https://towardsdatascience.com/how-neural-networks-solve-the-xor-problem-59763136bdd7

How Neural Networks Solve the XOR Problem

And why hidden layers are so important

Aniruddha Karajgi

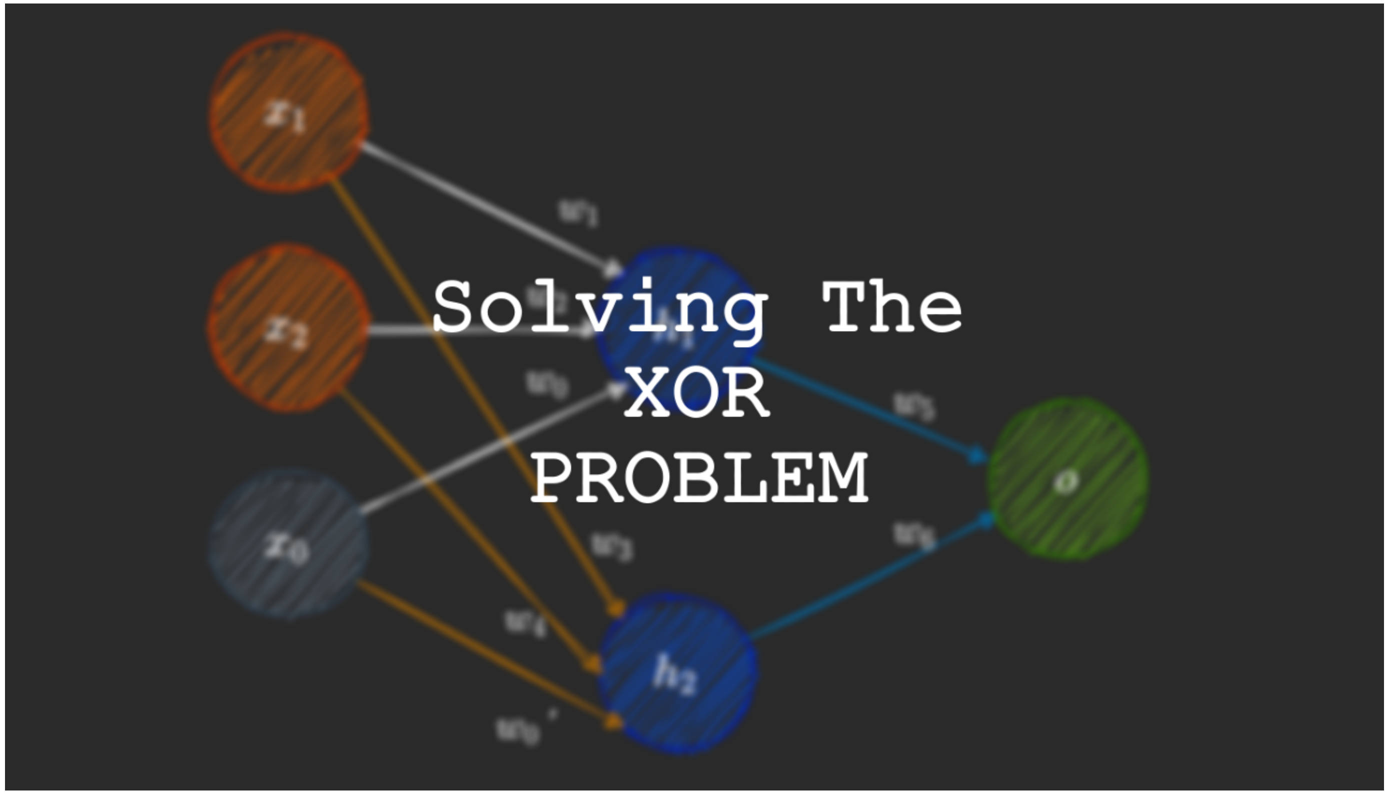

Image by Author

The perceptron is a classification algorithm. Specifically, it works as a linear binary classifier. It was invented in the late 1950s by Frank Rosenblatt.

The perceptron basically works as a threshold function — non-negative outputs are put into one class while negative ones are put into the other class.

Though there's a lot to talk about when it comes to neural networks and their variants, we'll be discussing a specific problem that highlights the major differences between a single layer perceptron and one that has a few more layers.

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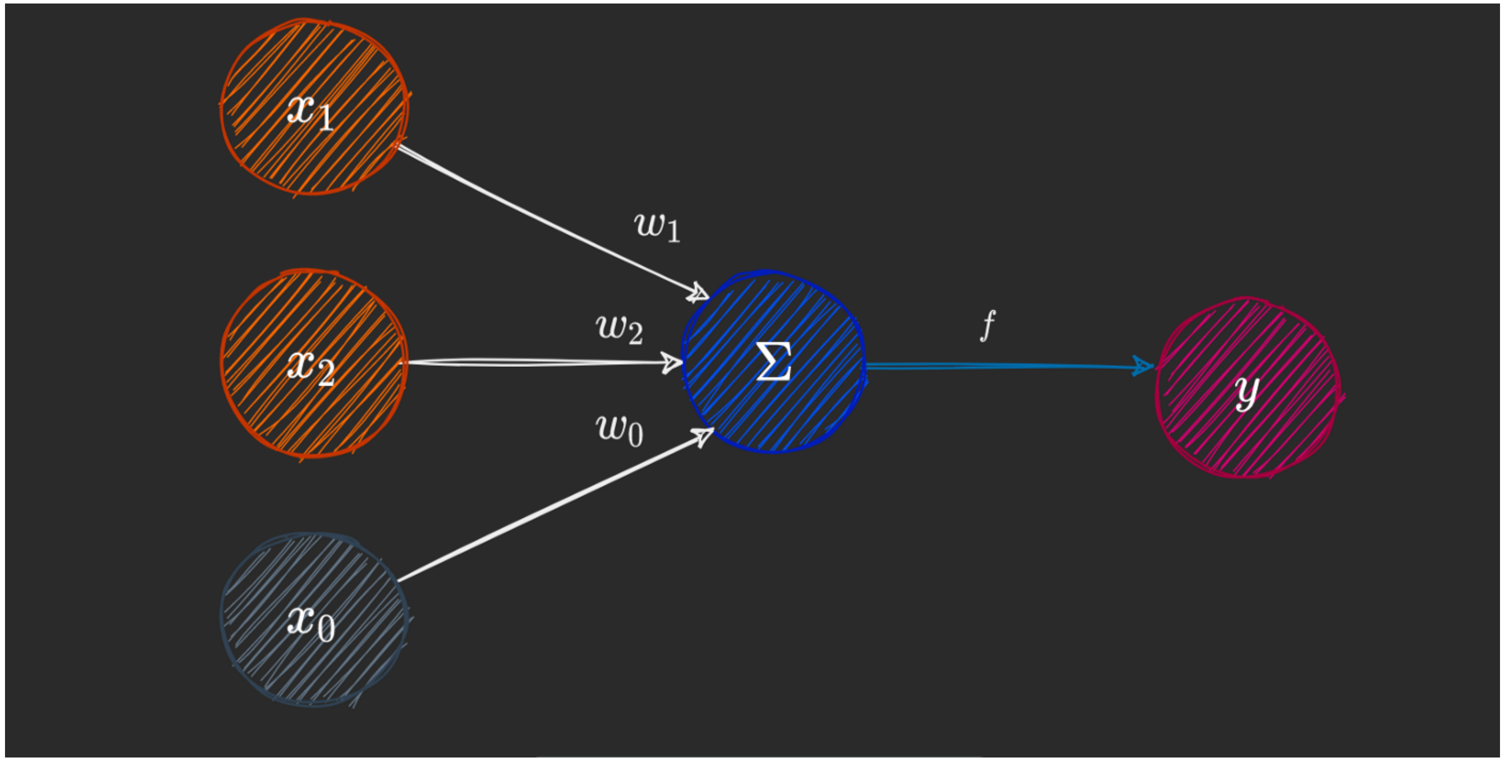
Structure and Properties

A perceptron has the following components:

- Input nodes
- Output node
- An activation function
- Weights and biases
- Error function



A representation of a single-layer perceptron with 2 input nodes — Image by Author using draw.io

Input Nodes

These nodes contain the input to the network. In any iteration — whether testing or training — these nodes are passed the input from our data.

Weights and Biases

These parameters are what we update when we talk about “training” a model. They are initialized to some random value or set to 0 and updated as the training progresses. The bias is analogous to a weight independent of any input node. Basically, it makes the model more flexible, since you can “move” the activation function around.

Evaluation

The output calculation is straightforward.

- Compute the dot product of the input and weight vector
- Add the bias
- Apply the activation function.

This can be expressed like so:

$$y = f(x_1 \cdot w_1 + x_2 \cdot w_2 + b)$$

This is often simplified and written as a dot- product of the weight and input vectors plus the bias.

$$y = f(w \cdot X + b)$$

Activation Function

This function allows us to fit the output in a way that makes more sense. For example, in the case of a simple classifier, an output of say `-2.5` or `8` doesn’t make much sense with regards to classification. If we use something called a sigmoidal activation function, we can fit that within a range of 0 to 1, which can be interpreted directly as a probability of a datapoint belonging to a particular class.

Though there are many kinds of activation functions, we’ll be using a simple linear activation function for our perceptron. The linear activation function has no effect on its input and outputs it as is.

Classification

How does a perceptron assign a class to a datapoint?

We know that a datapoint’s evaluation is expressed by the relation `wX + b`. We define a threshold (**θ**) which classifies our data. Generally, this threshold is set to 0 for a perceptron.

So points for which `wX + b` is greater than or equal to 0 will belong to one class while the rest (`wX + b` is negative) are classified as belonging to the other class. We can express this as:

$$Class_1 : w \cdot X + b \geq 0$$

$$Class_2 : w \cdot X + b < 0$$

Training algorithm

To train our perceptron, we must ensure that we correctly classify all of our train data. Note that this is different from how you would train a neural network, where you wouldn't try and correctly classify your entire training data. That would lead to something called overfitting in most cases.

We start the training algorithm by calculating the **gradient**, or Δw. Its the product of:

- the value of the input node corresponding to that weight
- The difference between the actual value and the computed value.

$$\Delta w = node \cdot (actual - computed)$$

We get our new weights by simply incrementing our original weights with the computed gradients multiplied by the learning rate.

$$w_{updated} = w_{old} + lr \cdot \Delta w$$

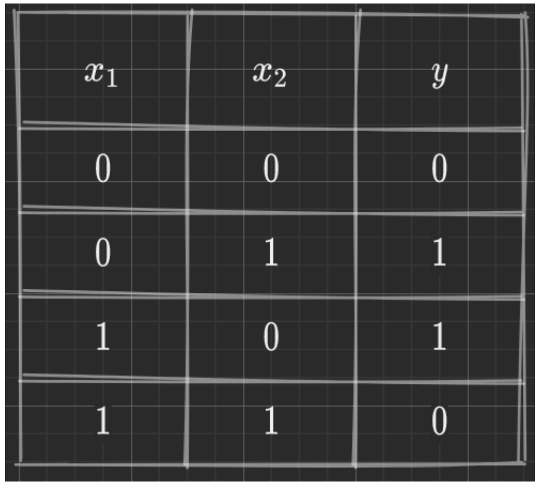
A simple intuition for how this works: if our perceptron correctly classifies an input data point, `actual_value − computed_value` would be `0` , and there wouldn't be any change in our weights since the gradient is now `0`.

