An Undergraduate's Explanation of the Multilayer Perceptron: Mathematical Concepts and a Python3 Implementation

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2022
January

1   Preamble

The purpose of the present document is to explain and implement the major mathematical constructs/concepts behind feedforward neural networks, specifically the multilayer perceptron. This includes the layers that compose such networks, the cost (aka loss, error, or objective) function and activation functions, the forward pass through the network, the computation of gradients via backpropagation (a concept that is often "handwaved" to the extreme or explained in so much detail as to be utterly confusing–at least in the author's experience), and the update of model parameters via mini-batch stochastic gradient descent. If the ideas such as *layer* and *backpropagation* are entirely unfamiliar to you, then the author encourages you to visit 3Blue1Brown's Deep Learning YouTube Series [1] and peruse the first few chapters of texts such as *Deep Learning* (free, online) [2], *Neural Networks and Deep Learning* (free, online) [3], *Hands-on Machine Learning with Scikit-Learn, TensorFlow and Keras 2ed* (buy) [4], and/or *Deep Learning with Python 2ed* (buy) [5]. The present document is not intended to be a comprehensive overview of neural networks nor an extremely in-depth explanation but rather a document that highlights certain concepts that the author found confusing or ambiguous when he was learning about neural networks.

The format of explanations in the present document will essentially alternate between mathematics and concrete implementations using the Python3 programming language with the NumPy library. Note that the implementations here are not intended to be optimal. If you would like optimal implementations, the author encourages you to use a machine learning API such as TensorFlow or PyTorch, the tutorials for which will abstract and make easily usable many of the concepts elucidated in the present document.

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2   Introduction

The neural network (function approximator) is just a chain of geometric transformations (functions) each parametrized by a weight matrix $W \in \mathcal{R}^{n_x \times n_h}$ and a bias vector $b \in \mathcal{R}^{n_h}$ on the input vector $x \in \mathcal{R}^{n_x}$. Note that n_x is the input size (i.e., output size of the previous layer in a network with L total layers) and n_h is the number of hidden units in the current layer. The following paragraphs will elucidate the claims in this sentence and notation.

The author assumes you know what a function is; however, the term *parametrized* is one that appears often in deep learning literature and should be well-understood by the student. Consider a generic quadratic function [6] as

$$f(x) = ax^2 + bx + c \tag{1}$$

The *variable* x is an *argument* to the function f that has *parameters* a, b, and c. The parameters determine the behavior of the function (e.g., the steepness of slope, intercepts, shape, etc.) while the variable can take on some range of values. When a variable that takes on a particular value is passed as an argument to the function with defined parameters, the result is some other value y if $y = f(x)$. This explanation of a function should not be anything new; however, the *parameters* are quantities of particular interest for neural networks since the parameters are the quantities that are *learned* by the neural network over time. What it means to learn parameters will be explaned later.

A neural network can be denoted as a function h with parameters W and b of a variable x. This statement can be compactly written as $h_{W,b}(x)$. The subscript with W and b means that the weights W and biases b are parameters of the neural network h. The claim that a neural network is a chain of functions is useful later during the updating of the parameters of the network. But to briefly illustrate the idea of chaining functions, the generic quadratic function in Equation 1 is decomposed into units called *atomic functions*.

$$g_a(x) = ax^2 \tag{2}$$
$$u_b(x) = bx \tag{3}$$
$$f_{a,b,c}(x) = g_a(x) + u_b(x) + c \tag{4}$$

The input x is not a single value as is conceived in the elementary formulations described above. Rather, the input x is a list of values referred to as a *column vector*. Each element of the vector is the value a particular feature, or independent variable, could take on. The shape of the vector x is important to understand since the functions and operations performed by the neural network (dot product, Hadamard product, addition, etc.) restrict their vector/matrix operands to particular shapes. When using the term *vector*, the author is always referring to a *column vector* unless otherwise specified. Also, note that $x \in \mathcal{R}^{n_x}$ indicates that x is a vector with n_x elements and the jth is a real number. For example, the below vector x is shown and a common vector operation known as transposition (converts a *column vector* to a *row vector* and is denoted with

a superscript of $\top$) is also shown.

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{(n_x)} \end{bmatrix} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_{(n_x-1)} \end{bmatrix} = \begin{bmatrix} x_0 & x_1 & x_2 & \cdots & x_{(n_x-1)} \end{bmatrix}^\top \tag{5}$$

Many programming languages assign the first element of a vector the index 0; this notation is shown above in addition to the more standard mathematical notation where the first element begins with the index 1. For the remainder of this document, the author will use the index 0 assumption since the author's implementation of the the neural network will use the Python programming language. If you wish to implement the same algorithms in a language such as R or Wolfram Mathematica, be wary of this index discrepancy.

Lastly, a weight matrix W_{jk} has weight edges between the kth input neuron and the jth hidden neuron of n_h total hidden neurons.

3 Equations

Here the author defines the operations that occur for a multilayer perceptron (MLP). Note that the MLP can sometimes refer to any class of feedforward neural network, that is a network that applies affine transformations and activation functions to input from a previous layer in the network. The affine transformation is simply $xW^\top + b$.

3.1 Single Hidden Layer Neural Network

$$\begin{aligned} NeuralNet_\theta(X) &= \sigma(ReLU(XW^{[1]} + b^{[1]})W^{[2]} + b^{[2]}) \\ &= \sigma(g(ReLU(w(X)))) \\ A^L &= NeuralNet_\theta(X) \qquad \text{Activation matrix } A \text{ for last layer } L \end{aligned} \tag{6}$$

where σ, $ReLU$, g, and w are defined as follows:

$$\begin{aligned} \sigma(t) &= \frac{1}{1 + e^{-t}} \\ ReLU(t) &= max(0, t) \\ g_{\theta^{[2]}}(A) &= AW^{[2]} + b^{[2]} \\ w_{\theta^{[1]}}(A) &= AW^{[1]} + b^{[1]} \\ u_{\theta^{[l]}}(A) &= AW^{[l]} + b^{[l]} \quad \text{General form of } g \text{ and } w \text{ for } l^{th} \text{ layer} \end{aligned} \tag{7}$$

3.2 Neural Network Prediction (Forward Pass)

$$\hat{y} \leftarrow NeuralNet_\theta(X) \tag{8}$$

3.3 Mean Squared Error Loss Function

$$\mathcal{L}_\theta(X) = \frac{1}{N} \sum_{i=1}^{N} (\hat{y}^{(i)} - y^{(i)})^2$$

$$= \frac{1}{N} \sum_{i=1}^{N} (a^{(i)} + y^{(i)})^2 \quad a^{(i)} \text{ is the activation vector of the last layer } L \text{ for the } i^{th} \text{ input} \tag{9}$$

3.4 Gradient Update

$$\theta_i \leftarrow \theta_i - \eta(\nabla_\theta \mathcal{L}_\theta(\hat{y}, y)) \tag{10}$$

References

[1] 3Blue1Brown: Grant Sanderson. *But What is a Neural Network — Chapter 1, Deep Learning*. YouTube. 2017. URL: https://www.youtube.com/watch?v=aircAruvnKk.

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[5] Francois Chollet. *Deep Learning with Python, Second Edition*. Manning Publications, 2021.

[6] nmasanta (https://math.stackexchange.com/users/623924/nmasanta). *What is the difference between variable, argument and parameter?* Mathematics Stack Exchange. URL: https://math.stackexchange.com/q/3562026.