

Mathematical Analysis of Multilayer Perceptron Training

Independent Study

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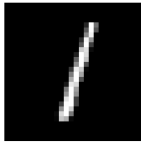
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Abstract

This paper provides a comprehensive mathematical derivation and implementation of a Multilayer Perceptron (MLP) for the classification of handwritten digits from the MNIST dataset, starting from fundamental principles. We begin by exploring the biological inspiration behind artificial neurons, establishing a clear mapping between biological and artificial neural components. We then develop the mathematical representation of a single artificial neuron, progressing to the construction of perceptron layers and the full MLP architecture. The necessity of hidden layers for non-linear separability is discussed, alongside the selection and application of appropriate activation functions. We detail the forward propagation process using matrix-vector notation, followed by an in-depth explanation of cost functions and the error backpropagation algorithm for gradient computation. Optimization and training techniques, including batch-based methods and strategies for improving convergence, are examined. We address the critical issue of regularization to mitigate overfitting and underfitting, including the influence of initialization strategies. Finally, we present the implementation of a fully functional MLP for MNIST classification, concluding with a discussion of extensions to deeper architectures and modern practices in neural network development. This work aims to provide a clear, step-by-step mathematical foundation for understanding and building MLPs from the ground up.

Introduction

The MNIST (Modified National Institute of Standards and Technology) dataset consists of 70,000 handwritten digit images (60,000 for training and 10,000 for testing). It is commonly used for training and evaluating machine learning models in image recognition tasks. Each image is a 28x28 pixel grayscale image, and the task is to classify the digit (0-9) represented by the image.



Sample MNIST digit 1



Sample MNIST digit 2



Sample MNIST digit 7

A Multilayer Perceptron (MLP) is a type of artificial neural network composed of multiple layers of nodes (neurons), each fully connected to the next layer. The MLP processes input data through a series of transformations, with the final layer producing an output. It is one of the fundamental types of neural networks and is used in a variety of applications, including image recognition.

In this paper, we aim to build the mathematical foundations necessary to understand and implement a Multilayer Perceptron (MLP) for the MNIST digit recognition task.

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Preliminaries

Here we will cover some basic mathematical concepts that will be used throughout the paper. These will be derived from first principles, so don't worry if you're not familiar with them.

Vectors

A vector in mathematics is an ordered list of numbers, represented as a bold lowercase letter, e.g. \mathbf{v} . A vector can be represented as:

$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$

We can refer to the first element as v_1 , the second as v_2 , and the i th element as v_i .

Each element of \mathbf{v} corresponds to a coordinate in some n -dimensional space, where n is just the number of elements in the vector. The vector points to the location of these coordinates in space. For example, take the vector in 2-dimensional space:

$$\mathbf{v} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

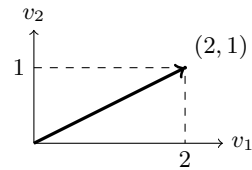


Figure 1: A 2-dimensional vector \mathbf{v}

The Transpose of a Vector

Consider a vector \mathbf{v} :

$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}.$$

The transpose of \mathbf{v} , denoted \mathbf{v}^T , is the same vector, but flipped on its side:

$$\mathbf{v}^T = [v_1 \quad v_2 \quad \dots \quad v_n].$$

The transpose of a vector is used to convert a row vector into a column vector, or vice versa.

Multiplying Vectors : The Dot Product

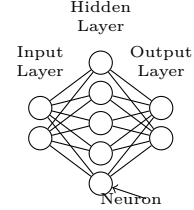
Say we have a vector $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, we say the dimension of this is 2×1 . In order to multiply \mathbf{x} with another vector we need the vector to be of dimension 1×2 .

Let $\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$. We note that the dimension of \mathbf{v} is 2×1 . We can use the transpose of \mathbf{v} to turn it into a 1×2 vector. Given two vectors \mathbf{w} and \mathbf{v} :

$$\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \quad \text{and} \quad \mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

1 Motivation for the Multilayer Perceptron

The perceptron is composed of multiple artificial neurons. Each of which makes a simple decision based on its inputs. These neurons are subsequently assembled into layers, with each layer functioning as a distinct 'area' of the brain. In this way, the Multilayer Perceptron serves as an abstract model inspired by the brain's structure.



