Evolving Quantum Circuits with Genetic Algorithms and through Exhaustive space search

Outline

- Technology
  - Constraints
- Design of new quantum primitives
- Evolutionary and Frame based Generator
- Exhaustive Search
- Results
- Future directions
- Possible projects - Homework

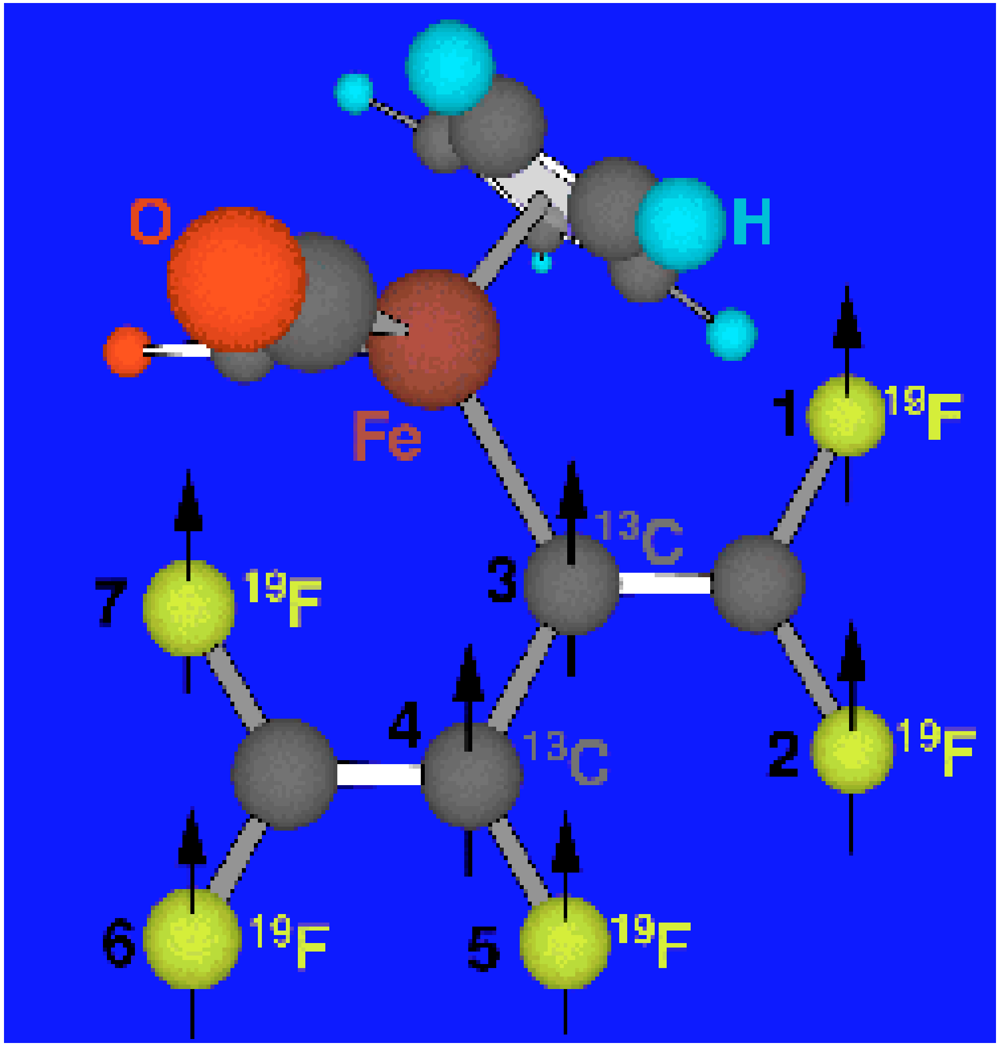
Technology for
Quantum Computing

What size of (binary) Quantum Computers can be build in year 2003?

- ***7 bits***

What size of (binary) Quantum Computers can be build in year 2003?

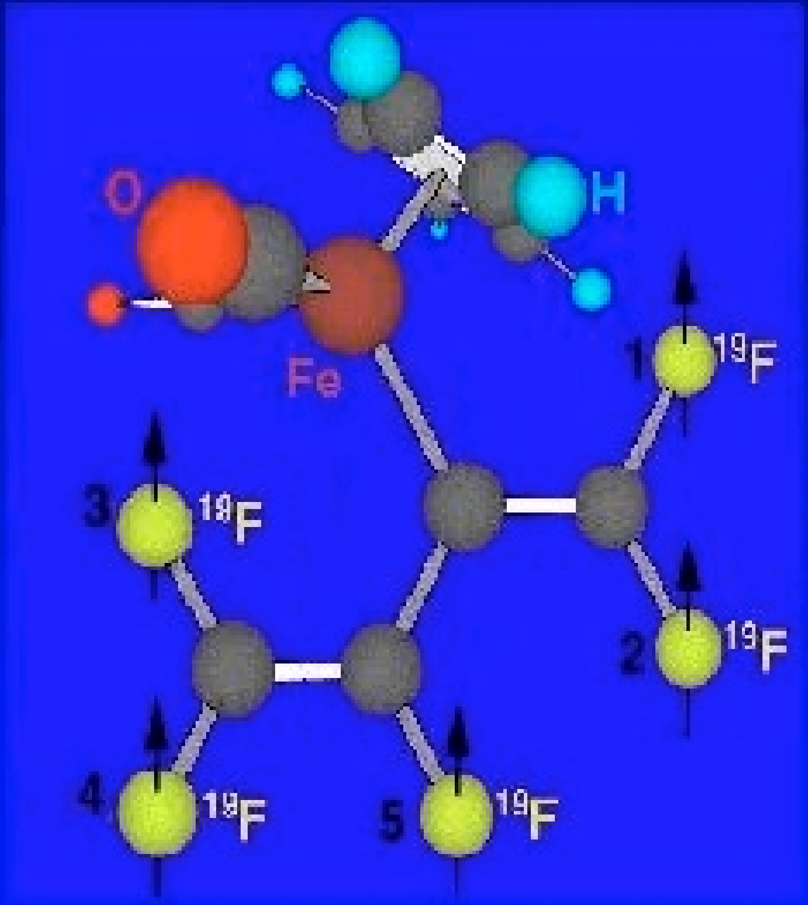
- ***7 bits***



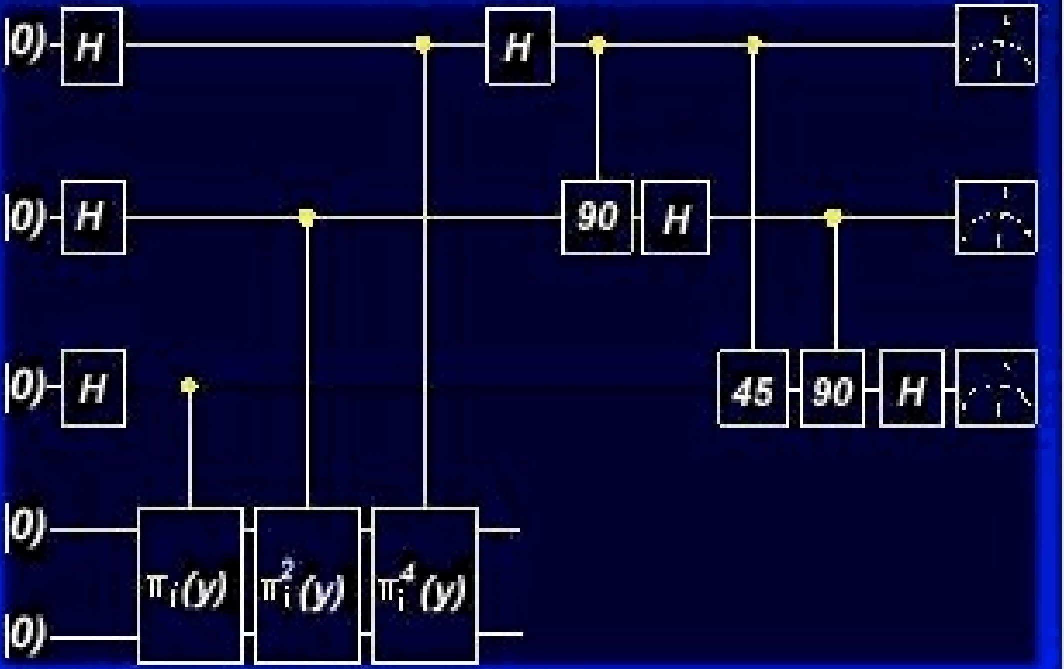
- dicarbonylcyclopentadienyl (perfluorobutadien-2-yl) iron ($C_{11}H_5F_5O_2Fe$)
- Each fluorine and 2 Carbones can be used for computation

5 qubit 215 Hz Q. Processor

(Vandersypen, Steffen, Breyta Yannoni, Cleve, and Chuang, 2000)



- The Molecule



- Quantum Circuit

T_2 > 0.3 sec ; ~ 200 gates

Source: IBM, Hot Chips Conference, 2000

Qbits, ¬ bits

- In binary quantum logic, the notation for the superposition is $\alpha|0> + \beta|1>$.
- These intermediate states cannot be distinguished, rather a ***measurement*** will yield that the qubit is in one of the basis states, |0>, or |1>.
- The ***probability*** that a measurement of a qudit yields state |0> is $|\alpha|^2$, and the probability is $|\beta|^2$ for state |1>. The **sum of these probabilites** is one. The absolute values are required, since in general, α and β are ***complex quantities.***

Quantum Circuit Synthesis is Technology dependent

Constraints based on the properties of physical implementation of quantum circuits(technology constraints, gate costs)

We would like to assume that any two quantum wires can interact, but we are limited by the **realization (layout) constraints**

Structure of atomic bonds in the molecule **determines neighborhoods** in the circuit.

This is similar to restricted routing in FPGA layout - *link between logic and layout synthesis* known from CMOS design **now appears in quantum.**

Decoherence plays an important role → minimization circuit length

Minimization of cascade's width but each bit counts **(more critical than in reversible synthesis)**

At first, we will be interested only in the so-called **"permutation circuits"** - their unitary quantum matrices are permutation matrices

One solution to layout constraint problem in quantum NMR computers is to take into account in logic synthesis phase only those gate and their placements that are ***technology-realizable***

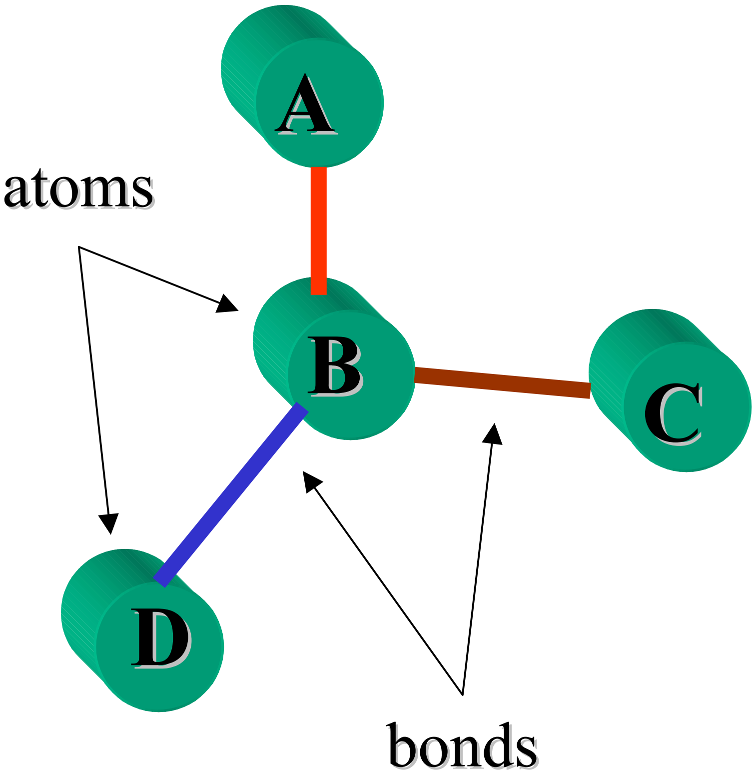
- Even if conceptually we use higher complexity gates, ultimately we have to build from 2-qubit gates.

