Tunable Quantum Neural Networks for Boolean Functions

Viet Pham Ngoc  
Imperial College London  
London, United Kingdom  
viet.pham-ngoc17@imperial.ac.uk

Herbert Wiklicky  
Imperial College London  
London, United Kingdom  
h.wiklicky@imperial.ac.uk

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Abstract

In this paper we propose a new approach to quantum neural networks. Our multi-layer architecture avoids the use of measurements that usually emulate the non-linear activation functions which are characteristic of the classical neural networks. Despite this, our proposed architecture is still able to learn any Boolean function. This ability arises from the correspondence that exists between a Boolean function and a particular quantum circuit made out of multi-controlled NOT gates. This correspondence is built via a polynomial representation of the function called the algebraic normal form. We use this construction to introduce the idea of a generic quantum circuit whose gates can be tuned to learn any Boolean functions. In order to perform the learning task, we have devised an algorithm that leverages the absence of measurements. When presented with a superposition of all the binary inputs of length $n$, the network can learn the target function in at most $n + 1$ updates.

1 Introduction

Artificial neural networks are a specific model of computation in which simple operations are performed by elementary structures called neurons. While a single neuron has a limited capability, the non-linearity introduced by its activation function and the fact that it is possible to build a network made of layers of neurons make it possible to approximate any functions [1]. This type of architecture has been successfully applied to different tasks ranging from image recognition to predictive maintenance but as the number of neurons and connections between neurons increases, so does the complexity. Given the importance gained by artificial neural networks, alleviating this complexity has become an active area of research which main axis are either proposing alternatives to classical algorithm [2] or developing dedicated hardware to accelerate the computations [3].

Another possible lead consists in the implementation of artificial neural networks on quantum computers with the expectation of a quantum speed-up. Given that the quantum versions of some other machine learning techniques, for supervised and unsupervised learning tasks alike, have exhibited a speed-up [4] this expectation seems reasonable. It is further strengthened by the tensor structure of artificial neural networks which is an inherent feature of quantum systems. In recent years, several architectures have been proposed to implement quantum artificial neural networks [5]. These propositions mimic to different degrees the functioning of the classical versions while taking advantage of quantum properties such as superposition to exponentially reduce the dimension of the state space [6] [7]. One persistent hurdle stemming from this approach is the implementation of the non-linear activation function. Most of the proposed solutions to overcome this difficult rely on the use of measurements to provide the non-linear behaviour at the cost of losing the quantum nature of the state.

Here we propose an alternative architecture devoid of measurement, thus preserving the quantum information, but that is still able to learn any Boolean function. This construction relies on the correspondence, introduced by [8] and most recently by [9], between the algebraic normal form of a Boolean function and a quantum circuit made of multi-controlled NOT gates acting on a single ancillary qubit. We provide a proof that this correspondence is correct and unique by building a group isomorphism between the set of Boolean functions and the set of the multi-controlled
NOT gates. This allows us to introduce a general quantum circuit which gates can be tuned in order to exactly learn any Boolean functions.

This circuit can be thought of as a neural network in the sense that each gate can only perform a simple operation while taking into account the outcome of the previous gate. The circuit taken as a whole is then able to compute complex Boolean functions. In order to train this network we present a novel algorithm. While [10] have introduced an algorithm to automatically build circuits similar to the ones presented in this paper, ours takes an approach that is more in the fashion of the training algorithms used with classical neural networks. Furthermore it takes advantage of the lack of measurements to reduce the number of updates needed until convergence. We show that provided with a superposition of all the inputs of length \( n \), our network can exactly learn the target function within \( n + 1 \) updates.

2 The Algebraic Normal Form of Boolean Functions

Let \( \mathbb{B} = \{0, 1\} \) the set of the Boolean values and \( \mathbb{B}^n \) the set of functions from \( \mathbb{B}^n \) to \( \mathbb{B} \). For \( u = (u_0, \ldots, u_{n-1}) \in \mathbb{B}^n \) we note \( 1_u = \{ i \in \{0, \ldots, n-1\} \mid u_i = 1 \} \subseteq \{0, \ldots, n-1\} \) and for \( x = (x_0, \ldots, x_{n-1}) \in \mathbb{B}^n \), \( x^u \) is defined by \( x^u = \prod_{i \in 1_u} x_i \). For \( u \in \mathbb{B}^n \), we introduce \( m_u : \mathbb{B}^n \to \mathbb{B} \) with \( m_u : x \mapsto x^u \). Let \( f \in \mathbb{B}^n \), then \( f \) has a unique polynomial representation of the form:

\[
 f = \bigoplus_{u \in \mathbb{B}^n} c_u^f m_u
\]

(1)

The notations introduced in (1) are as follow. The binary operator \( \oplus \) represents the logical operator XOR. The terms \( m_u \) are called monomials and the coefficients \( c_u^f \in \mathbb{B} \) indicate the presence or the absence of the corresponding monomial.

