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Part I

Introductory Block
Chapter 2

Neural networks as universal approximators, and the issue of depth

In Chapter 1 we discussed the chronological (and logical) development of neural networks, and saw how neural networks can be viewed as functions that can model almost any AI task. They can do so because they can operate on continuous-valued inputs, generate continuous valued outputs, and represent arbitrarily complex decision boundaries in continuous spaces. In this chapter, we will study the latter topic in greater detail: how neural networks represent arbitrarily complex decision boundaries.

To be able to accomplish “intelligent” tasks, it was believed that computing machines must emulate the human brain. The basic formalisms for neural networks were focused on realizing this goal. Over time, as the structure and functioning of neurons in the brain came to be better understood, direct analogies to those were created within mathematical frameworks. The perceptron, and later, networks of perceptrons emerged from these attempts.

2.1 The perceptron revisited

However, while neural networks sought to approximately mimic the networked structure of the brain, the scale of the brain’s structure in terms of the number of neurons was difficult to emulate due to computational and logistic limitations.
The reasons will become clearer as we learn more about these computational approximations, some of which we discussed in Chapter 1. We must note in this context that the human brain is a massive structure comprising billions of neurons. An average human brain has about 86 billion neurons!

Let us understand further how neural networks sought to mimic the structure of the brain. For this, we must first revisit the Perceptron. We saw in Chapter 1 that each neuron (fashioned after the neurons in the brain) can be approximated with a unit that “fires” or generates an output different from 0 when some function of its inputs exceeds some pre-set threshold. In electrical engineering terms, the perceptron is a threshold gate, and implements threshold logic. Fig. 2.1 recalls the basic perceptron from Chapter 1.

The perceptron in Fig. 2.1(a) is represented as a threshold unit that fires if the weighted sum of inputs and the “bias” $T$ is positive. This is a slightly different way of visualizing the perceptron. Here we first compute an affine combination of the inputs, which is a weighted sum of inputs plus a bias (which is $-T$), and this is then put through a thresholding activation function which outputs a 1 if the input is zero or greater (i.e. positive), and 0 otherwise.

Fig. 2.1(b) shows the “soft” perceptron, which uses a thresholding function (sometimes loosely referred to as the “squashing” function) – which is a sigmoid. A sigmoid is simply a smoothed version of the threshold function. Thus this version has a sigmoid activation instead of a threshold activation. The sigmoid renders the output to be continuous valued, lying between 0 and 1. Later in this chapter (and in future chapters) we will discuss the many benefits of replacing the threshold activation by a soft activation.

The sigmoid is not the only function that can enable soft activation. Some popular formulations of soft activations are shown in Fig. 2.2. Of the examples shown, the $tanh$ function is in fact simply a scaled and shifted version of the sigmoid. Note that an activation function need not even be a function that scales the vertical axis (i.e., it need not be a “squashing” function). The rectifier (or rectification) function shown in Fig. 2.2 represents one that is not such a function: it simply truncates negative values, but passes positive values through unchanged.
(a) A perceptron is a unit (depicted as a circle above) that receives many inputs. It has a weight associated with each incoming input. If the weighted sum of all of the inputs, i.e. the sum over all inputs of the product of the input and the corresponding weight, exceeds a threshold, the neuron fires, otherwise it doesn’t. Its operation can be expressed as an affine (upper expression) or a linear (lower expression) combination of inputs.

\[ z = \sum_i w_i x_i - T \]

\[ y = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{else} \end{cases} \]

(b) The perceptron with a soft thresholding function, highlighted in yellow (lower expression).

\[ z = \sum_i w_i x_i - T \]

\[ y = \frac{1}{1 + \exp(-z)} \]

Figure 2.1: Recap: Threshold logic in a perceptron
The softplus function is its smooth variant – it is differentiable everywhere. These are just a few examples of soft activation functions. We will discuss more of these later.

![Diagram of activation functions](image)

The **sigmoid**, **tanh**, **rectifier** and **softplus** activation functions.

Figure 2.2: Examples of some activation functions

For the purpose of this chapter, let us continue to assume the threshold activation, as it is somewhat easier to understand and intuitions developed from it generalize well.

### 2.2 Deep structures and the concept of depth

Fig. 2.3(a) shows a general “layered” network of neurons. Fig. 2.3(b) shows a “deep” neural network.

In a network of perceptrons, layering is not essential. We can have networks without explicit layers in them. A multi-layered perceptron, or an MLP, is a network of perceptrons wherein the neurons are generally arranged in layers, as shown in Fig. 2.3. When MLPs have many layers, they are said to be **deep** networks. In the section below we discuss the formal notion of depth in this context – what are the formal criteria for a network to qualify as a “deep” network?
(a) A multi-layered network of perceptrons.

(b) Deep layering in a network of perceptrons – a **deep** neural network.

Figure 2.3: The concept of layering and deep layering in a network of perceptrons
2.2.1 The formal notion of depth

In any directed graph with a source and a sink, the *depth* of the graph is simply the length of the path – i.e., the number of edges – on the longest path from source to sink. Fig. 2.4 shows some illustrative examples. In general, in any directed network of computational elements with input source nodes and output sink nodes, “depth” is the length of the longest path from a source to a sink.

![Diagram](image)

**Left:** There are 2 paths from source to sink. One is of length 2, another is of length 1. The depth of this graph is therefore 2. **Right:** This graph has paths of length 1, 2 and 3 from source to sink. The longest path is of length 3, so the depth of this graph is 3.

Figure 2.4: Explaining the notion of depth in deep structures

We apply the same criterion to defining depth in neural networks. In a neural network, the computation is generally carried out in a directed fashion – from input to output. The depth of a network is the length of the longest path, i.e. the maximum number of units (or neurons) from input to output.

As a more specific example, consider the networks shown in Fig. 2.5. The depth of the network in Fig. 2.5(a) is 3, since the longest path from the input to output is 3. Similarly, the depth of the network in Fig. 2.5(b) is 2, and that in Fig. 2.5(c) is 3.

