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Reversible Logic Synthesis Using a Non-blocking Order Search

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Reversible Logic Synthesis Using a Non-blocking Order Search

by

Alberto Patino

A thesis submitted in partial fulfillment of the requirements for the degree of

Master of Science
in
Computer Engineering

Thesis Committee:
Marek Perkowski, Chair
Xiaoyu Song
Christof Teuscher

Portland State University
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Abstract

Reversible logic is an emerging area of research. With the rapid growth of markets such as mobile computing, power dissipation has become an increasing concern for designers (temperature range limitations, generating smaller transistors) as well as customers (battery life, overheating). The main benefit of utilizing reversible logic is that there exists, theoretically, zero power dissipation.

The synthesis of circuits is an important part of any design cycle. The circuit used to realize any specification must meet detailed requirements for both layout and manufacturing. Quantum cost is the main metric used in reversible logic. Many algorithms have been proposed thus far which result in both low gate count and quantum cost.

In this thesis the AP algorithm is introduced. The goal of the algorithm is to drive quantum cost down by using multiple non-blocking orders, a breadth first search, and a quantum cost reduction transformation. The results shown by the AP algorithm demonstrate that the resulting quantum cost for well-known benchmarks are improved by at least 9% and up to 49%.
Dedication

I dedicate this thesis to my loving wife. Without her patience, support, understanding, and most of all love, the completion of this work would not be possible.
Acknowledgments

I would like to show my gratitude to my advisor, Dr. Marek Perkowski, whose passion for teaching guided me in my research. Also, I would like to thank Dr. Xiaoyu Song and Dr. Christof Teuscher for participating in the thesis committee.
# Table of Contents

Abstract ......................................................................................................................... i  
Dedication ....................................................................................................................... ii  
Acknowledgments ........................................................................................................... iii  
List of Figures .............................................................................................................. vi  
Glossary ........................................................................................................................... viii  
Chapter 1 ....................................................................................................................... 1  
  Introduction .................................................................................................................... 1  
Chapter 2 ....................................................................................................................... 5  
  Background .................................................................................................................... 5  
    2.1 Boolean Logic Overview ......................................................................................... 5  
    2.2 Basic Definitions .................................................................................................... 7  
      2.2.1 Reversible Logic Network Structure ............................................................... 7  
      2.2.2 Reversible Gates ............................................................................................. 10  
      2.2.3 Other Reversible Gates .................................................................................. 12  
      2.2.4 Positive Polarity Reed-Muller Expansion ....................................................... 13  
    2.3 Measuring Quality of Reversible Gates ............................................................... 15  
      2.3.1 Ancilla Bits ....................................................................................................... 15  
      2.3.2 Delay ................................................................................................................ 15  
      2.3.3 Quantum Cost .................................................................................................. 16  
Chapter 3 ....................................................................................................................... 17  
  Previous Work on Reversible Logic Synthesis ........................................................... 17  
    3.1 MMD (Maslov, Miller, and Dueck) ....................................................................... 17  
      3.1.1 Algorithm ......................................................................................................... 17  
      3.1.2 MMD Example ................................................................................................. 19  
    3.1.2 MMD with Bidirectional Search ...................................................................... 21  
    3.1.3 MMD Strengths and Weaknesses .................................................................... 24  
  3.2 Optimal Reversible Circuits .................................................................................... 25
List of Figures

Figure 1 Truth Table Example ................................................................. 6
Figure 2 EXOR Operation ................................................................ 6
Figure 3 Basic EXOR Operations ...................................................... 6
Figure 4 Reversible Specification ....................................................... 8
Figure 5 Non-Reversible Specification .............................................. 9
Figure 6 Non-Reversible Specification Realized by reversible Logic .......... 9
Figure 7 Reversible Logic Structure .................................................. 10
Figure 8 Tofolli Gates ....................................................................... 11
Figure 9 TOF(A) ............................................................................... 11
Figure 10 TOF(A,B) .......................................................................... 11
Figure 11 TOF(A,B,C) ....................................................................... 11
Figure 12 Fredkin Gates .................................................................... 12
Figure 13 Fred(A,B) .......................................................................... 12
Figure 14 FRED(C;A,B) .................................................................... 12
Figure 15 Peres Gate Operation .......................................................... 12
Figure 16 Kerntopf Gate Operation .................................................... 13
Figure 17 Delay Equation ................................................................. 15
Figure 18 Quantum Circuit showing stages. The arrow denotes a feedback loop.... 16
Figure 19 MMD Implementation Direction ........................................ 18
Figure 20 Example of applying MMD Basic Algorithm ..................... 19
Figure 21 MMD Synthesis Example .................................................... 20
Figure 22 Bidirectional Algorithm Gate Direction ............................ 21
Figure 23 Bidirectional Example - MMD Algorithm ......................... 22
Figure 24 Bidirectional Example - MMD Circuit .............................. 22
Figure 25 Bidirectional Example - Bidirectional Algorithm ............... 24
Figure 26 Bidirectional Example - Circuit Result ............................... 24
Figure 27 PPRM Example Specification ............................................ 26
Figure 28 PPRM Example Search Tree Diagram ............................... 27
Figure 29 PPRM Example Realized Circuit ....................................... 28
Figure 30 Specification - Template Matching Example .................... 29
Figure 31 Non-optimized Circuit ....................................................... 29
Figure 32 Optimized Circuit after Template Matching ....................... 30
Figure 33 3 Examples of Tofolli and Feynman Templates ................. 30
Glossary

**HD** – Hamming Distance, which is the amount of bits that differ between 2 binary specifications;

**QC** – Quantum Cost, which is a measurement of quality in a quantum circuit;

**GC** – Gate Count;

**CNOT** - Controlled NOT gate, also known as the Feynman gate;

**LSB** – Least Significant Bit
Chapter 1

Introduction

Since 1958, the semiconductor industry has successfully doubled the amount of transistors incorporated on an integrated-circuit every 2 years, but some experts argue that Moore’s Law may be coming to an end in the next one or two decades. Moving along with Moore’s law trend is the amount of heat dissipated in a single device. While some of the dissipation can be minimized with manufacturing optimization methods, other factors have yet to find a solution.

