \tanh(-1.71)\end{bmatrix} = \begin{bmatrix}1 \\ -0.94\end{bmatrix}$
- $\mathbf{s}^{(3)} = \begin{bmatrix}(1)(1) + (2)(-0.94)\end{bmatrix} = \begin{bmatrix}-0.88\end{bmatrix}$
- $W^{(3)} = \begin{bmatrix}1 \\ 2\end{bmatrix}$
- $\mathbf{x}^{(3)} = \begin{bmatrix}\sigma(-0.88)\end{bmatrix} = \begin{bmatrix}0.29\end{bmatrix}$

Check for Mastery

What are $\mathbf{x}^{(2)}$ and $\mathbf{s}^{(2)}$ when $x = 1$?

Forward Propagation (1/2)

Studying the above example gives general formulae for computing the output of a neural network with fixed weights:

- $\mathbf{x}^{(\ell)} = \begin{bmatrix} 1 \\ \theta(\mathbf{s}^{(\ell)}) \end{bmatrix}$
- $\mathbf{s}^{(\ell)} = (W^{(\ell)})^T \mathbf{x}^{(\ell-1)}$

So we get the chain:

$$\mathbf{x}^{(0)} \xrightarrow{W^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{W^{(2)}} \mathbf{s}^{(2)} \cdots \rightarrow \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}^{(0)})$$

Forward Propagation (2/2)

This chain of transformations is called the *forward propagation* algorithm.

Check for Mastery

In terms of the number of nodes V and weights E, what is the algorithmic complexity of forward propagation (in Big-O notation)?

Backpropagation (1/4)

We now know how NNs with fixed weights make predictions. But how do we train a neural network?

- Training data $\{(\mathbf{x_i}, y_i\}$
- Need to minimize some error function E on our training set over the weights $\mathbf{w} = (W^{(1)}, \ldots, W^{(L)})$
  - We'll use
    $$E(\mathbf{w}) = \frac{1}{N} \sum_i (h(\mathbf{x_i}; \mathbf{w}) - y_i)^2$$
    (mean squared error)
- This function can be *extremely* complicated to write algebraically
  - No closed form solution for minima

Check for Mastery

What tool/tools do we have available to find the minimum value?
Why don't we use sign as an activation function?

Backpropagation (2/4)

Train a neural network using a gradient descent algorithm called *backpropagation*:

- Recall the update step in gradient descent:

$$\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \nabla E(\mathbf{w}(t))$$

- Our total error is a sum of the errors e_n on each input $E(\mathbf{w}) = \frac{1}{N}\sum e_i$
  - $e_i = (h(\mathbf{x_i}; \mathbf{w}) - y_i)^2$
  - $\dfrac{\partial E}{\partial W^{(\ell)}} = \dfrac{1}{N} \sum \dfrac{\partial e_n}{\partial W^{(\ell)}}$
  - Can consider one data point at a time and add the results to get the total gradient

Backpropagation (3/4)

Backpropagation uses the chain rule to compute the partial derivatives of layer ℓ in terms of layer $\ell + 1$.

- The *sensitivity vector* of layer ℓ is

$$\delta^{(l)} = \frac{\partial e}{\partial \mathbf{s}^{(\ell)}}$$

- Then we can compute

$$\frac{\partial e}{\partial W^{(\ell)}} = \mathbf{x}^{(l-1)}(\delta^{(\ell)})^T$$

- For j in $1, \ldots, d^{(\ell)}$

$$\delta_j^{(\ell)} = \theta'(\mathbf{s}^{(\ell)})_j \times [W^{(\ell+1)}\delta^{(\ell+1)}]_j$$

Backpropagation (4/4)

- Can compute $\delta^{(\ell)}$ from $\delta^{(\ell+1)}$
- Must still compute $\delta^{(L)}$ to seed the process
  - Depends on the error function and the output activation function
  - In our case

$$\delta^{(L)} = 2(h(\mathbf{x_i}; \mathbf{w}) - y_i)h(\mathbf{x_i}; \mathbf{w})(1 - h(\mathbf{x_i}; \mathbf{w}))$$

- $W^{(\ell)} = W^{(\ell)} - \eta \frac{\partial E}{\partial W^{(\ell)}}$

Example: Backpropagation

Suppose our observation is $x = 2, y = 1$

- $\mathbf{x}^{(0)} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$; $\mathbf{s}^{(1)} = \begin{bmatrix} 0.1 & 0.3 \\ 0.2 & 0.4 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 0.7 \\ 1 \end{bmatrix}$; $\mathbf{x}^{(1)} = \begin{bmatrix} 1 \\ 0.6 \\ 0.76 \end{bmatrix}$
- $\mathbf{s}^{(2)} = \begin{bmatrix} -1.48 \end{bmatrix}$; $\mathbf{x}^{(2)} = \begin{bmatrix} 1 \\ -0.90 \end{bmatrix}$
- $\mathbf{s}^{(3)} = \begin{bmatrix} -0.8 \end{bmatrix}$; $\mathbf{x}^{(3)} = \begin{bmatrix} 0.31 \end{bmatrix}$

Example: Backpropagation

Backpropagation gives:

- $\delta^{(3)} = 2(0.31 - 1)(0.31)(1 - 0.31) = -0.30$;
  $\delta^{(2)} = (1 - 0.9^2)(2)(-0.30) = -0.114$; $\delta^{(1)} = \begin{bmatrix} -0.104 \\ 0.188 \end{bmatrix}$

Now we can find the partial derivatives

- $\frac{\partial e}{\partial W^{(1)}} = \mathbf{x}^{(0)}(\delta^{(1)})^T = \begin{bmatrix} -0.104 & 0.188 \\ -0.208 & 0.376 \end{bmatrix}$;
  $\frac{\partial e}{\partial W^{(2)}} = \mathbf{x}^{(1)}(\delta^{(2)})^T = \begin{bmatrix} -0.69 \\ -0.42 \\ -0.53 \end{bmatrix}$;
  $\frac{\partial e}{\partial W^{(3)}} = \mathbf{x}^{(2)}(\delta^{(3)})^T = \begin{bmatrix} -1.85 \\ 1.67 \end{bmatrix}$

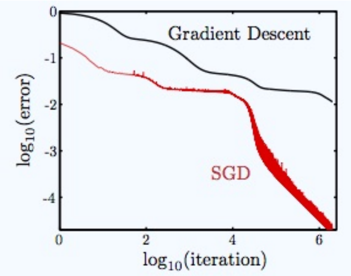
Stochastic Gradient Descent

Backpropagation finds the gradient at each observation, adds then up to find the total gradient

- $\nabla E(\mathbf{w}) = \frac{1}{N} \sum_i \nabla e_i(\mathbf{w})$
- $\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \nabla E(\mathbf{w}(t))$

Instead, update weights at each observation

- $\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \nabla e_i(\mathbf{w}(t))$



Afternoon Objectives

This afternoon's objectives are:

- Understand how neural networks can be used for regression and multi-class classification by using different loss functions and output activations
- Explain the properties/pros/cons of different activation functions
- Explain some methods to avoid overfitting
- Learn about some more complicated versions of neural networks
- Use Keras to build neural networks in Python

References

Books

- Y. S. Abu-Mostafa, M. Magdon-Ismail, H.-T. Lin *Learning From Data: A Short Course*