The 2D XOR problem

In the XOR problem, we are trying to train a model to mimic a 2D XOR function.

The XOR function

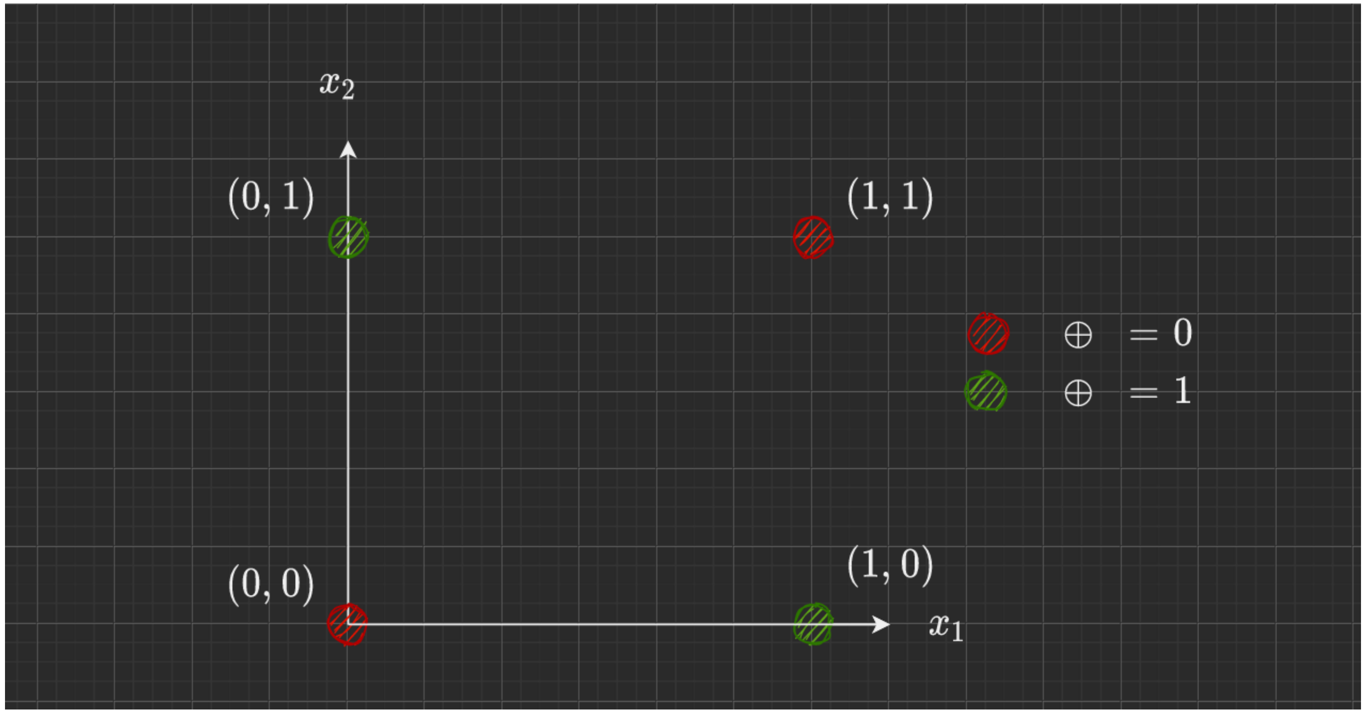
The function is defined like so:



x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0

The XOR Truth table — Image by Author

If we plot it, we get the following chart. This is what we're trying to classify. The ⊕ ("o-plus") symbol you see in the legend is conventionally used to represent the XOR boolean operator.



The XOR output plot — Image by Author using draw.io

Our algorithm —regardless of how it works — must correctly output the XOR value for each of the 4 points. We'll be modelling this as a classification problem, so `Class 1` would represent an XOR value of 1, while `Class 0` would represent a value of 0.

Attempt #1: The Single Layer Perceptron

Let's model the problem using a single layer perceptron.

Input data

The data we'll train our model on is the table we saw for the XOR function.

```
Data         Target
[0, 0]         0
[0, 1]         1
[1, 0]         1
[1, 1]         0
```

Implementation

Imports

Apart from the usual visualization (`matplotlib`and `seaborn`) and numerical libraries (`numpy`), we'll use `cycle` from `itertools` . This is done since our algorithm cycles through our data indefinitely until it manages to correctly classify the entire training data without any mistakes in the middle.

The data

We next create our training data. This data is the same for each kind of logic gate, since they all take in two boolean variables as input.

The training function

Here, we cycle through the data indefinitely, keeping track of how many consecutive datapoints we correctly classified. If we manage to classify everything in one stretch, we terminate our algorithm.

If not, we reset our counter, update our weights and continue the algorithm.

To visualize how our model performs, we create a mesh of datapoints, or a grid, and evaluate our model at each point in that grid. Finally, we colour each point based on how our model classifies it. So the `Class 0` region would be filled with the colour assigned to points belonging to that class.

The Perceptron class

To bring everything together, we create a simple `Perceptron` class with the functions we just discussed. We have some instance variables like the training data, the target, the number of input nodes and the learning rate.

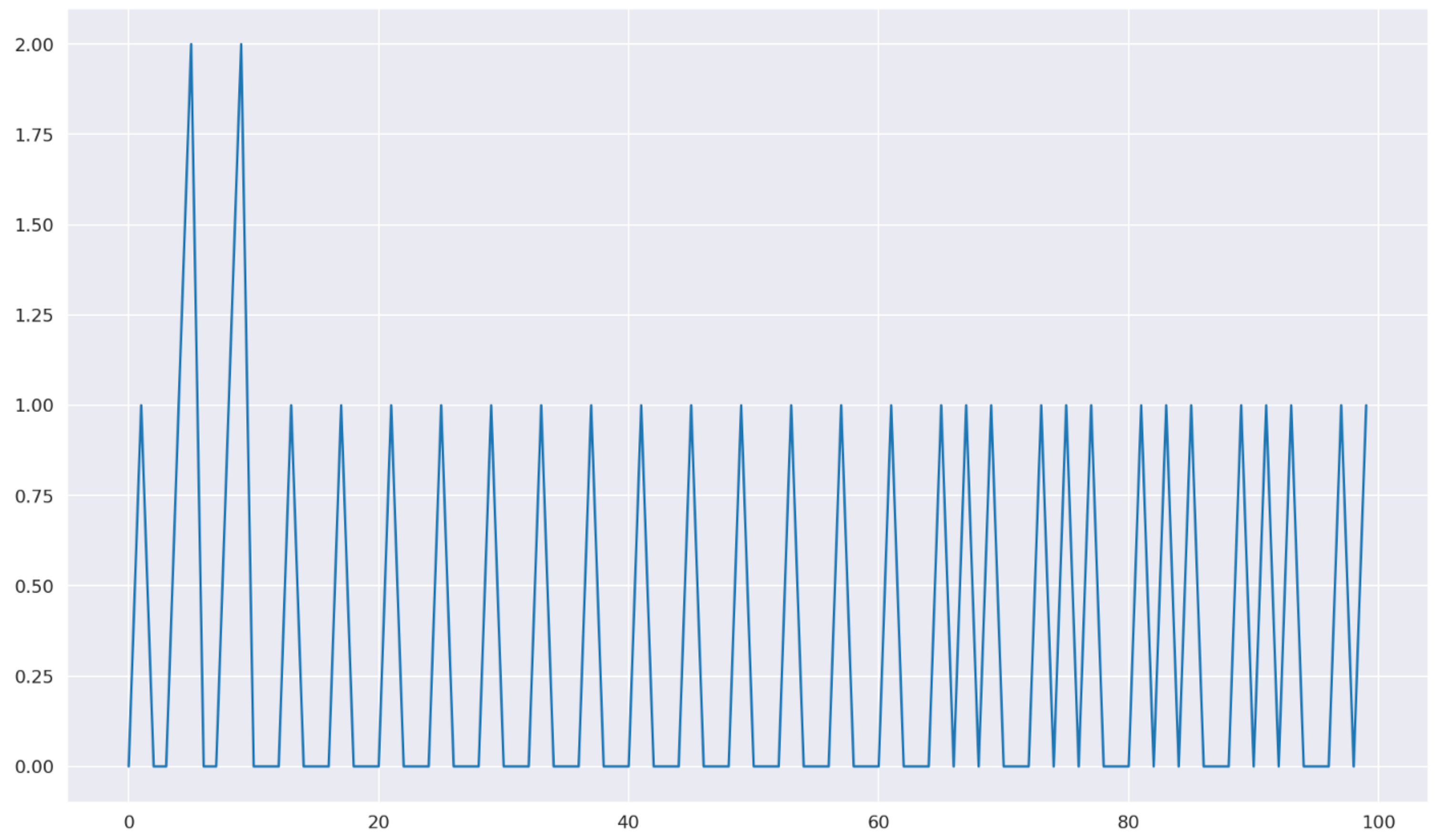
Results

Let’s create a perceptron object and train it on the XOR data.

You’ll notice that the training loop never terminates, since a perceptron can only converge on linearly separable data. Linearly separable data basically means that you can separate data with a point in 1D, a line in 2D, a plane in 3D and so on.

> A perceptron can only converge on linearly separable data. Therefore, it isn’t capable of imitating the XOR function.

Remember that a perceptron must correctly classify the entire training data in one go. If we keep track of how many points it correctly classified consecutively, we get something like this.