The notion of a “layer” can now be formalized in terms of depth as defined above: A *layer comprises the set of neurons in which all members have same depth from the input*. For example, in Fig. 2.5(d), all the green neurons have a depth 2, so they form a layer, which we will call the second layer. Note that there is also a direct path of length 1 from the input to these neurons, but they are not part of the first layer. The first layer is the set of neurons colored red, which are all at depth

---

1We often refer to perceptrons as neurons in this book, to be more generic
Figure 2.5: Explaining the notion of depth in MLPs
1 with respect to the input. The yellow neurons form layer 3, while the output neurons, in blue, are layer 4.

2.2.2 The multi-layer perceptron

In chapter I we presented a multi-layer perceptron as a network of perceptrons (or neurons). The nodes in such a network are individual perceptrons. The edges represent the connection between perceptrons, and each edge carries a weight. The network performs computations on some input, and produces an output. The inputs can be real valued, or Boolean stimuli. The outputs too can be Boolean or real valued. While we have largely discussed networks with a single output so far, a network can in fact have multiple outputs, or a vector of outputs, for any input. The perceptron network (or neural network) thus represents a function that embodies an input-output relationship between its inputs and outputs.

For us to understand the strengths and limitations of such networks much better, we must have an clear understanding of the types of input/output relationships that such networks can model, and the kinds of functions they can compute. The following sections attempt to build up our understanding of these aspects of MLPs.

2.3 MLPs as approximate functions

In Chapter I we have already seen that the MLP can compose, Boolean functions (operating on Boolean inputs and producing Boolean outputs), real-input category functions (that operate on real inputs and output Boolean values), and even real functions (which operate on real inputs and produce real outputs).

Some examples are shown in Fig. 2.6. Fig. 2.6(a) shows a network that models an ugly function of four Boolean variables. Fig. 2.6(b) graphs a function (in blue) and the piece-wise approximation for it that can be obtained from an
Figure 2.6: Examples of Boolean and continuous valued functions modeled by an MLP appropriately constructed network (See 1.4.10 for explanation).

An important question in this context is: can we always construct a network to compute any function, or are there limitations on the kinds of functions that can be modeled with a network (and if so, what are they)? We will learn the answers to these question in the sections that follow.

### 2.4 MLPs as universal Boolean functions

Multi-layer perceptrons can model any Boolean function: given a Boolean function, we can construct an MLP that computes it. The function can be arbitrarily complex, and over any number of variables. Does this imply that the MLP that models it must also be complex?

There are several ways of quantifying the complexity of a network. We will consider two: the number of layers in the network, and the number of neurons in the network.
2.4.1 The perceptron as a Boolean gate

We have seen that individual perceptrons can model Boolean gates. Fig. 2.7 shows examples of how a perceptron can model AND, NOT and OR gates.

The numbers on the edges represent weights, the numbers in the circles represent thresholds. The perceptron outputs a 1 if the total weighted input equals to, or exceeds the threshold. **Top left:** a perceptron that only outputs a 1 when both inputs are 1. This models an AND gate. **Top right:** This perceptron outputs a 1 when the input is 0 and vice versa. This models a NOT gate. **Bottom:** This perceptron outputs a 1 when either of the inputs is 1. This models an OR gate.

![Perceptron Diagram](image)

Figure 2.7: AND, NOT and OR gates modeled by a perceptron

Perceptrons can however model much more. A perceptron can model *generalized* gates. This is illustrated by the panels in Fig. 2.8. In Fig. 2.8[a], the perceptron is a generalized AND gate. It will fire only if $X_1, X_2, \ldots, X_L$ are all 1, and $X_{L+1}, X_{L+2}, \ldots, X_N$ are all 0.

To understand why this is so, consider the case when $X_1, X_2, \ldots, X_L$ are all 1 and the rest are 0. Then the total input is exactly $L$, and since the threshold is also $L$, the perceptron will fire. But now if we set any of the inputs from $X_{L+1}, X_{L+2}, \ldots, X_N$ to 1, then because those inputs have a weight of -1, the sum of all weighted inputs will become less than $L$, and the perceptron will not fire. So also, if any of the first $L$ bits becomes 0, the sum can never be $L$ or more, and the unit will not fire. Thus, this perceptron *only* produces an output of 1 when $X_1, X_2, \ldots, X_L$ are 1 and the rest are 0. In general, we can construct a gate that
(a) A generalized AND gate. This perceptron will only fire if $X_1$ through $X_L$ are 1 and $X_{L+1}$ through $X_N$ are 0.

(b) A generalized OR gate. This perceptron will only fire if any of the first $L$ inputs is 1 or if any of the remaining inputs is 0.

(c) A generalized majority gate. This perceptron will fire if at least $K$ inputs are of the desired polarity.

(d) Another generalized majority gate. This perceptron will fire only if the total number of $X_1$, $X_2$, $X_{L+1}$, $X_{L+2}$, $X_N$ that are 0 is at least $K$.

Figure 2.8: Generalized gates modeled by a perceptron
will only fire under the very specific condition that some chosen subset of inputs are 1, and the rest are 0, by choosing an appropriate threshold and appropriate weights to apply to the inputs.

In Fig. 2.8(b), the perceptron is generalized OR gate. It will fire if any of the first \( L \) inputs is 1, OR if any of the remaining inputs is 0. To understand this, let us assume that all of the first \( L \) inputs are 0 and all of the remaining inputs are 1 – the only condition under which it should not fire.

In this situation, there are \( N - L \) inputs with value 1, and all their weights are -1. Therefore, the total input is \( L - N \). Now, if even one of the inputs flips its value, the sum becomes \( L - N + 1 \), which is the threshold at which the perceptron fires. In other words, if any of the first \( L \) inputs becomes 1, or if any of the last \( N - L \) inputs becomes 0, the perceptron will fire, which is the required OR condition in this gate. If more of the inputs satisfy our condition, the sum will, of course, exceed the threshold of \( L - N + 1 \).

In Fig. 2.8(c), the perceptron is generalized majority gate. The perceptron shown will fire if at least \( K \) of the inputs are 1.

This is so because in the first case, all inputs have a weight of 1, and if at least \( K \) of the inputs are 1, the total weighted sum of inputs will equal or exceed the threshold \( K \). The perceptron will then fire. This gate is called a generalized majority gate because for \( K > N/2 \) the perceptron fires if the majority of inputs is 1.