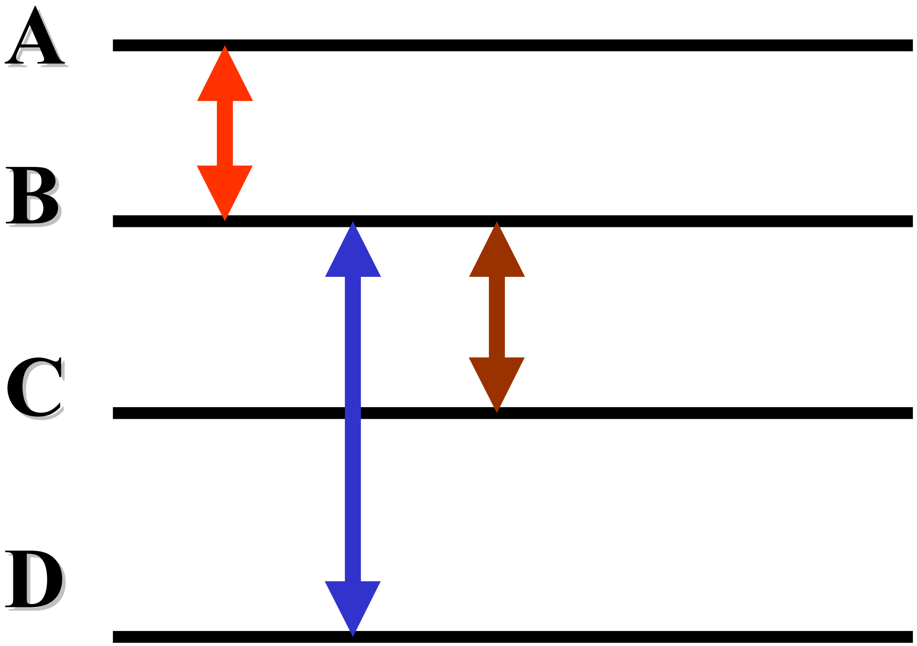
- Another possibility is to assume only primitives for the future algorithms are only 2-qubit gates then the optimal circuit will be the ***shortest***

- **Bottom line is that basic gate in quantum logic is a *2*2* (2-qubit gate).**

- **3*3 Toffoli, Fredkin, de Vos, Kerntopf, Margolus are not directly realizable as a primitive**

Molecule - Driven Layout and Logic Synthesis

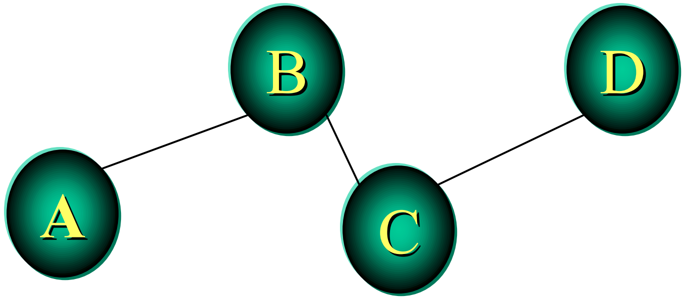


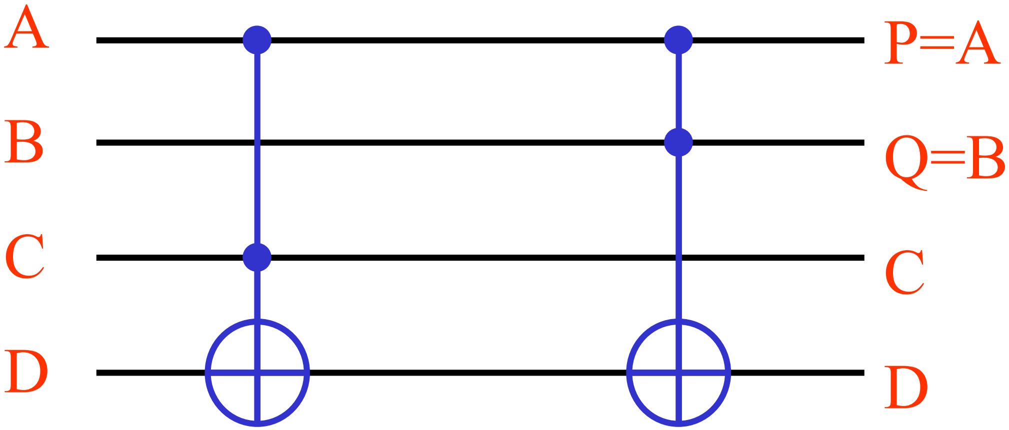


Allowed gate neighborhood for 2 q-bit gates

A schematics with two binary Toffoli gates

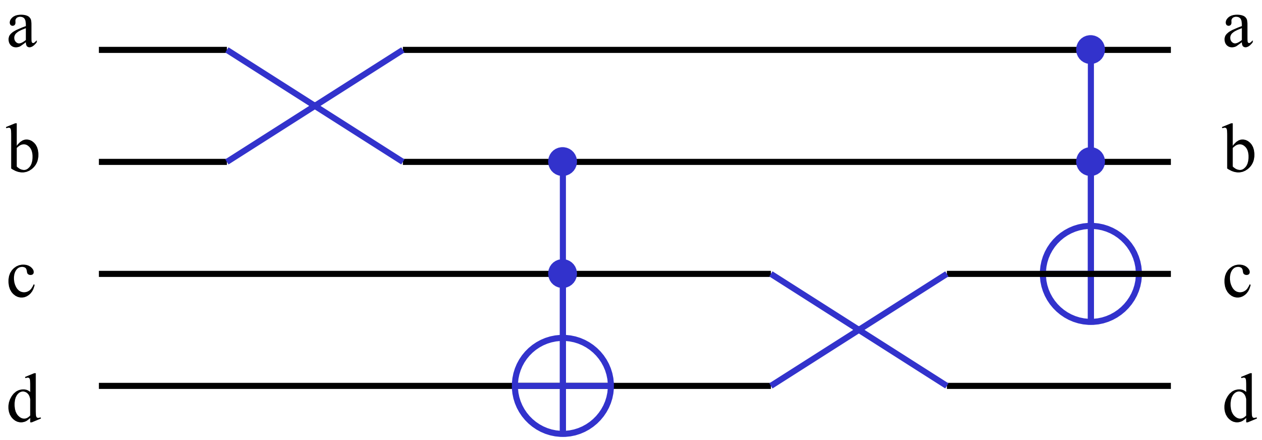
Quantum wires A and C are not neighbors

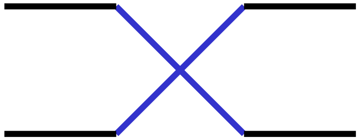




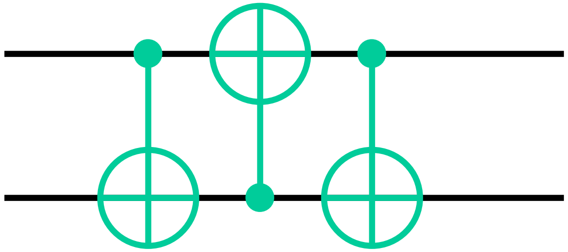
This is a result of our ESOP minimizer program, but this is not realizable in NMR for the above molecule, because there is no connection between A and C, for instance, in the molecule.

So we have to modify the schematics as follows

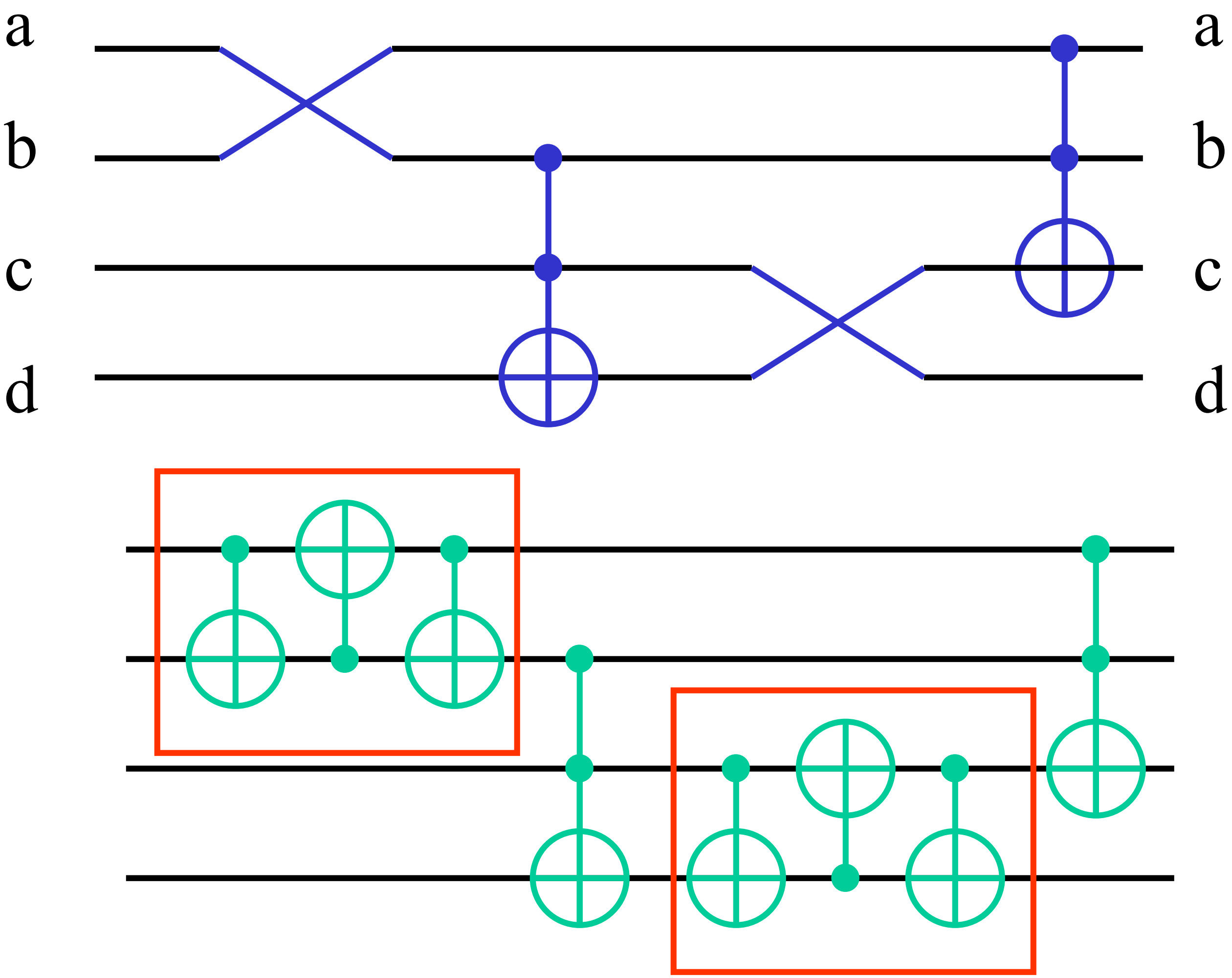




Costs 3
Feynman gates

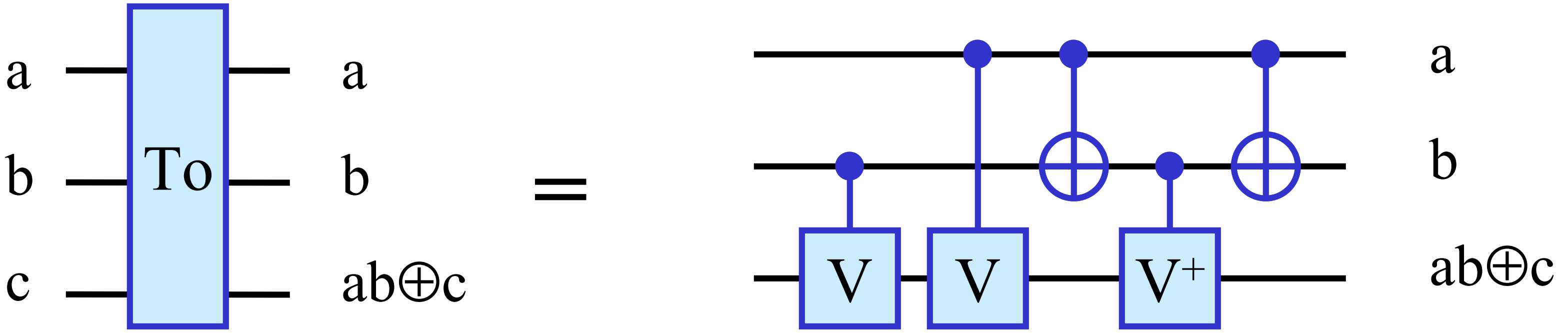


So we have to modify the schematics as follows



Design
of new (complex) quantum gates and their costs

Design a Toffoli Gate from 2-qbit quantum primitives



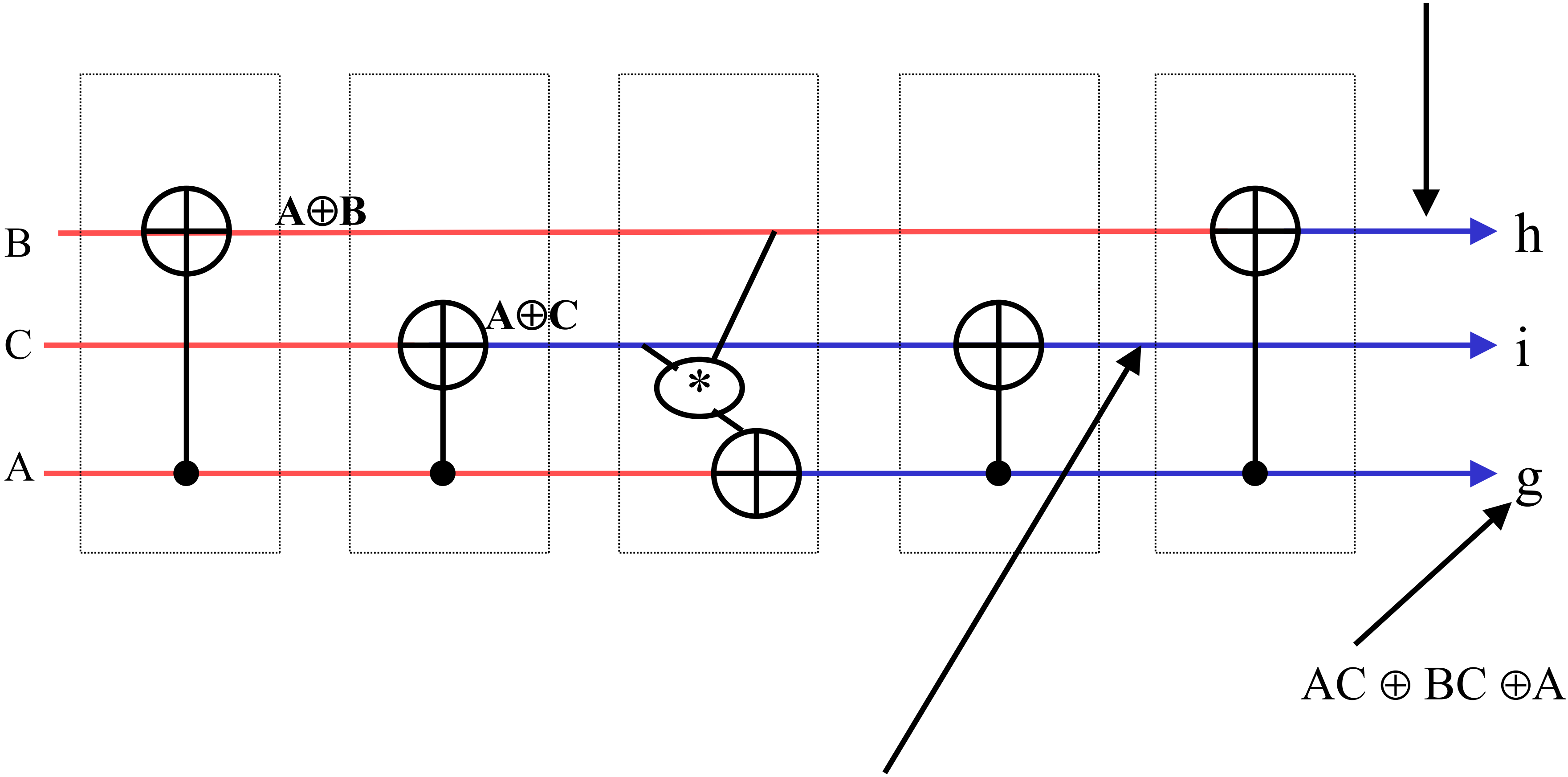
- V & V^+ are root square of NOT and its hermitian (complex) conjugate such as V*V =NOT