1.1 The Structure and Function of a Biological Neuron

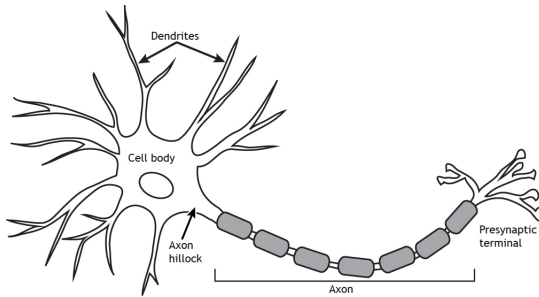
Neurons, the brain's fundamental processing units, transmit information throughout the nervous system. The human brain contains about 86 billion neurons [1], each comprising:

- **Dendrites:** Branch-like structures that receive input signals from other neurons.
- **Cell Body (Soma):** Combines incoming signals and determines whether the neuron should fire.
- **Axon:** Carries the electrical impulse (if the combined signal at the soma exceeds the threshold) to other neurons.
- **Synapse:** Junction between neurons; connects one neuron's axon to another's dendrites.
- **Firing Threshold:** The neuron fires only if the total input exceeds a certain threshold.

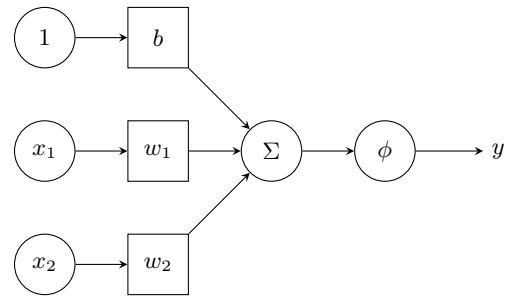
1.2 Mapping the Biological Neuron to the Artificial Neuron

The perceptron, proposed by Frank Rosenblatt in 1958 [3], is a simplified model of the biological neuron. Its components are:

- **Inputs:** x_1, x_2, \dots, x_n , analogous to dendrites.
- **Weights:** w_1, w_2, \dots, w_n , indicating each input's importance.
- **Summation:** $\sum w_i x_i + b$, analogous to the soma, with b as a bias term.
- **Activation Function (ϕ):** applies a mathematical function to the weighted sum to determine the output y , analogous to the neuron's firing mechanism.
- **Output:** The final signal from the perceptron.



(a) Human neuron [2]



(b) Artificial neuron

Figure 2: Comparison of biological and artificial neurons.

2 Artificial Neurons

2.1 Mathematical Representation

As we discussed, biological neurons receive multiple weighted signals and fire when the combined input surpasses a threshold. In the artificial neuron, we mathematically represent this process as follows:

2.1.1 Inputs and Weights as Vectors

We need some way to represent the list of inputs signals to the A.N (artificial neuron). We can do this by using a vector, which is a mathematical object that represents a list of numbers.

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

where each x_i represents an individual input signal.

Similarly, the weights associated with each input are also represented as a weight vector:

$$\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

Each weight w_i corresponds to the input x_i and represents the strength of that input's connection to the neuron - analogous to synaptic strength in a biological neuron. A larger magnitude of w_i indicates a stronger influence of x_i on the neurons output.

2.1.2 Weighted Sum

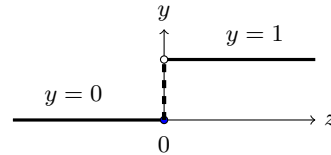
The neuron calculates a weighted sum of its inputs, analogous to the combined signals reaching the soma of a biological neuron. This summation, denoted as z , is defined as:

$$\begin{aligned} z &= w_1x_1 + w_2x_2 + \dots + w_nx_n + b \\ &= \sum_{i=1}^n w_ix_i + b \end{aligned}$$

