CPSC 4210 - Final Paper

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Abstract

his paper explores the use of genetic programming in conjunction with a shared cube representation of reversible cascades to minimize the gate count and quantum cost of arbitrary reversible circuits. Rather than optimizing for either quantum cost or cascade length, we utilize a feature vector approach to minimize both aspects. A recent approach by Nayeem and Rice provides a foundation for the shared-cube approach to reversible logic synthesis. Due to the complexity of these operations, we expand on this foundation, combining it with a genetic algorithm to yield a solution. This approach allows us to achieve a solution more quickly than by performing a brute-force search over the problem space. We demonstrate the use of a shared cube representation from Nayeem and Rice [2011] and apply an evolutionary algorithm to find optimized representations. We consider an implementation that uses a subset of the ordering rules in Rice and Nayeem [2011] as a guideline for implementing our mutation function. We present an implementation of this approach and selected examples using the Python programming language, and compare our results to those achieved in the literature as applied to Revlib benchmarks Wille et al. [2008].

1 Introduction

Reversible computing is a field that is rapidly gaining interest among researchers due to the potential to circumvent the fundamental limitations in energy efficiency and heat loss that are being faced by traditional irreversible computing designs. It has been suggested that within 20 years we will no longer be able to achieve further increases in performance or efficiency at a chip level in irreversible circuits (`frank 2005`) It has also been long known that reversible logic can lead to circuits with much lower power dissipation (`R. Landauer, 1961`) and in theory it is possible to design a reversible circuit capable of dissipating zero energy (`Bennett 1973`). Interest in reversible logic is also growing because it has been shown to be applicable to other fields such as optical computing (`P.Picton, 1991`), low power CMOS design (`W.C. Athas & L.J. Svensson, 1994`), nanotechnology (`R.C. Merkle, 1993`), and quantum computing (`A.N Al-Rabadi, 2004`).

2 Background

2.1 Unitary Matrices

Every quantum gate can be represented by a unitary transformation (in the form of a unitary matrix) whose entries are complex variables corresponding to the complex coefficients of a given particle's wave function. Unitary transformations allow us to perform actual computations with qubits since they can be realized using technologies like NMR, for instance: a qubit in an NMR machine undergoes state changes due to a changing magnetic field. These magnetic field changes are, in turn, represented by unitary matrices (Lukac et al. [2003]). Constructing useful quantum circuits in this way is analogous to early computer programmers who "programmed" massive machines like ENIAC by physically connecting relays and vacuum tubes with wires. How far we have come since then...

Definition 1. *A* **unitary matrix** *is an $n \times n$ matrix of complex coefficients which, when multiplied by its Hermitian, gives the identity matrix. Thus, for a unitary matrix U, it is true that $(U^T)^* = U^{-1}$ where $(\cdot)^*$ denotes complex conjugation.*

In addition, every 2×2 unitary matrix can be expressed using the following product (Barenco et al. [1995]). This representation is particularly useful since it corresponds to the exact rotation matrix which can be applied to the Bloch sphere representation of a qubit:

$$\begin{bmatrix} e^{i\delta} & 0 \\ 0 & e^{i\delta} \end{bmatrix} * \begin{bmatrix} e^{\frac{i\alpha}{2}} & 0 \\ 0 & e^{\frac{-i\alpha}{2}} \end{bmatrix} * \begin{bmatrix} \cos\theta/2 & \sin\theta/2 \\ -\sin\theta/2 & \cos\theta/2 \end{bmatrix} \times \begin{bmatrix} e^{i\beta/2} & 0 \\ 0 & e^{-i\beta/2} \end{bmatrix}$$

In order to create useful operations out of "quantum primitives", we can compose unitary transformations in order to come up with a permutation representation of a gate or cascade of gates. We can use the "Square-Root-of-NOT" gate to construct a NOT gate, for instance:

$$\sqrt{\text{NOT}} = \frac{1+i}{2}\begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix} \Rightarrow \sqrt{\text{NOT}} * \sqrt{\text{NOT}} = \left(\frac{1+i}{2}\right)^2 \begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix} * \begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

There are many other unitary matrices: more examples may be found in Lukac et al. [2003]. Gates such as the Pauli-X, Pauli-Y, Pauli-Z, are interesting examples to play around with.