- $V : \dfrac{(1+i)}{2}\begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix}$

C_V: q-bit 2 unchanged
unless q-bit 1 equals
to 1

Example: Optimal Solution to Miller Function

$(AC \oplus BC \oplus AB) \oplus (A \oplus B) = AC' \oplus AB \oplus BC'$



$AC \oplus BC \oplus AC$

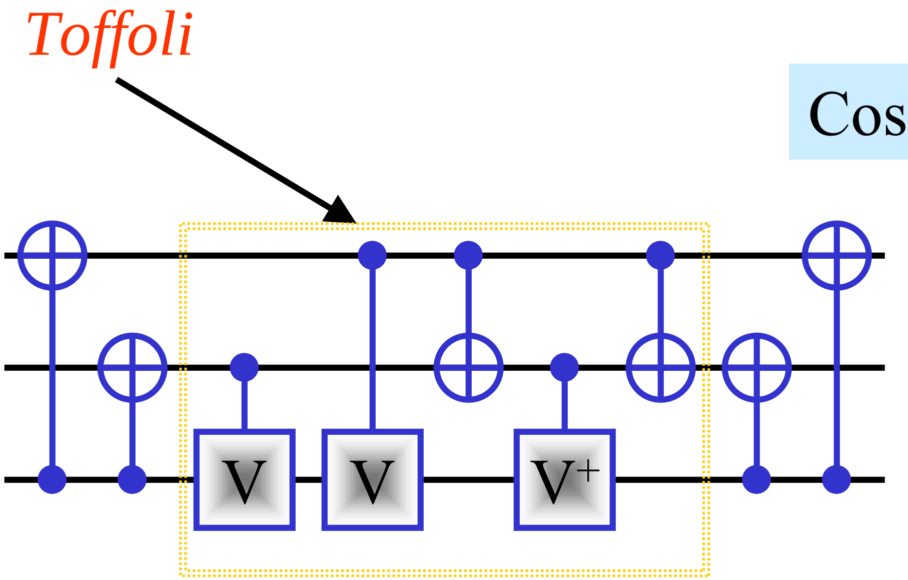
$(AC \oplus BC \oplus AB) \oplus (A \oplus C) = AC \oplus AB' \oplus B'C$

Cost = 1 Toffoli + 4 Feynman gates

Cost in Gates:

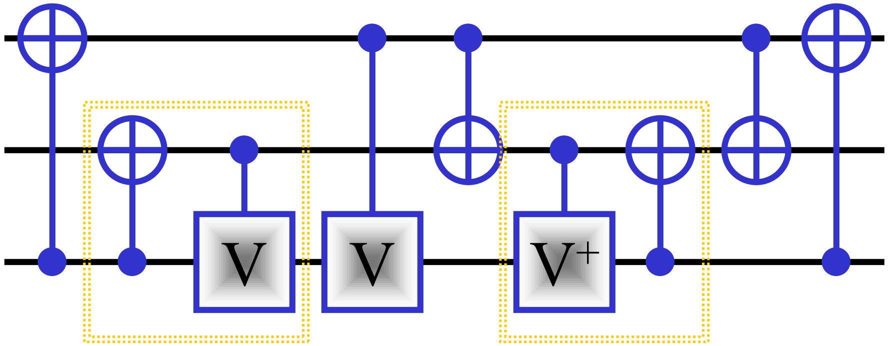
$4*1+5 = 9$

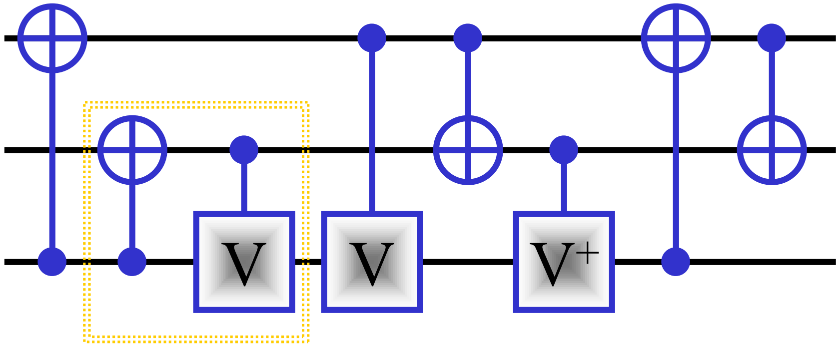
2-qubit quantum realization of Miller Gate



Cost in Gates: 9*1 = 9

Cost in Gates: 7*1 = 7



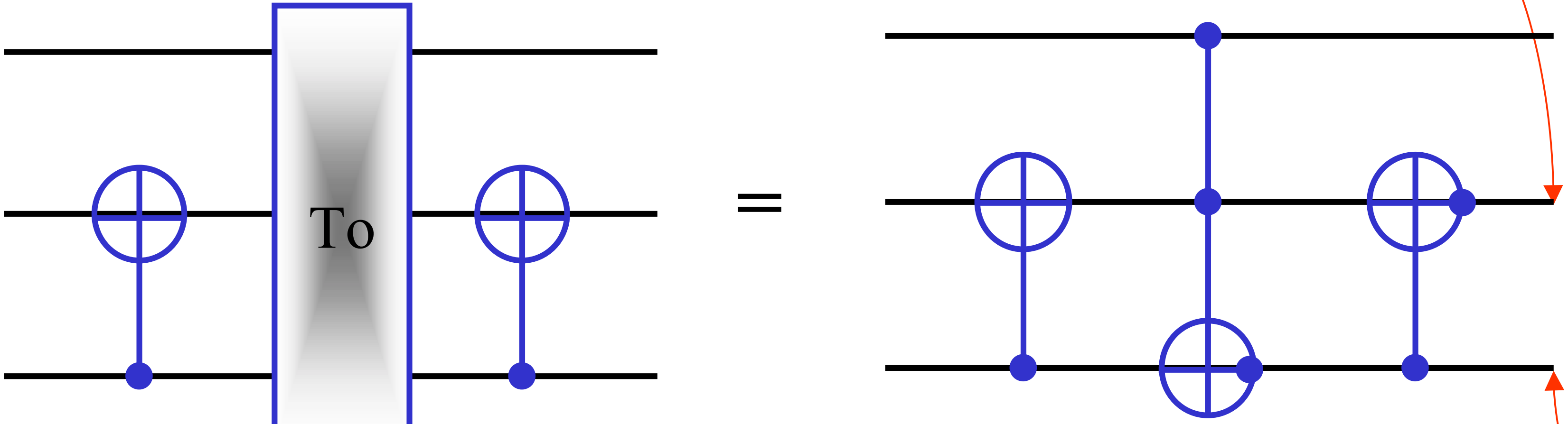


Cost in Gates: 7*1 = 7

Fredkin Gate build from Toffoli and Feynman gates

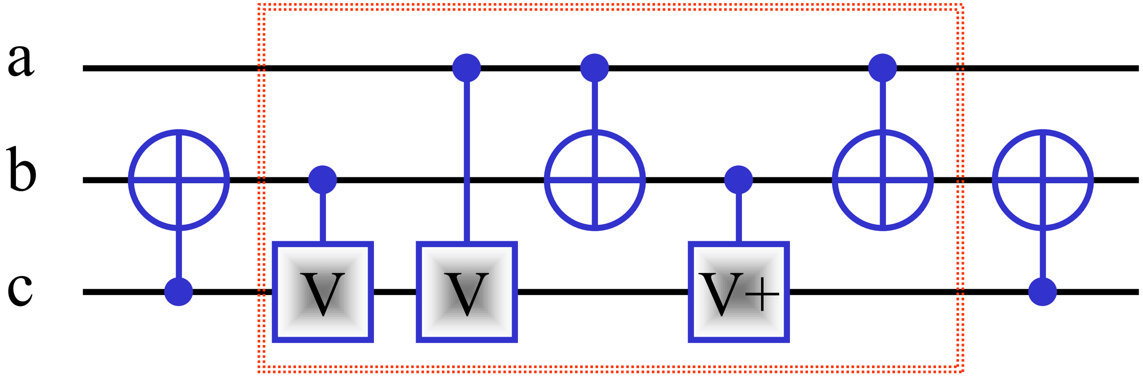
Cost in Gates: 2+5 = 7

$b \oplus c \oplus ab \oplus a'c = ac \oplus ba'$

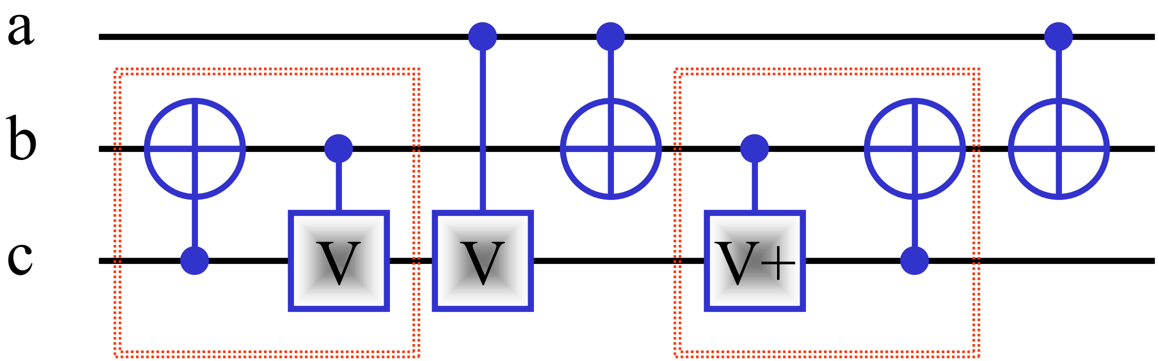


$c \oplus a(b \oplus c) = c \oplus ab \oplus ac = ca' \oplus ac$

Transforms



Cost in Gates: 7*1 = 7



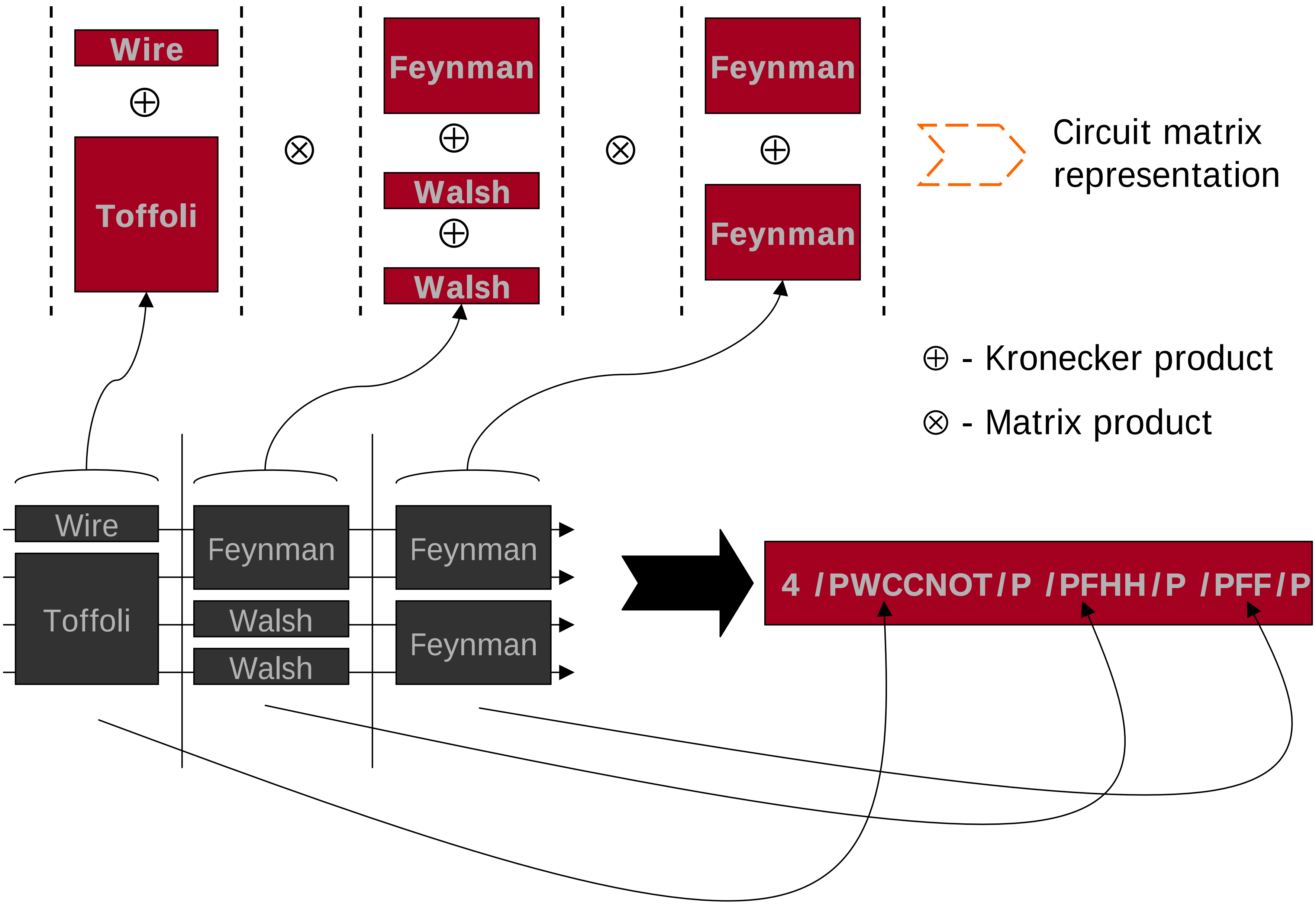
Cost in Gates: 5*1 = 5

Evolutionary and Frame-based gate generators

Genetic Algorithm

- ***A set of elements being modified according to evolutionary rules:***
  - Selection (based on the fitness function)
  - Crossing Over
  - Mutation
  - Replication
- ***These operators are made in generation steps***
- ***Process stops when the solution is found***
- ***Important in GA***
  - Encoding of the elements/individuals
    - Complex with a lot of parameters
    - Simple, task specific no parameters
  - Fitness function
    - Simple
    - Including layout specific constraints
    - Cost of gates