This representation is called the algebraic normal form (ANF). We are interested in the ANF as it shows the relation between the inputs and the outputs of a Boolean function while using two simple Boolean operations: the XOR as well as the AND. While there exist other polynomial representations, this particular form allows for an easy translation of a Boolean function into a quantum circuit as will be shown below. In Table 1 we have gathered the algebraic normal form of some well-known functions.

| \( f \) | \( \text{NOT}(x_0) \) | \( \text{AND}(x_0, x_1) \) | \( \text{XOR}(x_0, x_1) \) | \( \text{OR}(x_0, x_1) \) |
|---|---|---|---|---|
| ANF(f) | \( 0 \) | \( 0 \) | \( 1 \oplus x_0 \) | \( x_0 x_1 \) | \( x_0 \ominus x_1 \oplus x_0 x_1 \) |

Table 1: ANF of some Boolean functions

We now show that the set of Boolean functions possesses a group structure when fitted with the operator XOR and that a Boolean function has a unique algebraic normal form.

Lemma 2.1. Let \( f, g \in \mathbb{B}^n \), we define the operation \( f \oplus g \) as \( f \oplus g : x \mapsto f(x) \oplus g(x) \), then:

\( (\mathbb{B}^n, \oplus) \) is a finite commutative group where the identity element is the constant function \( 0 \) and each element is its own inverse.

Proof. These results stem from the properties of the operator XOR.

Let \( \mathcal{M} = \{ m_u \mid u \in \mathbb{B}^n \} \), then we have the following:

Theorem 2.1. Let \( \mathcal{A} \) be the subgroup of \( (\mathbb{B}^n, \oplus) \) generated by \( \mathcal{M} \), then:

\( \mathcal{A} = \mathbb{B}^n \)

Proof. The proof can be found in Appendix A.

Theorem 2.1 shows the existence as well as the uniqueness of the algebraic normal form of a Boolean function. It also shows that it is equivalent to consider a Boolean functions or its ANF. We now present a way to construct the ANF of a function called the Method of Indeterminate Coefficients (11). For the sake of clarity we use a simple example but the generalization is straight-forward. Let \( f \in \mathbb{B}^2 \) defined by Table 2

These values can be gathered in the vector \( v_f = (1, 0, 1, 1) \) and we are looking for the vector \( c = \)
Table 2: Truth table of $f$

$$
\begin{array}{c|cccc}
    x & 00 & 01 & 10 & 11 \\
    \hline 
    f(x) & 1 & 0 & 1 & 1 \\
\end{array}
$$

\(^T\) verifying $Ac = v_f$ where $A$ is the matrix such that $A_{x,u} = m_u(x)$. In our case:

$$
A = \begin{pmatrix}
1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 \\
1 & 1 & 1 & 1 \\
\end{pmatrix}
$$

It can be shown that $A = A^{-1}$ in $\mathbb{B}^{2 \times 2}$, hence $c = A v_f$ and $c = (1, 1, 0, 1)^T$. This leads to $f = m_{00} \oplus m_{01} \oplus m_{11}$ or equivalently $f(x_0, x_1) = 1 \oplus x_1 \oplus x_0 x_1$

3 From Algebraic Normal Form to Quantum Circuit

Using the ANF of a Boolean function, we show that we can easily design a quantum circuit expressing this function. We consider a quantum circuit operating on $n + 1$ qubits $|x_0, \ldots, x_{n-1}, q_r\rangle$ where the last qubit is the readout qubit and we are interested in a particular set of gates. Let $u \in \mathbb{B}^n$ and define $C_u$ as the multi-controlled $X$ gate that is acting on the readout qubit and controlled by the qubits $\{|x_i| \mid i \in 1_u\}$ where $1_u = \{i \in \{0, \ldots, n-1\} \mid u_i = 1\}$. Figure 1 represents the 4 possible gates for $n = 2$.

![Figure 1](image)

We now present some intermediary results that exhibit the correspondence existing between the algebraic normal form of a Boolean function and the quantum circuit able to compute this function over the ancillary qubit.

**Lemma 3.1.** Let $u \in \mathbb{B}^n$, then:

$$(x_0, \ldots, x_{n-1}, q_r) \in \mathbb{B}^{n+1}, C_u |x_0, \ldots, x_{n-1}\rangle |q_r\rangle = |x_0, \ldots, x_{n-1}\rangle |q_r \oplus m_u(x_0, \ldots, x_{n-1})\rangle$$

**Proof.** The proof can be found in Appendix B.

**Lemma 3.2.** Let $C = \{C_u \mid u \in \mathbb{B}^n\}$ and $A_Q$ the subgroup of the unitary group $U(n+1)$ that is generated by $C$, then: $A_Q$ is a finite commutative group whose identity element is the Identity matrix and where each element is its own inverse.