2.1.3 Activation Function and the Bias Term

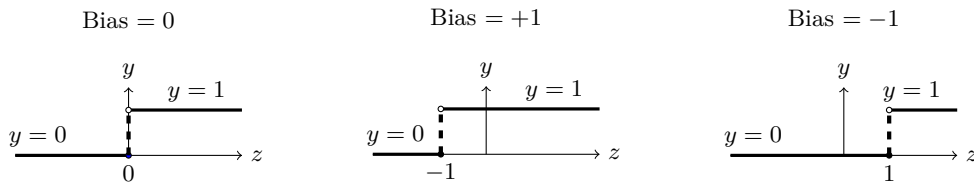
To determine the output of the artificial neuron, we use an activation function. Analogous to the threshold firing of a biological neuron, the activation function, denoted ϕ , decides whether the neuron should fire based on the weighted sum of its inputs, z . In the artificial neuron, we use a simple step function as the activation function:

$$y = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$



Although, in practice we often use a different activation function, such as the sigmoid or ReLU function, the step function is a good starting point for understanding the basic concept of an activation function.

The bias term, b , is introduced to shift the activation threshold. Biologically, this is analogous to the neuron's resting membrane potential, which influences how easily the neuron will fire.



2.2 Learning

The core idea of learning is, given an unfavorable outcome, we look back and try to figure out what we could've done differently to achieve a better outcome. We can only do this if we know how wrong our decision was, and what we should have done instead.

Consider, for a moment, getting a college test result back. If we wanted to get 90% on the test and only got 40%, we know we need to give a much higher weight to studying next time. Whereas, if we got 88% we know we're on the right track, and only need to make minor adjustments.

In an artificial neuron, we can compare the difference between the correct output and the output produced by the neuron. The larger the error, the greater need for adjustment. The learning rate η controls how sensitive we are to these errors. A high learning rate means we make large adjustments, while a low learning rate means we make small adjustments.

The question then becomes, why not always use a high learning rate? Let's revisit the college test scenario. Imagine you aimed for 90% but only scored 40%. A large error signal indicates a significant adjustment is needed. With a high learning rate, you would react very strongly to this error. You might drastically increase your study time, perhaps even overcompensating and studying excessively. This could lead to burnout or neglecting other important aspects of life. Conversely, with a low learning rate, even with a 40% score, your adjustment would be small. You might only slightly increase your study time, potentially not enough to significantly improve your score on the next test. The learning rate, therefore, is a delicate balance. It needs to be high enough to enable learning in a reasonable time, but low enough to prevent wild oscillations or overreactions to errors. The learning rate, is something we can adjust to find the right balance between making large adjustments when we are far off, and making small adjustments when we are close to the correct answer.

Mathematically, we can represent the learning process as follows. We define the error as the difference between the predicted result and the actual result. This error indicates how far off our prediction was from the correct answer, and can be positive (overprediction) or negative (underprediction)

$$\text{Error} = y_{\text{actual}} - y_{\text{predicted}}$$

We then define how much we should change the weight of each input (x_i) as:

$$\Delta w_i = \eta \times \text{Error} \times x_i$$

Here, η is the learning rate, controlling our sensitivity to errors. The multiplication by x_i is important because it scales the weight adjustment by the magnitude of the input x_i . Inputs with larger values have a proportionally larger influence on the output, and therefore their weights should be adjusted more significantly for a given error. We also calculate the change for the bias term as: We also calculate how much we should change the bias term as:

$$\Delta b = \eta \times \text{Error}$$

The intuition behind these adjustments is that if the prediction is consistently too low, we increase weights and bias to make firing easier (like studying more). If consistently too high, we decrease them to make firing harder (like studying less). We then update the weights and bias as follows:

$$w_i = w_i + \Delta w_i$$

$$b = b + \Delta b$$

2.3 What does the Artificial Neuron Actually do? - Example: Mushroom Classification

Imagine we're in a field filled with all kinds of mushrooms. Some have dozens of little white spots, and tall stems. While others have very few spots and short stems. You know from past experience that the mushrooms with many spots are poisonous, while the ones with few spots are safe to eat.

But there's a catch. Sometimes we find mushrooms that are hard to classify - they have medium length stems, or only a few spots. Where exactly do we draw the line between poisonous and safe mushrooms? You may not know from a glance, and you certainly don't want to eat a poisonous mushroom to find out.

This is exactly the problem the artificial neuron helps solve. It learns to draw a line in the mushroom field that separates the poisonous mushrooms from the safe ones.