Similarly, the perceptron in Fig. 2.8(d) is another example of a generalized majority gate. It will fire only if the total number of \( X_1, X_2, \ldots, X_L \) that are 1 and \( X_{L+1}, X_{L+2}, \ldots, X_N \) that are 0, is at least \( K \).

Thus we see that the perceptron is a very versatile unit, and can model complex Boolean functions. It is probable that such examples and reasoning led Rosenblatt to believe that perceptrons could model all Boolean functions, without exception. However, this is not the case. In spite of such versatility, the perceptron cannot model the XOR function. There is in fact no combination of weights and
threshold for which it will compute an XOR.

(a) Example of a perceptron network that computes the XOR.

(b) A more compact MLP that can compute an XOR.

Figure 2.9: Examples of MLPs modeling XOR functions

In fact, to compute an XOR we must use a network of perceptrons, or a multilayer perceptron as we discussed in Chapter 1. For example, Fig. 2.9(a) shows a network that computes the XOR. It is a network of 3 perceptrons, with one hidden layer whose outputs we do not directly see. It has one output perceptron. The computation performed by this structure is rather obvious: the first perceptron (on top), in the hidden layer computes \((X \lor Y)\). The perceptron at the bottom in the hidden layer computes \(((\neg X) \lor (\neg Y))\). The final (output) perceptron ORs the outputs of the two hidden-layer perceptrons to yield \((X \oplus Y)\).

This is of course not the only way to build an MLP to compute an XOR. Fig. 2.9(b) shows a more compact way of building an MLP to compute an XOR. This uses only two perceptrons, uses 5 weights and 2 thresholds, and now the weights are also not all 1.

Since MLPs can compose any Boolean gate, and any network of Boolean gates, MLPs are, in fact, universal Boolean functions. For any Boolean function there is always an MLP that can compute it.

Although MLPs are universal Boolean functions, it is important to know how complex the network must be in order to compute any given Boolean function.
(a) A multi-layered MLP can model any function, such as the one shown on top. An MLP that computes this function has two layers.

(b) A deep network. The depth of a network is relevant to its ability to compute a given Boolean function.

Figure 2.10: MLPs as universal Boolean functions
In the example shown in Fig. 2.10(a), we see that in order to construct the function shown, we must use 7 neurons in three layers. If we had a more complex function, of a larger number of inputs, how can we determine the number of layers that an MLP would need to compute it?

To understand this, let us consider the example shown in Fig. 2.11. Any Boolean function can be expressed as a truth table, that explicitly lists every possible combination of input variables and the corresponding outputs as a table. In the example shown in Fig. 2.11, columns in blue represent all combinations of input variables, and the yellow column on the right hand side lists the corresponding output for each row. Note that we need not enter every combination of inputs in the table. It is sufficient to only list all the input combinations for which the output is 1. For the other combinations, the output is implicitly 0.

### Truth Table

<table>
<thead>
<tr>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>$X_4$</th>
<th>$X_5$</th>
<th>$Y$</th>
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<td>0</td>
<td>0</td>
<td>1</td>
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$Y = \bar{X}_1\bar{X}_2X_3X_4\bar{X}_5 + \bar{X}_1X_2\bar{X}_3X_4X_5 + \bar{X}_1X_2X_3\bar{X}_4\bar{X}_5 + X_1\bar{X}_2\bar{X}_3\bar{X}_4X_5 + X_1\bar{X}_2X_3\bar{X}_4X_5 + X_1X_2\bar{X}_3\bar{X}_4X_5$

Any Boolean function can be represented as a truth table. The columns in blue represent all combinations of input variables, and the yellow column on the right hand side lists the corresponding output for each row. The function that this truth table represents is shown below the table.

Figure 2.11: Boolean function as a truth table and its disjunctive normal form

The function that the truth table in Fig. 2.11 represents is in fact expressed below it in a disjunctive normal form (DNF form or DNF formula).
The DNF formula has *clauses*: each clause represents one of the combinations for which the output is 1, i.e. one of the rows of the truth table. Thus the first clause in the DNF form shown in Fig. 2.11 – \((\text{NOT } X_1) \text{ AND } X_2 \text{ AND } X_3 \text{ AND } X_4 \text{ AND } (\text{NOT } X_5)\) – represents the first row in the truth table. Note that by definition, \((\text{NOT } X_1)\) becomes true when \(X_1\) is 0. Thus the first clause indicates that the output is 1 when \(X_1\) is 0, \(X_2\) is 0, \(X_3\) is 1, \(X_4\) is 1 and \(X_5\) is 0. The second clause similarly represents the second row in the truth table: \((\text{NOT } X_1) \text{ AND } X_2 \text{ AND } (\text{NOT } X_3) \text{ AND } X_4 \text{ AND } X_5\). The third clause represents the third row: \((\text{NOT } X_1) \text{ AND } X_2 \text{ AND } X_3 \text{ AND } (\text{NOT } X_4) \text{ AND } (\text{NOT } X_5)\). The fourth clause represents the fourth row: \(X_1 \text{ AND } (\text{NOT } X_2) \text{ AND } (\text{NOT } X_3) \text{ AND } (\text{NOT } X_4)\) and \(X_5\), and so on. Since the truth table lists only six combinations for which the output is 1, the DNF formula shown has exactly six clauses, one representing each of the combinations in the truth table, and its interpretation is that the function that it represents takes a value of 1 if any of the clauses is true.

Once we have this representation, we can use it to build an MLP to compute it, using perceptrons that model generalized AND gates and OR gates. The perceptrons that model the first to sixth clauses are shown in Fig. 2.12.

Finally, as shown in Fig. 2.13 the MLP has one output perceptron that ORs the outputs of the six clauses. Thus we now have an MLP that computes exactly the Boolean formula shown in the example of Fig. 2.11. An interesting point to note is that this network only has one hidden layer, wherein each neuron computes one of the clauses in the DNF formula for the function. In fact, since any Boolean function can be expressed as a truth table, and thereby in DNF form, it can be modeled by an MLP with only one hidden layer. A *one-hidden-layer MLP is a universal Boolean function*!