2.2 Permutation Matrices

Definition 2. *A* **permutation matrix** *P is an $n \times n$ matrix created by permuting the rows of the identity matrix I_n. It is the case that $P * P^T = P^T * P = I$ and that $det(P) = 1$.*

Rather than deal with extremely large and unwieldy unitary transformations all the time, we can use permutation matrices, as described by Williams [1999]. These are a powerful tool, since an $n \times n$ permutation matrix can be used to represent a $2^n \times 2^n$ unitary operation. Additionally, since permutation matrices are sparse, they can be computed with and stored

more efficiently than full matrices. As an aside, some unitary matrices are also permutation matrices (such as the NOT gate), but the gates which are "true quantum primitives", as described in Lukac et al. [2003] are only unitary.

In brief, permutation matrices encode the rows of a circuit or gate's truth table. Given the truth table for a CNOT gate, for instance, it is quite simple to construct its permutation matrix: we begin by encoding the inputs and outputs of the gate as decimal numbers, and create a mapping between them. Then, we use this mapping to construct the permutation matrix, using the following rule:

$$P = [p_{ij}] \text{ where } p_{ij} = \begin{cases} 1 & \text{if } i = n \text{ and } j = M(n) \quad \forall n \in \mathbb{Z}_k \\ 0 & \text{otherwise} \end{cases}$$

In this case, $k = 2^w$ where w is the "width" of the gate, or the number of inputs. Since CNOT has a width of 2, that means $k = 2^2 = 4$, in this case.

a	b	a'	b'
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

$\rightarrow$

n	$M(n)$
0	0
1	1
2	3
3	2

$\rightarrow \quad P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

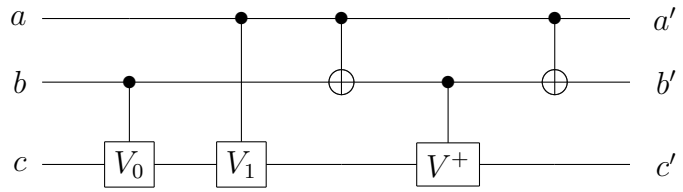
A useful property of permutation matrices is that they allow us to "compose" permutations. In order to do this, we use the following identity: $P_{\sigma\circ\pi} = P_\pi * P_\sigma$. Note that the order of the matrix multiplication matters, as matrices do not typically commute under multiplication. Having this composition operator makes it easy to represent cascades in a unique way. We can check that two cascades realize the same function if their output permutation matrices are identical. This provides circuit designers with an efficient way to "equate" cascades and determine which is "better".

2.3 Quantum Cost

Since we can represent operations on qubits using unitary transformations (which conveniently correspond to exactly one quantum operation each), we can devise a metric called "quantum cost" in order to determine whether the transformations we perform constitute an efficient synthesis of a given operation. In an NMR system, each electromagnetic pulse to which we subject a qubit has a cost: whether it is the amount of energy required to create the pulse, or the risk of the qubit decohering into a useless state (through vibrations, or other environmental perturbations), these factors may be treated as unitless "cost" variables which must be taken into account.

As quantum cost is a unitless quantity which corresponds directly to the number of unitary operations in a quantum circuit, it is a very useful metric for calculating the efficiency of an

implementation of a circuit. In order to determine the quantum cost of a gate or cascade, we need to break it down into "quantum primitives" (unitary transformations). For instance, we can break down a 3-input Toffoli gate like so:



Of course, it is not immediately obvious why this construction gives us a Toffoli gate. Note that the $\sqrt{\text{NOT}}$ gates (and their Hermitian friend) do not get activated unless their control lines are 1.

So, if we pass $a = 0$ and $b = 0$ through our gate, c remains unchanged, as do a and b. If $a = 0$ and $b = 1$, then the gate that gets applied to c will be $V_0 * V^+ = I$, which is the identity, so c will be unchanged. If $a = 1$ and $b = 0$, then the gate that gets applied to c will be $V_1 * V^+ = I$, so c will be unchanged, and finally, if $a = 1$ and $b = 1$, c will be inverted because the gate that gets applied will be $V_0 * V_1 = \text{NOT}$. And thus, we have shown that a 3-input Toffoli gate may be simulated by at least five quantum primitives, and so it has a quantum cost of 5. This result is due to DiVincenzo and Smolin [1994].