It has been shown by Landauer’s Principle that a circuit which is logically reversible will, in principle, be thermodynamically reversible as well. He showed that for every bit lost, $kT \cdot \log_2$ joules of heat is generated. While this amount is relatively small today, Zhirnov shows the difficulties in removing heat as CMOS (Complementary metal–oxide–semiconductor) density increases, which has made research in this area an important topic.

A circuit that results in no data lost is called reversible, hence would solve the problem discussed by Landauer and will make this technology important in the semiconductor world. Bennett showed that zero heat dissipation would only be possible if a circuit was compromised of only reversible gates.
The most well-known application for reversible logic is quantum computing. For any algorithm to be efficient, the execution time should not grow exponentially as the number of inputs increase; instead, it should ideally grow as a polynomial function. It has been shown that quantum computing is able to achieve this with some exponentially hard problems, such as factorization (Shor’s Algorithm). Quantum computation must be done using reversible logic. Thus, research into the synthesis of reversible logic is important as this could be the key factor resulting in more powerful computers.

There have been a number of synthesis algorithms for reversible logic proposed in recent years. Miller et al. introduced a transformation based algorithm (AKA MMD) in which steps were based on a truth table so that no transformation would affect previous ones. Agrawal and Jha proposed a search algorithm using ESOP PPRM minimization techniques. Kentopf introduced an algorithm based on shared binary decision diagrams with complemented edges. Maslov recently introduced two algorithms using Reed-Muller spectra.

This thesis is organized as follows:

• In Chapter 2, the basic concepts of reversible object are defined and discussed. This includes basic Boolean logic, reversible gates, and
intermediate Boolean formulas. Popular methods to measure the quality of a circuit design are also introduced.

- The next chapter, Chapter 3, explains existing synthesis algorithms. Maslov’s MMD algorithm is explained in great detail as well as its strengths and weaknesses. This section is important to understand as these concepts are an integral part of the later chapters.

- Chapter 4 explains the new algorithm AP researched for this thesis. First, the basic concept is explained, then, more complex algorithms are added on to show how effective each step is. We also briefly touch on how this algorithm compares to MMD.

- Chapter 5 will show the results yielded from the new algorithm. The well known quality check of checking all 3-variable function specifications will be compared against other algorithms. The weakness of this quality check will be discussed and new/better quality checks will be proposed, which will look at larger circuits. Also, it will be shown that the AP Algorithm generates circuits with low quantum costs when compared to other well known algorithms.

- The chapter Further Research will point the direction for further research in the reversible logic synthesis area.

- Finally, the conclusion will summarize the work discussed in this thesis.
My contributions to reversible logic technology are the following:

- The AP algorithm which uses an MMD like algorithm which uses Hamming Distance as a metric to yield more efficient results.
- A search variant which explores many different circuits which result in the same circuit output.
- An algorithm which will compute all the possible vectors which can be taken in the same cycle that will maintain a non-blocking vector ordering.
- A quantum cost reduction transformation that adds an extra ancilla bit and reduces the size of the gates needed to complete the synthesis.
Chapter 2

Background

2.1 Boolean Logic Overview

Boolean logic is a logical algebra developed by George Boole where all arguments and results of operators result in true or false. The most common application of this type of math is in computer architecture and general digital logic design.

Single-output Boolean logic functions of n variables are specified in the form of truth tables, which have n+1 columns and $2^n$ rows. The columns are broken up into n inputs and 1 output. The rows include all the combinations of the binary input values in order to specify the complete behavior of the logic. Notice that the size of a truth table is susceptible to explosion as the amount of inputs increases. This creates an issue in computer programs as memory can quickly reach its limitation.
The main three gates used is classic Boolean logic are the AND, OR, and NOT gates. The inputs to these gates are logical 1’s and 0’s. From these gates, any Boolean formula can be derived. The logical operation exclusive disjunction, AKA exclusive-or, can be derived and is extremely powerful. The operation of this function will output ‘True’ when exactly one of the inputs is true, while all others are false. The truth table for this function is shown in Figure 2 followed by some basic operations for this gate in Figure 3, which is the basis of reversible logic gates.
2.2 Basic Definitions

2.2.1 Reversible Logic Network Structure

There are quite a few rules that make reversible logic synthesis more challenging than traditional binary logic synthesis. The following definitions outline these differences.

**Definition 2.1.** A binary logic gate is reversible if the function it computes is bijective, that is; each binary input pattern is mapped to a unique binary output pattern. Thus, the circuit must have an equal amount of inputs and outputs.

As an example, the specification of a 3-input 3-output function from Figure 4 is a reversible specification. Notice that every single-output function from a multi-input multi-output reversible function can always be in the form of $x' = x \oplus f(x, y, z)$. 
Definition 2.2. Every output of a gate that is irrelevant to the circuit functionality will be considered a garbage signal.

Let us consider the specification in Figure 5, which will be realized using reversible logic. As specified in Definition 2.1, there must be an equal amount of inputs and outputs. Since one output is considered, there will be at least 3 garbage outputs in the realized circuit. In this case, a single ancilla bit is used, which means there are 5 inputs and 4 garbage outputs as shown in Figure 6.
**Definition 2.3.** A gate output can only be used once in the next level of gates. In other words, the total fanout of a gate in a reversible circuit is equal to one.

**Definition 2.4.** A reversible circuit is acyclic. Figure 7 shows the structure of a reversible circuit.
2.2.2 Reversible Gates

As definition 2.1 suggests, reversible logic does not use traditional logic gates (AND, OR, XOR etc.). Instead, a new set is used with the following characteristics.

**Definition 2.5.** For the function variables \{x_1, x_2, \ldots, x_n\}, a Toffoli gate will use this notation: \( \text{TOF}(C; t) \), where \( C = \text{Control bits} = \{x_{i1}, x_{i2}, \ldots, x_{in}\} \) and \( t = \{x_j\} \) and \( C \cap t = \emptyset \) (empty set). The function of this gate will invert bit \( x_j \) iff all variables in set \( C \) are logically equal to ‘1’.