This leads us to a related question: while any Boolean function can be modeled an MLP with just one hidden layer, how large must that layer be, i.e. how many neurons must it contain? Since the one-hidden-layer MLP is derived from the DNF formula for the Boolean function, the equivalent question is – what is the smallest DNF formula (i.e. the DNF formula with the fewest clauses) that can model the function? To determine this, we must reduce the Boolean function to
The networks for computing successive terms in the disjunctive normal form.

Figure 2.12: Construction of MLPs corresponding to a DNF/truth table

\[ Y = \overline{X}_1 \overline{X}_2 X_3 X_4 \overline{X}_5 + \overline{X}_1 X_2 \overline{X}_3 X_4 X_5 + \overline{X}_1 X_2 X_3 \overline{X}_4 \overline{X}_5 + \overline{X}_1 X_2 X_3 X_4 X_5 + X_1 X_2 \overline{X}_3 \overline{X}_4 X_5 \]

\[ Y = \overline{X}_1 \overline{X}_2 X_3 X_4 \overline{X}_5 + \overline{X}_1 X_2 \overline{X}_3 X_4 X_5 + \overline{X}_1 X_2 X_3 \overline{X}_4 \overline{X}_5 + \overline{X}_1 X_2 X_3 X_4 X_5 + X_1 X_2 \overline{X}_3 \overline{X}_4 X_5 \]

\[ Y = \overline{X}_1 \overline{X}_2 X_3 X_4 \overline{X}_5 + \overline{X}_1 X_2 \overline{X}_3 X_4 X_5 + \overline{X}_1 X_2 X_3 \overline{X}_4 \overline{X}_5 + \overline{X}_1 X_2 X_3 X_4 X_5 + X_1 X_2 \overline{X}_3 \overline{X}_4 X_5 \]

\[ Y = \overline{X}_1 \overline{X}_2 X_3 X_4 \overline{X}_5 + \overline{X}_1 X_2 \overline{X}_3 X_4 X_5 + \overline{X}_1 X_2 X_3 \overline{X}_4 \overline{X}_5 + \overline{X}_1 X_2 X_3 X_4 X_5 + X_1 X_2 \overline{X}_3 \overline{X}_4 X_5 \]

The final network for computing the complete disjunctive normal form.

Figure 2.13: The complete MLP for the DNF/truth table

\[ Y = \overline{X}_1 \overline{X}_2 X_3 X_4 \overline{X}_5 + \overline{X}_1 X_2 \overline{X}_3 X_4 X_5 + \overline{X}_1 X_2 X_3 \overline{X}_4 \overline{X}_5 + \overline{X}_1 X_2 X_3 X_4 X_5 + X_1 X_2 \overline{X}_3 \overline{X}_4 X_5 \]
its minimal form. We discuss this below.

2.4.2 Reducing the Boolean function

(a) A Karnaugh map. It represents a truth table as a grid. Filled boxes represent input combinations for which output is 1; blank boxes have an output of 0. Adjacent boxes can be “grouped” to reduce the complexity of the DNF formula.

(b) Reducing the DNF by grouping filled boxes (3 groups or clauses emerge in this example). The single-hidden layer MLP that computes the Boolean function for this truth table has only 3 neurons in the hidden layer, each of which computes one of these clauses. The black dots in the input layer represent $W$, $X$, $Y$ and $Z$ from left to right.

Figure 2.14: The Karnaugh map and its role in reducing DNFs to minimal forms

Fig. 2.14 shows an alternative representation of a truth table. This representation is called a *Karnaugh map*. A Karnaugh map is a way of representing bit patterns such that bit patterns that differ by only one bit are always arranged next to one another. The example in Fig. 2.14(a) is a Karnaugh map over four variables: $W$, $X$, $Y$ and $Z$. The four rows represent the four combinations of $W$ and $X$. Observe that adjacent rows differ by only one bit. The four columns represent the four combinations of $Y$ and $Z$. Observe again that adjacent columns differ by only one bit. Thus all combinations of the four variables can be placed on a $4 \times 4$ grid. Any grid cell differs from its neighbors by only one bit. Also, the rightmost edge is “connected” to the leftmost edge because patterns in the rightmost column and leftmost column differ by only one bit. For instance the rightmost box in the first row, representing 0010 differs by only one bit from the
leftmost box in this row, which represents 0000. Thus they can be considered to be “connected” — i.e. are neighbors, and the row represents a “cycle.” The top row is connected to the bottom row in the same manner, since 0010 differs from 1010 by only one bit. The square grid in Fig. 2.14(a) is in fact a torus, and represents a topologically correct representation of all patterns of the 4 variables used.

The Karnaugh map in the example shown takes the place of a 4-variable truth table: the 16 boxes represent the 16 possible combinations of the 4 input variables. The boxes highlighted in yellow represent input combinations for which the output is 1. For the function represented by this Karnaugh map, there are 7 input combinations that produce the output 1. A naïve DNF would thus have 7 clauses.

To reduce the size of that DNF, the neighboring boxes that are filled can be grouped. This is shown in Fig. 2.14(b). In this, the four boxes in the first column all produce the output 1. If the combination $YZ$ takes the value 00, it doesn’t matter what $WX$ is, the output is always 1. They can therefore be grouped into the DNF clause $(\text{NOT } Y)$ AND $(\text{NOT } Z)$. Similarly, the two neighboring second row elements shown in the figure too produce the output 1, which means for $WX = 01$, if $Y = 0$, the output is 1 and $Z$ can be ignored. This gives us the second group which comprises the DNF clause $(\text{NOT } W)$ AND $X$ AND $(\text{NOT } Y)$. In the fourth column, the two filled boxes are actually neighbors, as explained earlier, and can be grouped into the clause $(\text{NOT } X)$ AND $Y$ AND $(\text{NOT } Z)$. As a matter of fact, we could group all four corners together and get an even simpler clause $(\text{NOT } X)$ AND $(\text{NOT } Z)$.

With this grouping, the original 7-entry truth table can now be reduced to only 3 groups, with a corresponding 3-clause DNF. The reduced DNF formula is shown in Fig. 2.14(b). The figure also shows the reduced perceptron network for this function, which needs only 3 hidden units. Thus, reduction of the DNF reduces the size of the one-hidden-layer network needed to model the corresponding Boolean function. In other words, so long as the entries in the truth table can be grouped based on neighborhood, the DNF formula that expresses it can be
made smaller, and the resulting network too will be small. When the DNF for-

made smaller, and the resulting network too will be small. When the DNF for-
mula is minimal, the network that represents it will be the smallest one required
to compute the corresponding Boolean function.