2.4 ESOP Cube-list Representations

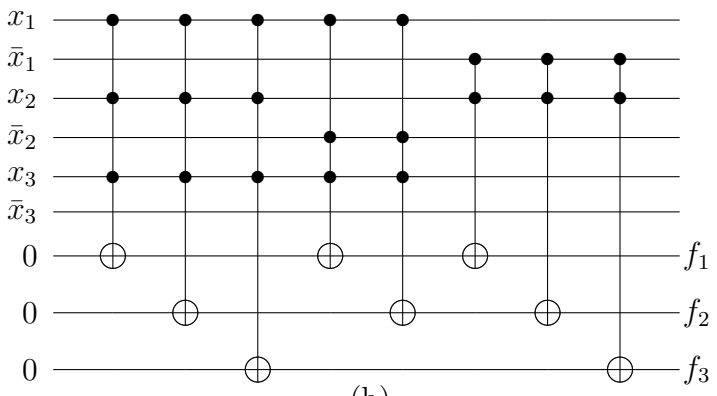
Any boolean function can be represented by an exclusive-or sum-of-products (ESOP) expression.This is particularly useful for reversible logic synthesis since there are existing algorithms for converting any ESOP expression into a cascade of reversible toffoli gates, thus generating a reversible circuit to implement your original function.

In reversible circuit design ESOP expressions are often written as a cube-list. A cube list is an $n \times m$ matrix with m, the number of product terms in the ESOP expression, and $n = i + j$ where i is the number of input variables and j is the number output variables. Each of the m rows in the matrix are the individual cubes that make up the cube list and represent one of the products from the ESOP expression.

Each cube in the list takes the general form: $x_1x_2...x_if_1f_2...f_j$, where each of the elements $x_1..x_i$ represent an input variables and each element $f_1..f_j$ represents an output variable. For each cube in the cube list a 1 is written in cube position x_k , $k \in \{1, 2, ..., i\}$ if the variable x_k is in the ESOP product for that row, a 0 is written if the negation $\bar{x}_k$ is present, and a '$-$' nis written if x_k is not present in that product term for that cube. For each element, f_p, $p \in 1, 2, ...j$, a 1 is written if that output variable contains the product represented by the input portion of the list and a 0 otherwise. See figure *draw figure 1* for an example.

x_1	x_2	x_3	f_1	f_2	f_3
1	1	1	1	1	1
1	0	1	1	1	0
0	1	–	1	1	1

(a)



(b)

Figure 1: A (a) the cube-list and (b) resulting circuit.

Given an ESOP represented as a cube list in this way Fazel et al. [2007] proposed a method of reversible logic synthesis that implements the function as a reversible circuit using only Toffoli gates. In this method an empty cascade with $2i + j$ lines is created. Two input lines are given for every input variable where one line corresponds to the variable x_k, the 2^{nd} line corresponds to its negation, $\bar{x}_k$, and the remaining j lines correspond to the output variables. For every output line f_p, a Toffoli gate is placed with its target on line f_p and a control for that target is placed on the input line x_k if there was a 1 in the cube for the corresponding variable, or on the negation line of x_k if there was a 0 in the cube for x_k, see figure (draw figure 2). This method allows a cube-list to be quickly and efficiently transformed into a reversible cascade and allows for the synthesis of rather large functions.

2.5 ESOP Cube-list Ordering Rules

Modifications to the above method with the use of inverters instead of a negation line, careful ordering of cubes to reduce the number of not gates and and sharing cubes between output lines have both reduced the number of lines and the number of gates required to implement these circuits see *[To add citations for these papers]*. In Nayeem and Rice [2011] a number of rules were proposed that manipulate the cube-list representation to create a new cube-list with the same output as the first one, depending on the rule and the state of the cube that the rule is being applied to these rules may increase or decrease the number of cubes in the list.

[To add brief description of ordering rules as these are to be used in our mutation function ...]

2.6 Genetic Algorithm

The Genetic Algorithm is a search heuristic that was introduced and investigated by John Holland (1975) and his students (DeJong, 1975). The algorithm attempts to mimic the

evolutionary process of natural selection (Mitchell, 1996) by modelling the concepts of individuals in a population, fitness and selection, crossover, and mutation that are found in the biological reproduction of organismsMitchell [1996].

The basic idea is that over a number of generations an individual that is the solution to a problem can evolve out of the latest generation of the individuals in the population. While there are a many variations on this theme, the basic algorithm is as follows:

1. Generate an initial population of 'individuals' that represent potential solutions to the problem.
2. Evaluate each individual's Fitness
3. Until a solution is found or a maximum number of generations have passed, repeat the following:
   (a) Select individuals to reproduce.
   (b) Apply crossover
   (c) Apply mutation
   (d) Evaluate each individual's fitness.

2.6.1 Representation

Representation of the individuals in a population is critical to the successful application of this algorithm and is perhaps the most challenging aspect of implementing it. Since the model is based on biology, each individual is often represented as some type of string which the mutation and crossover functions can be applied to.