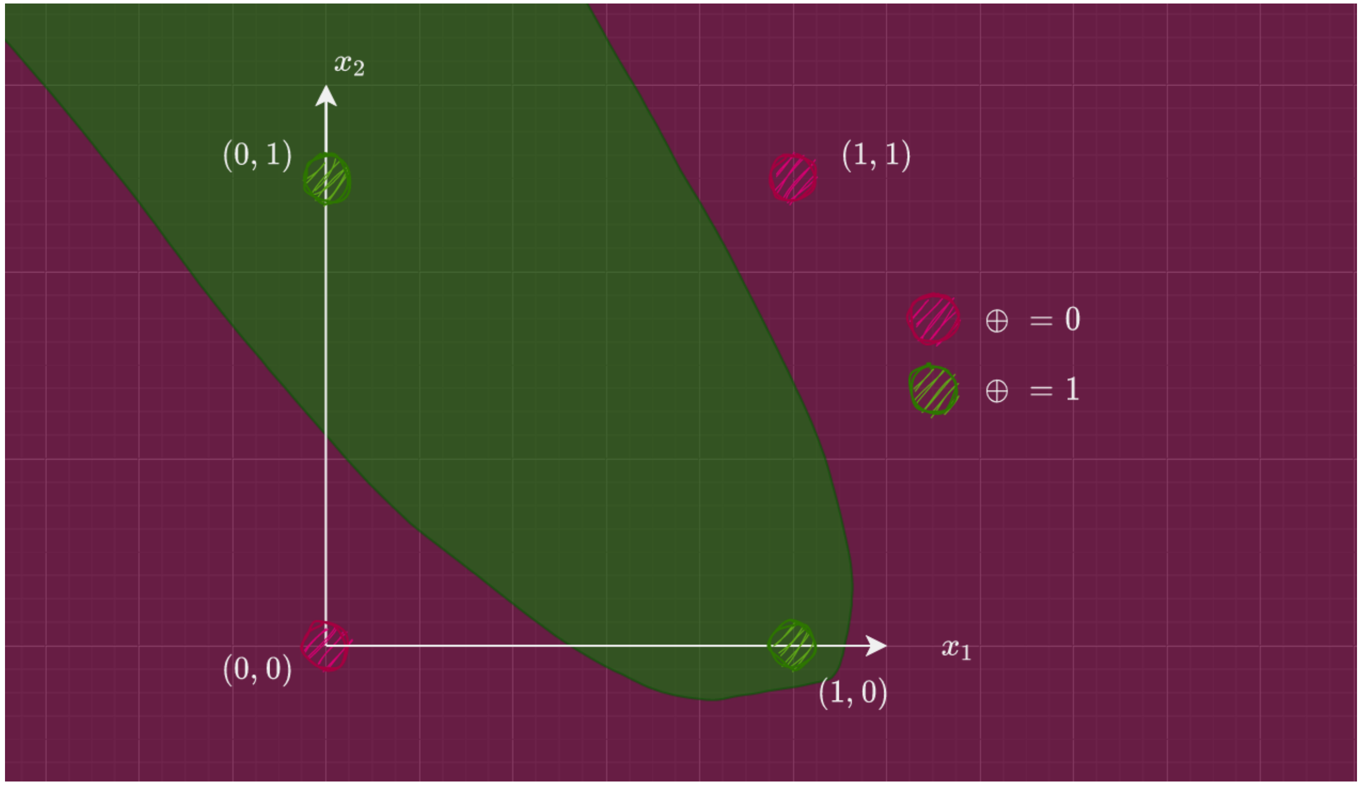
The value of correct_counter over 100 cycles of training — Image by Author

The algorithm only terminates when `correct_counter` hits 4 — which is the size of the training set — so this will go on indefinitely.

The Need for Non-Linearity

It is clear that a single perceptron will not serve our purpose: the classes aren't linearly separable. This boils down to the fact that a single linear decision boundary isn’t going to work.

Non-linearity allows for more complex decision boundaries. One potential decision boundary for our XOR data could look like this.



A potential non-linear decision boundary for our XOR model — Image by Author using draw.io

The 2d XOR problem — Attempt #2

We know that the imitating the XOR function would require a non-linear decision boundary.

> But why do we have to stick with a single decision boundary?

The Intuition

Let’s first break down the XOR function into its AND and OR counterparts.

The XOR function on two boolean variables A and B is defined as:

$$XOR(A, B) = A \cdot \overline{B} + B \cdot \overline{A}$$

Let’s add `A.~A` and `B.~B` to the equation. Since they both equate to 0, the equation remains valid.

$$XOR(A, B) = A \cdot \overline{B} + B \cdot \overline{A} + (A \cdot \overline{A} + B \cdot \overline{B})$$

Let’s rearrange the terms so that we can pull out `A` from the first part and `B` from the second.

$$XOR(A, B) = (A \cdot \overline{A} + A \cdot \overline{B}) + (B \cdot \overline{A} + B \cdot \overline{B})$$

Simplifying it further, we get:

$$XOR(A, B) = (A + B) \cdot (\overline{A} + \overline{B})$$

Using DeMorgan's laws for boolean algebra:`~A + ~B = ~(AB)` , we can replace the second term in the above equation like so:

$$XOR(A, B) = (A + B) \cdot (\overline{AB})$$

Let's replace A and B with x_1 and x_2 respectively since that's the convention we're using in our data.

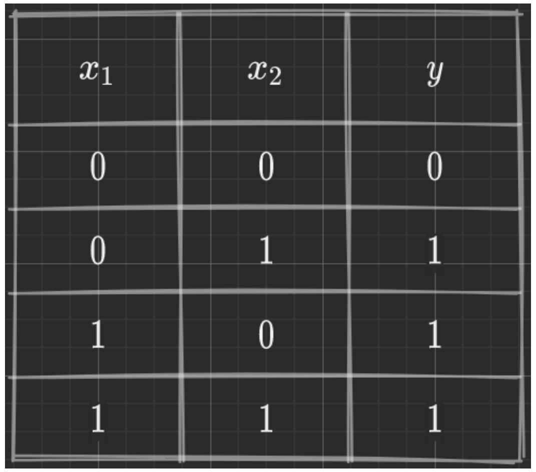
$$XOR(x_1, x_2) = (x_1 + x_2) \cdot (\overline{x_1 x_2})$$

The XOR function can be condensed into two parts: **a NAND and an OR**. If we can calculate these separately, we can just combine the results, using **an AND gate.**

Let's call the OR section of the formula part I, and the NAND section as part II.

Modelling the OR part

We'll use the same Perceptron class as before, only that we'll train it on OR training data.