(a) A different Karnaugh map. This
map cannot be reduced further.

(b) A Karnaugh map in 3 dimensions. This
map also cannot be reduced further.

Figure 2.15: Examples of irreducible Karnaugh maps

In this context, it is interesting to note the examples of Karnaugh maps given in
Fig. 2.15. These give us an idea of how large the one-layer Boolean MLP can get,
in the worst case. Why is this so? Smaller Boolean MLPs are possible through
the process we have just discussed because we can group adjacent highlighted
cells in a Karnaugh map. However, this may not always be possible. With a little
thought, it is easy to see that the one arrangement of cells in a Karnaugh map
in which cells simply cannot be grouped together is the checkerboard pattern, as
shown in Fig. 2.15. In the examples shown, alternate entries are highlighted in
red in the rows and columns, representing an output of 1 for the corresponding
input patterns (the input variables are indicated in each example). The pattern
ensures that no two cells can be grouped. These also represent the largest irre-
ducible DNFs. The DNF corresponding to Fig. 2.15[a] would have half as many
clauses as the product of the number of rows and columns \((16/2 = 8\) in this
example). The corresponding MLP would have 8 neurons in its hidden layer.
Fun facts 4.1: Karnaugh maps or K-maps

Boolean functions can be expressed in two ways: in their disjunctive normal form (DNF) (more explicitly, canonical disjunctive normal form (CDNF)) and in their conjunctive normal form (CNF) (more explicitly, canonical conjunctive normal form (CCNF)).

The CDNF is also called the minterm canonical form and the CCNF is called the maxterm canonical form. Other canonical forms exist, such as the algebraic normal form, Blake canonical form etc which we will not discuss.

A minterm expression uses logical ANDs – products of variables. A max-term expression uses logical ORs – sums of variables. These are dual concepts. They are have a complementary (or symmetrical) relationship with each other (they follow De Morgan’s laws).

The Sum of Products (SoP or SOP) is a sum of minterms: a disjunction (OR) of minterms. The Product of Sums (PoS or POS) is a product of maxterms: a conjunction (AND) of maxterms.

Karnaugh maps [1], or K-maps, are used to simplify or minimize complex logic expressions. They are useful in many applications that implement Boolean logic (among others): in circuits that use logic gates, software design etc.

K-maps can use minterm or maxterm expressions. Accordingly, they have two forms: SoP and PoS forms. In the examples above, we have used the SoP form, which is practically realized in hardware implementations using AND gates in the minterms, which are aggregated (summed) by an OR gate. A PoS form would be its alternative, and would use OR gates in the maxterms, which would all be aggregated by an AND gate. In MLPs, the perceptrons used would do the exact equivalent of these operations.
How do we make a K-map for a large (even or odd) number of variables? It is not easy. The problem arises due to neighborhood: two bit patterns are neighbors if they differ in no more than one bit. So, for instance, 0011, 1010, 0110 and 0000 are all immediate neighbors of 0010. To properly display this neighborhood pattern we will need a 2D map, since a linear map will allow no more than 2 neighbors for any cell. But now when we go up to 5 or 6 variables, each bit pattern will have up to six neighbors. This will require a 3-dimensional grid, with the caveat that the grid is not cuboidal, but in fact a hard-to-visualize four-dimensional torus, since the left and right faces of the cube are neighbors, as are the front and back, and top and bottom. In general, with \( N \) variables, the K-map equivalent may be viewed either as a hypercube in \([N/2]\)-dimensional space with opposite faces being neighbors, or a hypertorus in even higher dimensional space.

Popular visualizations will instead show “unfolded” versions of the map, which lay “slices” of the hypercube next to one another in a manner that captures the neighborhood along 4 of the bits, leaving higher-dimensional neighborhood relations to the imagination of the viewer. For example, such a visualization of a K-map for 8 variables is shown below:
2.4.3 Width of a one-hidden-layer Boolean MLP

Fig. 2.15 shows a 3-dimensional version of the Karnaugh map of six input variables: $U, V, W, X, Y$ and $Z$. In this case, 32 neurons would be required in the hidden layer for a one-hidden-layer MLP that computes the corresponding Boolean function.
This reasoning can be generalized. If we have a Boolean function over $N$ variables, and construct a one-hidden-layer MLP to compose the corresponding DNF formula, we will need a maximum of $2^{N-1}$ neurons in the hidden layer. The size of the network (in terms of the neurons required) is thus exponential in $N$, the number of inputs.

However, this applies only to a one-hidden-layer MLP. An obvious question in this context is: what would the size of the network be if we allowed multiple hidden layers? We discuss this next.

### 2.4.4 Size of a deep MLP

The function represented by each checkerboard patterned Karnaugh map in the example above is actually just an XOR, as shown in Fig. 2.17. The four-variable function corresponding to the map on the left is $W \oplus X \oplus Y \oplus Z$, where the symbol “⊕” represents the XOR operation. Similarly, the six-variable function corresponding to the map on the right is $U \oplus V \oplus W \oplus X \oplus Y \oplus Z$.

\[
O = W \oplus X \oplus Y \oplus Z \\
O = U \oplus V \oplus W \oplus X \oplus Y \oplus Z
\]

The Karnaugh maps shown represent XOR functions. **Left:** $W \oplus X \oplus Y \oplus Z$, **Right:** $U \oplus V \oplus W \oplus X \oplus Y \oplus Z$.

Figure 2.17: Karnaugh maps representing XOR functions

Recall that we can compose a single XOR function using an MLP with 3 perceptrons, or in fact even only 2 perceptrons, as shown in Fig. 2.9. Fig. 2.18[a] recalls the 3-perceptron case.
Now let us consider Fig. 2.18(b). For the Karnaugh map shown in Fig. 2.18(b), the corresponding function is shown below it. For this function, we can construct the MLP as a series of XOR MLPs as shown on the right of the Karnaugh map. In this MLP, the first 3 neurons compute $W \oplus Y$. The next 3 neurons compute the XOR of the result of this with $Y$, and the final three neurons XOR this output with $Z$. Since the function shown includes only 3 XORs, we need 3 neurons per XOR. Thus we need only 9 neurons when we build a deep MLP for it. Recall that the one-hidden-layer MLP for this, shown in the previous example, also needed 9 neurons – one each for each of the 8 clauses, and one final OR neuron. The current XOR scheme does not present any advantage in this case. However, as we shall see in the subsequent example, when we have a larger number of inputs to contend with, the enormous difference and advantage of using a deep structure becomes apparent.