Lets define the two inputs to our neuron as:

$$x_1 = \text{number of spots} \quad \text{and} \quad x_2 = \text{length of the stem}$$

The artificial neuron then forms a linear combination of these inputs:

$$z = \sum_{i=1}^2 w_i x_i + b = w_1 x_1 + w_2 x_2 + b$$

where our weights scale the importance of each input. The neuron then decides whether the mushroom is poisonous or not:

$$y = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

where, $y = 1$ means the mushroom is poisonous, and $y = 0$ means it is safe to eat. The perceptron learns the weights w_1 and w_2 to draw the best line that separates the two classes of mushrooms.

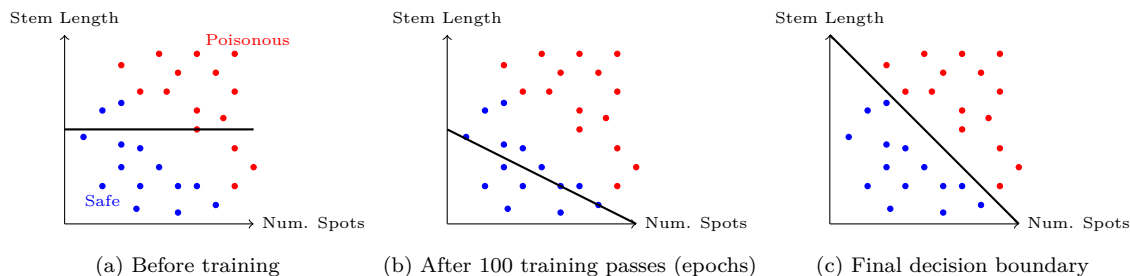


Figure 4: Artificial Neuron learning to separate safe and poisonous mushrooms.

We refer to this line as the decision boundary, as it separates the two classes of mushrooms. We now have a simple model, that given the number of spots and the length of the stem, can predict whether a mushroom is poisonous or safe to eat. This is the essence of what an artificial neuron does - it learns to draw decision boundaries in the input space to separate different classes of data.

3 A Layer of Neurons

3.1 Recap of the Single Neuron and Intro to Layers

The artificial neuron is a simple unit, like a tiny decision maker. It takes inputs representing different features (think stems and spots of mushrooms), it gives these features different weights (importance), adds them up, applies a little tweak (a bias) and runs it through an activation function (like a yes/no switch) to decide what to output. It learns by tweaking these weights and biases to make better decisions on examples its given.

Now, instead of one neuron working alone, we introduce a layer of neurons, each of them looking at the same inputs but looking at them in different ways, for example one might focus on the color of the mushroom, while another might focus on its size. Together, these neurons can work together to make more complex decisions, where we can consider multiple features at once.

3.2 The XOR Problem

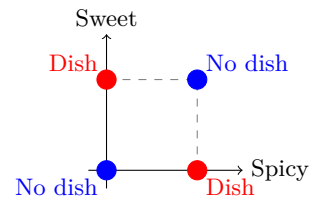
A single artificial neuron can separate data with only one straight line—great if your data is linearly separable. But some datasets require more complex boundaries. One classic example is the XOR (exclusive OR) problem: how do we classify data points that should be labeled “1” if they satisfy exactly one condition (but not both), and “0” otherwise?

Analogy: A Chef and Two Flavors

Imagine a chef wants to create a dish that is appealing only if it is *either* sweet *or* spicy, but not both (that combination clashes) and not neither (too boring). This is precisely the XOR condition: the dish is appealing if it is sweet *or* spicy, but not both. The chef needs to find the right balance of flavors to create a dish that satisfies this condition.

Sweet	Spicy	Dish
No	No	No (boring dish)
No	Yes	Yes (sweet dish)
Yes	No	Yes (spicy dish)
Yes	Yes	No (flavours clash)

(a) XOR truth table

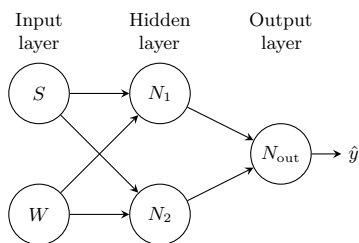


(b) Visualization of XOR: Red = 1, Blue = 0

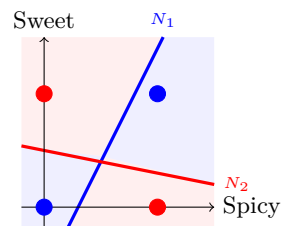
Figure 5: The XOR problem

As we can see, we can’t split this data with a single straight line so that all the red points are one side and all the blue points are on the other side. This is where a single neuron fails. We need a more complex decision boundary. To solve this problem we can use multiple neurons in the same layer, where each neuron draws its own boundary and the final decision is made by combining the outputs of these neurons.