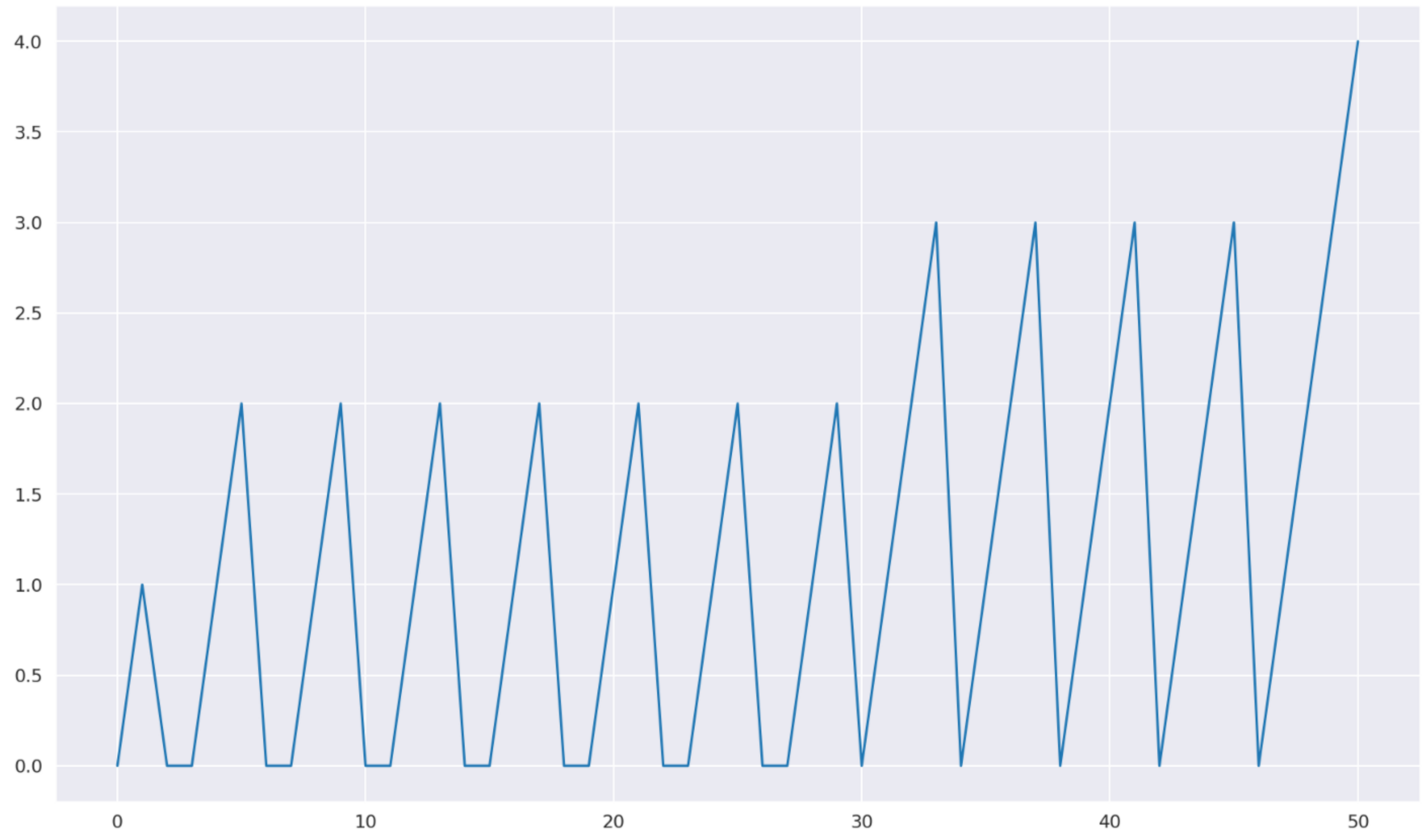


x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	1

The OR truth table — Image by Author using draw.io

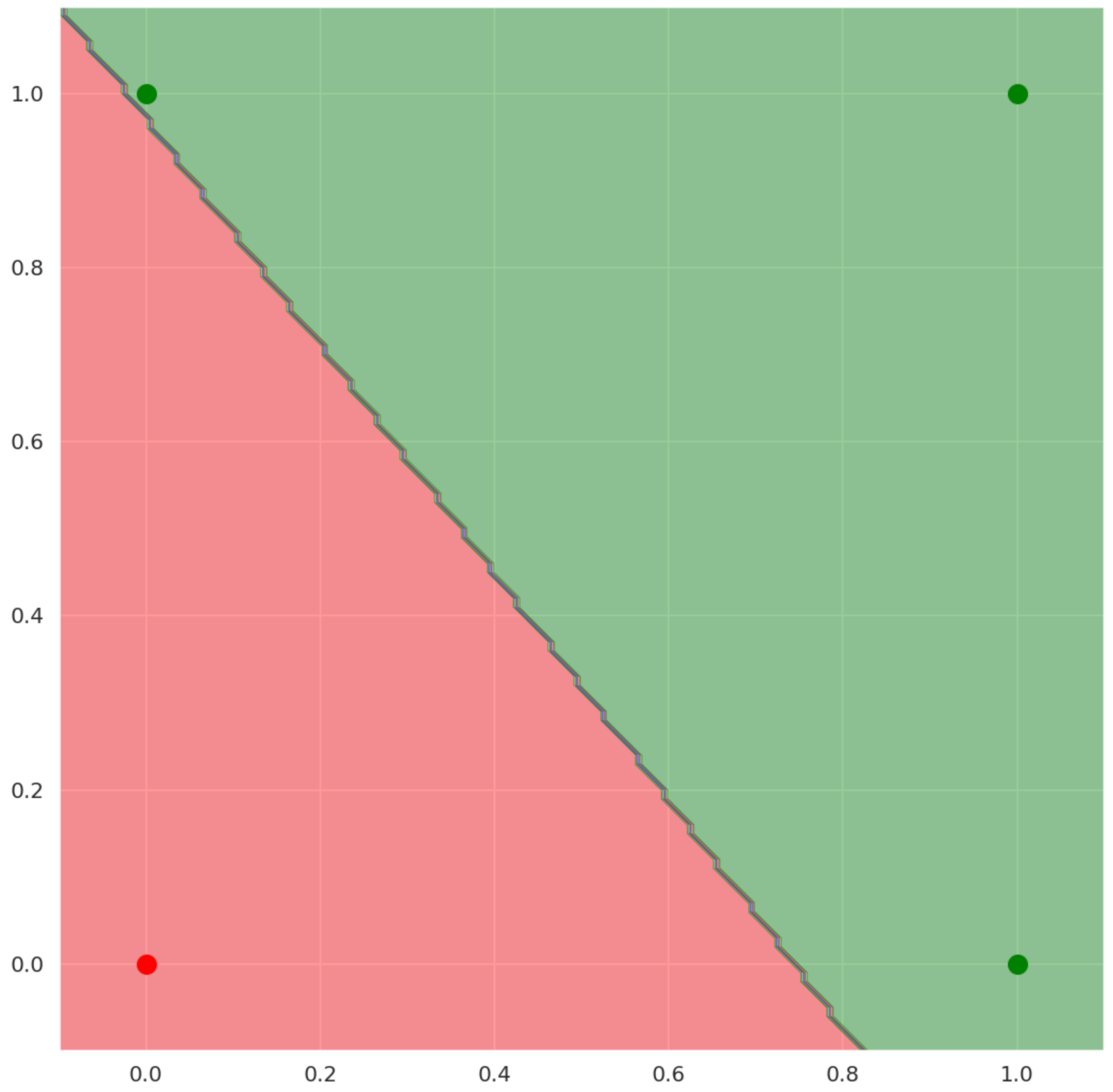
This converges, since the data for the OR function is linearly separable. If we plot the number of correctly classified consecutive datapoints as we did in our first attempt, we get this plot. It's clear that around iteration 50, it hits the value 4, meaning that it classified the entire dataset correctly.

> correct_counter measures the number of consecutive datapoints correctly classified by our Perceptron



The correct_counter plot for our OR perceptron — Image by Author

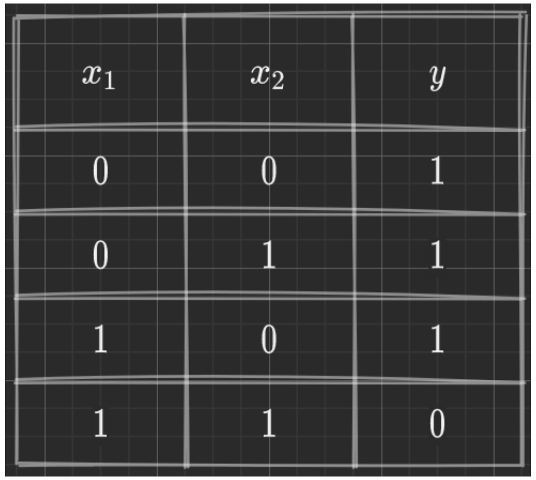
The decision boundary plot looks like this:



The Output plot of our OR perceptron — Image by Author

Modelling the NAND part

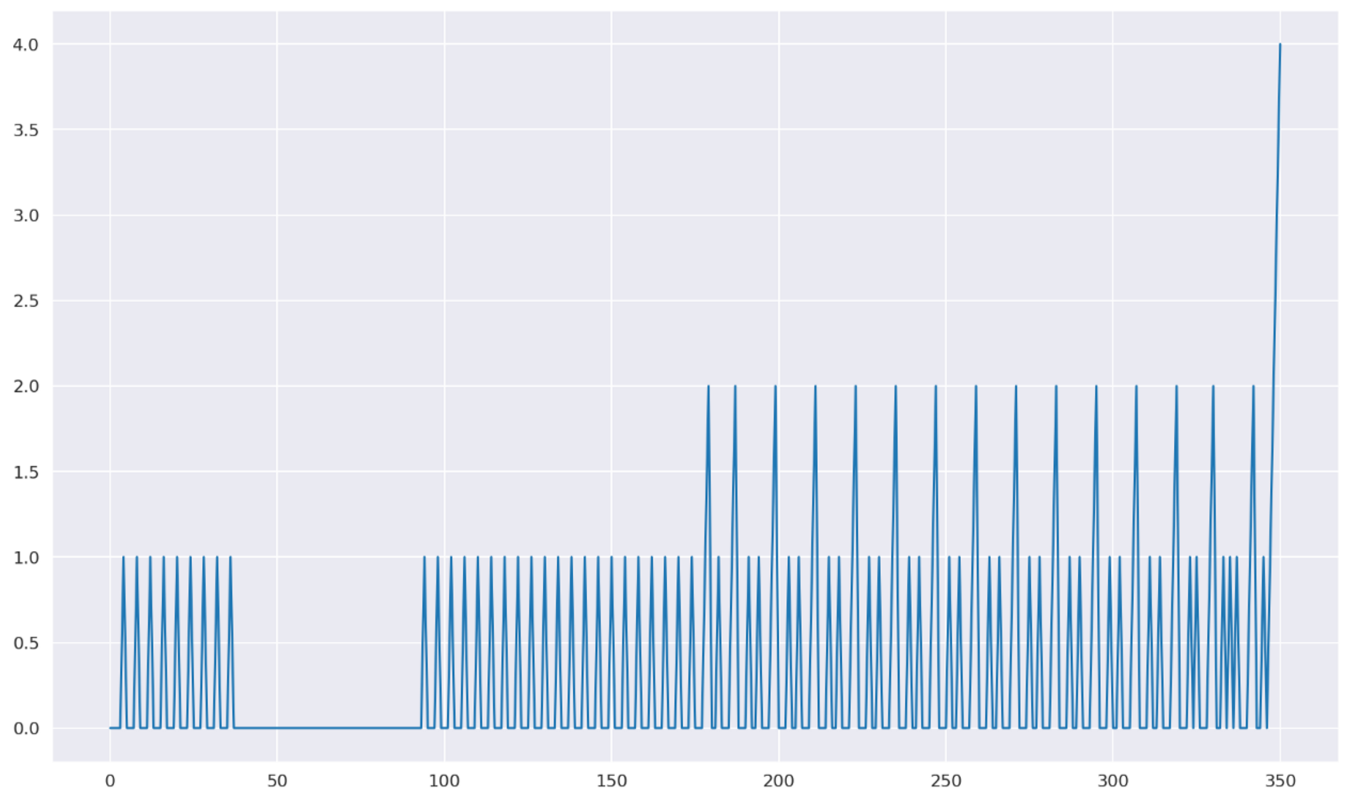
Let’s move on to the second part. We need to model a NAND gate. Just like the OR part, we’ll use the same code, but train the model on the NAND data. So our input data would be:

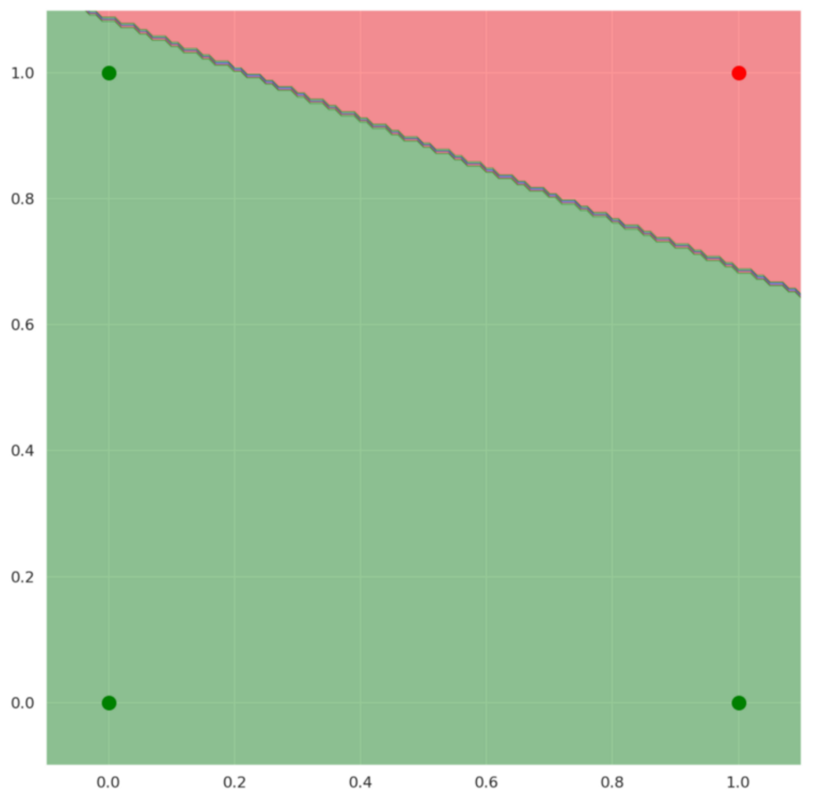


x_1	x_2	y
0	0	1
0	1	1
1	0	1
1	1	0

The NAND Truth table — Image by Author using draw.io

After training, the following plots show that our model converged on the NAND data and mimics the NAND gate perfectly.