Now consider Fig. 2.19. The Karnaugh map shown in this figure represents a function over 6 variables, and has 5 XORs in the corresponding function, as shown. In this case, the deep MLP would only require 15 neurons, whereas the one-hidden-layer network required 65 neurons, as explained earlier.

This requirement can be generalized for $N$ input variables. The XOR of $N$ input variables will require $3(N - 1)$, or even only $2(N - 1)$ neurons (if we use the two-neuron model for the XOR) when built in this manner.

To summarize the differences between a one-hidden-layer Boolean MLP and a deep Boolean MLP, we see that more generally, when we have an XOR of $N$ inputs, a naïve single-hidden-layer MLP will require $2^{N-1} + 1$ neurons, which is exponential in $N$, whereas a deep network will require only $3(N - 1)$ perceptrons, which is linear in $N$. In addition, the $3(N - 1)$ neurons can be arranged in only $2\log_2(N)$ layers. This is explained through the example in Fig. 2.20.

Let us first focus on Fig. 2.20(a). We note that the XOR is associative. This means that we can group the operations in any way, and the output will still be the same. So, as shown in Fig. 2.20(a), we can first compute the XORs of pairwise groupings of the variables. That gives us $N/2$ XOR’ed outputs. We then XOR the outputs, also in a pairwise fashion, and continue to do this until we
(a) Recap: XOR using an MLP with 3 percep- trons.

\[ O = W \oplus X \oplus Y \oplus Z \]

(b) An XOR needs 3 percep- trons. This network will require \(3 \times 3 = 9\) percep- trons.

Figure 2.18: Composing an MLP from Karnaugh maps with XORs
An XOR needs 3 perceptrons. The network shown in this figure will require \(3 \times 5 = 15\) perceptrons. More generally, the XOR of \(N\) variables will require \(3(N-1)\) perceptrons.

Figure 2.19: Estimating the size of deep MLPs from Karnaugh maps

have a single output. At each stage, this strategy reduces the number of variables by 2. There are \(\log_2 N\) such stages. Each stage requires 2 layers to compute the XOR. Thus we obtain a total of \(2 \log_2 N\) layers.

In Fig. 2.20(b), each pair of layers that produces a set of variables that must be further XOR’d downstream is highlighted in a blue box. The same rules about the size of the net apply from there on.

2.4.5 The challenge of depth

The key point to be noted here is that if we terminate the net after only a few layers, say \(K\) layers as shown in Fig. 2.21, we must still compute an XOR over \(2^{-K/2} N\) variables, which will require an exponentially-sized network. In general, as we reduce the size of the net below the minimum depth for an XOR-based network, the number of neurons required to compute the function grows rapidly. For any fixed depth network, the number of neurons that are required will still grow exponentially with the number of inputs. Also, very importantly, if we use fewer than the minimum required neurons, we will not be able to model
(a) Only $2 \log_2 N$ layers are needed and can be obtained by pairing terms: 2 layers per XOR. The final output is given by $O$.

(b) Each pair of layers that produces a set of variables that must be further XOR’ed downstream is highlighted in a blue box.

Figure 2.20: How $3(N - 1)$ neurons can be arranged in only $2\log_2(N)$ layers.
the function at all! In fact, for an XOR, if we use a total of even one neuron below the minimum requirement, the error incurred in computing the function will be 50%.

Using only K hidden layers will require $O(2^{CN})$ neurons in the $K^{th}$ layer, where $C = 2^{((K-1)/2)}$, since the output can be shown to be the XOR of all the outputs of the K-1th hidden layer. In other words, reducing the number of layers below the minimum will result in an exponentially sized network to express the function fully. A network with fewer than the minimum required number of neurons cannot model the function.

![Diagram](image)

$O = X_1 \oplus X_2 \oplus \cdots \oplus X_N$

$= Z_1 \oplus Z_2 \oplus \cdots \oplus Z_M$

Figure 2.21: Illustrating the challenge of depth

### 2.4.6 The actual number of parameters in the network

Fig. 2.22(a) illustrates another important point: it is not really the number of neurons in the network that governs network size, but the number of connections. The number of parameters in the network is the number of weights. In the example in Fig. 2.22(a), it is 30.

However, for now we can still think in terms of the number of neurons because networks that require an exponential number of neurons require an exponential number of weights.

In summary, deep Boolean MLPs that scale linearly in size with the number of inputs, can become exponentially large if they are recast using only one hidden layer. The problem gets worse: if we have any function that can eventually be expressed as the XOR of a number of intermediate variables, as shown in Fig. 2.22(b), from that point on we need depth. If we have a fixed depth from that
(a) The actual number of parameters in a network is the number of connections. In this example, there are 30. This is the number that really matters in software or hardware implementations. Networks that require an exponential number of neurons will require an exponential number of weights.

(b) If we have a fixed depth from any point, the network can grow exponentially in size from there.

Figure 2.22: Relating the number of parameters (connections) and the network size.
point on, the network can grow exponentially in size. Having a few extra layers can greatly reduce the size of a network.

2.4.7 Depth vs size in Boolean circuits

The XOR function we have discussed in the examples above is really a parity problem. It can actually be shown that any Boolean parity circuit of depth $d$, based on AND, OR and NOT gates, with even unbounded input, must have size $2^{n^{1/d}}$ [6]. Alternately stated, $\text{parity} \notin AC^0$ (set of constant-depth polynomial-size circuits of unbounded fan-in elements) – i.e., the parity function does not belong to the class of functions that can be implemented with fixed depth networks with only a polynomial number of units. It will require an exponential number of units or gates.

