

Extending the Design Space of Dynamic Quantum Circuits for Toffoli based Network

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Abstract—Recent advances in fault tolerant quantum systems allow to perform non-unitary operations like mid-circuit measurement, active reset and classically controlled gate operations in addition to the existing unitary gate operations. Real quantum devices that support these non-unitary operations enable us to execute a new class of quantum circuits, known as *Dynamic Quantum Circuits (DQC)*. This helps to enhance the scalability, thereby allowing execution of quantum circuits comprising of many qubits by using at least two qubits. Recently DQC realizations of multi-qubit *Quantum Phase Estimation (QPE)* and *Bernstein–Vazirani (BV)* algorithms have been demonstrated in two separate experiments. However the dynamic transformation of complex quantum circuits consisting of Toffoli gate operations have not been explored yet. This motivates us to: (a) explore the dynamic realization of Toffoli gates by extending the design space of DQC for Toffoli networks, and (b) propose a general dynamic transformation algorithm for the first time to the best of our knowledge. More precisely, we introduce two dynamic transformation schemes (dynamic-1 and dynamic-2) for Toffoli gates, that differ with respect to the required number of classically controlled gate operations. For evaluation, we consider the *Deutsch–Jozsa (DJ)* algorithm composed of one or more Toffoli gates. Experimental results demonstrate that dynamic DJ circuits based on dynamic-2 Toffoli realization scheme provides better computational accuracy over the dynamic-1 scheme. Further, the proposed dynamic transformation scheme is generic and can also be applied to non-Toffoli quantum circuits, e.g. BV algorithm.

Index Terms—Dynamic quantum circuit, mid-circuit measurement, quantum algorithms.

I. INTRODUCTION

With recent technological advancements, developments in quantum computing [1] has picked up. Lately IBM introduced the concept of *mid-circuit measurement* that allows the designers to measure the outcome of a quantum circuit in the intermediate stages of execution based on which the rest of the gate operations in a circuit are executed [2]. This enables application of non-unitary operations like *active reset*, *mid-circuit measurement* and *classically-controlled gate operations* along with unitary quantum operations such as *Hadamard*, *Phase*, and *Controlled-NOT* within the coherence time of qubits. More importantly, all the unitary and non-unitary gate operations are conducted over two qubits, i.e. an entire quantum algorithm can be realized using two qubits only. This provides a new class of quantum circuits, called *Dynamic Quantum Circuits (DQC)*.

DQC shows a great promise in scaling down the number of qubits in any quantum circuits. In fact, large-scale traditional

quantum circuits with many qubits can be transformed into two-qubit dynamic circuits thanks to the availability of non-unitary operations. Such scalability is evident from the two different experiments conducted recently on *Quantum Phase Estimation (QPE)* [3] and *Bernstein–Vazirani (BV)* [2] algorithms, where many qubit QPE and BV circuits are transformed into their respective dynamic versions using only two qubits. But several complex quantum circuits (e.g., realization of *Deutsch–Jozsa* [4], *Grover’s search* [5], *Shor’s factorization* [6] algorithms) composed of Toffoli gates are yet to be realized as dynamic circuits, keeping the design space of dynamic circuits largely unexplored.

This motivates us to: (a) investigate the dynamic realization of Toffoli gates by expanding the design space of DQC for Toffoli networks, and (b) propose a general dynamic transformation algorithm. To this end, we introduce two versions of dynamic transformation (*dynamic-1* and *dynamic-2*) for Toffoli gates. The two approaches differ from one another in terms of number of required non-unitary operations. For evaluation, *Deutsch–Jozsa (DJ)* algorithm composed of one or more Toffoli gates have been used. Results show that dynamic DJ circuits using dynamic-2 Toffoli realization gives better computational accuracy over the dynamic-1 version. Also our proposed transformation scheme is generic and can be applied to non-Toffoli quantum circuits, e.g. BV algorithm as demonstrated in experimental evaluation.