2.6.2 Fitness and Selection

The fitness function allows us to measure how close the solution represented but any specific individual is to the desired output solution. Each individual is evaluated and ranked according to its fitness, and then according to the selection criteria some are chosen for crossover and mutation

2.6.3 Crossover

Crossover tries to model the process of sexual reproduction in nature. after parent individuals are selected from the population of the previous generation, the 'genes' of these individuals are combined to make one or more child individuals (go to listed example)

2.6.4 Mutation

The mutation operation models mutation of the genes in organisms. For selected individuals individual 'genes' are randomly changed in some way (whether through addition, deletion, or swapping with another type of 'gene' (add example)

2.6.5 Parameter Variations

2.6.6 Previous Applications of the Genetic Algorithm to Reversible Logic Synthesis

2.7 Old GA material

2.7.1 String Representation and Fitness Function

String representation and fitness functions are the two critical components of the GA. For better understanding let's take an example of biological chromosomes. We can represent chromosomes as binary bit strings, where each gene is made up of a certain number of 0's or 1's. For example, we represent a chromosome of 6 genes, where each gene has 4 binary bits. 0001 1100 1001 1010 0110 0000 So far, that just looks like a bunch of zeros and ones, doesn't it? Which doesn't make a lot of sense, for this is where encoding comes in. We use encoding to represent information in the form of an arrangement of binary bits. For example, 0001 may represent the number 1, 0010 may represent the number 2 and 1010 may represent the '+' addition operator and so on. If we come up with a sensible encoding pattern, then our chromosomes will end up meaning something useful. So it is vital that we choose appropriate representation method and encoding pattern for our problem solution to ensure accuracy and quality of the result.

The fitness function allows us to rate how close an individual from the population is to the ideal solution. We use this function just before the crossover stage, so we can chose the two most suitable individuals to split and swap genes with.

2.7.2 Selection, Crossover and Mutation

As we mentioned earlier that the fitness function helps us chose the two fittest individuals in the population, however it's not recommended to simply search through the population and pick the two fittest members. Instead, we use probability. We assign a higher probability of an individual being selected, proportional to that individual's fitness. So essentially, if an individual is fitter according to our fitness function, then it has a higher chance of being chosen. By doing this, less fit individuals still have a chance of crossing over their genetic material, albeit less likely.

Crossover stage is similar to reproduction in nature. We combine genes from two individuals in the population to make 1 or more new individuals (children). We pick two individuals with highest fitness value from the population, split them at random generated point (depend on problem at hand), swap the fragments with each other and create the new generations. Consider following two binary strings, A: 1010 1100 0001 1000 1111 0000 and B: 1011 0011 1010 1111 0000 1110. Now using randomly chosen crossover point, we would get following crossover.

A: 1010 1100 0001 X 1000 1111 0000
B: 1011 0011 1010 X 1111 0000 1110

Swapping fragments with A and B would produce two offspring AB and BA.

AB: 1010 1100 0001 1111 0000 1110
BA: 1011 0011 1010 1000 1111 0000

After crossover stage, we can apply the mutation. This operation can be optional. Certain times we can get the desire solution by just using crossover but often times mutation is used to provide some variation in population. Typically mutation rate is applied with less than 1

Once the process of selection, crossover and mutation is complete, we can evaluate the fitness of new population. We repeat this process until our desire solution is found or simply we have reached the termination limit – that could be certain amount of generation has passed or computing power has reached.

Pseudo code for Genetic Algorithm

Choose initial population
Evaluate each individual's fitness
Repeat until solution is found or enough generation has passed
    Select best-ranking individuals according to it's fitness to reproduce
    Apply crossover
    Apply mutation
    Evaluate each individual's fitness

2.8 Parallelization

Parallelization is an approach to computational problem solving where the computation is divided into smaller subproblems and each sub-problem is computed simultaneously. The results of each sub-problem are then combined to get the final result of the whole computation.

The process of parallelizing a computation can be taken at different levels, from the bit level on a single machine to distributed computing over multiple machines (such as cluster or grid computing).

multiple threading and processes A common approach is to split a computation into into multiple threads or processes where it can be concurrently worked on by different processors on the same cpu (references)

Grid Computing add basic definition: which is each node is generally loosely coupled, generally heterogeneous.

3 Our Approach

This section will detail our approach to the genetic algorithm, including the planned use of the cube reordering rules in our mutation function and a general description of our sofware and the hardware it runs on

3.1 Revsim: Reversible Logic Simulator

3.1.1 Overview

Representing reversible circuits in a way that we could both easily simulate them and process them through a genetic algorithm was one of the first challenges we faced. There have been a number of reversible approaches to circuit synthesis using the genetic algorithm *(*references lukac, etc) but after conducting a preliminary review, none of them offered the flexibility and extensibility that we were seeking. We set out to develop a software suite that could would allow us to simulate any number of reversible circuits and let us manipulate those circuits at the gate level. We will provide a brief overview and description of the development of our software below.