There are some caveats that must be noted in this context:

1. **Caveat 1:** Not all Boolean functions have such clear depth vs. size trade-off. Claude Shannon proved that for an $N > 2$, there exists a Boolean function of $N$ variables that requires at least $2^N/N$ Boolean gates. In fact he showed that for large $N$, almost all $N$-input functions require more than $2^N/N$ gates, regardless of depth. In fact, if all Boolean functions over $N$ inputs could be computed using a circuit that is polynomial in $N$, then $P = NP$. Regardless, for working purposes we can retain the lesson that as a network gets deeper, the number of neurons required to represent a function can fall exponentially. This is why we need depth.

2. **Caveat 2:** So far we have considered a simple “Boolean circuit” analogy for explanations. But an MLP is actually a threshold circuit, not just a Boolean circuit. It is composed of threshold gates, which are far more versatile than Boolean gates. For instance, a single threshold gate can compute the majority function, but a circuit of bounded depth, composed of Boolean gates would require an exponential number of them.
In summary, of this section, we see that an MLP is a universal Boolean function, but can represent a given function only if it is sufficiently wide and sufficiently deep. Depth can be traded off for (sometimes) exponential growth of the width of the network. The optimal width and depth of a network depend on the number of variables and the complexity of the Boolean function it must compute, where the term “complexity” refers to the minimal number of terms in DNF formula required to represent it.

Recap 4.1

- Multi-layer perceptrons are Universal Boolean Machines.
- Even a network with a single hidden layer is a universal Boolean machine – however, a single-layer network may require an exponentially large number of perceptrons.
- Deeper networks may require far fewer neurons than shallower networks to express the same function, and can therefore be exponentially smaller in size.

Info box 4.1

Formally, the class of Boolean circuits is a subset of the class of Threshold circuits. This means that for \( N \) inputs we can, in fact compose a depth-2 threshold circuit for parity using only \( O(2^N) \) weights. But a network of depth \( \log(N) \) will still only require \( O(N) \) weights. More generally, even for threshold circuits, for large \( N \), for most Boolean functions, a threshold circuit that has size polynomial in \( N \) at an optimal depth \( d \) can become exponentially large at \( d - 1 \). Other formal analyses of neural networks generally view them as arithmetic circuits – circuits that compute polynomials over any field.
2.5 MLPs as universal classifiers

We have already seen how an MLP can operate as a Boolean function over real inputs. A Boolean function will effectively partition the input space into regions where in some regions it outputs a 0, and in other regions it outputs a 1. So we see that the function that computes the output is a classifier, and therefore the MLP effectively becomes a classifier, and computes a classification boundary.

MLPs are also universal classifiers. In Chapter 1, we discussed this briefly. Let us recall the examples given in Section 1.4.9 in Figs. 1.33 - 1.36. Through these examples, we saw that MLPs can actually compute very complex decision boundaries. The examples showed that given an arbitrary decision boundary, we can construct an MLP that captures it arbitrarily accurately. In our examples the MLPs that composed these functions were deep, but is this a requirement? We will understand this requirement in more detail in this section.

Let us reconsider the complex decision boundaries shown in Fig. 1.36b. We now refer to Fig. 2.23.

In the example shown in Fig. 2.23a, the decision boundary shown is a complex one. It can be partitioned into many sub-regions, for each of which a subnet can be composed. Finally, all the subnets must be OR’d by a perceptron. This same mechanism can be used to compose any decision boundary, regardless of how complex it is.

The MLP composed for the example in Fig. 2.23a has two hidden layers. Let us see how this can be done with just one hidden layer, and what the consequences of doing so might be. To understand how, we refer to Fig. 2.23b, which shows a double pentagon. How can we compose the decision boundary for this with only one hidden layer? To learn how to do this in turn, let us start with the polygon net shown in Fig. 2.24a. This is a simple diamond-shaped decision boundary. We can compose a net for this with four hidden perceptrons, as shown in the figure. The sum of their outputs is 4 inside the diamond. In the regions shown outside the diamond shaped boundary, the sum is not 4. It is 3 within the strips shown in
(a) An arbitrary decision boundary (left) can be composed in a piece-wise fashion by an MLP (right).

(b) A relatively simpler decision boundary (left) and the corresponding MLP (right) that can compose it.

Figure 2.23: Composition of MLPs for complex decision boundaries
yellow, and 2 in the intermediate regions, as shown. The regions where the sum is not 4 in fact extend all the way to infinity and actually represent infinite area.

![Diagram of polygon nets](image)

(a) The polygon net. Composing a diamond.

(b) Composing a pentagon.

(c) Composing a hexagon.

Figure 2.24: Composition of an MLP for the double pentagon

If we try to compose a pentagon instead, as shown in Fig. 2.24(b), we would have hidden 5 perceptrons. The sum of their outputs would be 5 within the pentagon, and 4 within the triangular shaped finite-area regions shaded yellow. Moreover, the yellow shaded regions are smaller than the inner pentagonal region. Also, outside these two types of regions, the regions in which the sum is 3 or 2 have
infinite area.

Extending this analogy, we try to compose a hexagon in Fig. 2.24. We see that the region where the sum is 6 is within the hexagon, and the finite regions where the sum is 5 are each relatively smaller compared to the hexagon itself. Smaller, in fact than their analogs in the case of the pentagonal decision boundary. This is an important observation, as we will see below.

Let us now focus on the 3-dimensional plots, which show the sum of the outputs of the hidden-layer neurons (prior to the application of a threshold to obtain an actual decision boundary), while considering polygons of greater numbers of sides, as in Fig. 2.25. The examples shown include a heptagon, a polygon with 16 sides, one with 64 sides and one with 1000 sides.

If we compose a heptagon, we obtain the plot shown in Fig. 2.25. The plot shown is a 3-dimensional one, with the height showing the sum. The sum is 7 in the central peaky region, the area where the sum is 6 is adjacent to it and is smaller, the region where the sum is 5 is shown by the 7-pointed star in the plot, and it too has finite area. Elsewhere the sum is either 4 or 3.

Figs. 2.25(b)-(d) show similar plots for polygons with 16, 64 and 1000 sides, and can be similarly interpreted: there are increasing numbers of finite-area regions with increasing number of sides, and those in turn are smaller and smaller in size, relative to the central region.