**Proof.** This is a direct consequence of Lemma 3.1 and Theorem 2.1.

We now introduce the group morphism $\Phi: \mathcal{A} \to A_Q$ such that:

$$\forall u \in \mathbb{B}^n, \Phi(m_u) = C_u$$

This morphism leads to the following Lemma:

**Lemma 3.3.** Let $f \in \mathbb{B}^n$ then:

$$\forall (x_0, \ldots, x_{n-1}, q_r) \in \mathbb{B}^{n+1}, \Phi(f) |x_0, \ldots, x_{n-1}\rangle |q_r\rangle = |x_0, \ldots, x_{n-1}\rangle |q_r \oplus f(x_0, \ldots, x_{n-1})\rangle$$

**Proof.** It suffices to take the ANF of $f$ and apply $\Phi$. Lemma 3.1 then allows to conclude.
The resulting circuit is depicted in Figure 2. We can check that we do have \( \Phi(f) \) whose values are provided in Table 3. Applying the Method of Indeterminate Coefficients yields the algebraic normal form of \( f \):

\[
f(x_0, x_1, x_2) = x_1 \oplus x_0 \oplus x_1 x_2 \oplus x_0 x_2 \oplus x_0 x_1 x_2
\]

Now applying the isomorphism \( \Phi \) to \( f \), we get:

\[
\Phi(f) = C_{010}C_{100}C_{011}C_{101}C_{111} = C_{111}C_{101}C_{100}C_{011}C_{010}
\]

The resulting circuit is depicted in Figure 2. We can check that we do have \( \Phi(f) |x\rangle |0\rangle = |x\rangle |f(x)\rangle \) for \( x \in \mathbb{B}^3 \).

These preliminary results lead to the concept of a generic quantum circuit. This circuit is made of gates whose action on the readout qubit can be tuned so that the resulting circuit is able to express any given Boolean function.

### 4 Tunable Quantum Neural Network

As previously, we work with a quantum circuit operating on \( n+1 \) qubits \( |x_0, \ldots, x_{n-1}\rangle |q_r\rangle \). We recall that for \( u \in \mathbb{B}^n \), \( C_u \) is the multi-controlled \( X \) gate, controlled by the qubits \( \{|x_i\rangle : i \in I_u\} \) and \( I_u = \{i : u_i = 1\} \). We introduce \( G_u \) the tunable quantum gate whose value can either be \( I \), the identity gate, or \( C_u \). \( G_u \) can be seen as the quantum version of the neuron as it performs simple local computations. Let \( TNN \) be the tunable quantum neural network, \( TNN \) is defined by:

\[
TNN = \prod_{u \in \mathbb{B}^n} G_u
\]

We have shown with Lemma 3.2 that the gates \( C_u \) commute together and \( I \) commuting with all matrices, it comes that the order in which the product is done does not change the overall circuit. Tunable neural networks for different values of \( n \) are pictured in Figure 3. For \( n \in \mathbb{N} \) such a circuit contains \( 2^n \) gates. Each gate having two possible values, there exists in total \( 2^{2^n} \) different circuits, meaning that the set of all the tuned circuit is \( \mathcal{A}_Q \).

### 5 Learning Algorithm

Given such a circuit and a Boolean function, \( f \in \mathbb{B}^{2^n} \), we introduce a learning algorithm resulting in a correctly tuned neural network that is able to express \( f \). We first outline a general version of the algorithm and then discuss the details further. This algorithm intends to use quantum superposition in order to reduce the number of updates performed during the learning phase. Let \( |\Psi\rangle \) be such superposition:

\[
|\Psi\rangle = \sum_{x \in \mathbb{B}^n} a_x |x\rangle |0\rangle
\]
Where the last qubit is the readout qubit.

Suppose further that given a superposition, we are able to identify some of the states present in this superposition. More precisely, given a network \( \mathcal{TNN} \) and \( |\Psi'\rangle = \mathcal{TNN} |\Psi\rangle \), we are able to identify all the states of the form \( |x\rangle |1 \oplus f(x)\rangle \) in \( |\Psi'\rangle \). Let us call this operation \( qt(f) \left( |\Psi'\rangle \right) \), then

\[
qt(f) \left( |\Psi'\rangle \right) = \{ x \in \mathbb{B}^n \mid a_x \neq 0, \mathcal{TNN} |x\rangle |0\rangle = |x\rangle |1 \oplus f(x)\rangle \}
\]

The goal of the operator \( qt \) is thus to identify the inputs for which the output by the circuit is different from that of the target function. For now we assume that we have \( a_x \neq 0 \), for all \( x \).