There are three forms where the Toffoli gate will be used: an inverter gate denoted by \( \text{TOF}(x_j) \), the CNOT gate denoted by \( \text{TOF}(x_{i1}; x_j) \), commonly referred to as a Feyman gate, and the original Tofolli gate denoted by \( \text{TOF}(x_{i1}, x_{i2}, \ldots, x_{in}; x_j) \). An example of the gates discussed are shown in Figure 8. The equivalent functions in traditional logic are shown in Figures 9, 10, and 11.
Definition 2.6. For the function variables \( \{ x_1, x_2, \ldots, x_n \} \), a Fredkin gate will use this notation: \( \text{FRED}(C; s) \), where \( C = \text{Control bits} = \{ x_{i_1}, x_{i_2}, \ldots, x_{i_m} \} \) and \( t = \{ x_{s_1}, x_{s_2} \} \) and \( C \cap t = \emptyset \). The function of this gate will swap bits \( x_{s_1}, x_{s_2} \) iff all variables in set \( C \) are logically ‘1’.

A Swap gate denoted by \( \text{FRED}(x_j) \), and the original Fredkin gate denoted by \( \text{FRED}(x_{i_1}, x_{i_2}, \ldots, x_{i_m}; x_{s_1}, x_{s_2}) \). Figure 12 will show the graphic notation for these two gates. The equivalent gates using Toffoli gates are shown in Figures 13 and 14.
2.2.3 Other Reversible Gates

The following is a brief overview of other gates that have been developed in previous research.

The Peres gate\textsuperscript{11} can accomplish the same task as the CNOT gate and a 3-bit Toffoli gate, with an operation defined in Figure 15.

\[
\begin{align*}
    a' &= a \oplus b \\
    b' &= b \\
    c' &= c \oplus ab
\end{align*}
\]
The most common form of this gate is the 3-bit version defined in Figure 15, but it can be extended to include multiple control lines. The 3-bit gate has a quantum cost of 4.

The Kerntopf gate is a 3-bit gate with the operations defined in Figure 16. It has the maximum number of subfunctions (cofactors). The usefulness of this gate is still yet to be practically assessed as there are not many algorithms implemented in software that include Kerntopf gate.

\[
a' = 1 \oplus a \oplus b \oplus c \oplus ab \\
b' = 1 \oplus b \oplus c \oplus ab \oplus bc \\
c' = 1 \oplus a \oplus b \oplus ac
\]

Figure 16 Kerntopf Gate Operation

2.2.4 Positive Polarity Reed-Muller Expansion

Any Boolean function can be converted into an xor sum of products. The positive-polarity Reed-Muller expansion only uses variables which are uncomplemented. PPRM is a canonical expression in the form:

\[
f(x_1, x_2, ..., x_n) = a_0 \oplus a_1 x_1 \oplus a_2 x_2 \oplus ... \oplus a_n x_n \oplus a_{12} x_1 x_2 \oplus ... \oplus a_{n-1} x_{n-1} x_n \oplus ... \oplus a_{12...n} x_1 x_2 ... x_n
\]

Where \( a_i \in \{0,1\} \), and \( x_i \) are all uncomplemented variables.
PPRM is easily obtained from the xor sum of products by replacing any complemented variable $x$ with $x \oplus 1$ and reducing the expression using laws of Boolean logic. From this form, along with the use of well known Boolean algebra methods the PPRM form can be realized. One motivator for using PPRM is the fact that this form is unique and easy to minimize by eliminating redundant expressions.

To illustrate this, let us take the expression:

$$a' = \overline{a} \oplus b \oplus \overline{ab} \oplus \overline{ab} \oplus a.$$  

Now taking the PPRM form we can easily identify redundant expressions:

$$a' = a \oplus 1 \oplus b \oplus b(a \oplus 1) \oplus a(b \oplus 1) \oplus a$$

$$a' = a \oplus 1 \oplus b \oplus ab \oplus b \oplus ab \oplus a \oplus a$$

$$a' = a \oplus 1$$

The PPRM representation is an extremely powerful tool to use in software to efficiently minimize equations as shown by the Agrawal and Jha algorithm\(^8\) for reversible function specification.
2.3 Measuring Quality of Reversible Gates

2.3.1 Ancilla Bits

Ancilla bits are additional inputs that are not part of the original specification. These bits are added in hopes to reduce the circuit complexity or realize a non-reversible function. They come in the form of a constant logical 1 or 0.

It is ideal to keep the number of ancilla bits minimal due to the added circuit complexity of having more inputs. In addition, the cost of adding ancilla bits could outweigh the cost savings of reducing gate count of quantum cost.

The addition of ancilla bits cannot always be avoided. For instance, any non-reversible specification will always need ancilla bits as it is otherwise impossible to synthesize as a circuit with reversible gates.

2.3.2 Delay

The delay\(^{12}\) of a quantum circuit is defined with the equation in Figure 17.

\[ \text{depth} \times \Delta \]

*Figure 17 Delay Equation*

Where \(\Delta\) is dependent of the process technology and the depth is the number of stages in the circuit. Stages in a quantum circuit are dependent on the number of gates required to synthesize of specification. Figure 19 shows how the number of stages is defined.
2.3.3 Quantum Cost

The quantum cost in a popular measurement used to compare different reversible or logical circuits. The quantum cost of a reversible circuit is defined as the number of primitive quantum gates needed to implement a reversible specification.

There are 2 methods that can be used to determine the quantum cost of a reversible logic. First, the circuit can be realized using primitive quantum gates (1 x 1 and 2 x 2 gates) and then count the number of gates needed. Second, the circuit can be realized using well know reversible gates whose quantum cost has already been determined and the cost of each individual gates is summed. In this thesis, the latter will be used.