The rest of the paper is organized as follows. Section II presents a brief background on traditional quantum circuits. A brief survey of DQCs and the challenges are discussed in Section III. Section IV discusses the proposed method and experimental evaluation is presented in Section V. Finally, Section VI provides the concluding remarks.

II. BACKGROUND

In this section, we briefly discuss about quantum circuits, quantum gates and the necessary background required to make the paper self-contained.

A quantum circuit consists of a number of qubits in a traditional computing model [1], on which sequence of gate operations are performed. A quantum gate G_i that operates on m qubits can be represented by a $2^m \times 2^m$ unitary matrix. Generally, a qubit exists either in $|0\rangle$ or $|1\rangle$ basis states, or in a state called superposition as represented by the state vector

$\psi = \alpha|0\rangle + \beta|1\rangle$, where α and β are complex coefficients or amplitudes such that $|\alpha|^2 + |\beta|^2 = 1$. Finally, when we measure a qubit, the state $|\psi\rangle$ settles down into one of the basis states $|0\rangle$ or $|1\rangle$, with probabilities $|\alpha|^2$ and $|\beta|^2$ respectively. All quantum operations are unitary except the qubit measurement operation.

Typically, quantum circuits consist of various gates such as multiple-control Toffoli gates that are decomposed into 1- and 2-qubit basic quantum gates like *Hadamard* (H), *NOT* (X), *Phase* (T/T^\dagger), and *Controlled-NOT* (CX) from the *Clifford+T gate library* [1]. Consider a 3-qubit circuit shown in Fig. 1 realizing the function $\mathcal{F}(a, b) = a + b$, where q_0^D and q_1^D are the data or control qubits and q_0^A is an answer or a target qubit.

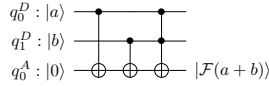


Fig. 1: 3-qubit realization of $\mathcal{F}(a, b) = a + b$

The circuit consists of the following operations

$$CX(q_0^D, q_0^A), CX(q_1^D, q_0^A), C^2X([q_0^D, q_1^D], q_0^A),$$

where $CX(q_{i \in \{0,1\}}^D, q_0^A)$ indicates an inversion operation on the target qubit q_0^A if the control qubit $q_{i \in \{0,1\}}^D$ is in state 1. The Toffoli gate, $C^2X([q_0^D, q_1^D], q_0^A)$ inverts the target qubit q_0^A if both the control qubits q_0^D and q_1^D are at logic 1. The Clifford+T realization of the C^2X operation is shown in Fig. 2. This decomposed circuit structure can be inserted in place of the C^2X gate shown in Fig. 1. As a result, we obtain a 3-qubit quantum circuit composed of only Clifford+T gates that can be implemented on a real quantum device [7].

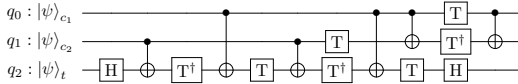


Fig. 2: Clifford+T realization of 3-qubit Toffoli circuit

To determine whether the function $\mathcal{F}(a, b) = a + b$ is completely balanced or constant using DJ algorithm [4], we need to incorporate operations like

$$X|q_0^A\rangle \cdot H|q_0^A\rangle \cdot H^{\otimes 2}|q_0^D q_1^D\rangle \cdot U(\mathcal{F}(a+b)) \cdot H^{\otimes 2}|q_0^D q_1^D\rangle,$$

where $X|q_0^A\rangle$ and $H|q_0^A\rangle$ indicate NOT and Hadamard operations respectively on answer qubit q_0^A , and $H^{\otimes 2}|q_0^D q_1^D\rangle$ represents Hadamard operations on data qubits q_0^D and q_1^D .