Circuit Encoding

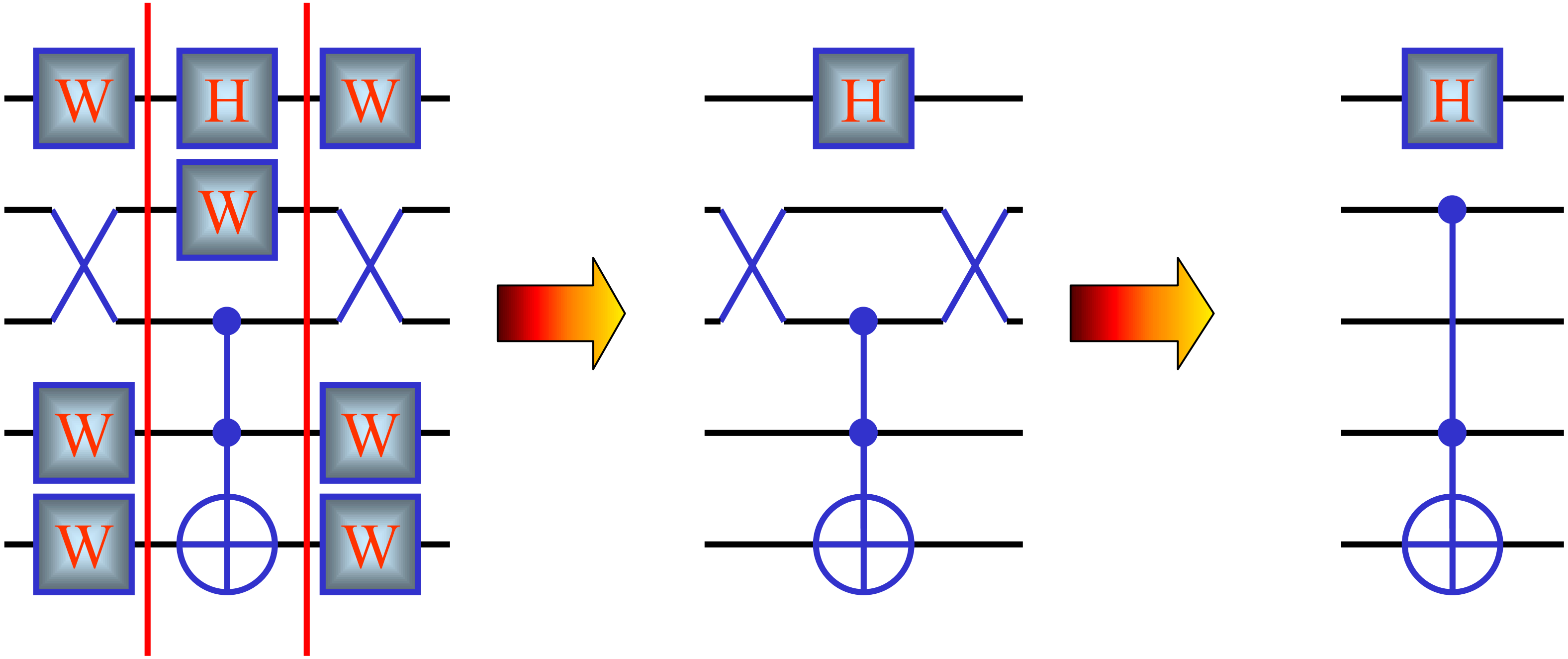


⊕ - Kronecker product

⊗ - Matrix product

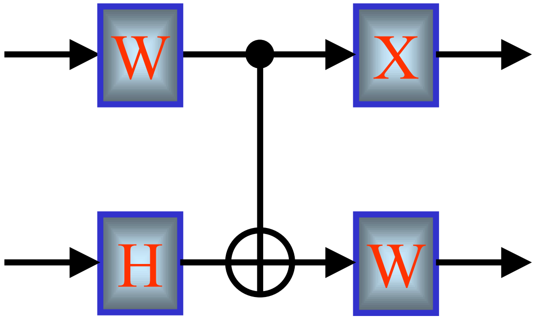
GA for quantum circuit synthesis

- Set of elements: randomly generated q-circuits encoded in string representation



5PWSWWPPHWCPPWSWWP

Example



Pauli X gate $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

Wire $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Hadamard gate $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

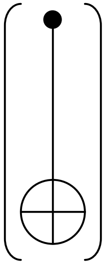
$$|0\rangle \rightarrow (|0\rangle + |1\rangle)/\sqrt{2}$$

$$|1\rangle \rightarrow (|0\rangle - |1\rangle)/\sqrt{2}$$

XOR or CNOT $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

$$|j\rangle|k\rangle \rightarrow |j\rangle|j \oplus k\rangle$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \tfrac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad \begin{pmatrix} W \\ \\ H \end{pmatrix} \Rightarrow \tfrac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \oplus \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



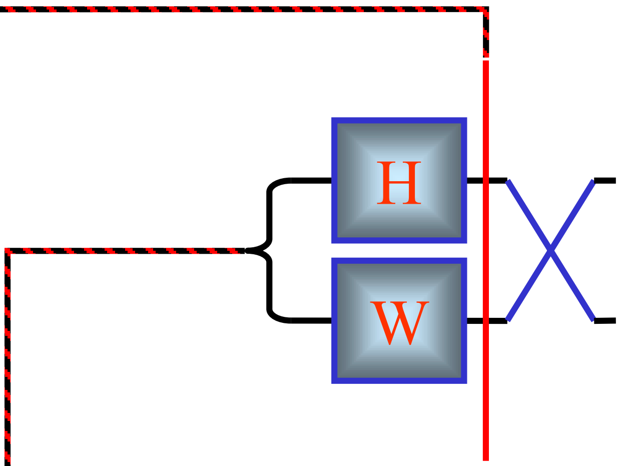
$$\Rightarrow \tfrac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \oplus \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \quad \begin{pmatrix} X \\ \\ W \end{pmatrix}$$

$$\Rightarrow \tfrac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{bmatrix}$$

Evaluation

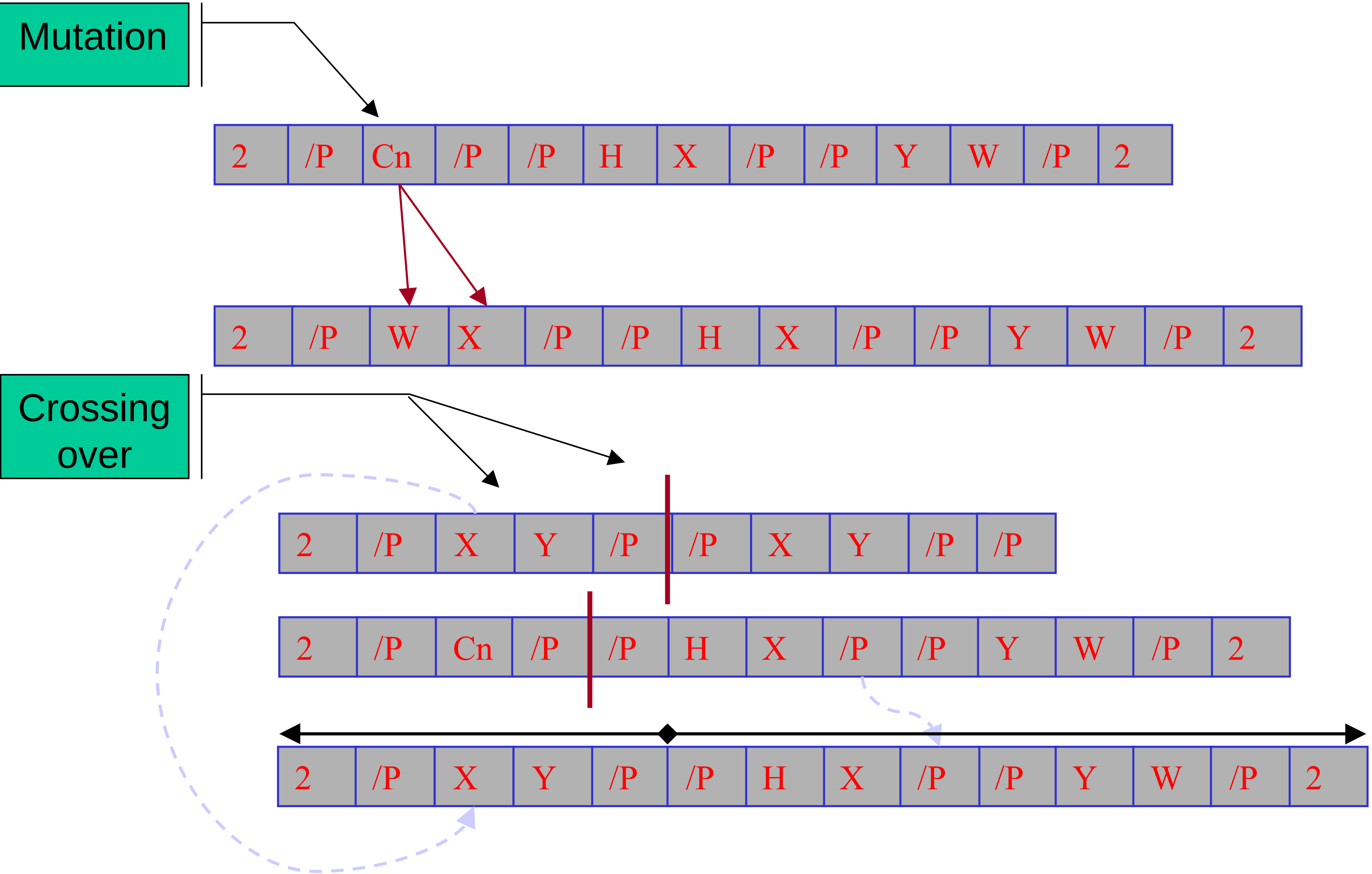
Calculation

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\\ 1 & 0 & -1 & 0\\ 0 & 1 & 0 & -1\end{bmatrix} * \begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1 & 0 & 0\\ 0 & 0 & 1 & 1\\ 1 & -1 & 0 & 0\\ 0 & 0 & 1 & -1\end{bmatrix}$$



$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix} \oplus \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & 1 & 0\\ 0 & 1 & 0 & 1\\ 1 & 0 & -1 & 0\\ 0 & 1 & 0 & -1\end{bmatrix}$$

Operations



Mutation

2 /P Cn /P /P H X /P /P Y W /P 2

2 /P W X /P /P H X /P /P Y W /P 2

Crossing over

2 /P X Y /P /P X Y /P /P

2 /P Cn /P /P H X /P /P Y W /P 2

2 /P X Y /P /P H X /P /P Y W /P 2

Overview

Mutation	Gates Blocks	Position (block/circuit)
Cross-Over*	Segments	Experimental (unitary matrices)
Reproduction	Circuits	Best gates Best Circuits

* - for circuits having only same number of I/O

GA's settings

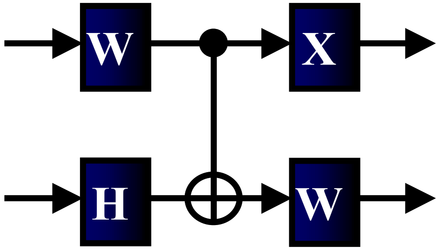
- SUS, Roulette wheel
- Fitness:

$$F_i = \frac{1}{1 + error_i} - \Lambda_i$$

$$error = \sum_{i=1}^{n} \sum_{j=1}^{2^n} \left| U_{ij} - S_{ij} \right| \quad S,U \in U(2^n)$$

Goal:

$$\tfrac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{bmatrix}$$



Fitness:

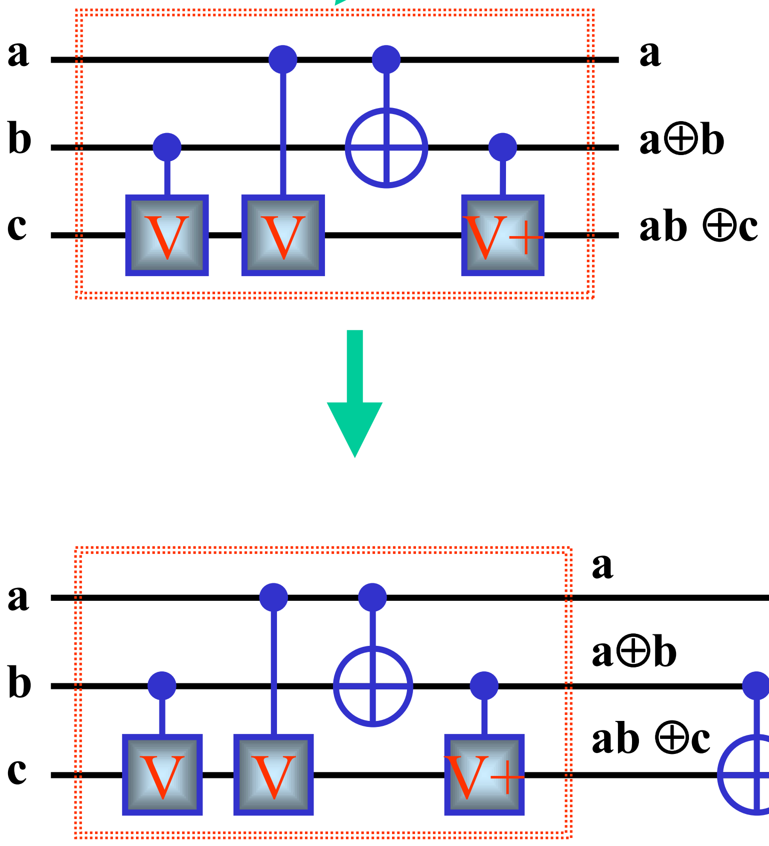
$$\tfrac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix}$$

$$\Lambda_i = 0$$

$$F_i = \frac{1}{1 + \tfrac{2}{Ni}} \approx 0.88$$

Frame-based search starting from Peres gate

- Peres gate - the cheapest 3-qubit gate



Adding Feynman gates on all possible pairs of wires on which Feynman is realizable

