

CPSC 4210 - Final Paper

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Abstract

This 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 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 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:

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

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.

$$\begin{array}{c|c|c|c} a & b & a' & b' \\ \hline 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{array} \rightarrow \begin{array}{c|c} n & M(n) \\ \hline 0 & 0 \\ 1 & 1 \\ 2 & 3 \\ 3 & 2 \end{array} \rightarrow P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

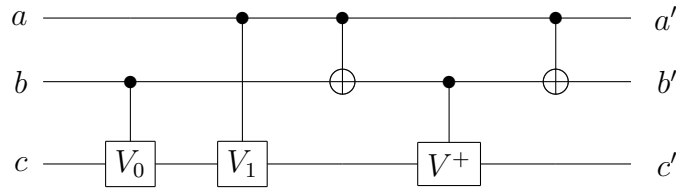
A useful property of permutation matrices is that they allow us to “compose” permutations. In order to do this, we use the following identity: $P_{\sigma \circ \pi} = P_\pi * P_\sigma$. Note that the order of the matrix multiplication matters, as matrices do not typically commute under multiplication. 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”.

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].

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 , $k \in \{1, 2, \dots, i\}$ 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 '-' is written if x_k is not present in that product term for that cube. For each element, f_p , $p \in 1, 2, \dots, j$, 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.

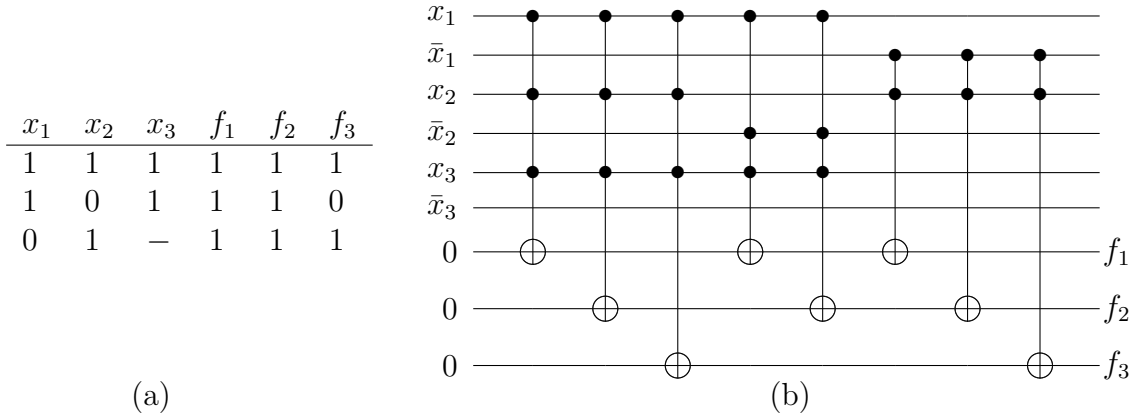


Figure 1: A (a) the cube-list and (b) resulting circuit.

Given an ESOP represented as a cube list in this way [To add citation: Fazel et al.] 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.

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 *[to add citation for (nayeem/rice - ordering techniques)]* 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 ...]

Genetic Algorithm

Genetic Algorithm refers to a model introduced and investigated by John Holland (1975) and by students of Holland (DeJong, 1975). It is a search heuristic that mimics the process of natural evolution [To add citation Book: *An Introduction to Genetic Algorithms*, Mitchell, Melanie (1996)]. It works by simulating nature's behavior of 'survival of the fittest' to evolve towards a solution. The process of finding solution using GA is based on natural selection, crossover and mutation. So basically, GA selects a population of strings, which encodes the possible solution, combines them with crossover and mutation based on a fitness function to produce individuals that are more fit and closer to the solution.

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 choose the two most suitable individuals to split and swap genes with.

Selection, Crossover and Mutation

As we mentioned earlier that the fitness function helps us choose 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

6 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 software and the hardware it runs on

7 Experimental Results

This section will detail our results

8 Conclusion

This section will detail our conclusion

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