III. DYNAMIC QUANTUM CIRCUIT (DQC)

This section motivates our work and triggers an investigation of the design space for DQCs. To this end, we briefly review the current design status of the DQCs. Subsequently, the open questions and challenges for designing this new class of quantum circuits are discussed.

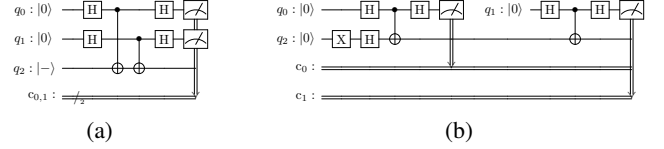


Fig. 3: (a) A BV circuit and (b) its DQC

A. Current Design Status

The circuit model discussed in the previous section has become a standard for designing quantum circuits to be executed on real quantum devices. Typically, the design of quantum circuits involves (1) the applications of 1- and 2-qubit gates on multiple qubits to realize the desired functionality, (2) measuring the states of all the qubits, and (3) storing these states in the classical registers to obtain the results. However, the desired result may be obtained with low probability due to the presence of noise in the real quantum device with limited computing resources. Recently, IBM introduced the concept of DQC [3] that allows the designers to guide the outcome based on the intermediate results of the circuit. Besides employing all the 1- and 2-qubit gates used to design traditional quantum circuits, this new class of quantum circuits additionally utilizes new computation primitives such as active-reset (comprising of a classically controlled X operation based on the measurement result of a qubit), mid-circuit measurement (enabling estimation of a qubit's state during computation) and classically controlled quantum operations (representing unitary operations on a qubit based on classical register value). Unlike traditional quantum circuit that needs at least n qubits to implement any n -qubit quantum algorithm, the DQC requires at least two qubits to realize the corresponding algorithm. The support of underlying technology enables quantum circuits comprising of a distinct set of *data* and *answer* qubits to be re-described using a single data qubit and equal number of answer qubit for executing on such platforms. The description can be transformed in a straightforward way when the input quantum circuit comprises of only independent set of 1- and 2-qubit operations that involve at most a single data qubit and one answer qubit that can be executed in arbitrary order.

For example, consider the BV circuit to find out a 2-qubit hidden string 11 using two data qubits (q_0 and q_1) initialized to $|0\rangle$ state, and an answer qubit (q_2) initialized to $|- \rangle$ ($= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$) state (see Fig. 3a). The corresponding DQC can be realized using a pair of data and answer qubits (i.e. 2 qubits only) in two iterations as shown in Fig. 3b. An iteration involves all the operations between a reset and a measurement on data qubit. The first and second iterations include execution of all the operations between qubits q_0 and q_2 , and between q_1 and q_2 , respectively, with an execution of reset operation on a data qubit after the first iteration. Lately, the concept of DQC is applied on the QPE algorithm [3].

B. Open Questions and Challenges

Realizing n -qubit quantum algorithms using only 2-qubit circuits shows a great potential of scaling down the number

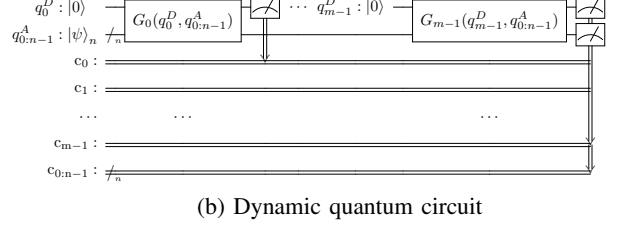
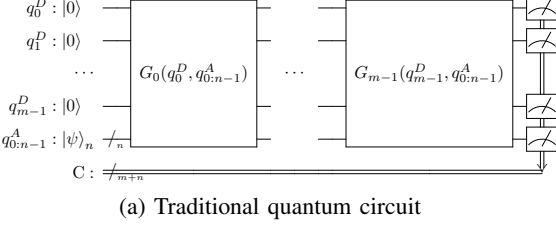


Fig. 4: Dynamic realization of a traditional quantum circuit

of qubits – still a limited resource while achieving the desired functionality. Thus far, BV and QPE algorithms are considered for dynamic realizations, in which the resulting DQCs obtained from the respective traditional quantum representations depict different scenarios. In cases of dynamic BV circuits, we can interchange the iterations (e.g., first and second iterations in Fig. 3b), which in turn changes the order of execution of a set of gates in one iteration with that of another iteration without affecting the desired functionality. However, in case of QPE algorithm, such change in the order of execution of iterations is not possible as the iterations are gate-dependent.