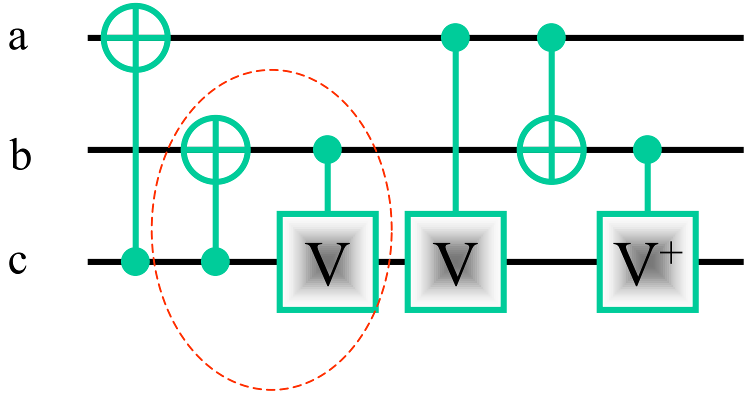
$a \oplus b \oplus ab \oplus c = (a+b) \oplus c$

$C=0 \Rightarrow (A+b)$

$C=1 \Rightarrow (a+b)' = a'b'$

Other frame search examples

a)



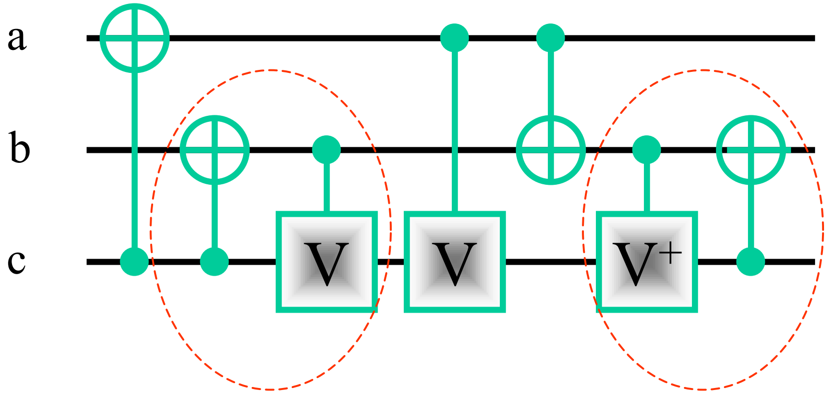
$A = a \oplus c$

$B = a \oplus b$

$C = ab \oplus ac \oplus bc$

Cost in Gates: **_5*1 = 5_**

b)



$A = a \oplus c$

$B = a'b \oplus a'c \oplus bc$

$C = ab \oplus ac \oplus bc$

Cost in Gates: **_5*1 = 5_**

Exhaustive Search

Exhaustive gate search

- Searching all gates in a very limited space of permutation 10^{15}-10^{18}
- Up to 7 segments circuits
- 3 I/O circuits
- Comparing to gates such as Toffoli, Fredkin, de Vos, Kerntopf, etc.

Exhaustive gate search

- Idea: to look for all possible equivalent gates in a certain category
- Using specified gates in different technologies
- Find the minimal possible cost of the gate

Results

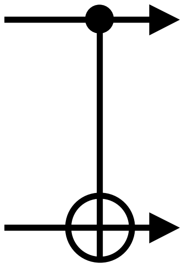
Unitary gate search examples

No starting set restriction

$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Generations: 10

Mutation rate: 0.3

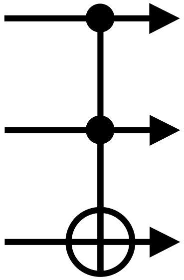


$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Generations: 20

Mutation rate: 0.3

Other gates search

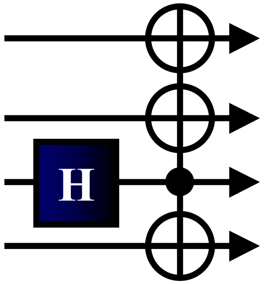


$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Generations: 100

Mutation rate: 0.4

Random circuit search

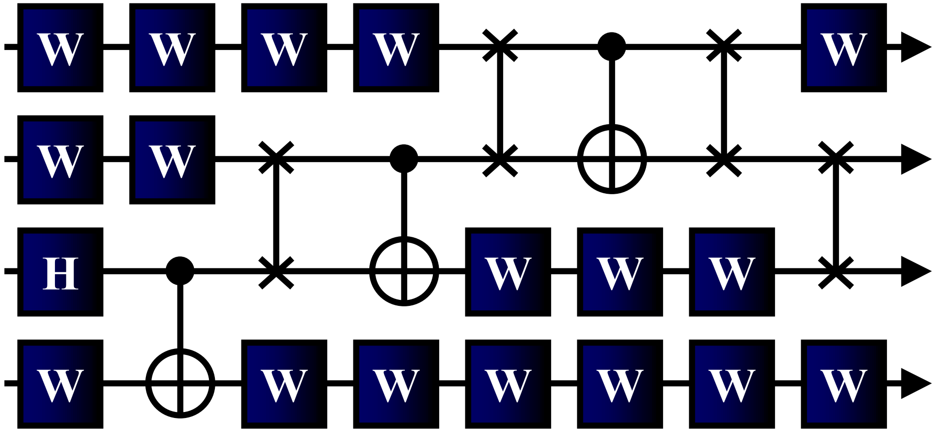


EPR producing circuit

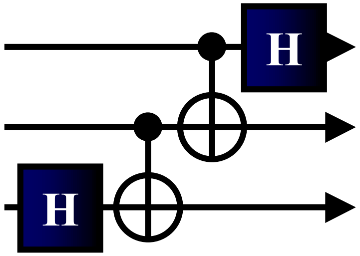
Generations: 450

Mutation: 0.3

4 /PWWHW/P /PWWF/P /PWSW/P /PWFW/P /PSWW/P /PFWW/P /PSWW/P /PWSW/P



Random circuit search

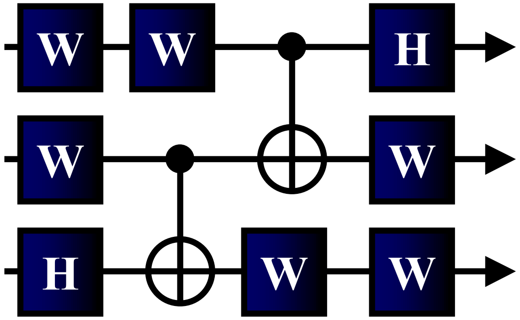


"Send" circuit

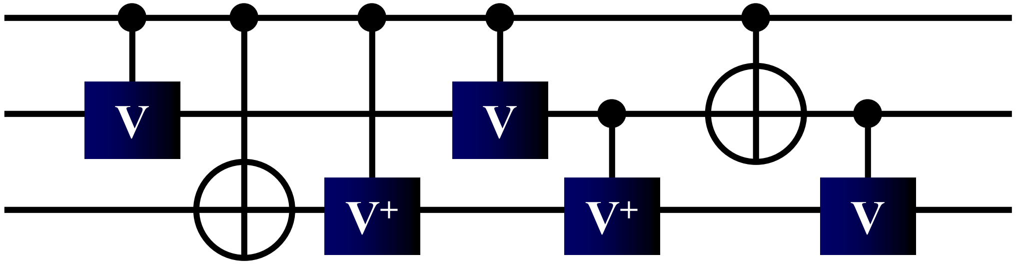
Generations: 150

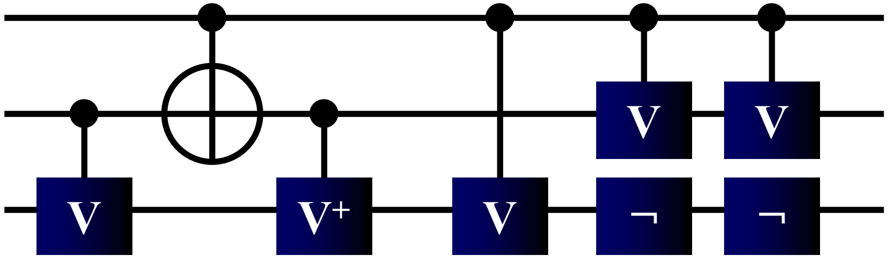
Mutation: 0.3

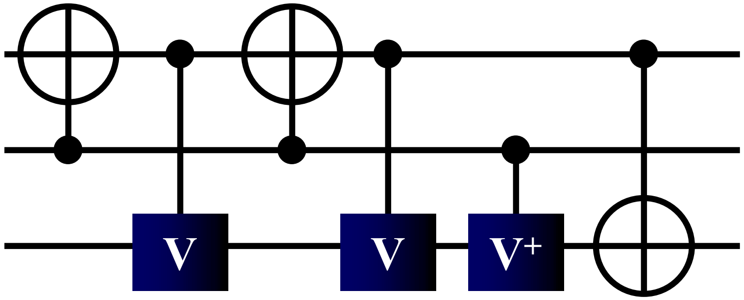
3 /PWWH/P /PWF/P /PFW/P /PHWW/P



Examples for Toffoli







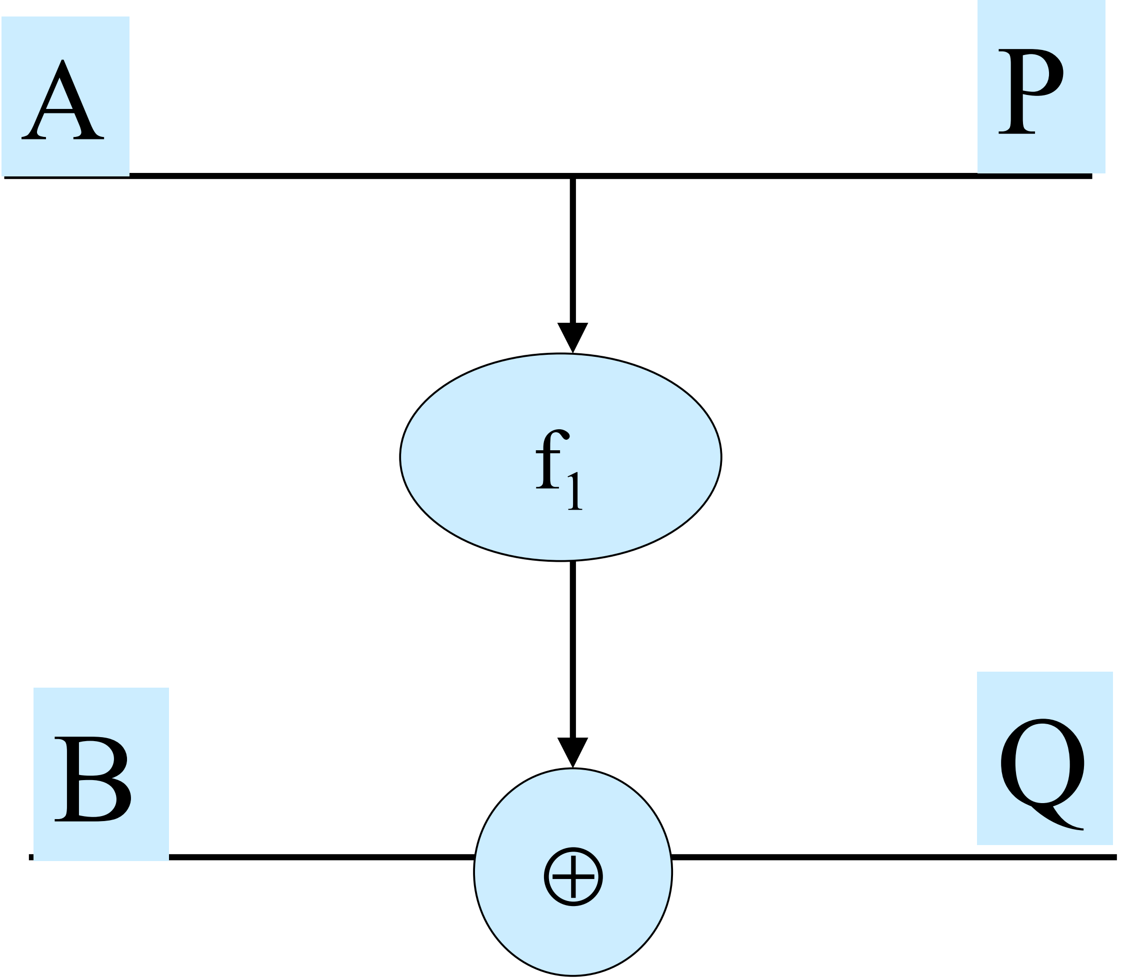
Experimental results

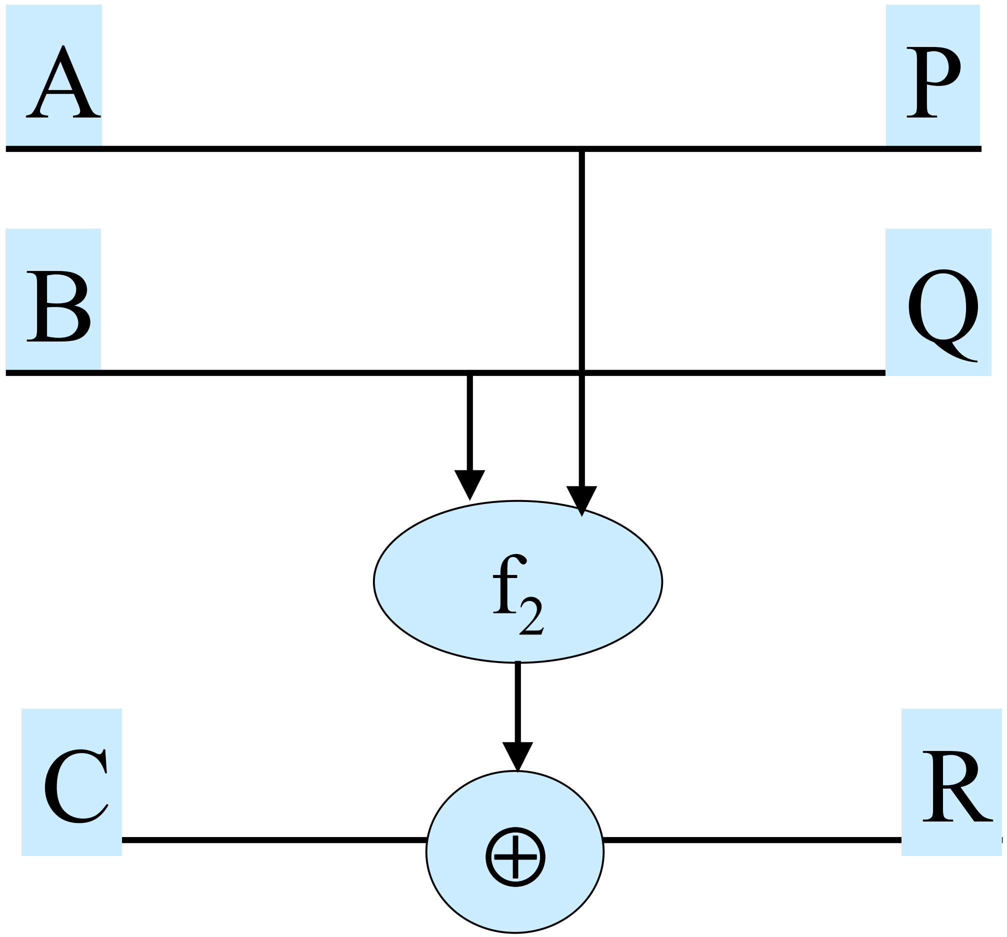
Number of inputs per q-gate	**Number of generations**	**pM**	**pC**	**Real time (average 20 runs)**	**pM<0.2 Number of generations**	**Real time (average 20 runs)**	**Population size**
1 - input	<50	0.4	0.6	< 30 seconds	<100	< 1 minute	50
2 - inputs	<50	0.6	0.4	< 30 seconds	<100	< 1 minute	50
3 - inputs	50 - 200	0.6	0.6	<1 minute	<200	< 3 minutes	60

Experimental results (cont.)