Figure 18 Quantum Circuit showing stages. The arrow denotes a feedback loop.
Chapter 3

Previous Work on Reversible Logic Synthesis

3.1 MMD (Maslov, Miller, and Dueck).

3.1.1 Algorithm

MMD algorithm\textsuperscript{10} is currently the most popular synthesis algorithm for reversible circuits. This method has been proven to be 100% convergent, that is, for every circuit it is able to find a solution. The solution is guaranteed to yield a circuit size of less than or equal to \((n - 1)2^n + 1\).

The basic MMD algorithm can be completed in these steps\textsuperscript{7}:

1. If \(f(0) \neq 0\), then invert all the outputs that currently are logical 1’s using a CNOT gate for each. This will ensure that \(f^+(0) = 0\).
2. Consider all other input/output combinations in order from \(i\) to \(2^n\). If \(f^+(i) = i\), no transformation is needed. Otherwise, a transformation is needed in order to make \(f^{++}(i) = i\). The following sub-steps will accomplish this:
   a. Consider all positions in \(f^+\) where a transformation from \(0 \rightarrow 1\) is needed, for each of these, a Toffoli gate is needed whose target line is that very position and the control lines are all lines that are currently a logical 1.
b. Consider all positions in $f^+$ where a transformation from 1 → 0 is needed, for each of these, a Toffoli gate is needed whose target line is that very position and the control lines are all lines that are currently a logical 1.

Each gate derived from this algorithm in implemented from output to input. If Gate $m$ is that last gate which ensures that $f^+ (2^n - 1) = 2^n - 1$, then the first gate in the circuit will be gate $m$.

![Gate Implementation Direction](image)

**Figure 19  MMD Implementation Direction**

The main thing to note is this algorithm is that any Tofolli gate implemented in $f(i)$ will not affect any of the transformations that occurred in the previous steps. In other words, once a row as successfully transformed $f^+ (i) \rightarrow i$, it will remain that value regardless of what gate is implemented for the completion of the algorithm. This is known as “control line blocking”.

18
### 3.1.2 MMD Example

Figure 20 shows how the MMD basic algorithm in applied. In order to fully understand this algorithm, each step will be discussed in closer detail. The notation is as follows: C is the target line, 1 is a control line, X indicates this line is not used in the gate.

- Step i in the algorithm shows that since $f^+(0) = 0$, then no NOT gates will be used in this circuit.
- In the output column, $f^+(1) \neq 1$ and the Hamming Distance is equal to 2. Therefore, it will take 2 transformations (2 gates from step i and step ii) to have $f^+(1) = 1$. In this instance, only transformations for $1 \rightarrow 0$ is needed so the order does not matter. C11 and XC1 gates are used.
• Now, in step ii column we see that $f^+(2) \neq 2$. Since the Hamming Distance is 1, then only one gate in needed for this transformation. A Feynman gate C1X is applied.

• In step iii, $f^+(3) \neq 3$ and the Hamming Distance in 1. A Feynman gate C11 is applied in step iv.

• In step iv, $f^+(4) \neq 4$ and the Hamming Distance in 2. In this instance, both transformations are from $0 \to 1$, therefore order does not matter. Toffoli gate 1C1 and Feynman gate 1XC are applied.

• In step vi, $f^+(5) \neq 5$ and the Hamming Distance is equal to 1. The Toffoli gate 1C1 is applied.

• Now we see that $f^+(6) = 6$ and $f^+(7) = 7$. The algorithm is complete and no more transformations are needed.

Figure 21 shows the circuit which resulted from the above synthesis. The gate count is equal to 7 and the total quantum cost is 17. Observe that the circuit was built from outputs to inputs.

![Figure 21](image)
3.1.2 MMD with Bidirectional Search

Introduced by Maslov\textsuperscript{7} is an MMD variant, the bidirectional method, and is a natural progression of the original MMD algorithm as it addresses the weakness that MMD only synthesizes the circuit from one direction, back to front. In this method, for each step, it will be determined which direction (Figure 22) to synthesize based on the Hamming Distance.

![Bidirectional Algorithm Gate Direction](image)

*Figure 22 Bidirectional Algorithm Gate Direction*

To illustrate how the bidirectional synthesis works, let us analyze the following circuit specification using both traditional MMD and bidirectional MMD. The MMD method yields a circuit with 9 gates and a quantum cost of 21 as shown in Figures 23 and 24.
Using the bidirectional synthesis method, let us analyze the first 5 steps (Figure 25) to understand the main differences between the traditional MMD and the bidirectional method:

- **Step i** – As seen above, the traditional MMD method would naively synthesize the output side to match the input side. Notice that the HD = 3 in this case. Attempting to change the input side, we see that the HD = 1, and therefore, it is the better choice. Only one CNOT gate is needed.
• Step ii and iii – In order to synthesize the binary equivalent of 1, both directions show a HD of 2. The input choice is chosen because it has a smaller number of one’s which could yield smaller gates.

• Step iv - Looking at the binary equivalent of 3 from both directions, we see that the input side has a HD=1 and the output side has a HD=2. Therefore, we chose the input side.

The bidirectional algorithm yields a circuit (Figure 26) which is 1 gate less than what MMD resulted. Clearly, the benefits of using a bidirectional method are realized.
### 3.1.3 MMD Strengths and Weaknesses

The most important attributes of the MMD algorithm are that it is fast and that it is 100% convergent. On top of this, there are many additional steps in the algorithm that have been added or can be added to realize circuits that are closer to optimal.
One important attribute that lacks in this algorithm is the fact that it is not scalable. As more and more variables are added into a specification, the memory requirements grow exponentially. Also, there is a lack of search. We have seen in many algorithms that it is impossible to know which step is the best gate selection step, therefore, it is important to check all directions and get more than one result. Then all results are analyzed and the most optimal is used.

3.2 Optimal Reversible Circuits

In 2003, Shende\textsuperscript{13} proposed an algorithm that resulted in a guaranteed optimal circuit for any reversible logic specification. This algorithm requires the generation of all optimal k-gate circuits as k increases for a logical specification π. This is done using a depth first search technique in which additional gates will be added after each step and checked for completion, if not, the process will continue. Once the first correct circuit is discovered, the depth of the search will be limited to that amount of gates.