4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
50
100
150
200
250
300
350



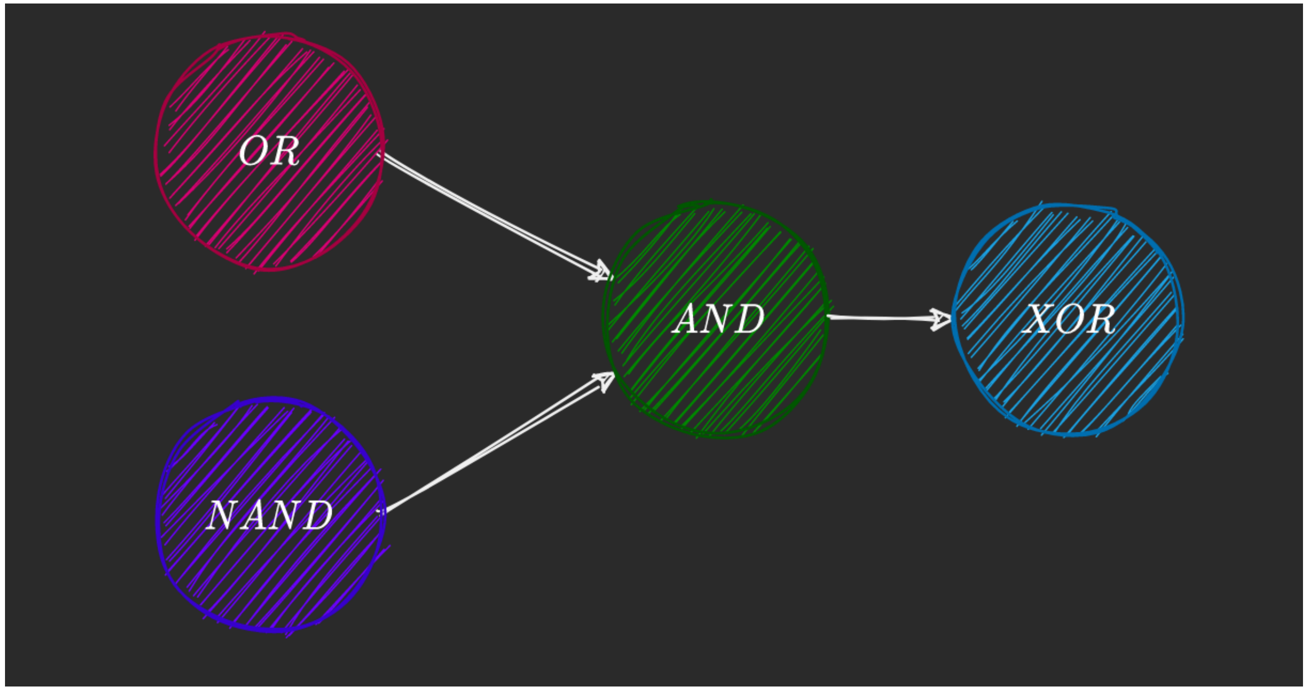
Decision boundary and correct_counter plots for the NAND perceptron — Image by Author

Bringing everything together

Two things are clear from this:

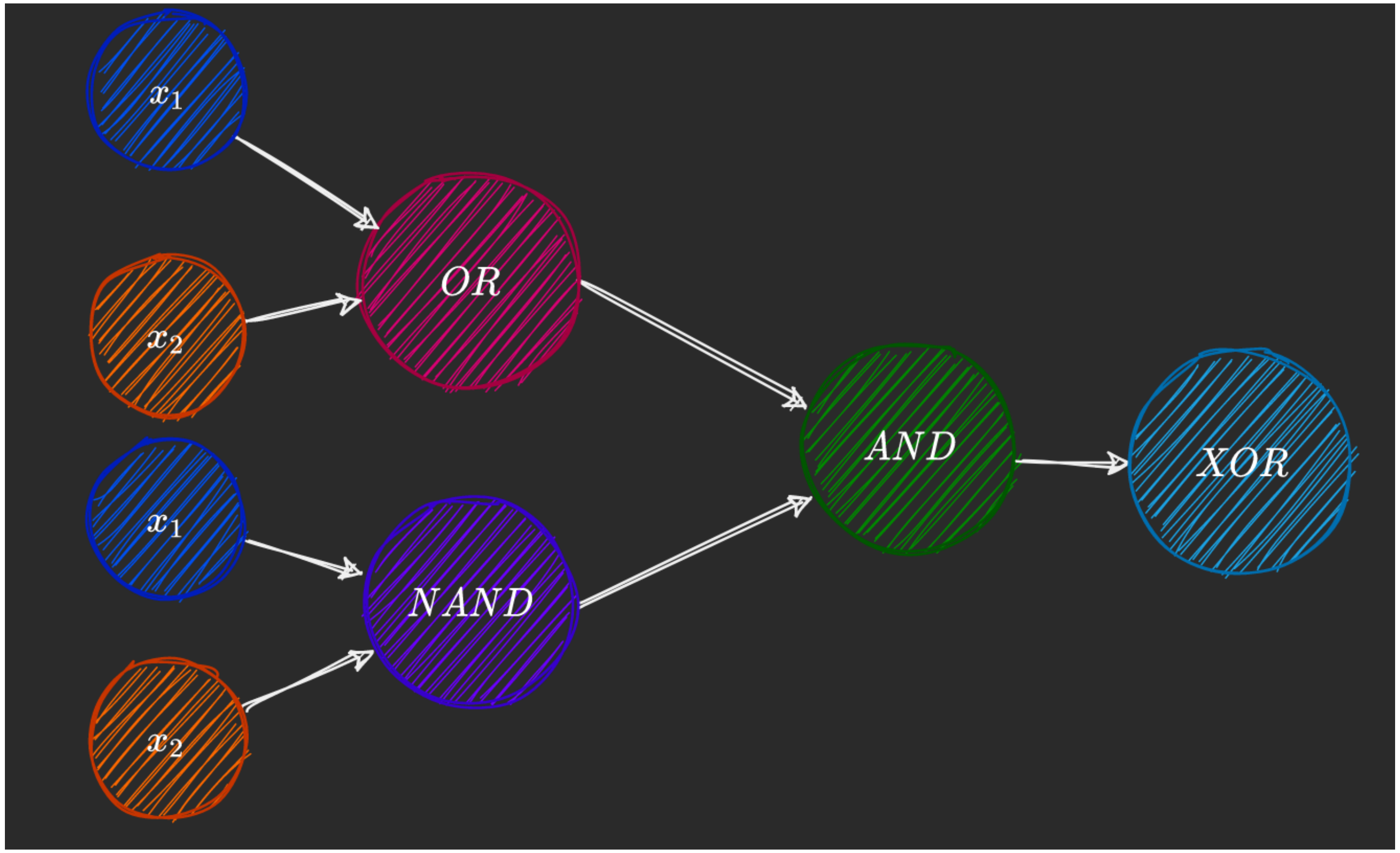
- we are performing a logical AND on the outputs of two logic gates (where the first one is an OR and the second one a NAND)
- and that both functions are being passed the same input (x1 and x2).

Let's model this into our network. First, let's consider our two perceptrons as black boxes.



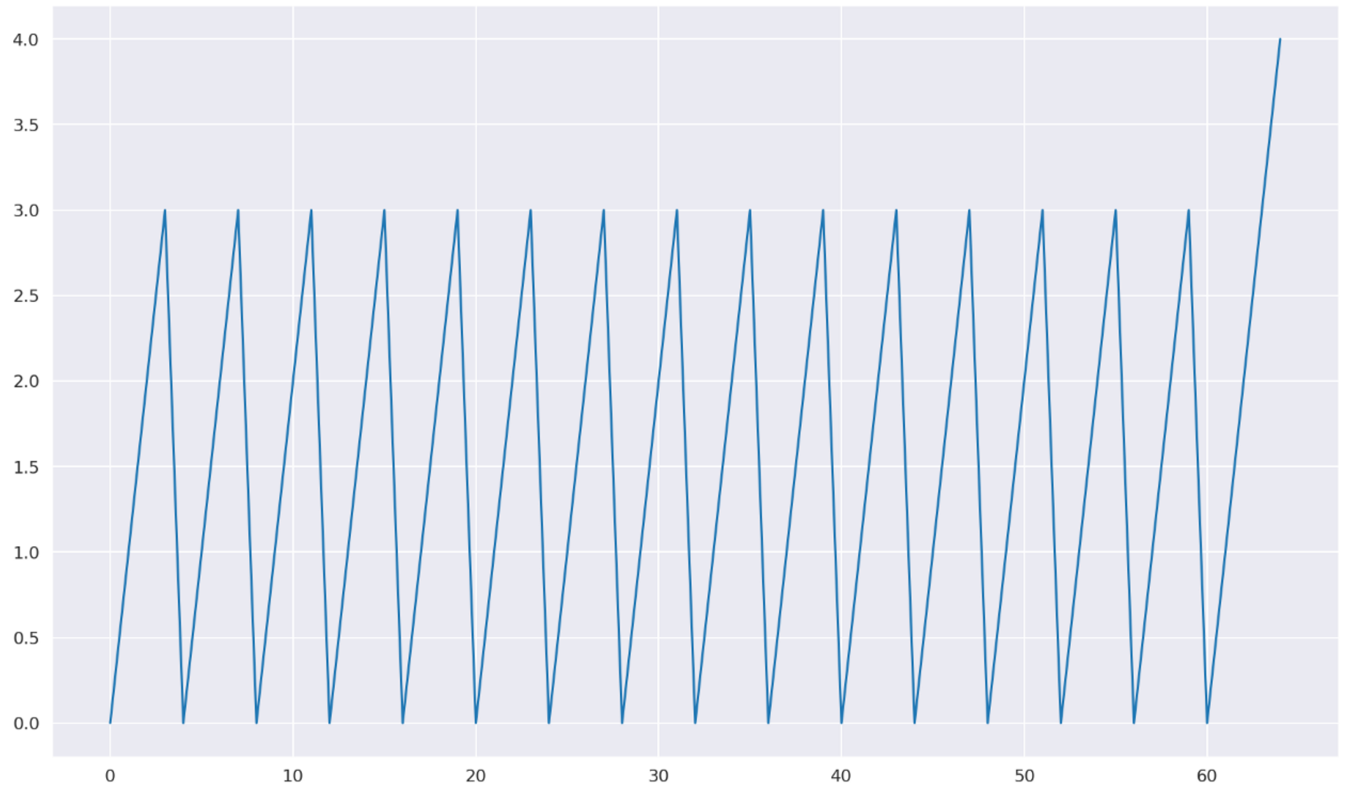
The plan for our model — Image by Author using draw.io

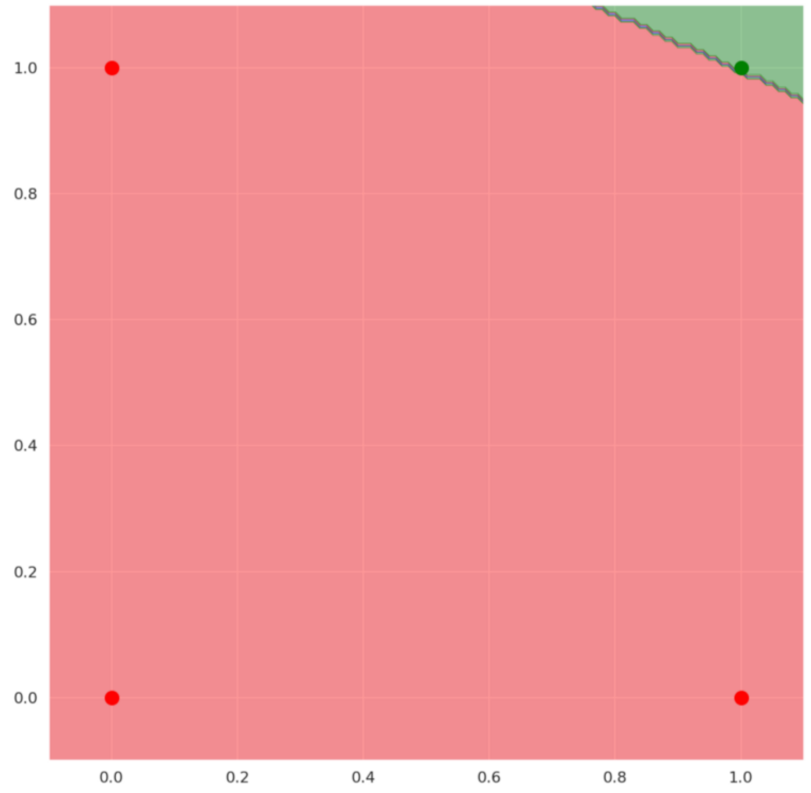
After adding our input nodes x_1 and x_2, we can finally implement this through a simple function.