Problem searched	Solution found F1/F6	Time of search in number of generations F1/F6
Toffoli	YES/YES	<2000 / <50000
Fredkin	YES/YES	<1000 / <75000
Margolus	YES/NO	<1000 / <100000

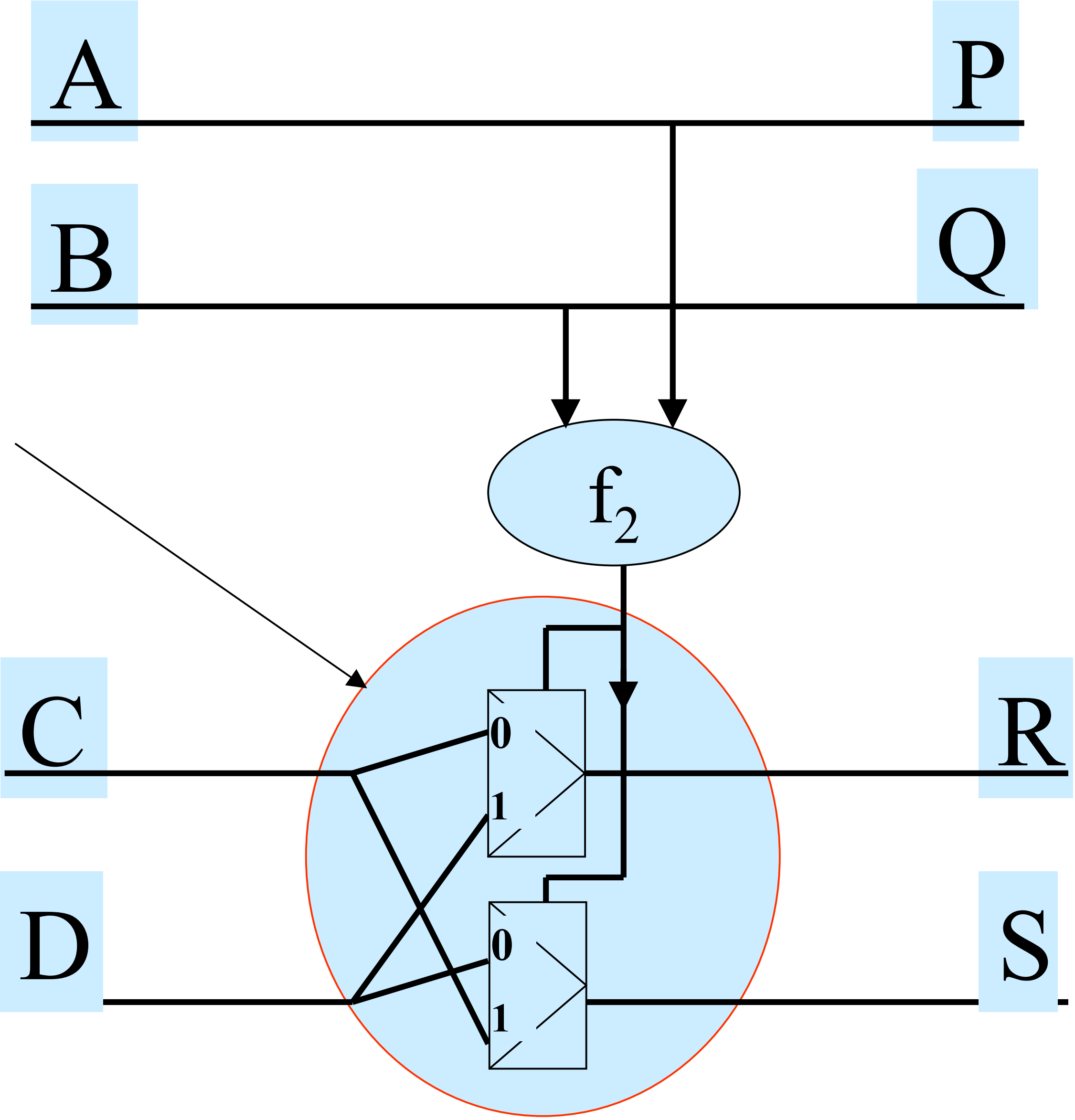
Generalized Feynman Gate



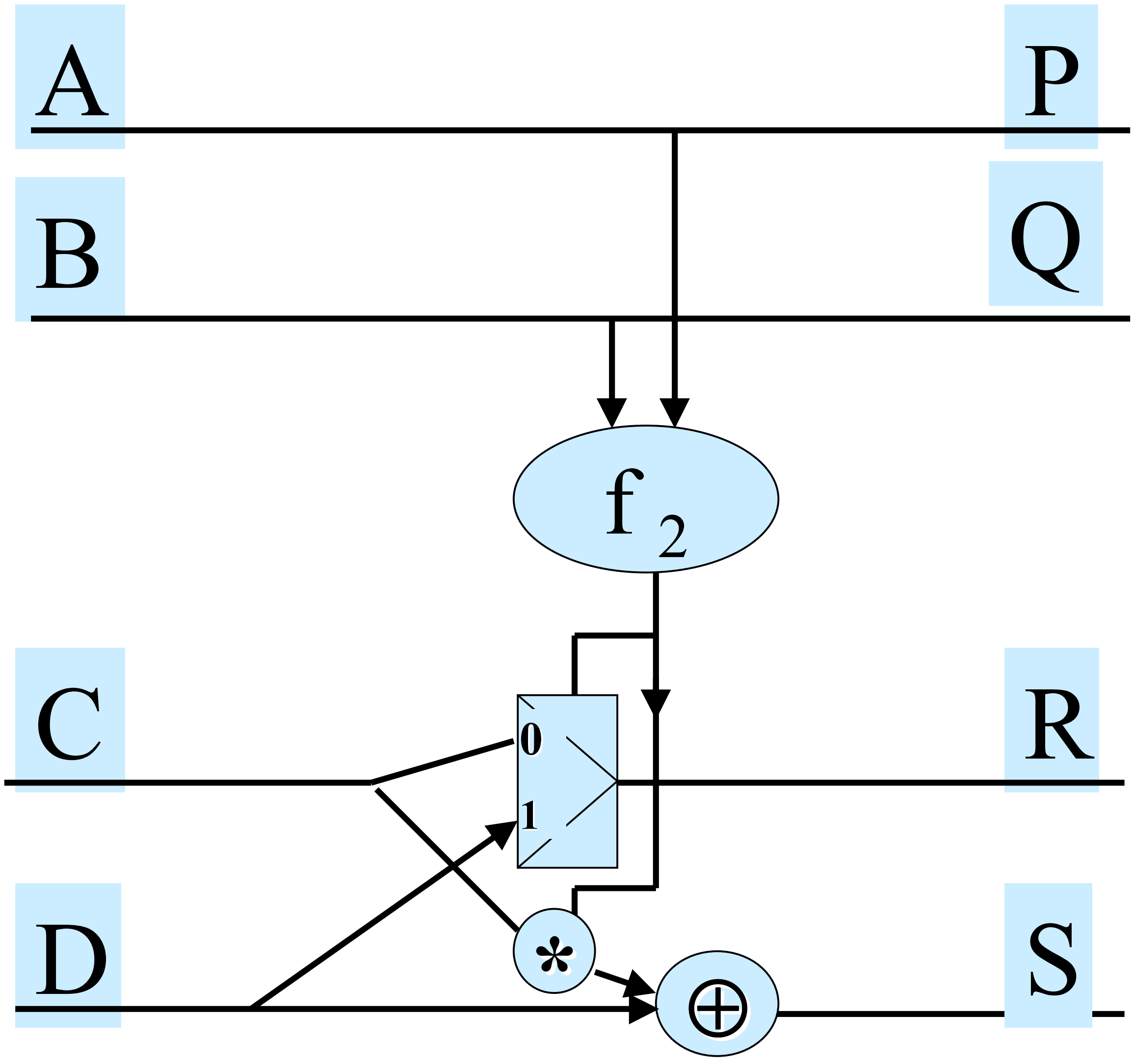


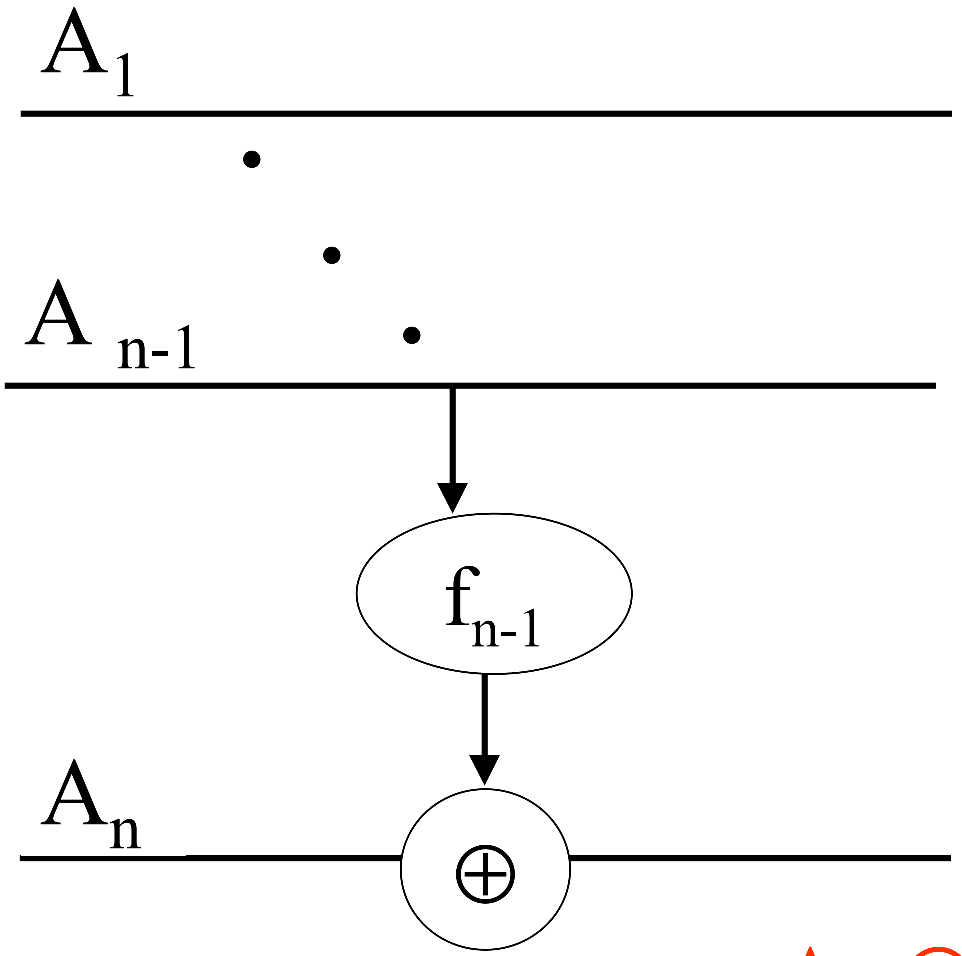
Generalized Ternary 3*3 Toffoli Gate

Generalized 4*4 Fredkin Gate



Generalized 4*4 Kerntopf Gate

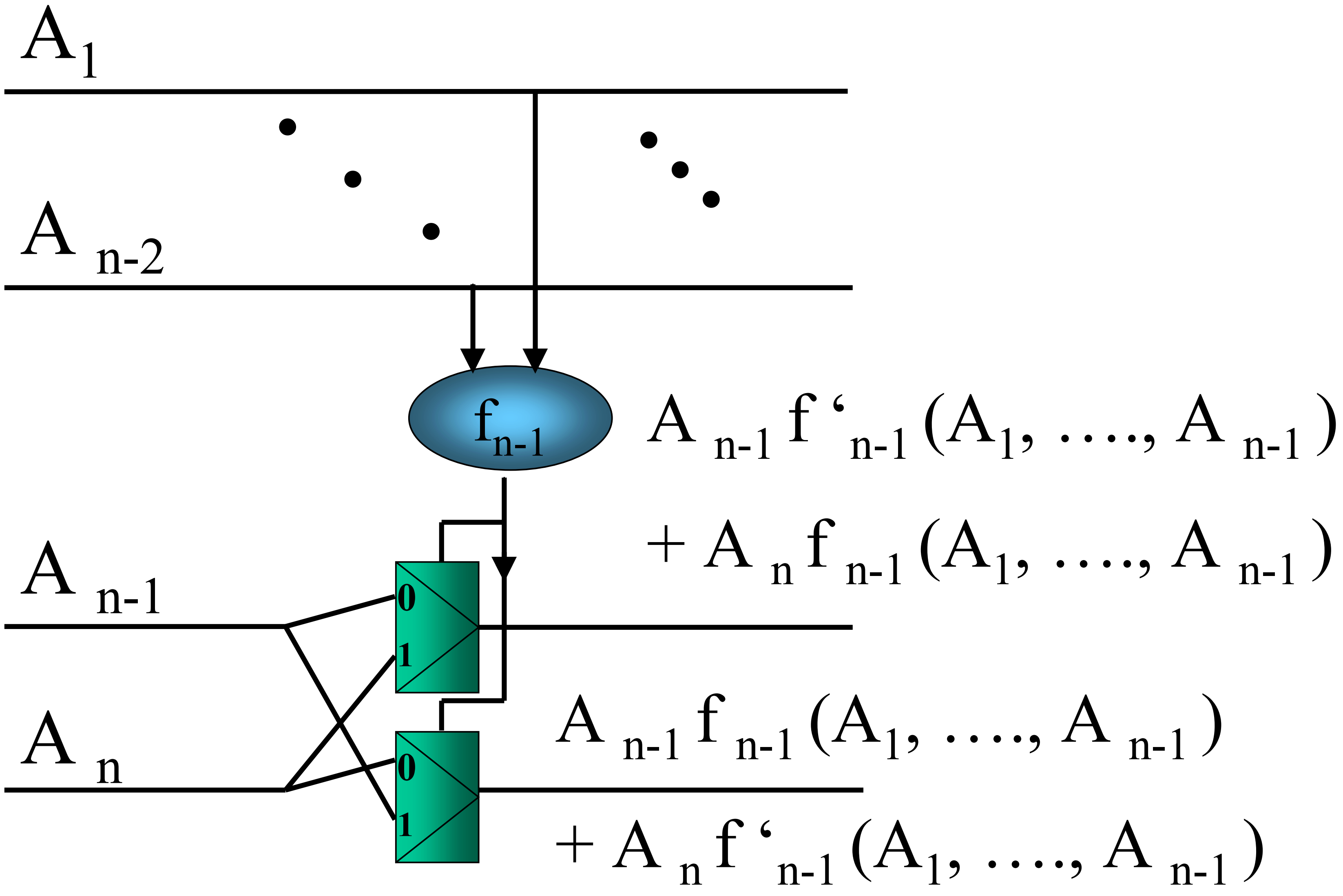




Generalized n*n Toffoli Gate

$A_n \oplus f_{n-1}(A_1, \ldots, A_{n-1})$

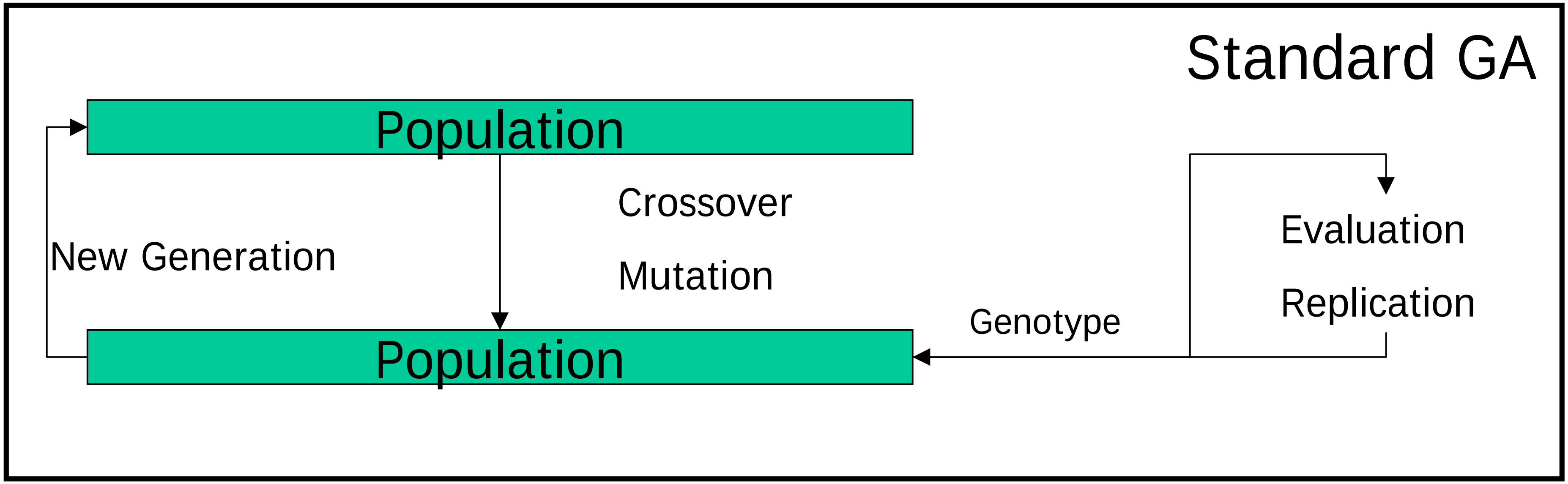
Generalized n*n Fredkin Gate



$$A_{n-1}\, f'_{n-1}(A_1, \ldots, A_{n-1}) + A_n\, f_{n-1}(A_1, \ldots, A_{n-1})$$

$$A_{n-1}\, f_{n-1}(A_1, \ldots, A_{n-1}) + A_n\, f'_{n-1}(A_1, \ldots, A_{n-1})$$

Future Perspectives



Standard GA

Population

Crossover

Mutation

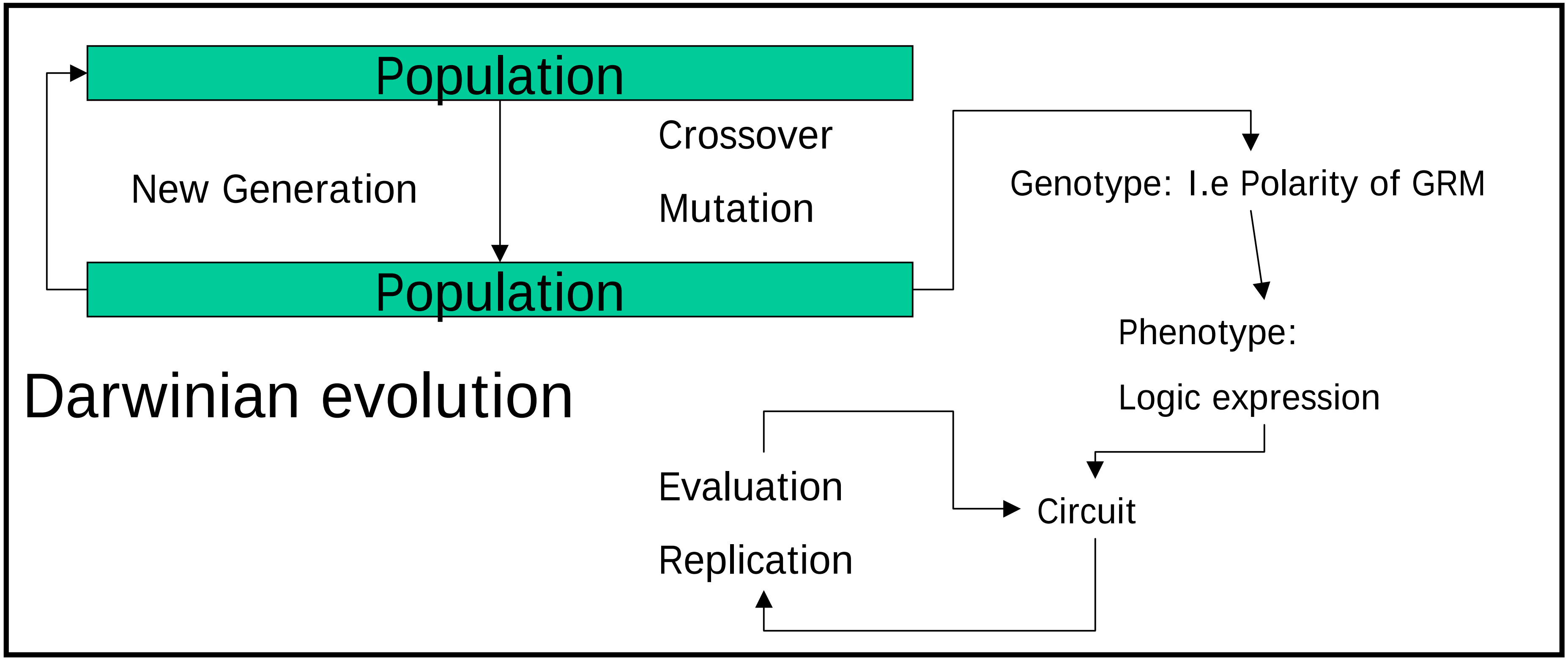