We start with \( \mathcal{TNN}^{(0)} \) the circuit where all the gates are initialised with \( I \). For \( k \in \mathbb{N} \), \( \mathcal{TNN}^{(k)} \) is the circuit resulting from the \( k \)-th update. We denote \( E^{(k)} = qt(f) \left( \mathcal{TNN}^{(k)} |\Psi\rangle \right) \) that is the set of the inputs for which the output by \( \mathcal{TNN}^{(k)} \) is erroneous. For example \( E^{(0)} = f^{-1}(\{1\}) \). Given these notations, we define the update rule as follow:

- Determine \( E^{(k)} \)
- For \( u \in E^{(k)} \) switch the value of the corresponding gate \( G_u \), resulting in \( \mathcal{TNN}^{(k+1)} \)

The algorithm terminates when we reach an updated circuit \( \mathcal{TNN}^{(h)} \) such that \( E^{(h)} = \emptyset \). The learning algorithm can be summarised as shown in the Algorithm 1

**Algorithm 1: Learning algorithm**

\[
\begin{align*}
\mathcal{TNN} &\leftarrow I; \\
E &\leftarrow qt(f)\left( |\Psi\rangle \right); \\
\text{while } E \neq \emptyset \text{ do} \\
&\text{for } u \in E \text{ do} \\
&\quad G_u \leftarrow G_u C_u; \\
&\text{end} \\
&\mathcal{TNN} \leftarrow \prod_{u \in \mathbb{B}^n} G_u; \\
&\mathcal{TNN} |\Psi\rangle \leftarrow \mathcal{TNN} |\Psi\rangle; \\
&\mathcal{TNN} |0\rangle \leftarrow |x\rangle |1 \oplus f(x)\rangle; \\
&\text{end} \\
\end{align*}
\]

5.1 Example

Let us run this algorithm on an example. We want to tune the circuit in order for it to express the function introduced in Example 3.1. We remind that the values of \( f \) are gathered in Table 3. Let \( |\Psi\rangle \) be the superposition we are working
with:

$$|\Psi\rangle = \sum_{x \in \mathbb{B}^n} a_x |x\rangle |0\rangle$$

We start with the circuit $TNN^{(0)} = Id$ and

$$|\Psi^{(1)}\rangle = TNN^{(0)} |\Psi\rangle = \sum_{x \in \mathbb{B}^n \atop f(x)=0} a_x |x\rangle |0\rangle + \sum_{x \in \mathbb{B}^n \atop f(x)=1} a_x |x\rangle |0\rangle$$

Performing $qt(f)(|\Psi^{(0)}\rangle)$ then yields $E^{(0)} = \{010, 100, 111\}$. We thus have to switch the value of the gates $G_{010}$, $G_{100}$ and $G_{111}$ resulting in $TNN^{(1)}$ as depicted in Figure 4.

![Figure 4: TNN(1), the circuit obtained after the first update](image)

Continuing the algorithm: $|\Psi^{(1)}\rangle = TNN^{(1)} |\Psi\rangle$ with

$$|\Psi^{(1)}\rangle = \sum_{x \in \mathbb{B}^n \atop f(x)=0} a_x |x\rangle |0\rangle + \sum_{x \in \mathbb{B}^n \atop f(x)=1} a_x |x\rangle |1\rangle + a_{011} |011\rangle |1\rangle + a_{101} |101\rangle |1\rangle$$

Once again we perform $qt(f)(|\Psi^{(1)}\rangle)$ and get $E^{(1)} = \{011, 101\}$. Applying the update rule, we switch the gates $G_{011}$ and $G_{101}$, resulting in $TNN^{(2)}$ as represented in Figure 5. Applying $TNN^{(2)}$ to $|\Psi\rangle$ now yields:

![Figure 5: TNN(2), the circuit obtained after the second update](image)

And $E^{(2)} = qt(f)(|\Psi^{(2)}\rangle) = \emptyset$ which is the termination condition of the algorithm. Applying $\Phi^{-1}$, the inverse of the isomorphism introduced in Section 3, we get $\Phi^{-1}(TNN^{(2)}) = \tilde{f}$ where

$$\tilde{f}: (x_0, x_1, x_2) \mapsto x_1 \oplus x_1 x_2 \oplus x_0 \oplus x_0 x_2 \oplus x_0 x_1 x_2$$

As this is the algebraic normal form of $f$ we conclude that $\tilde{f} = f$ and we have tuned the circuit properly.

### 5.2 Proof of Termination and Correctness of the Algorithm

We show here that the algorithm will terminate after at most $n + 1$ updates. Let $x \in \mathbb{B}^n$, we denote by $T_x$ the set of gates that can be triggered by $|x\rangle |q_r\rangle$ and $w_H(x) = |1_x|$ the Hamming weight of $x$. We then notice that:

**Lemma 5.1.** $\forall x \in \mathbb{B}^n$, $T_x \subset \{G_x\} \cup \{G_u \mid w_H(u) < w_H(x)\}$

**Proof.** The proof can be found in Appendix C.

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6
Lemma 5.1 shows that if $TNN = \prod_{u \in B^n} G_u$ then for $x \in \mathbb{B}^n$ we have:

$$TNN |x⟩ |q_r⟩ = G_x \prod_{u \in \mathbb{B}^n \wedge w_H(u) < w_H(x)} G_u |x⟩ |q_r⟩$$

We will use this result to show the following:

**Lemma 5.2.** Suppose that all the inputs are present in the superposition $|Ψ⟩$, that is $a_x \neq 0$ for $x \in \mathbb{B}^n$. Then after the $k$-th update, the gates controlled by at most $k - 1$ qubits will not be updated anymore.