Adding input nodes — Image by Author using draw.io

Finally, we need an AND gate, which we'll train just we have been.


4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
10
20
30
40
50
60

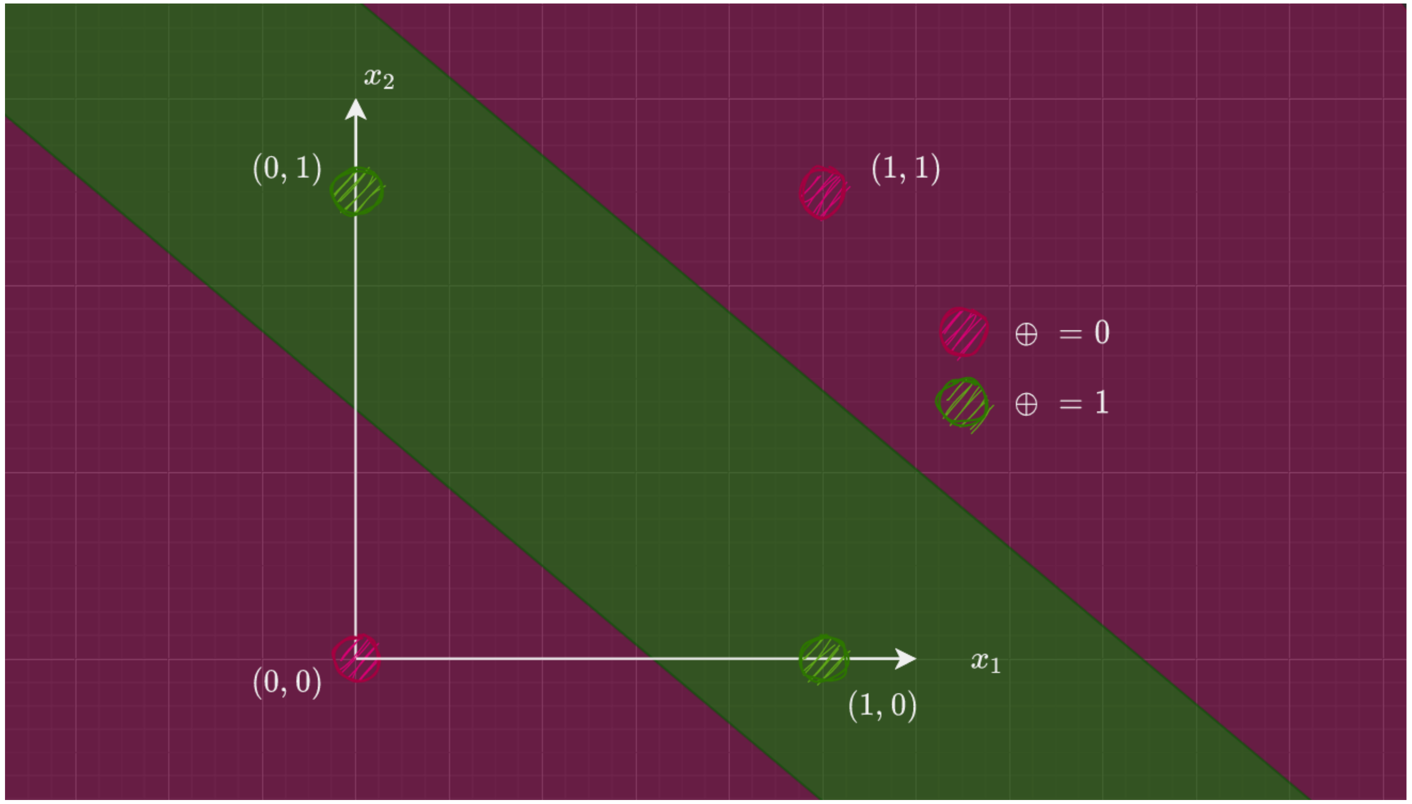


The correct_count and output plots of our AND perceptron. — Image by Author

What we now have is a model that mimics the XOR function.

If we were to implement our XOR model, it would look something like this:

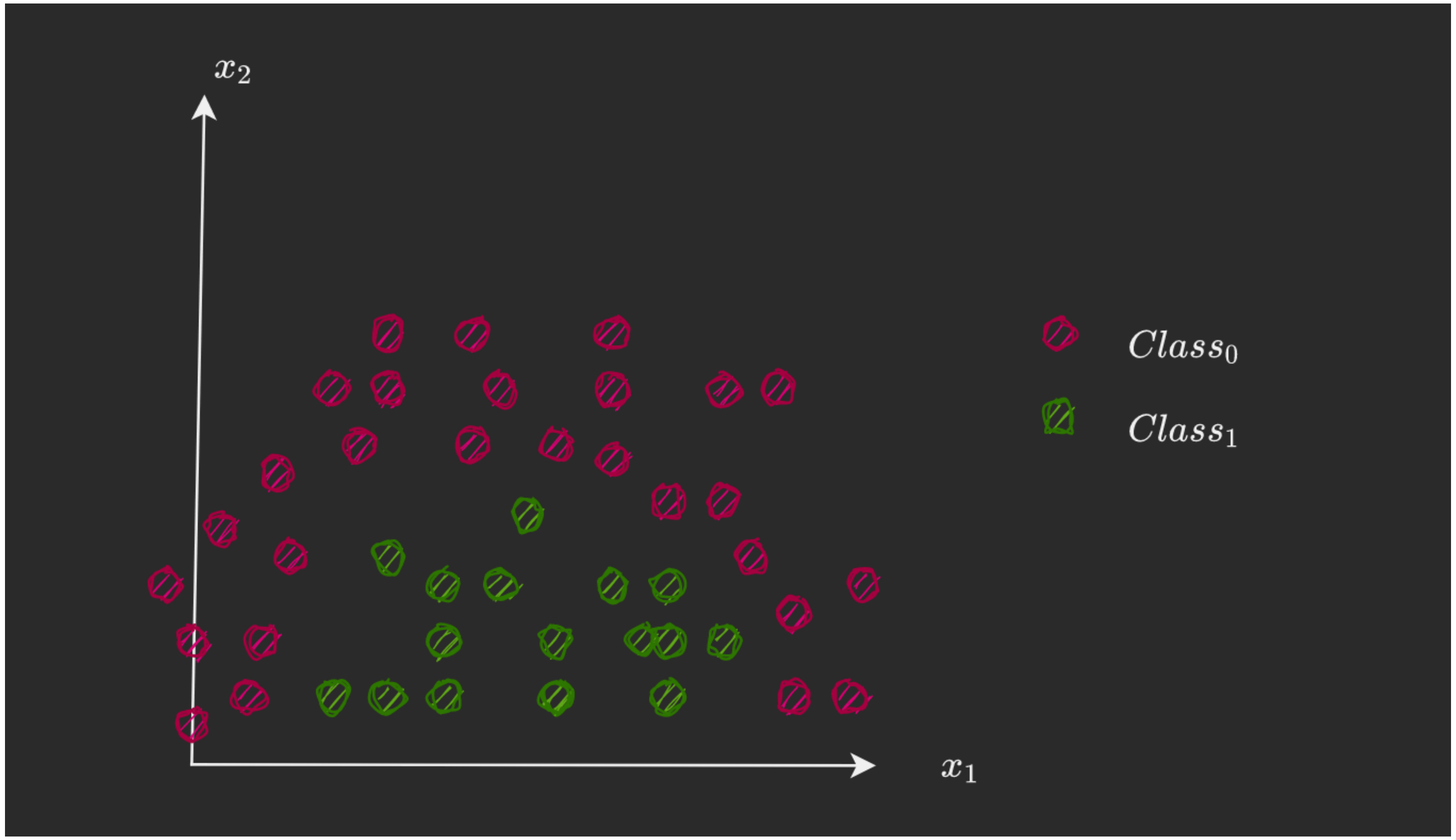
If we plot the decision boundaries from our model, — which is basically an AND of our OR and NAND models — we get something like this:



The Output plot of our 2nd Attempt, showing a correct classification on our XOR data— Image by Author using draw.io

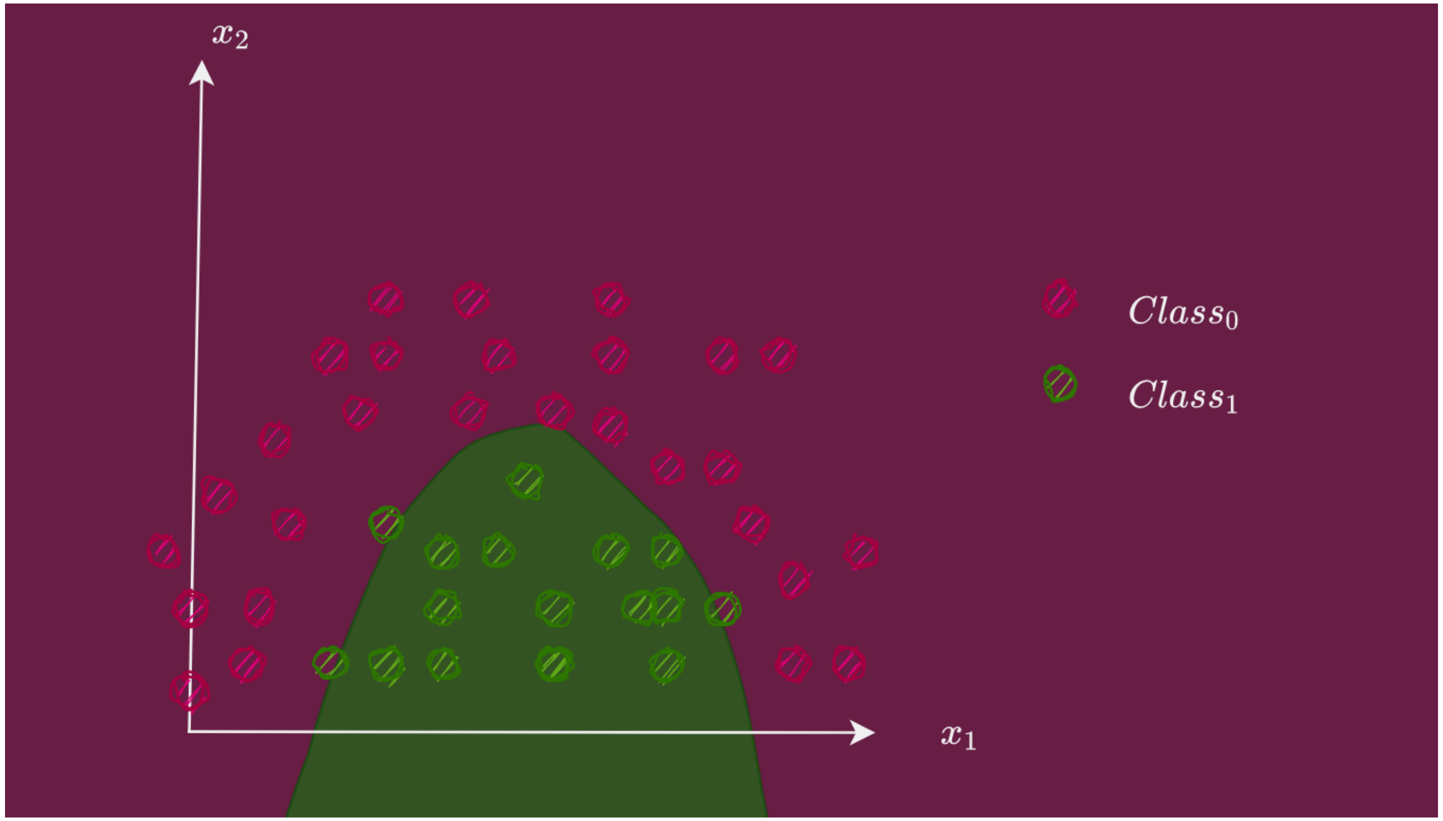
> Out of all the 2 input logic gates, the XOR and XNOR gates are the only ones that are not linearly-separable.