While this algorithm is convergent as well guaranteeing the optimal result, it requires $\Theta(2^n!)$ memory space. Therefore, this algorithm can only work for, at most, 4-variable specifications. This limitation makes the algorithm an unrealistic solution to synthesizing reversible logic, but it does give a bound of how well an algorithm can perform.
3.3 PPRM Algorithm

3.3.1 Algorithm

Agrawal and Jha developed an algorithm that uses the Reed-Muller expansion for each individual output. During each step there exists n equations; where n is the amount of inputs in the specification. Using the fact that all gates result in the equation of \( x' = x \oplus f \) (variables not \( x \)), any possible gate that can be extracted from the equation is done this way and implemented into all equations. This process is repeated until a specification is discovered, there exists no more possible gates to be included, or an infinite loop has been entered.

3.3.2 PPRM Algorithm Example

To understand the algorithm, the specification in Figure 27 will be analyzed:

<table>
<thead>
<tr>
<th>Input A</th>
<th>Input B</th>
<th>Input C</th>
<th>Output A'</th>
<th>Output B'</th>
<th>Output C'</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 0 0</td>
<td>1 0 0</td>
<td>1 1 0</td>
<td>0 0 1</td>
<td>1 1 0</td>
<td>0 0 0</td>
</tr>
<tr>
<td>0 0 1</td>
<td>1 1 0</td>
<td>0 1 1</td>
<td>0 0 0</td>
<td>0 0 1</td>
<td>0 0 0</td>
</tr>
<tr>
<td>0 1 0</td>
<td>0 0 1</td>
<td>1 0 0</td>
<td>0 0 0</td>
<td>0 0 1</td>
<td>0 0 0</td>
</tr>
<tr>
<td>0 1 1</td>
<td>1 0 0</td>
<td>1 1 0</td>
<td>0 0 0</td>
<td>0 0 1</td>
<td>0 0 0</td>
</tr>
<tr>
<td>1 0 0</td>
<td>1 1 0</td>
<td>0 1 1</td>
<td>0 0 0</td>
<td>0 0 1</td>
<td>0 0 0</td>
</tr>
<tr>
<td>1 0 1</td>
<td>0 1 0</td>
<td>1 1 1</td>
<td>0 0 0</td>
<td>0 0 1</td>
<td>0 0 0</td>
</tr>
<tr>
<td>1 1 0</td>
<td>1 0 1</td>
<td>0 0 1</td>
<td>0 0 0</td>
<td>0 0 1</td>
<td>0 0 0</td>
</tr>
<tr>
<td>1 1 1</td>
<td>0 1 0</td>
<td>1 1 1</td>
<td>0 0 0</td>
<td>0 0 1</td>
<td>0 0 0</td>
</tr>
</tbody>
</table>

Figure 27 PPRM Example Specification
The first step is to convert the table into equations in the form of PPRM (Section 2.2.4). From these equations, 3 different gates are implemented. Note that we cannot apply a change to line with variable C because the equation does not have the variable as a standalone.

The graph in Figure 29 shows only the first iterations of the algorithm which finds a circuit rather quickly. The completed circuit (Figure 30) is identifiable by the section where both sides of the equations are equal. This algorithm will continue its search to see if there is a more optimal solution.
3.3.3 Strengths and Weaknesses of the Agrawal and Jha Algorithm

PPRM algorithm is stronger than other known methods due to the fact that it has a search involved rather than stopping at the first result. Agrawal and Jha were able to achieve near optimal results for all 3-variable specifications.

This algorithm was able to show full convergence on 3 and 4 variable functions, but its evaluation found that a large number of 5-variable functions were unable to converge. This could be due to time or memory constraints. Not being able to show convergence on larger function is detrimental to the actual usage of this algorithm in a real world environment.

3.4 Template Matching

3.4.1 Overview

In the previous section, some algorithms were discussed and the only one which achieves guaranteed optimal results can only synthesize circuits which have at most 3-4 variable inputs. This is the main motivation behind template matching; a local optimization that can be applied to any circuit.
Basically, template matching analyzes a circuit and tries to find a specific sequence of gates that can achieve the same logical results with lesser cost and no adverse affects. This algorithm is very flexible since both the optimal and non-optimal sequences live on an outside database.

3.4.2 Template Matching Example

As an example, consider the reversible logic specification in Figure 31. The circuit that realizes the specification is TOF(a,b,c), TOF(b,c), TOF(a,b,c). The quantum cost of this circuit (Figure 32) is 7 and a gate count of 3. The equations that are associated with this specification are \( a' = a \); \( b' = a \oplus b \); \( c' = (c \oplus ab) \oplus a(a \oplus b) \).

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>b</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
</tr>
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<td>0</td>
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Figure 30 Specification - Template Matching Example

Figure 31 Non-optimized Circuit
The equation for $c'$ can be reduced using simple Boolean algebra: $c' = \lnot(c \oplus ab) \oplus (a \oplus ab) = c \oplus a$. It is clear at this point that the circuit can be realized using the sequence of gates: TOF($a,b$), TOF($a,c$), which is the optimized version of this specification. This sequence of gates has a gate count of 2 and a quantum cost of 2. This circuit is shown in Figure 33.

![Figure 32 Optimized Circuit after Template Matching]

Figure 34 shows some well known 2 and 3 variable templates.

![Figure 33 3 Examples of Tofoli and Feynman Templates]

### 3.4.3 Strengths and Weaknesses

Template matching has been shown to dramatically improve the size and cost of reversible circuits. Maslov\(^7\) reported close to a 6% improvement when applied to the MMD algorithm. This optimization result along with the fact that it can be
applied to any current and future algorithm makes this algorithm an extremely powerful one.