**Proof.** The proof can be found in Appendix [C](#).

From Lemma 5.2 stems the following corollary:

**Corollary 5.1.** $∀k > 0, E^{(k)} \subset \mathbb{B}^n \setminus \{x \in \mathbb{B}^n \mid w_H(x) < k\}$

**Proof.** Let $k > 0$ and suppose there exist an $x \in \mathbb{B}^n$ such that $w_H(x) = s < k$ and $x \in E^{(k)}$. Then according to the update rule, the gate $G_x$ will be updated which is in contradiction with Lemma 5.2.

We recall that the process terminates whenever a circuit $TNN^{(h)}$ such that $E^{(h)} = ∅$ is reached. The previous results then allow us to prove:

**Theorem 5.1.** When presented with a superposition of all possible inputs, the process will terminate after at most $n + 1$ updates.

**Proof.** The proof can be found in Appendix [C](#).

We have effectively shown that the learning process will halt after at most $n + 1$ updates. We now have to prove that when it terminates, the resulting circuit is well-tuned. Let $TNN$ be the final circuit and $E = qt(f)(TNN |Ψ⟩)$, then by the halting condition, we have $E = ∅$ and we can show:

**Theorem 5.2.** We recall that $Φ$ is the isomorphism introduced in Section [C](#) that transforms a Boolean function into the quantum circuit corresponding to its algebraic normal form. Then:

$E = ∅ \Rightarrow TNN = Φ(f)$

**Proof.** The proof can be found in Appendix [C](#).

So far, we have demonstrated that when presented with a superposition of all the possible inputs, the learning algorithm terminates after at most $n + 1$ updates of the circuit. Additionally, when it stops the resulting circuit is correctly tuned. But these results are conditioned to our ability to identify the states corresponding to a wrong input-output relation. We thus have to detail a way to perform the operation that we have denoted $qt$.

### 6 The operation $qt$

Let $TNN$ be a tunable circuit and $|Ψ⟩$ be a state superposition of the form $|Ψ⟩ = \sum_{x \in \mathbb{B}^n} a_x |x⟩ |0⟩$. We remind that we want to define an operator $qt$ such that for a Boolean function $f \in \mathbb{B}^n$ we have:

$$qt(f)(TNN |Ψ⟩) = \{x \in \mathbb{B}^n \mid a_x \neq 0, TNN |x⟩ |0⟩ = |x⟩ |1 \oplus f(x)⟩\}$$

So let us take $f \in \mathbb{B}^n$ and define $F(f)$ such that:

$$∀x \in \mathbb{B}^n \begin{cases} F(f) |x⟩ |f(x)⟩ = |x⟩ |0⟩ \\ F(f) |x⟩ |1 \oplus f(x)⟩ = |x⟩ |1⟩ \end{cases}$$

$F(f)$ performs a permutation on the usual computational basis, hence it is a unitary operation. Let $|Ψ'⟩ = TNN |Ψ⟩$, then

$$F(f) |Ψ'⟩ = \sum_{x \in \mathbb{B}^n} a_x |x⟩ |1⟩ + \sum_{x \in \mathbb{B}^n} a_x |x⟩ |0⟩$$

$$TNN|x⟩|0⟩=|x⟩|1\oplus f(x)⟩ \quad \text{and} \quad TNN|x⟩|0⟩=|x⟩|f(x)⟩$$
Measuring the read out qubit, the probability \( P_1 \) of it being in state \( |1\rangle \) is:

\[
P_1 = \sum_{x \in B^n} |a_x|^2
\]

The resulting circuit is given in Figure 6. In order to fully implement \( q_t \) we thus need to accurately estimate \( P_1 \) and reconstruct the sum resulting in this estimation. The way both of these tasks can be performed depends on the superposition we are using.

### 6.1 Building a Suitable Superposition

Suppose we can accurately estimate \( P_1 \), we want to build a set of amplitude \( \{a_x \in \mathbb{C} \mid x \in B^n\} \) such that there exist a unique subset \( S \subset B^n \) verifying:

\[
P_1 = \sum_{x \in S} |a_x|^2
\]

This can be done using the uniqueness of the binary decomposition. For \( x \in B^n \) we note \( x_{10} \) its conversion in the decimal system and we consider the following superposition \( |\Psi\rangle \):

\[
|\Psi\rangle = \frac{1}{\sqrt{2^{2n} - 1}} \sum_{x \in B^n} \sqrt{2^{x_{10}}} |x\rangle |0\rangle
\]

The uniqueness of the binary decomposition yields:

\[
\forall S, S' \subset B^n, S \neq S' \iff \frac{1}{2^{2n} - 1} \sum_{x \in S} 2^{x_{10}} \neq \frac{1}{2^{2n} - 1} \sum_{x \in S'} 2^{x_{10}}
\]

Which is what we aimed for. Nonetheless we remind that when tuning, the gates controlled by the least number of qubits are tuned to their definitive value early in the process. We want to reflect this particular behaviour in the superposition by granting a large amplitude to inputs with a small Hamming weight. We can then switch to a superposition where inputs with a large Hamming weight have a large amplitude. To do so, for \( h \in \{0, \ldots, n\} \) and \( x \in B^n \) such that \( w_H(x) = h \), we introduce \( o_h(x) \) the lexicographic order of \( x \) among the elements of \( B^n \) whose Hamming weight is \( h \). We illustrate this set of functions for \( n = 4 \) with Figure 7.