New Generation

Population

Genotype

Evaluation

Replication



Population

Crossover

Mutation

New Generation

Population

Genotype: I.e Polarity of GRM

Phenotype:

Logic expression

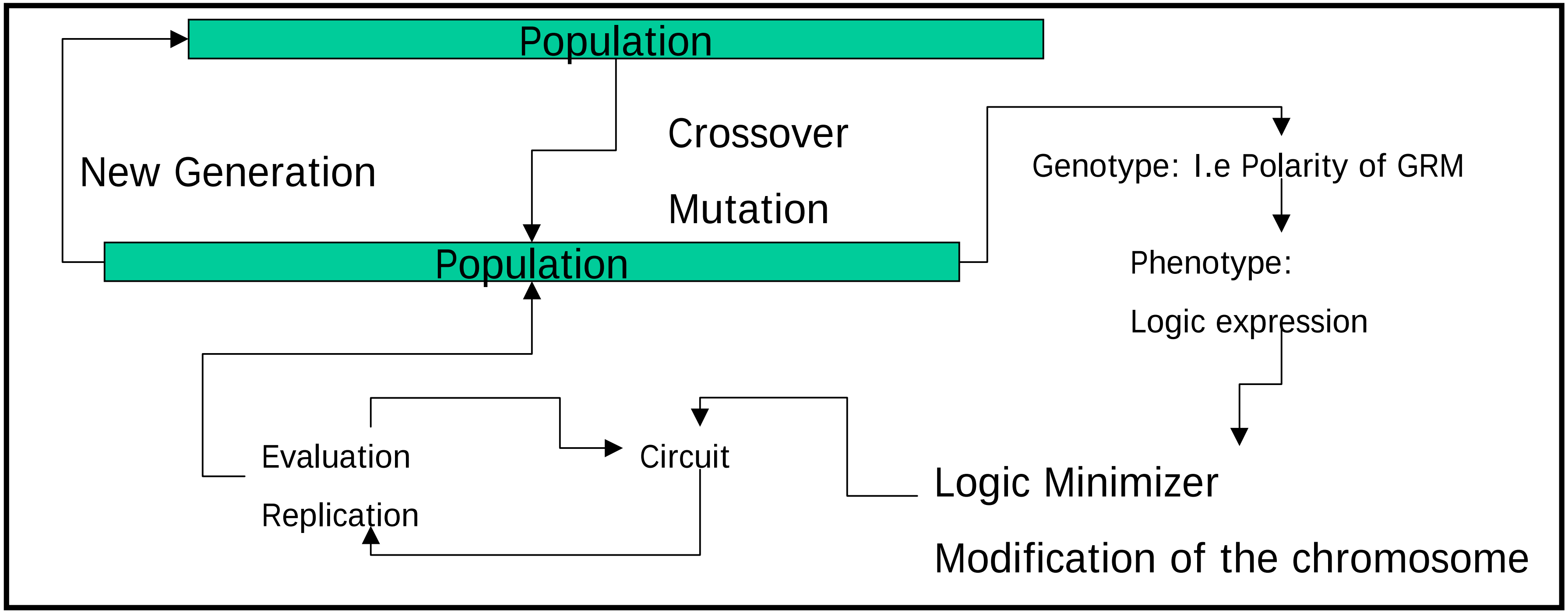
Darwinian evolution

Evaluation

Replication

Circuit

Lamarckian optimization



Population

Crossover

Mutation

New Generation

Population

Genotype: I.e Polarity of GRM

Phenotype:

Logic expression

Evaluation

Replication

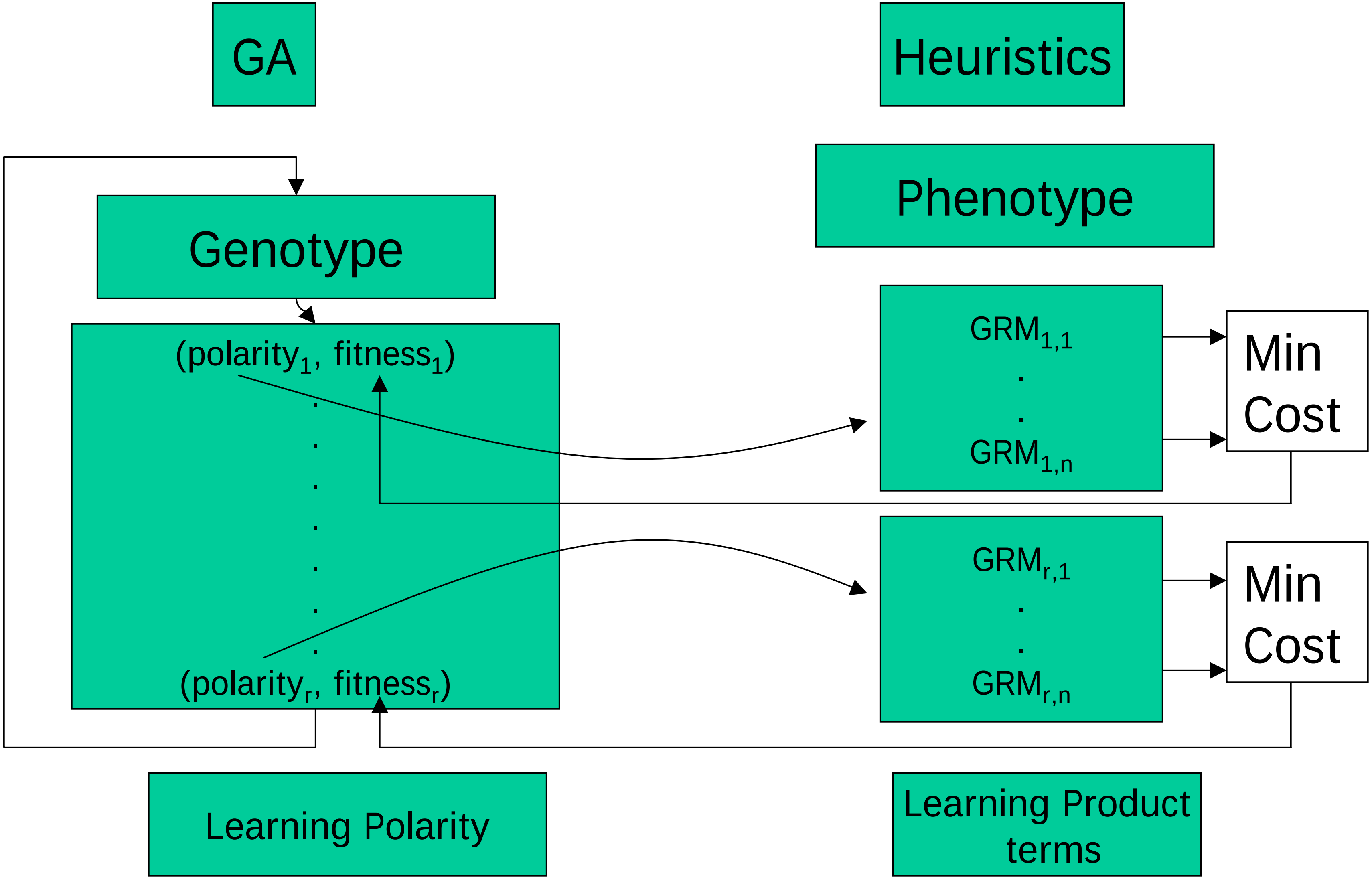
Circuit

Logic Minimizer

Modification of the chromosome

- An alternative approach to this problem can be the use of Lamarckian approach to the GA.
  - When a solution is found, the genotype is modified in order to be more precise for a given term-wise polarity set and the given function.
  - Consequently the search for this individual will induce smallest search space