With such distinct scenarios, this new class of quantum circuits raises new questions: (1) how can we efficiently realize DQCs from complex traditional quantum circuits consisting of Toffoli gates, and (2) what will be the computational accuracy of dynamic quantum circuits? These questions open new design challenges for realizing efficient DQCs. The ideas based on BV and QPE algorithms are not sufficient enough to address these issues. Therefore, we extend the ideas to transform the traditional quantum circuits primarily consisting of Toffoli gates to DQCs. More precisely, we address the challenges and issues that can be associated with the transformation of Toffoli-based traditional circuits into the dynamic ones. To do this, we first investigate the dynamic realization of Toffoli gate and then determine a systematic approach to transform any Toffoli-based or Toffoli-free traditional quantum circuits into respective DQCs. Consequently, we explore the design space of the DQCs that largely remain unexplored till date.

IV. PROPOSED DQC TRANSFORMATION

In this section, we first introduce the general idea of our proposed method to generate DQCs from the corresponding traditional quantum circuits. We further show the dynamic transformation of Toffoli gate and then present dynamic realization of DJ algorithm [4] with an example.

A. General Idea

A traditional quantum circuit can be transformed into a DQC by performing dynamic realizations of a set of quantum operations in an iterative fashion with a limited number of qubits. To transform a n -qubit quantum circuit to its equivalent realization using at least 2 qubits, the following cases need to be considered:

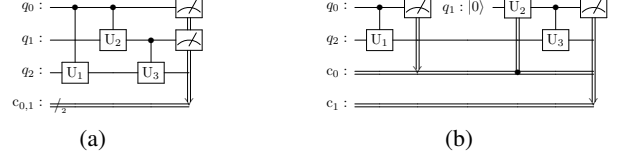


Fig. 5: Gate dependency in DQC transformation

Case 1. In dynamic realization the number of iteration plays a significant role to determine the performance of the resulting DQC and is lower bounded by the size of the input data qubits. More precisely, given a traditional quantum circuit comprising of m data qubits ($q_{i \in \{0, \dots, m-1\}}^D$) and n answer qubits ($q_{i \in \{0, \dots, n-1\}}^A$) as depicted in Fig. 4a, a dynamic realization composed of $n + 1$ qubits can be obtained with a minimum of m iterations, as shown in Fig. 4b provided all the quantum operations $G_{i \in \{0, \dots, m-1\}}$ are independent and involve at most one data qubit $q_{i \in \{0, \dots, m-1\}}^D$.

Case 2. Interaction between data qubits restricts the order in which they are to be considered in each iteration. For example, the quantum circuit with two data qubits q_0 and q_1 and one answer qubit q_2 contains a CU_2 operation between two data qubits q_0 and q_1 as shown in Fig. 5a.

Since the data qubit q_0 in the network acts as the control input in CU_2 operation, a dynamic description using one data and one answer qubit must consider the operations between q_0 and q_2 in early iteration as shown in Fig. 5b.

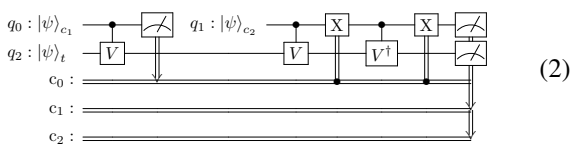
Considering the above ideas and constraints, we propose *Algorithm 1* to obtain DQC from its traditional version.