This allows us to recursively construct the following function:

\[
p(x) = \begin{cases} 
0 & \text{for } x = (0, \ldots, 0) \\
\left(\max_{w_H(y)=h-1} p(y)\right) + o_h(x) & \text{for } w_H(x) = h > 0
\end{cases}
\]

For \( n = 4 \), we have computed the values of \( p \) in Table 4.
This function allows us to define the following superpositions:

$$|\Psi_\downarrow\rangle = \frac{1}{\sqrt{2^n-1}} \sum_{x \in \mathbb{B}^n} \sqrt{2^{n-1-p(x)}} |x\rangle |0\rangle$$

And similarly:

$$|\Psi_\uparrow\rangle = \frac{1}{\sqrt{2^n-1}} \sum_{x \in \mathbb{B}^n} \sqrt{2^p(x)} |x\rangle |0\rangle$$

The reason we introduce these superposition is that it is impossible to exactly determine $P_1$. We thus want to minimize the impact of any estimation errors. By working with $|\Psi_\downarrow\rangle$ first, we are more likely to correctly identify the inputs with small Hamming weight for which the output by the circuit is not that of the target function. By the update rule and Lemma 5.4, we can be confident that, despite the estimation incertitude, the gates controlled by a small number of qubits can still be tuned to their definitive value early in the training process. Once these gates have been correctly tunes, we can switch to $|\Psi_\uparrow\rangle$ in order to tune the gates controlled by a large number of qubits.

### 6.2 Estimating $P_1$

In this section we discuss a way to estimate $P_1$ accurately enough to identify the inputs for which the output by the circuit are wrong. For now, we consider the superposition $|\Psi_\downarrow\rangle$. Let $f \in \mathbb{B}^n$ be the target function, $\text{TNN}$ the circuit being tuned and $F(f)$ the permutation we introduced earlier. Then a measurement of the read-out qubit of $|\Psi_\downarrow\rangle$ can be modelled by a Bernoulli process where the probability of measuring $|1\rangle$ is $P_1$. We want to determine the number of samples $s$ needed in order to estimate $P_1$ within a margin of error $\epsilon$.

Let $X$ be the random variable representing the outcome of the measurement, then $X$ has a Bernoulli distribution and we have

$$P(X = 1) = P_1$$

Suppose that the number of samples is large enough, then a 95% confidence interval CI [12] for $P_1$ is given by:

$$\text{CI} = \left[ P_1 - z_{0.025} \sqrt{\frac{P_1(1-P_1)}{s}}, P_1 + z_{0.025} \sqrt{\frac{P_1(1-P_1)}{s}} \right]$$

This means that we want:

$$\epsilon = z_{0.025} \sqrt{\frac{P_1(1-P_1)}{s}}$$

Or

$$s = \frac{P_1(1-P_1)}{\epsilon^2 z_{0.025}^2}$$

Given that $z_{0.025} = 1.96$ we can approximate with $z_{0.025} = 2$. And the term $P_1(1-P_1)$ taking its maximum value when $P_1 = \frac{1}{2}$ we can write:

$$s = \frac{1}{16\epsilon^2}$$

To determine $\epsilon$, remind that during the learning process we use two different superpositions $|\Psi_\downarrow\rangle$ and $|\Psi_\uparrow\rangle$ where the amplitude is larger for inputs with small and large Hamming weight respectively. This means that it suffices to determine $P_1$ up to a margin equal to:

$$\epsilon = \frac{2^{2n}}{2^{2n} - 1} \approx \frac{1}{2^{2n-1}}$$

This in turn yields

$$s = 2^{2n-4}$$
While the number of samples needed to obtain the required accuracy can seem quite large, this scale can be explained by the fact that the operation performed by $q_t$ is similar to quantum state tomography. This process aims at reconstructing a quantum state by performing measurements on copies of this state. The number of copies needed to achieve this task to a precision $\epsilon$ then scales in $O\left(\frac{1}{\epsilon^2}\right)$ \[13\].

6.3 Retrieving $E$

Suppose we have $s$ samples as specified previously, and among this samples, the read-out qubit has been measured in the state $|1\rangle$ $N_1$ times, then $P_1 = \frac{N_1}{s}$. We recall that $E = \{ x \in B^n \mid F(TNN) |0\rangle = |x\rangle |1\rangle \}$ which is the set of inputs for which the output computed by the tunable circuit $TNN$ is wrong. We then have:

$$P_1 = \frac{1}{2^{2^n} - 1} \sum_{x \in E} 2^{2^n} - 1 - p(x)$$

Thus:

$$\sum_{x \in E} 2^{2^n} - 1 - p(x) \approx \frac{N_1(2^{2^n} - 1)}{s}$$

The uniqueness of the binary decomposition then allows us to retrieve $E$ as required.