Unfortunately, this extra step does take a longer time to apply as the number of inputs increase as well as the gate count. Also, it is very difficult to have a database with every single scenario which could be reduced to a more optimal circuit. Furthermore, this algorithm requires several passes as when you change the circuit, it is possible that another optimization has been uncovered.
Chapter 4

AP Algorithm

4.1 Motivation

The main motivation behind this new algorithm created by me and called AP is to close the gap that MMD has left open. As shown by Stedman\textsuperscript{14}, the natural binary order actually falls into a subset of orderings that have the characteristics of “control line blocking”. It was also shows that an exhaustive search of these orderings results in a more efficient circuit. Unfortunately, an exhaustive search is not a good option as the number of inputs increases because the number of orders grows exponentially as shown in Figure 34.

![Figure 34 Input/Search Relationship](image-url)
4.2 AP Algorithm Overview

This algorithm follows the same high level flow as in MMD. The difference is that there exists another level of intelligence instead of following a pre-defined binary ordering. Before executing another iteration of the MMD algorithm, the software checks all the options possible in order to maintain a non-blocking order.

Minimizing the amount of gates needed to synthesize this portion of the circuit is the primary decision maker, which is done by choosing the combination that has the smaller Hamming Distance. This is true due to the fact that there is a direct correlation between the Hamming Distance and the amount of gates needed to synthesize the circuit. In the case of tie, the input which contains the smallest amount of logical 1’s will be chosen, which will minimize the quantum cost of the gate. Figures 35 and 36 are examples showing how Hamming Distance and number of logical 1’s affects the circuit.

Assume that these are the only 2 options for the next iteration of the circuit. Option 2 clearly has a smaller Hamming Distance (HD) and will ultimately be the chosen option. The decision to use the option with the smaller Hamming Distance is justified as both synthesized circuits are shown below and option 2 is clearly the smaller circuit.
The basic AP algorithm (intermediate improvement to MMD) is as follows:

1. If $f(0) \neq 0$, then invert all the outputs that currently are logical 1’s using a cnot gate for each. This will ensure that $f^+(0) = 0$.

2. Consider all the current options available. Calculate the Hamming distance for each of these options and choose the one with the smallest HD. If more than one options has the smallest HD calculation, randomly choose one.

3. If $f^+(i) = i$, then no transformation is needed. Otherwise, a transformation is needed in order to make $f^{++}(i) = i$. The following sub-steps will accomplish this:
a. Consider all positions in $f^+$ where a transformation from $0 \rightarrow 1$ is needed, for each of these, a Toffoli gate is needed whose target line is that very position and the control lines are all lines that are currently a logical 1.

b. Now consider all positions in $f^+$ where a transformation from $1 \rightarrow 0$ is needed, for each of these, a Toffoli gate is needed whose target line is that very position and the control lines are all lines that are currently a logical 1.

4. Consider the current option. Determine what options have been uncovered and consider them in step 2. If all $f^+(i) = i$, the algorithm in complete.

Note that directly after step 1, there are certain options that are open immediately. These options include all vectors that have exactly one logical one while all other positions have logical zeros. Therefore, any circuit description which has $n$ inputs will have $n$ options available immediately after step 1.

4.3 Discovering New Options

The main module in the AP algorithm is the one pertaining to discovering what are the options available to use in the next iteration (see step 4 above). In order to accomplish this, a history of every transformation must be kept in tables
separated by the number of logical 1’s in the transformation. The algorithm to discover new options follows.

Assume the number of logical 1’s in the current choice is $x$.

1. Consider the current transformation and let $p$ be all the positions where there is a logical 1 and $q$ be all the positions where there is a logical 0.

2. For all the previous transformations taken with $x$ logical 1’s, consider only transformations in which the number of differences in logical 1 positions is only 1. Refer to these transformations as a subset $p$ (which now includes the current transformation).

3. Consider subset $p$, for each position $p$, count the number of logical 1’s.
   
a. If the count is less than $x$ for any of the positions, then no new options have been uncovered. There is no need to continue.

4. Consider subset $p$, for each position $q$, count the number of logical 1’s.
   
a. If the count is greater or equal to $x$, then a new option has been uncovered where there is a logical one is all positions $p$ and a logical 1 located in the current position under consideration.

Figure 37 shows an example showing how the algorithm works in practice. Consider that the current transformation that took place is vector 11100 and the table shown below is the history of transformations taken place that have an equal amount of logical ones.
As mentioned in step 3, we must consider all the positions in which there exists a logical 1. In this case, we will be considering positions 1, 2, and 3. In order to have a possibility of uncovering a new option, the count for all of these positions must be equal to or greater than 3. As illustrated, the count for position 3 is only 2 and therefore, no new options have been discovered.

Let us now consider a similar example (Figure 39) to show how the algorithm will work when new options can be discovered.

In this example, the result from step 3 will show that all the positions in vector $p$ have a logical 1 count of greater or equal to 3. Step 4 requires the algorithm
to analyze all other positions (positions 4 and 5). From the table above, we see that position 4 is only one, and therefore, no new option will be uncovered with a logical 1 in that position. Position 5, on the other hand, has a value which is greater or equal to 3, and therefore, will result in a new option uncovered with a logical 1 is that position along with logical 1’s in all positions in position p (Position 1, 2, and 3). The new result is vector “11101”.

4.4 AP Algorithm Example

Figure 40 shows an example that demonstrates how the AP algorithm works. For continuity, we will use the same example that was used in Chapter 3 which outlines the basic MMD algorithm.

- In Step 1, no action is needed as $f^+(0) = 0$.
- Since step 2 is the first iteration in which we must choose among options, we must consider all possible vectors that contain exactly one logical 1. Option “010” and “100” both have a HD = 1, therefore we will randomly choose binary vector “100 “and make the transformation.
- At this point, no new options are uncovered.
- Step 3 will consider the remaining options. Between the 2 options available, option “010” has the smaller HD and therefore will be used in the following transformation.
• The history of transformation now contains “100” and “010” which uncovers a new option “110”.

• In Step 4, consider the 2 options available and automatically take the option with HD = 0, which requires no transformation.