B. Dynamic Transformation of Toffoli Operation

The operational dependency of individual gate operations in any traditional quantum circuit influences the number of iterations in the resulting dynamic realization. Higher the operational dependency, more will be the iterations. For the purpose of illustration, we consider the Toffoli netlist shown in Fig. 2. Here, the gate operations $CX(q_i, q_j)$ and $T(q_j)/T^\dagger(q_j)$ are not commutative, i.e.

$$q_i : \text{---} \bullet \text{---} \quad q_j : \text{---} \oplus \text{---} \quad \neq \quad q_i : \text{---} \oplus \text{---} \quad q_j : \text{---} \bullet \text{---} \quad \text{and} \quad q_i : \text{---} \bullet \text{---} \quad q_j : \text{---} \oplus \text{---} \quad \neq \quad q_i : \text{---} \oplus \text{---} \quad q_j : \text{---} \bullet \text{---}$$

As a result, a dynamic realization of the Toffoli network shown in Fig. 2 requires at least 4 iterations to conduct the initial four CX operations in sequence. As each iteration ends



C. DQC Transformation of DJ Algorithm

The DJ algorithm is used to determine whether a function is balanced or constant on a quantum computer in a single execution. For an n -qubit function \mathcal{F} the algorithm requires n data qubits ($\{q_0^D, q_1^D, \dots, q_{n-1}^D\}$), an answer qubit (q_0^A), and an n -bit classical register (C). Using the proposed dynamic transformation scheme we show the dynamic transformation of a 2-input function $\mathcal{F}(a, b) = a + b$ (see Fig. 1) as an example. Initially, the function $\mathcal{F}(a, b) = a + b$ is described in the following way:

$$\hat{\mathcal{U}}_{\mathcal{F}(a+b)} = \begin{array}{c} q_0^D : |a\rangle \\ q_1^D : |b\rangle \\ q_0^A : |0\rangle \end{array} \quad \text{(6)}$$

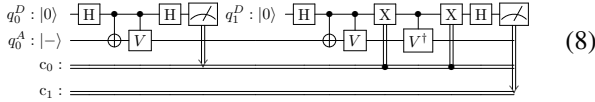
Since the gate operations $CV(q_{i \in \{0,1\}}^D, q_0^A)$ and $CX(q_{i \in \{0,1\}}^D, q_0^A)$ are commutative, the operations from the network presented in Eqn. (6) can be reordered in the following way.

$$\hat{\mathcal{U}}_{\mathcal{F}(a+b)} =$$

(7)

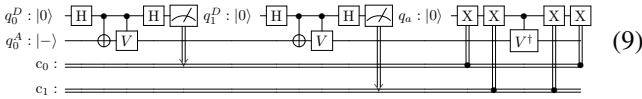
Using dynamic scheme for realizing Toffoli operation defined in Eqn. (2), the transformed DQC realizing the DJ algorithm for the function $\mathcal{F}(a + b)$ applying Algorithm 1 is presented below.

$$\text{Dynamic_DJ_Algorithm}(\mathcal{F}(a + b)) =$$



Similarly, considering the dynamic scheme defined in Eqn. (4) for Toffoli realization, the dynamic representation of the DJ algorithm for the function $\mathcal{F}(a + b)$ using Algorithm 1 is as follows.

$$\text{Dynamic_DJ_Algorithm}(\mathcal{F}(a + b)) =$$



Performance evaluation of the proposed dynamic transformation scheme and the environment considered for the evaluation are presented in next section.