7 Conclusion and Discussion

In this paper we have presented a method that allows to compute any Boolean function by building a corresponding quantum circuit simply made out of multi-controlled NOT gates. We have also provided a novel proof of the existence as well as the uniqueness of this correspondence. From this followed our approach to quantum neural network wherein the multi-controlled gates are the elementary components performing limited computations. Still by building a circuit, or network, made out of these gates we are able to compute any Boolean functions. Furthermore, the absence of measurement in this architecture means that it is possible to work with a superposition of inputs. This ability is leveraged by the learning algorithm we have designed. When learning with a certain superposition of all the possible inputs of length $n$, the training terminates in at most $n + 1$ updates of the circuit.

Nevertheless, because of the superposition, we need to perform quantum state tomography at each updating step. This process requires a significant number of copies of the state outputted by the quantum neural network and thus represents a bottleneck in our approach. One way to cope with this problem could be to restrain the states present in the superposition to the ones corresponding to inputs with a certain Hamming weight. By reducing the number of states within the superposition, the margin of error is increases and thus the number of copies needed for the tomography decreases. More specifically, when performing the $k$-th update, one could consider a superposition made of the states corresponding to inputs with Hamming weight equal to $k - 1$.

Thanks to its ability to handle superpositions, this architecture could be used in a Probably Approximately Correct (PAC) learning framework \[14\]. In the quantum version, we are provided with a superposition of the form $\langle \phi \rangle = \sum_{x \in B^n} \sqrt{D(x)} |x\rangle |c(x)\rangle$ where $c: B^n \to B$ is the target function or concept, belonging to a class $C$ and $D$ is an unknown distribution over $B^n$. Let $h$ be the function computed by the neural network $TNN$, then the error is defined by $	ext{err}_D(c, h) = P_{x \sim D} (c(x) \neq h(x))$. Now suppose we feed $|\phi\rangle$ to $TNN$, then $|\phi'\rangle = TNN |\phi\rangle$ and by noting $p_1$ the probability of measuring the read-out qubit of $|\phi'\rangle$ in the state $|1\rangle$, we get $p_1 = \text{err}_D(c, h)$. An algorithm is said to $(\epsilon, \delta)$-PAC learn $C$ when $P(\text{err}_D(c, h) \leq \epsilon) \geq 1 - \delta$ for all concept $c \in C$ and distribution $D$ \[15\]. The interest then lies in finding conditions on $C$ and designing an algorithm able to $(\epsilon, \delta)$-PAC learn $C$ while requiring a number of copies of $|\phi\rangle$ as low as possible.

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Appendices

A Proofs from Section 2

Proof of Theorem 2.7 The commutativity of $\oplus$ and the fact that for $u \in \mathbb{B}^n$, $m_u = m_u^{-1}$ yield

$$\mathcal{A} = \left\{ \bigoplus_{u \in \mathbb{B}^n} c_u m_u \mid \forall u \in \mathbb{B}^n, c_u \in \{0, 1\} \right\}$$

Let $\{c_u\}_{u \in \mathbb{B}^n}$ and $\{d_u\}_{u \in \mathbb{B}^n}$ such that $\bigoplus_{u \in \mathbb{B}^n} c_u m_u = \bigoplus_{u \in \mathbb{B}^n} d_u m_u$, then

$$\bigoplus_{u \in \mathbb{B}^n} (c_u \oplus d_u) m_u = 0$$
Suppose now that there exist $u \in \mathbb{B}^n$ such that $c_u \neq d_u$ and denote $D = \{ u \in \mathbb{B}^n \mid c_u \neq d_u \}$, then:

$$\bigoplus_{u \in \mathbb{B}^n} (c_u \oplus d_u) m_u = \bigoplus_{u \in D} m_u = 0$$

Take $u_0 \in D$ of minimal Hamming weight, that is such that $|1_{u_0}|$ is the smallest among $D$, then

$$\bigoplus_{u \in D} m_u(u_0) = m_{u_0}(u_0) = 1 \neq 0$$

So $D = \emptyset$ which leads to $|A| = 2^n$, hence $A = \mathbb{B}^n$.

\section*{B Proofs from Section 3}

\subsection*{Proof of Lemma 5.1} Let $(x_0, \ldots , x_n-1, q_r) \in \mathbb{B}^{n+1}$. $C_u$ being the gate controlled by the qubits $\{|x_i| \mid i \in 1_u\}$, it will only swap the state of the readout qubit when all the controlling qubits are in the state $|1\rangle$, meaning:

$$C_u |x_0, \ldots , x_{n-1}\rangle |q_r \oplus \prod_{i \in 1_u} x_i\rangle = |x_0, \ldots , x_{n-1}\rangle |q_r \oplus m_u(x_0, \ldots , x_{n-1})\rangle$$

\subsection*{Proof of Theorem 3.1} Let $f, g \in A$ such that $\Phi(f) = \Phi(g)$, then from Lemma 3.3:

$$\forall (x_0, \ldots , x_n-1) \in \mathbb{B}^n, |x_0, \ldots , x_n-1\rangle |f(x_0, \ldots , x_n-1)\rangle = |x_0, \ldots , x_n-1\rangle |g(x_0, \ldots , x_n-1)\rangle$$

That is $f = g$.