Baldwinian learning



GA

Heuristics

Phenotype

Genotype

(polarity_1, fitness_1)

.
.
.
.
.
.
.

(polarity_r, fitness_r)

$\text{GRM}_{1,1}$
.
.
$\text{GRM}_{1,n}$

Min Cost

$\text{GRM}_{r,1}$
.
.
$\text{GRM}_{r,n}$

Min Cost

Learning Polarity

Learning Product terms

Projects and Homework

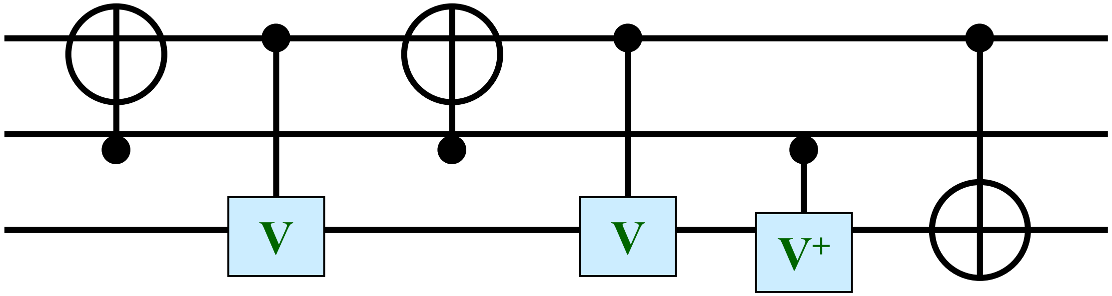
General directions

- All results from a GA should be averaged over 20 runs
- All details, files, precisions can be either asked directly or by email on lukac242@netscape.net
- Exceptionally good or bad results should be denoted apart
- All steps during exploration and experimentation should be precisely written down in a log book

Statistical analysis of non linearity in synthesized circuits

- **During synthesis fitness of circuits is highly non linear and non proportional to the distance from the final gate**
- **Goal: analyze a set of known gates (provided) and make a statistical analysis on the changes of the fitness function of the gates**
- **Finally establishing a table of results where the known gates will be represented as curves of fitness function**

Example



0.7	**0.39**	**0.33**	**0.76**	**0.18**	**1**
0.7	0.4	0.4	0.8	0.3	0
1	2	3	4	5	6

- Fitness
- Error
- Cost

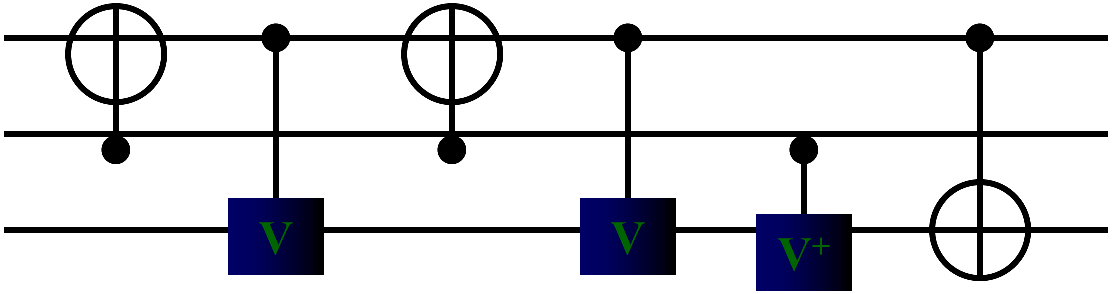
Evolving Fitness function for QC synthesis

- Inversely to the classical approach the goal is to synthesize a set of parameters fitting on the non linearity present in the fitness function evaluating quantum circuits
- Parameters evolved can be either taken from already existing fitness function or a completely new fitness function can be evolved

Evolving Fitness function for QC synthesis

Project 2

- Example



- Circuit

$$f = \alpha\left(1/_{error}\right)\Pi\,\beta(Cost)$$

- Fitness

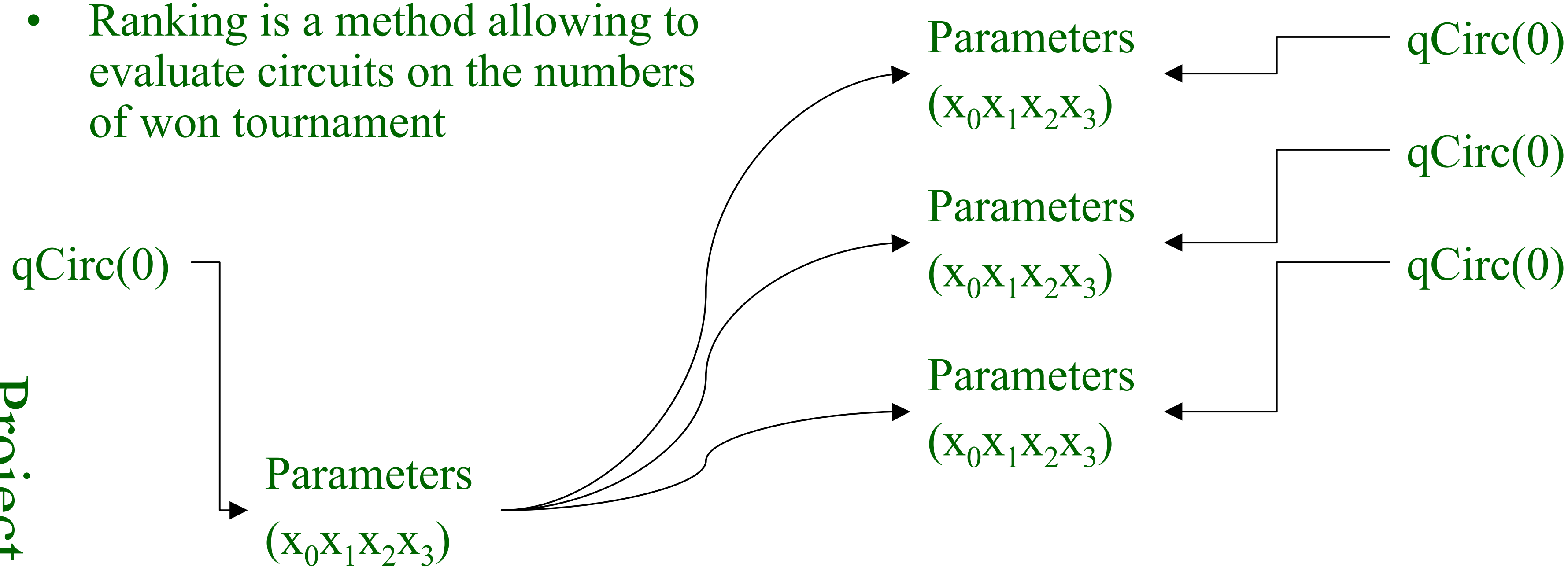
- **Encode parameters α,β,Π into chromosome Π is arbitrary function such as +, -, *, /, etc.**
- **Evolve them according to your own selected strategy**
- **You can choose any fitness function you want but minimum 2 parameters**

Pareto optimality GA and QC synthesis

- We want to test how will a GA with Pareto optimal evaluation evolve new quantum circuits.
- Minimal parameters are the size of the circuit and the error as a measure of the distance from the goal. More parameters can be used as cost, complexity, etc.
- Use ranking method to select the best individuals to the next generation

Pareto optimality GA and QC synthesis

- Evolving circuit according to more than one parameter.
- Ranking is a method allowing to evaluate circuits on the numbers of won tournament



qCirc(0)

Parameters

$(x_0x_1x_2x_3)$

Parameters

$(x_0x_1x_2x_3)$

Parameters

$(x_0x_1x_2x_3)$

Parameters

$(x_0x_1x_2x_3)$

qCirc(0)

qCirc(0)

qCirc(0)

Project 3

•All individuals are compared to all other in the population

•Mutation, Crossover as in standard GA

Comparing all parameters one to one

Fitness assigning on the number of won fights

$$\text{if} \sum_i (X_0 - X_j) \geq i \quad Rank_0{+}{+},\ \forall X = [x_0, \ldots x_i]$$

$$\text{else}\ Rank_0$$

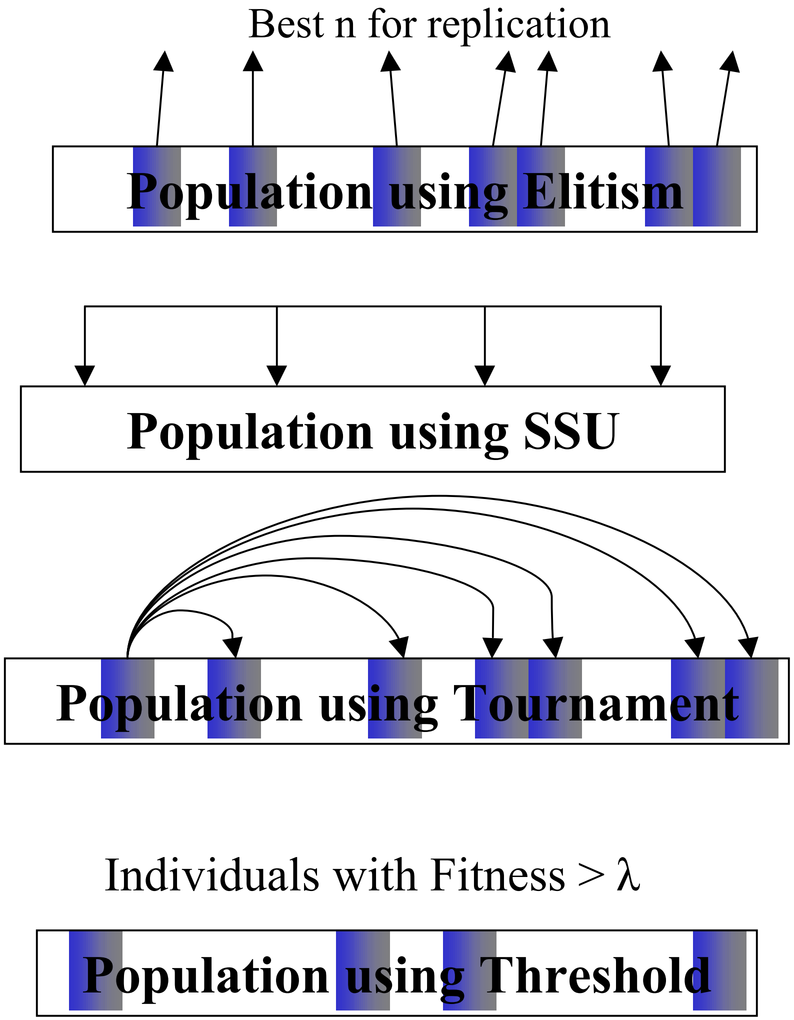
6	2	4	12	0	3

Exploring GA for QC by modifying parameters and settings

- By modifying parameters of the GA for QC synthesis it is possible to modify the behavior of the algorithm
- Here the goal is to explore in a methodic way combinations of parameters in the GA and observe the different behavior (deception, premature convergence)
- Parameters to be modified can be all such as mutation or crossover probability, population size, selection criteria, etc.

Exploring GA for QC by modifying parameters and settings

- Parameters to modify
  - Probabilities
    - Mutation
    - Crossover
    - Selection threshold
  - Selection pressure
    - Elitism
    - Roulette wheel
    - Universal Stochastic Sampling
    - Tournament
    - Threshold
  - Mixed generations
    - Comparing children with parents
  - Genetic operators
    - Mutation
      - Normal, bitwise, inversion,
    - Crossover
      - Normal, Double, Multi-point, Multi-parent



Best n for replication

Population using Elitism

Population using SSU

Population using Tournament

Individuals with Fitness > λ

Population using Threshold

Exhaustive search of Q-circuits

- Works by enumerating all possibilities of gates
  - Permutations
  - Wire allocations
  - Def: number of wires, number of blocks
- Goal: Make an extensive research for specified gates using this software.
- Classification according to different criteria:
  - Distance from the goal
  - Complexity
  - Cost

Using GAq

- A console interface
  - Input: file
  - Output: file
- All commands through the input file
- Available Monday on the class Web Page
  - Download the zipped package
    - Contents: exe file, source file, documentation and user’s manual

!!!!GOOD LUCK!!!!