• In Step 5, there is only one available option in order to maintain a non-blocking order. This option is used to make the transformation.

• At this point, the entire transformation is complete. The result is shown in Figure 40 and 41.
Figure 40  Transformations taken during AP Basic Algorithm

<table>
<thead>
<tr>
<th>Input</th>
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<tbody>
<tr>
<td>A B C</td>
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<table>
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Figure 41  Synthesized Circuit using Basic AP Algorithm

The circuit synthesized (Figures 41 and 42) shown above has a gate count of 5 and a quantum cost of 7. Compared to the basic MMD algorithm, this is a significant improvement.

4.5 AP Search

In step 2 of the previous section, notice there were 2 options with an HD = 1. In the basic algorithm, the option was chosen at random. By using randomness in an algorithm, it is not easy to know if the transformation used results in the most efficient circuit.

In this section, we introduce an AP Search Algorithm which is based on the basic algorithm above. The search is a breadth-first search, illustrated in Figure 42,
and each node signifies a situation in which a random choice needed to be made due to equivalent HD.

![MMDS Search Diagram](image)

**Figure 42.** MMDS Search Diagram.

Figure 43 and 44 is the same example we used in the previous section. We will not go through all the nodes in the search, but show what the results will be, if in step 2 we would actually take the other option that was available.
Figure 43  AP Search Algorithm Detailed Steps

Figure 44  AP Search Algorithm Transformation Table

Figure 45  Synthesized Circuit using AP Search Algorithm
The synthesized circuit resulting from the search algorithm is shown in Figure 45. The gate count is 3 while the quantum cost is equal to 3. This is clearly the best most reduced solution for this synthesis benchmark function.

Figure 46 is a summary of the synthesis methods for Basic MMD, Basic AP Algorithm, AP Search on a single 3-variable circuit. Clearly, using a search results in a better result as both the Gate Count and Quantum Cost are reduced.

![Comparison of MMD, AP Algorithm, and AP Algorithm Search.](image)

4.6 Quantum Cost Reduction

The AP algorithm, as is, works to reduce the overall gate count by minimizing the HD for every step in the algorithm. While reducing the gate count can
significantly reduce the quantum cost, there is some transformation which can be introduced into the AP algorithm to further reduce the quantum cost by adding a single ancilla bit.

Let us analyze an example of a single step in the AP algorithm. Assume that the next step is to transform the output from \(71_{10}\) to \(47_{10}\), which are decimal equivalents of a binary vector. By XORing these 2 numbers and counting the logical ones, we see that the HD is 3 which means it will take 3 gates to properly complete the transformation and have a quantum cost of 302. All figures in this section assume that the LSB (least significant bit) is variable ‘a’.

![Figure 47 Circuit synthesized without QC Reduction](image)

Notice that the gates in this transformation (Figure 48) use variables \(<a, b, c>\) as control lines. Since the quantum cost for Toffoli gates go up exponentially as the number on inputs increases, it would be prudent to use smaller gates even if it increases the amount of gates needed for the transformation. This notion justifies the idea of combining the control lines in order to reduce the size of gates. This is known as the Perkowski transformation.
The algorithm is as follows:

- For any transformation in the AP algorithm, the first gate in the transformation will have control lines in all places where the input and output have common logical ones and the target bit is the ancilla bit of logical zero.
- The next gates will actually perform the transformation which is needed and will follow a similar method to the explained in the original AP algorithm above. The difference is that the common logical one’s will no longer be control bits and a control line is added which is the ancilla bit.
- The last gate will be the same gate as the first in the transformation. This will return the ancilla bit to zero to enable it to be used in future transformations of this kind.

To see the benefits of the Perkowski transformation, we will apply it to the example at the beginning of this section. There are three common logical one bits between the input and output, which means the first and last gate will be a 4-input Toffoli gate (T4(a,b,c,0)). The next gates perform the transformation using the ancilla bit instead of the common logical one bits. Finally, we return the ancilla bit to zero. The gate below shows the circuit which now has a gate count of 5 and a quantum cost of 57. This transformation alone reduces the overall circuit, shown in Figure 48, by 245.
Assuming we are transforming a circuit which has x inputs, y common logical one bits between the inputs and outputs, and an HD of z. The z gates needed in the main transformation will have y - 1 less control bits compared to the original transformation rules. Therefore, any transformation which has only 1 common logical one will not have any quantum cost optimization and should follow the original transformations. Also, if a transformation only has an HD of 1, then the gate needed for this transformation would be y + 1 in the original transformation method. Since the Perkowski transformation applies 2 extra gates with the same quantum cost, using the Perkowski transformation would actually yield a larger quantum cost.

Therefore, the Perkowski transformation should only be applied when the current transformation has an HD \( \geq 2 \) and the common logical one bits \( \geq 2 \).

To understand how much improvement the QC minimization technique results in, it was applied to a large number of benchmarks. The result shown in
Figure 50 clearly shows that the QC reduction provides much improvement to the AP algorithm. In the case of an HWB18 benchmark, there is a 90% improvement of QC.

Note that the improvement grows as the number of inputs increase, which is mostly due to the fact that the Toffoli gates QC increases exponentially as the amount of control bits grows. You have to characterize all these benchmarks, tell the source, how big is each of them in terms of number of variables and rows.
Chapter 5

Results

5.1 3-Variable Results

One of the most common tests used to measure the quality of an algorithm is how it performs across all 40,320 specifications for 3-variable functions. While this test is not a good indication of the overall performance due to its lack of size, it does serve as a gross check against other methods. The results here only serve to see how close we can get to the optimal results$^9$.

In Figure 50, we compare the AP algorithm vs. other well known methods as well as the optimal circuits. Also included in the table is the progression of the algorithm to illustrate how each addition to the algorithm includes the total gate count.
Figure 50  Results of applying all 3-variable functions to a number of algorithms.

The results clearly show that using a bi-directional search with MMDS yields the best results. Unfortunately, this AP algorithm does not create more optimized gates when compared to other algorithms, but it does come somewhat close to optimal results.