Now let $G \in A_Q$, then from Lemma 3.2

$$G = \prod_{u \in \mathbb{B}^n} C_u^G$$

With $\alpha_u^G \in \{0, 1\}$ for $u \in \mathbb{B}^n$. Now let $f = \bigoplus_{u \in \mathbb{B}^n} \alpha_u^G m_u$, then $f \in A$ and we have

$$\Phi(f) = G$$

So $\Phi$ is an isomorphism from $A$ to $A_Q$.

\section*{C Proofs from Section 5}

\subsection*{Proof of Lemma 5.1} This comes from the fact that for $G_u$ to be triggered by $x$, we must have $1_u \subset 1_x$ which leads to $w_H(u) \leq w_H(x)$. Suppose now that $w_H(u) = w_H(x)$. Because $|1_u| = w_H(u)$ and $|1_x| = w_H(x)$, necessarily we have $1_u = 1_x$ that is $u = x$.

\subsection*{Proof of Lemma 5.2} We show this result by induction over $k$. As previously, $\text{TNN}^{(k)} = \prod_{u \in \mathbb{B}^n} G_u^{(k)}$ is the circuit obtained after the $k$-th update.

$k = 1$

According to Lemma 5.1, we have $\text{TNN}^{(0)} |0, \ldots , 0\rangle |0\rangle = G_{0...0}^{(0)} |0, \ldots , 0\rangle |0\rangle$.

We now apply the update rule: if $(0, \ldots , 0) \in E^{(0)}$ then we switch the value of $G_{0...0}^{(0)}$, else, we keep it the same. Let us denote $G_{0...0}$ the resulting gate.

Following the first update we have

$$\text{TNN}^{(1)} |0, \ldots , 0\rangle |0\rangle = G_{0...0} |0, \ldots , 0\rangle |0\rangle = |0, \ldots , 0\rangle |f(0, \ldots , 0)\rangle$$

This means that $(0, \ldots , 0) \notin E^{(1)}$ and by the update rule: $G_{0...0}^{(2)} = G_{0...0}$. An induction then leads to

$$\forall s \geq 1, G_{0...0}^{(s)} = G_{0...0}$$
This proves the case $k = 1$.

Let $\text{TNN}^{(k)} = \prod_{u \in B^n} G_u^{(k)}$ be the circuit resulting from the $k$-th update. According to the induction hypothesis we have:

$$\text{TNN}^{(k)} = \prod_{w_H(u) \geq k} G_u^{(k)} \prod_{w_H(u) < k} G_u$$

Where $G_u$ is the final value of the gate controlled by $u$.

Let $x \in B^n$ such that $w_H(x) = k$, Lemma 5.1 yields:

$$\text{TNN}^{(k)} |x\rangle |0\rangle = G_x^{(k)} \prod_{w_H(u) < k} G_u |x\rangle |0\rangle = G_x^{(k)} |x\rangle |q\rangle$$

We apply the update rule: if $G_x^{(k)} |x\rangle |q\rangle = |x\rangle |1 \oplus f(x)\rangle$ we switch the value of $G_x^{(k)}$, else, we keep it the same. Either way, we denote $G_x$ the value resulting from the $k+1$-th update. We thus have:

$$\text{TNN}^{(k+1)} |x\rangle |0\rangle = G_x \prod_{w_H(u) < k} G_u |x\rangle |0\rangle = G_x^{(k+1)} |x\rangle |q\rangle = |x\rangle |f(x)\rangle$$

The update rule then states that this gate will not change value during the $k+2$-th update and an induction shows that it will not change anymore.

This being true for all $x \in B^n$ such that $w_H(x) = k$, we have shown the induction hypothesis for $k+1$. 

\[\square\]

**Proof of Theorem 5.2.** By definition of $E$, the fact that $E = \emptyset$ means that

$$\forall x \in B^n, \text{TNN} |x\rangle |0\rangle = |x\rangle |f(x)\rangle$$

By construction, we have $\text{TNN} = \prod_{u \in B^n} G_u^{\alpha_u}$ with $\alpha_u \in \{0, 1\}$ thus $\text{TNN} \in A_Q$. Let $\tilde{f} = \Phi^{-1}(\text{TNN})$, then by Lemma 3.3 we must have

$$\forall x \in B^n, \text{TNN} |x\rangle |0\rangle = |x\rangle |\tilde{f}(x)\rangle$$

This means that for $x \in B^n$, we have $\tilde{f}(x) = f(x)$, thus $\tilde{f} = f$ and $\text{TNN} = \Phi(f)$. 

\[\square\]