Returning to the chef analogy: the chef might hire two sous-chefs. One sous-chef checks sweetness (N_1); the other checks spiciness (N_2). Their “votes” are then combined in a final decision. In neural network terms, each neuron in the hidden layer focuses on a specific aspect of the input; then the outputs are aggregated by the next neuron. This layering of simpler decisions leads to richer, non-linear decision boundaries—enabling the network to classify the XOR data correctly.



(a) Architecture of the chef analogy



(b) Decision boundaries

Figure 6: A layer of neurons for the XOR problem

4 Why stop at one layer?

The XOR problem (chef analogy) is a small illustration on non-linearly separable problems. Most real world tasks have layers of complexity that dwarf the XOR example. For example:

- **Image Recognition:** Deciding whether a cat or dog involves thousands or millions of pixels. A single layer of neuron cannot capture the patterns of edges, shapes, and textures that define a cat or dog.
- **Natural Language Processing:** Understanding a sentence involves understanding the meaning of each word, the context in which they are used, and the relationships between them. A single layer of neurons cannot capture the complexity of language.

4.1 The Power of Chaining Layers

Just having one layer of neurons is like having a single sous-chef in the kitchen. They can only focus on one aspect of the dish. To create a complex dish, the chef needs multiple sous-chefs, each focusing on different aspects of the dish. Similarly, to solve complex problems, we need multiple layers of neurons, each layer focusing on different aspects of the input data. This is the essence of deep learning: using multiple layers of neurons to learn complex patterns in data.

One way to overcome these limitations is to chain multiple layers of neurons so that the output of one layer becomes the input of the next. For example, in image recognition, one layer might learn to respond to simple edges or colors, while the next layer might take these edges as inputs and learn to detect more complex shapes, like corners and textures, a third layer might combine these shapes into an understanding of objects like a cat's ear, or a dog's nose. This chaining of layers is what gives deep learning its name. When we talk about hidden layers, we refer to the layers

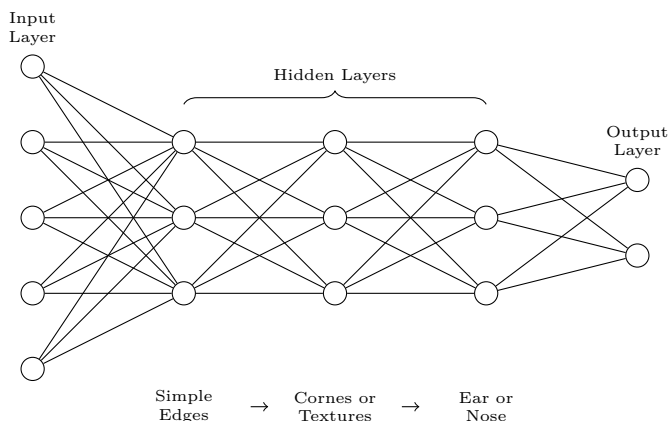


Figure 7: A deep neural network for image recognition

of neurons between the input and output layers. These layers are called hidden because we don't directly observe their outputs, but rather they are intermediate processing steps. Networks with one or more hidden layers are often called multi-layer perceptrons (MLPs). The more layers we add, the deeper the network becomes, and the more complex patterns it can learn - at a cost of more computational resources and longer training times.

4.2 Forward Pass : The Flow of Information

The forward pass is the process by which we transform raw inputs step by step through each layer until we produce a final output.

Revisiting our chef's examples, where the inputs may be spiciness (S) and sweetness (W). In the first hidden layer, each neuron does the following:

Weighted Sum

References

- [1] Azevedo et al. Equal numbers of neuronal and nonneuronal cells make the human brain an isometrically scaled-up primate brain, 2009.
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- [3] F. Rosenblatt. The perceptron: A probabilistic model for information storage and organization in the brain, 1958.