5.2 Proposal for Better Quality Check

The current quality check of using all 3-variable specifications is not enough to check the overall quality of an algorithm because the circuits are too small. Using specifications with a larger number of inputs will ensure that any proposed algorithm has the ability to create optimized results for all kinds of specifications. The challenge is that we cannot synthesize all specifications for circuits with more than 3
inputs, because the amount of specifications explodes. The solution to this problem is to create random specifications and compare the average gate count across them. Some would argue that this is problematic, because creating random specifications means that different algorithms will not be able to ensure that the results are due to the algorithm or the random specification that was used. In order to ensure that this is not an issue, for each x-variable experiment, a large amount of specifications needs to be included in the sample (i.e., 40,000 specifications). The resulting gate counts will create a bell curve with a relatively small standard deviation. Unless any algorithm can show a significant different in the average gate count, then we can consider the results as equal.

Figures 51, 52 and 53 are the gate count results for reversible specifications with inputs that are larger than 3.
Figure 51. Results of applying 40K random 4-variable functions in the AP Algorithm

Figure 52. Results of applying 40K random 5-variable functions in the AP Algorithm
5.3 Benchmarks

The AP algorithm was applied to a number of benchmarks that were used in both MMD and MP\textsuperscript{15} algorithms. Quantum Cost is the main parameter used to compare the different algorithm since it expresses the actual cost of implementation.

Due to the fact that the size of the circuits grows exponentially as the number of inputs increases, it was decided to show the results as the percentage quantum cost compared to the MMD baseline. For instance, for the HWB4 benchmark, Alhagi, Hawash and Perkowski\textsuperscript{15} show an increase of 30% compared to MMD and the AP algorithm shows a decrease of about 50% compared to MMD.
Of the 10 benchmarks used the AP algorithm shows that it produces better results for 9 of them. The exact results are shown in Figure 54.

![AP Algorithm QC Comparison](image)

Figure 54. AP Algorithm QC Analysis (MMD and ALHAGI)

### 5.4 Runtime

A good property of any CAD tool is a minimal runtime. The graph from FIGURE 55 shows that the AP algorithm can successfully provide results within 10 minutes for up to 16 variables. The time to synthesize will grow linearly with the amount of searches requested. Unfortunately, as the amount of inputs increases, the time to synthesize grows exponentially, which significantly limits this algorithm’s ability to synthesize specifications that require input variables greater than 18 input variables.
Figure 55 shows the results of running the hidden-weighted benchmark across many different sizes.
Chapter 6

Conclusion

The thesis starts off by analyzing previous work accomplished by Maslov et al and Jha et al to synthesize reversible specifications. Part of this analysis includes an understanding of the strengths and weaknesses of each algorithm in order to lay the groundwork for a new algorithm which can provide better results.

Chapter 4 introduces the AP algorithm which uses the same underlying concepts as those used in MMDS, but improves synthesis by exploring more than one non-blocking order and by prioritizing lower Hamming Distance transformations. These 2 additions successfully reduce the overall gate count, which directly reduces the quantum cost.

Unfortunately, this reduction in quantum cost is not enough. Section 4.4 introduces the Perkowski transformation which can perform the same transformation per cycle, but at the cost of adding an extra Ancilla bit and 2 Toffoli gates.

Next, the results of the AP algorithm are compared against MMD\textsuperscript{7}, RELOS\textsuperscript{8}, and the MP algorithm\textsuperscript{15}. The results show the AP algorithm significantly reduces the quantum cost. Also, the current quality check of checking all 3 variable specifications is challenged. A new check is proposed to randomly select a large sample of $n > 3$. 

variable reversible function specifications. The AP algorithm results should serve as a baseline for future algorithms since this is the first algorithm to report these types of results.

The AP algorithm successfully provides 4 out of the 4 highly desirable properties which make a good CAD tool:

1. **Reliability**: The AP algorithm will 100% convergent which means that it will always provide a solution even if it is not optimal.

2. **Quality**: Optimal or near-optimal networks are the goal of synthesis reversible specifications. The results of the AP algorithm show significant reduction in quantum cost, which has been shown to be one of the most desirable quality indicators.

3. **Runtime**: The time needed to synthesize is relatively small. While the runtime is extremely dependant on the amount of transformation needed as well as the amount of searches requested. Keeping the searches below 50, we see a runtime of just 1 hour for functions using 15 input variables. It is important to note that this time grows exponentially as the amount of inputs increases, which is not desirable.

4. **Scalability**: This algorithm has the ability to synthesize functions of up to 20 input variables. The main limiting factor is the size of the truth tables which need to be stored in memory.
Chapter 7

Further Research

The AP algorithm successfully drives down the quantum cost of the synthesized circuits by applying a single Ancilla bit. This method can be recursively applied to any cycle in the synthesis process for this algorithm. For instance, assume we are transforming the output from $193_{10}$ to $252_{10}$. The AP algorithm, without adding any transformation, will result in a circuit, shown in Figure 56, with quantum cost of 251.

As discussed in section 4.4, a transformation can be used which will add an extra Ancilla bit which will effectively reduce the quantum cost to 130. This circuit is shown in Figure 57.

The next logical step would be to analyze the gates which are not used to transform the single Ancilla bit to see if we can continue adding transformations and add more Ancilla bits. The process should continue until no more transformations can be accomplished. Figures 58 and 59 show the resulting circuits when more ancilla bits are applied. Figure 60 shows the final circuit with the maximum transformations. The circuit illustrates that by adding up to 4 ancilla bits, a circuit with quantum cost of 61 can be achieved.
Figure 56  No Transformation with quantum cost of 251

Figure 57  Transformation with 1 Ancilla bit with Quantum cost of 130

Figure 58  Transformation with 2 Ancilla bit with Quantum cost of 95
As with the most improvements to a circuit, it does not come free. In this case, the extra ancilla bits must be added for every transformation to be added. There has been little to no research done on the actual cost of extra Ancilla bits. This type of research is critical to the future research in synthesizing quantum circuits.
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