Though our model works, it doesn’t seem like a viable solution to most non-linear classification or regression tasks. It’s really specific to this case, and most problems can’t be split into just simple intermediate problems that can be individually solved and then combined. For something like this:



A binary classification problem in two dimensions — Image by Author using draw.io

A potential decision boundary could be something like this:



A potential decision boundary that fits our example — Image by Author using draw.io

We need to look for a more general model, which would allow for non-linear decision boundaries, like a curve, as is the case above. Let’s see how an MLP solves this issue.

The Multi-layered Perceptron

The overall components of an MLP like input and output nodes, activation function and weights and biases are the same as those we just discussed in a perceptron.

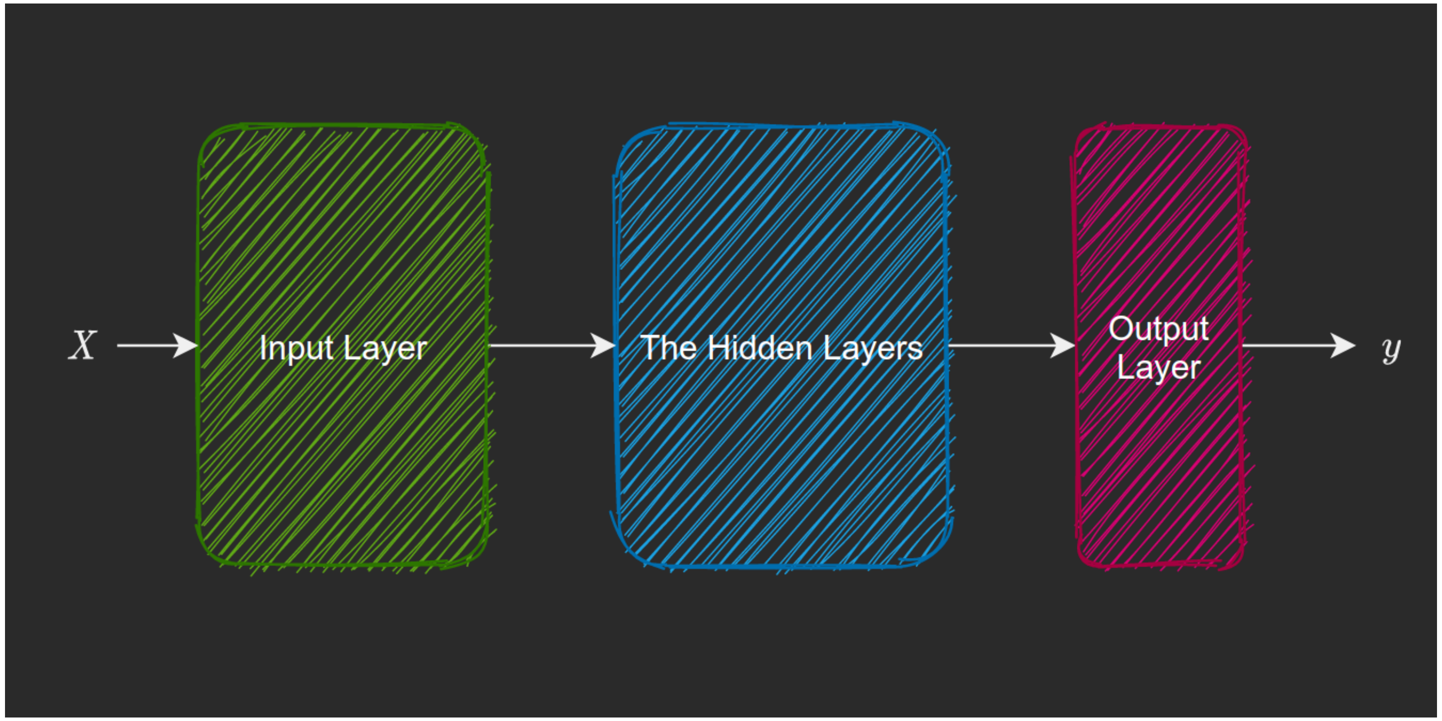
> The biggest difference? An MLP can have hidden layers.

Hidden layers

Hidden layers are those layers with nodes other than the input and output nodes.

> An MLP is generally restricted to having a single hidden layer.

The hidden layer allows for non-linearity. A node in the hidden layer isn’t too different to an output node: nodes in the previous layers connect to it with their own weights and biases, and an output is computed, generally with an activation function.



The general structure of a multi-layered perceptron — Image by Author using draw.io

Activation Function

Remember the linear activation function we used on the output node of our perceptron model? There are several more complex activation functions. You may have heard of the `sigmoid` and the `tanh` functions, which are some of the most popular non-linear activation functions.

> Activation functions should be differentiable, so that a network’s parameters can be updated using backpropagation.

Training algorithm

Though the output generation process is a direct extension of that of the perceptron, updating weights isn’t so straightforward. Here’s where backpropagation comes into the picture.

Backpropagation is a way to update the weights and biases of a model starting from the output layer all the way to the beginning. The main principle behind it is that each parameter changes in proportion to how much it affects the network’s output. A weight that has barely any effect on the output of the model will show a very small change, while one that has a large negative impact will change drastically to improve the model’s prediction power.

> **Backpropagation** is an algorithm for update the weights and biases of a model based on their gradients with respect to the error function, starting from the output layer all the way to the first layer.

The method of updating weights directly follows from derivation and the chain rule.

There's a lot to cover when talking about backpropagation. It warrants its own article. So if you want to find out more, have a look at this excellent article by Simeon Kostadinov.

Understanding Backpropagation Algorithm

Learn the nuts and bolts of a neural network's most important ingredient

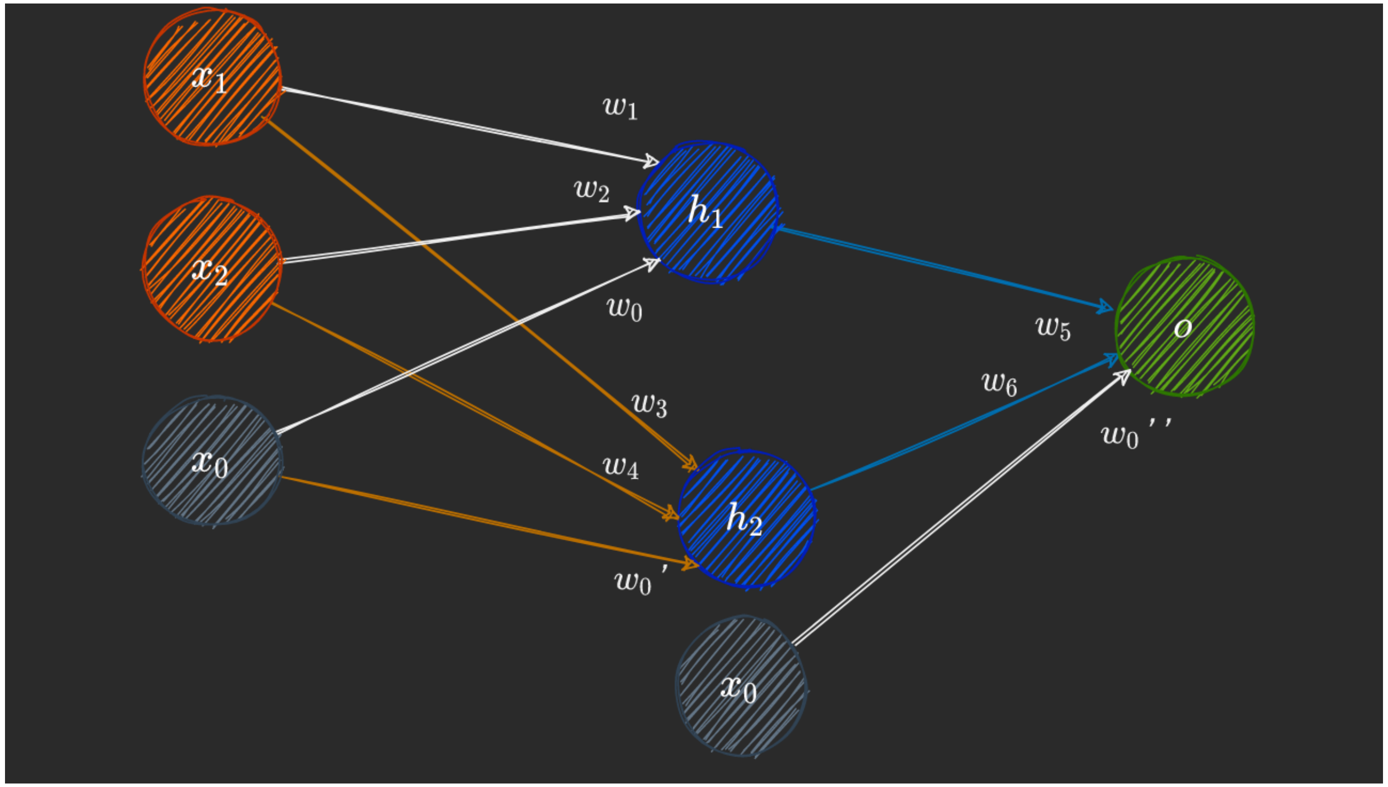
Attempt #3: the Multi-layered Perceptron

The architecture

There are no fixed rules on the number of hidden layers or the number of nodes in each layer of a network. The best performing models are obtained through trial and error.