3.1.2 Explanation of Simulator Design

We first developed an initial version of our circuit simulator using a functional but once we had conducted some initial experimentation and testing we decided to refactor our code using an object oriented approach.

Fig (7.1) shows the basic class structure of our software. Conceptually a gate has a number of input lines, output lines, controls and targets. The abstract Gate class formalizes this basic representation of a gate and is subclassed to create the various types of gates and their implementations.

As you can see from Fig (7.2) There are three main types of gates that we have represented in our simulator: Single Target gates, such as the the Toffoli, Multiple Target gates, like the Fredkin or Swap, and Same Target gates such as the inverter where the target and the control are on the same line.

The Cascade class is used to represent a reversible cascade of gates. It provides the primary functionality for modelling and modifying our reversible circuits, and is used other classes such as the Truth Table and Genetic Algorithm classes as described below.

The Truth Table class allows us to generate the truth tables of our reversible cascade and compare all or part of the truth table from one circuit with another. Since we have to propagate values across each gate in the cascade to generate the output values and need to generate all 2^n entries in the truth table, the process of generating the truth table is linear in the number of gates of the circuit is exponential in the number of variables

Our simulation software also has a number of classes that provide additional extensibility. For example there are input/output classes that allow us to directly read from and write to files in the revlib.org's .real file format. Our initial GA implementation required us to manually enter each goal cascade that we wanted to test against, but using these helper

classes we were able to implement the ability to parse any .real file and use its target output function in the fitness calculations for our Genetic Algorithm. (more below) We also developed an experimental Shared Cube class that allows us to generate and use the shared cube representation that we were initially going to use to represent individuals in our genetic algorithm so that we could apply a number of the rule based transformations from (ref: jackies paper on rule transformations) but after implementing it we decided on using the representation described below.

3.1.3 Description of Our Genetic Algorithm

Representation. We initially explored using a Shared Cubes representation for the individuals in used in our algorithm however while we initially thought that the transformational rules in [reference] would be useful in implementing mutation we found the difficult to implement in the context of our genetic algorithm and we not able to discover an appropriate method of implementing crossover using the shared cube representation. Instead we settled on using the cascade representation from our Cascade class which stores the list of gates used in the circuit for the individuals in our populations.

Our Algorithm initially reads in a circuit that specifies the desired output behaviour and then creates the initial population as copies of the initial circuit that have been mutated from the initial circuit up to a maximum number of mutations specified in the initial conditions.once the initial population is generated, the cycle of fitness evaluations, selection mutation and crossover repeat until one of two terminal conditions are reached, either a fitness of 1.0 or a maximum number of generations.

Fitness and Selection. Our fitness metric was a weighted measure of how closely the truth table of the current individual matched the truth table of the of the desired output behaviour. It basically performs an exhaustive comparison and so the number of comparisons needed are approximately exponential in the number of variables (linewidth) of the circuit.

Crossover. Our implementation of crossover selects the best two individuals as parents and creates two child individuals. The first child has the first half of the gates from parent 1 and the second half from parent 2 while the second child has the first half of the gates from parent 2 and the second half from parent 1, The children are then added to the population for the next iteration of the algorithm.

Mutation. The mutation function randomly selects a certain number of gates and will either replace or remove them from the cascade of the individuals it it being applied to.

Parameter Variations. Our initial parameters

3.1.4 Parallelization

We found that with larger circuits processing time became significantly longer so we looked at a few ways to parallelize our simulations in order to gather a larger dataset of results in a shorter period of time.

Grid Computing. We first spent some time adapting our software so that we could run it across the university of Lethbridge's HTcondor computing grid. Because we needed to test a number of circuits across a set of variable initial parameters one of the key challenges we faced was automating the task of creating the HTcondor job submissions. We were able to script a solution that allows us to automatically take a batch of any number reversible circuits in .real format and output a set of submission-ready executables that we could run across the HTcondor grid. This provided a significant increase in the speed we were able to generate tests and obtain results.

Parallelization of large circuits. Even using condor we still faced the problem that that the processing time for runs of our genetic algorithm with large circuits was significantly longer. In order to mitigate this we began experimenting with spitting the processing of each individual circuit into multiple processes that we can run concurrently on each of the processors of the machine running the job. Preliminary tests have been promising. *DOUBLE CHECK THIS STATEMENT!!! is is really promising??*

4 Experimental Results

This section will detail our results

5 Conclusion

This section will detail our conclusion

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