As we see from Fig. 2.26, as we increase the number of sides of an N-sided polygon, the area within which the sum of the outputs of the hidden-layer neurons lies between \( N/2 \) and \( N \) keeps shrinking. In the limit, as \( N \) becomes very large and tends to infinity, we get

\[
\sum_i y_i = N \left( 1 - \frac{1}{\pi} \arccos \left( \min \left( 1, \frac{\text{radius}}{|x - \text{center}|} \right) \right) \right) \tag{2.1}
\]

This is a closed-form expression for the sum of the outputs of the hidden-layer – basically the value of the sum at the output unit, as a function of distance from center, as \( N \) increases. For small radius, it is a near-perfect cylinder, with value
(a) Composing a heptagon.  
(b) Composing a polygon with 16 sides.  
(c) Composing a polygon with 64 sides.  
(d) Composing a polygon with 1000 sides. As we consider the sums in the different regions, a pattern emerges as N (the number of sides of the polygon) increases beyond 6.

Figure 2.25: Composition of MLPs for polygons with increasing numbers of sides: a 3-D perspective
When we compose a polygonal decision boundary of a very large number of sides, increasing the number of sides reduces the area outside the polygon that have $N/2 < \sum y_i < N$.

Figure 2.26: Limiting case for MLP composition of a polygonal decision boundary: 3-D perspective
within the cylinder and $N/2$ outside of it. Its height quickly tapers off to $N/2$ as we move away from the center of the cylinder.

Let us now compose a circle using the same process as we described above. This example is shown in Fig. 2.27(a). Using a very large number $N$ of neurons in the hidden layer, we find that the sum of the outputs of the first-layer neurons will compose a cylinder with value $N$ inside the cylinder, and value $N/2$ outside. If we add a bias term, as shown in Fig. 2.27(b), that subtracts $N/2$ out of the sum, we obtain a one-hidden layer network wherein the sum of the outputs of the hidden-layer neurons is exactly $N/2$ within the cylinder, and 0 outside.

An interesting question arises in this context: what happens when we have more than one circle, as might be in the case of disjoint decision boundaries? To answer this, we consider Fig. 2.27(c): if we compose two sets of hidden-layer neurons, each one composing a cylinder at a different location, and if we sum the outputs of both sets of neurons, the result will have two cylinders, each of height $N/2$ within the decision regions, and 0 elsewhere. Consequently, if the output neuron has a threshold of $N/2$, the result will be a decision boundary with two disconnected circles!

Now we come to an interesting application for this observation: creating arbitrarily shaded decision boundaries! We will discuss this next.

### 2.5.1 Composing an arbitrarily shaped decision boundary

If we want to compose an arbitrarily shaped decision boundary (e.g. the double pentagon shown in Fig. 2.28(a)) using only one hidden layer, we can do so by approximating it as a union of many small circles, and by including one subset of hidden neurons for each circle in the aggregate MLP. This approximation can be made arbitrarily precise, by filling it with more, and smaller, circles. We can thus approximate the double pentagon in Fig. 2.28(a) to arbitrary precision using only one hidden layer, though this will require an impossibly large number of neurons in the hidden layer.
(a) The “circle” net (MLP that models a circular decision boundary). It needs a very large number of neurons. The sum is $N$ inside the circle, $N/2$ almost everywhere outside.

(b) Same as above with a bias term included. The sum is now $N/2$ inside the circle. The circle itself can be at any location.

(c) The “sum” of two “circle” subnets is exactly $N/2$ inside either circle, and 0 almost everywhere outside.

Figure 2.27: Composition of MLPs for a circular decision boundary
(a) Approximating an arbitrarily shaped decision boundary with circles. We can approximate the double pentagon to arbitrary precision using only one hidden layer in the corresponding MLP, though this will require an impossibly large number of neurons in the hidden layer. More accurate approximation with greater number of smaller circles can achieve arbitrary precision.

(b) An MLP with more layers requires fewer neurons to model the same classification boundary and as MLP with just one layer. With two layers, the MLP requires 13 neurons to model the decision boundary shown on the left.

Figure 2.28: Composition of MLPs for an arbitrarily shaped decision boundary
Thus, we see that MLPs can capture any classification boundary. Even a one-layer MLP can model any classification boundary, as we see in Fig. 2.28(a). In other words, regardless of the decision boundary, we can always compose an MLP, or even a one-hidden layer MLP, that captures the decision boundary. **MLPs are therefore universal classifiers.**

Fig. 2.28(b) illustrates a final point, relating to depth in the context of a universal classifier. Simply making the network deeper can result in a massive reduction in the number of neurons required to model the function. For the double pentagon shown, a one-hidden layer network will require an impossibly large number of neurons, but if we do it with two hidden layers, we only need 13 neurons!

This of course raises the issue of optimal depth for an MLP. A lot of formal analyses has been done on the topic of optimal network size and depth. These analyses typically view the networks as instances of arithmetic circuits, and approach the problem as one of computing polynomials over any field. Multiple hypotheses have been offered for this: for example, according to Valiant et. al. [2, 3], a polynomial of degree $n$ requires a network (or circuit) of depth $\log^2(n)$, to keep the circuit from blowing up. A shallower network cannot suffice. The majority of functions are very high (possibly infinite) order polynomials. Bengio et. al. [4] show a similar result for sum-product networks, but only consider two-input units, as shown in Fig. 2.29. This has been generalized by Mhaskar et. al. [5] to all functions that can be expressed as a binary tree. Analysis of optimal depth and size of arithmetic circuits is an ongoing research topic. From our perspective, it is sufficient to remember that when neural nets get deeper, they can get much smaller, sometimes exponentially smaller, to compute the same function.
“Shallow vs deep sum-product networks,” (From [4]). For networks where layers alternately perform either sums or products, a deep network may require an exponentially fewer number of layers than a shallow one.

Figure 2.29: Sum product network

**Fun facts 5.1: Depth in sum-product nets**

**Theorem 5:** A certain class of functions $F$ of $n$ inputs can be represented using a deep network with $O(n)$ units, whereas it would require $O(2^{\sqrt{n}})$ units for a shallow network.

**Theorem 6:** For a certain class of functions $G$ of $n$ inputs, the deep sum-product network with depth $k$ can be represented with $O(nk)$ units, whereas it would require $O(n - 1)^k$ units for a shallow network.

To be continued.....
Bibliography