> The architecture of a network refers to its general structure — the number of hidden layers, the number of nodes in each layer and how these nodes are inter-connected.

Let's go with a single hidden layer with two nodes in it. We'll be using the sigmoid function in each of our hidden layer nodes and of course, our output node.



The final architecture of our MLP — Image by Author using draw.io

Implementation

The libraries used here like NumPy and pyplot are the same as those used in the Perceptron class.

The training algorithm

The algorithm here is slightly different: we iterate through the training data a fixed number of times — `num_epochs` to be precise. In each iteration, we do a forward pass, followed by a backward pass where we update the weights and biases as necessary. This is called backpropagation.

The sigmoid activation function

Here, we define a sigmoid function. As discussed, it's applied to the output of each hidden layer node and the output node. Its differentiable, so it allows us to comfortably perform backpropagation to improve our model.

Its derivate its also implemented through the `_delsigmoid` function.

The forward and backward pass

In the forward pass, we apply the `wX + b` relation multiple times, and applying a sigmoid function after each call.

In the backward pass, implemented as the `update_weights` function, we calculate the gradients of each of our 6 weights and 3 biases with respect to the error function and update them by the factor `learning rate * gradient`.

Finally, the classify function works as expected: Since a sigmoid function outputs values between 0 and 1, we simply interpret them as probabilities of belonging to a particular class. Hence, outputs greater than or equal to 0.5 are classified as belonging to `Class 1` while those outputs that are less than 0.5 are said to belong to `Class 0`.

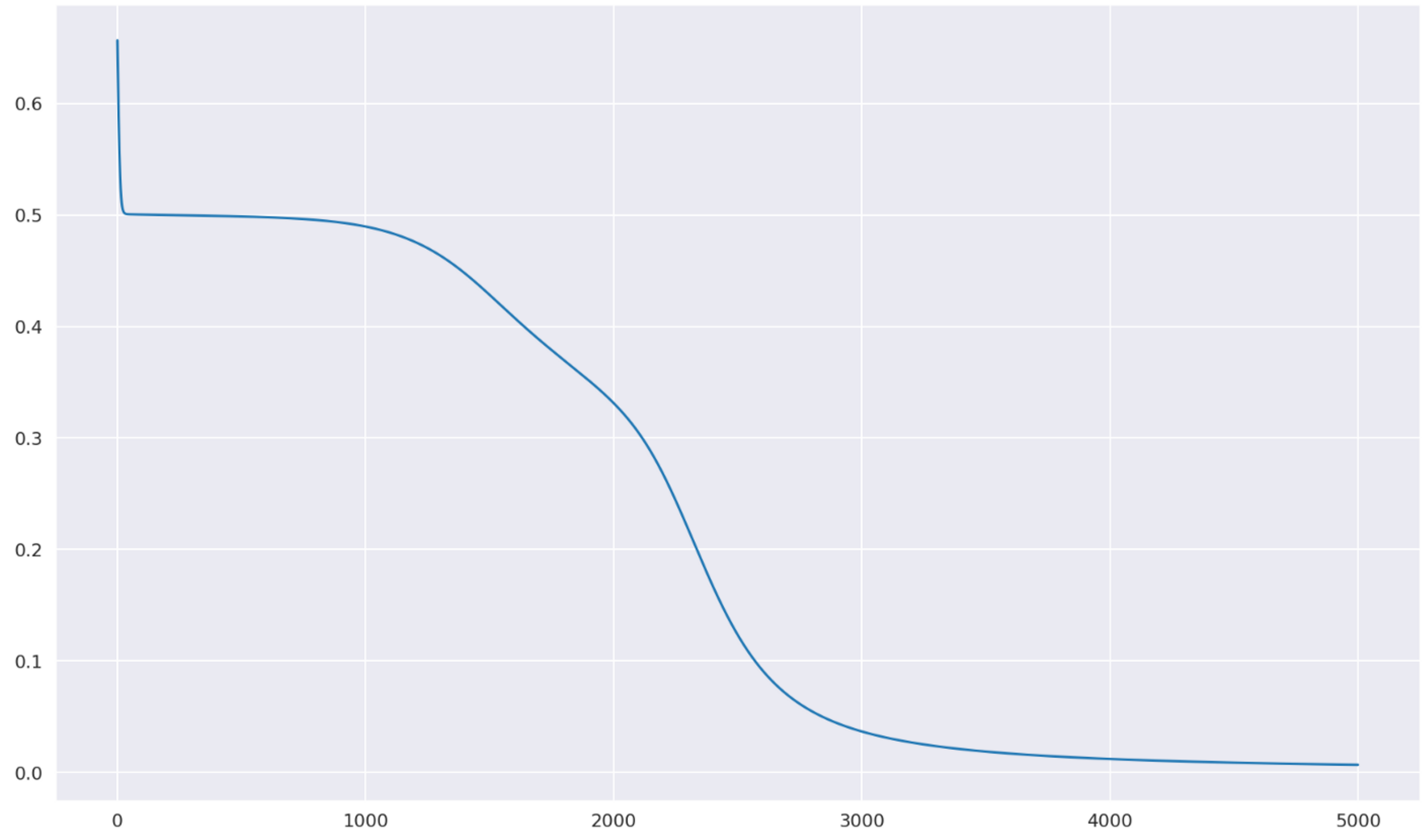
The MLP class

Let's bring everything together by creating an MLP class. All the functions we just discussed are placed in it. The `plot` function is exactly the same as the one in the `Perceptron` class.

Results

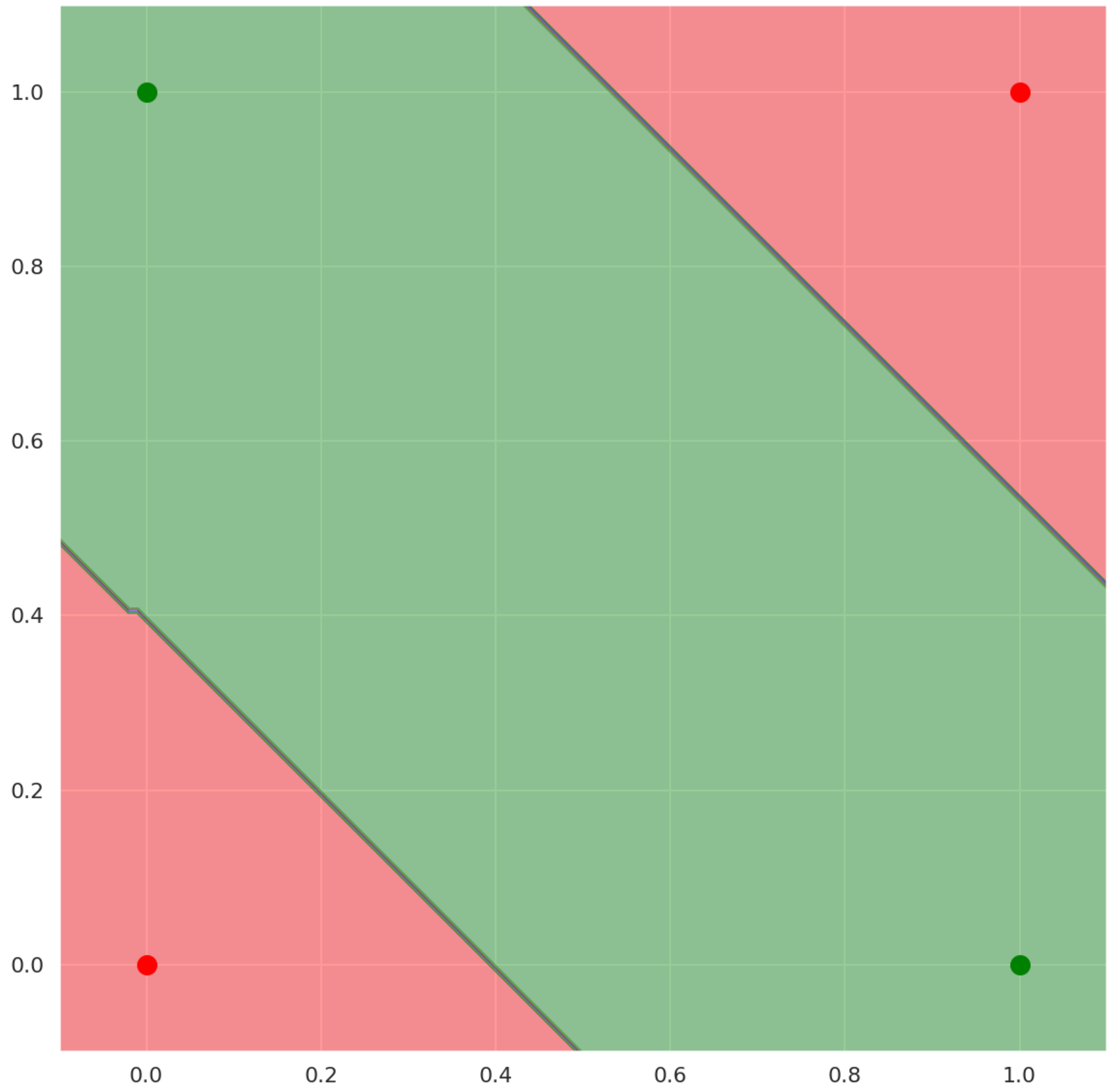
Let’s train our MLP with a learning rate of `0.2` over `5000` epochs.

If we plot the values of our loss function, we get the following plot after about 5000 iterations, showing that our model has indeed converged.



The Loss Plot over 5000 epochs of our MLP — Image by Author

A clear non-linear decision boundary is created here with our generalized neural network, or MLP.



The Decision Boundary plot, showing the decision boundary and the classes — Image by Author

Note #1: Adding more layers or nodes

Adding more layers or nodes gives increasingly complex decision boundaries. But this could also lead to something called overfitting — where a model achieves very high accuracies on the training data, but fails to generalize.

A good resource is the Tensorflow Neural Net playground, where you can try out different network architectures and view the results.

Tensorflow - Neural Network Playground

It's a technique for building a computer program that learns from data. It is based very loosely on how we think the...

playground.tensorflow.org

Note #2: Choosing a loss function

The loss function we used in our MLP model is the Mean Squared loss function. Though this is a very popular loss function, it makes some assumptions on the data (like it being gaussian) and isn't always convex when it comes to a classification problem. It was used here to make it easier to understand how a perceptron works, but for classification tasks, there are better alternatives, like **binary cross-entropy loss.**

How to Choose Loss Functions When Training Deep Learning Neural Networks - Machine Learning Mastery

Deep learning neural networks are trained using the stochastic gradient descent optimization algorithm. As part of the...

machinelearningmastery.com

Conclusion

Neural nets used in production or research are never this simple, but they almost always build on the basics outlined here. Hopefully, this post gave you some idea on how to build and train perceptrons and vanilla networks.

Thanks for reading!