V. EXPERIMENTAL EVALUATION

The proposed approach discussed in Section IV has been implemented on top of the *IBM's Qiskit* tool [9]. We conducted an extensive case study to evaluate the effectiveness of our proposed approach and compare the circuit complexities and performances of the dynamic quantum realizations with that of the traditional realizations. For this purpose, we considered few

well-known quantum algorithms such as BV [2], and DJ [4] as benchmarks. These algorithms are good fit for evaluating the effectiveness of our proposed scheme as they either contain Toffoli gates or are Toffoli-free circuits, thereby showcasing the various circuit structures that are efficiently handled by our proposed scheme. All the experiments have been conducted on a machine equipped with an AMD Ryzen 7 PRO 5850U processor running at 1.90 GHz and having a 48 GB RAM with Windows 10 Pro operating system.

A. Results of Non-Toffoli Circuits

In Table I, the results for the Toffoli free quantum circuits are provided. The first column represents the name of the benchmark. The second, third and fourth columns of Table I provide the details of the number of qubits (*Qubit count*), number of gates (*Gate count*) and the circuit depth (*Depth*), respectively for traditional circuits and their corresponding dynamic realizations. For dynamic realizations, depth measure includes measurement and reset operations.

We confirm that all the resulting DQCs obtained from their traditional realizations using the proposed algorithm are functionally equivalent to the corresponding traditional circuits. To do this, we simulated the traditional and corresponding dynamic realizations 1024 times using *IBM's AER Simulator tool* [10]. The simulation results show that the probability of expected outcome obtained from the traditional circuit and the resulting DQC are exactly same in all the cases, thereby establishing the correctness of our approach.

With respect to the circuit complexity, Table I clearly shows that a slight increase in the gate count in case of DQCs, while the circuit depth increases by almost $3\times$ of the traditional realizations. Nevertheless, this can be compensated by the number of qubits required to realize the DQCs. More precisely, all the benchmarks require at most 5-qubits to realize the desired functionalities traditionally, whereas the same functionalities can be dynamically realized using only 2-qubits.

B. Results of Toffoli-based Circuits

Table II summarizes the results of quantum circuits consisting of multiple 2-control Toffoli operations (i.e. C^2X gates). The first column indicates the names of the benchmarks. The number of qubits, total number of gates and the number of circuit depths for traditional circuits and their two different dynamic representations (*dynamic-1* and *dynamic-2*) are provided in the second, third and fourth columns, respectively. Dynamic-1 and dynamic-2 are the dynamic realizations of all the 9 benchmarks that are obtained by substituting the Toffoli operations with their corresponding dynamic representation schemes defined in Eqn. (2) and (4), respectively.

Compared to the traditional quantum circuits, the proposed dynamic realizations increase the gate count and the circuit depth due to the presence of additional classically-controlled gate operations. The traditional circuits and the two different types of dynamic circuits, dynamic-1 and dynamic-2, for all the considered benchmarks are simulated 1024 times in *IBM's AER Simulator tool* [10]. The resulting probabilities of the

TABLE I: Results of Toffoli-free quantum circuits

Benchmark	Qubit count		Gate count		Depth	
	tradi.	dyna.	tradi.	dyna.	tradi.	dyna.
BV_111	4	2	11	13	6	15
BV_110	4	2	8	10	5	13
BV_101	4	2	8	10	5	12
BV_011	4	2	8	10	5	12
BV_100	4	2	5	7	4	10
BV_010	4	2	5	7	4	10
BV_001	4	2	5	7	4	9
BV_1111	5	2	14	17	7	20
BV_1110	5	2	11	14	6	18
BV_1101	5	2	11	14	6	17
BV_1011	5	2	11	14	6	17
BV_0111	5	2	11	14	6	17
BV_1010	5	2	8	11	5	15
BV_1001	5	2	8	11	5	14
BV_0110	5	2	8	11	5	15
BV_0101	5	2	8	11	5	14
BV_1000	5	2	5	9	4	12
BV_0100	5	2	5	8	4	12
BV_0010	5	2	5	8	4	12
BV_0001	5	2	5	8	4	11
DJ_CONST_0	3	2	6	7	3	7
DJ_CONST_1	3	2	7	8	3	7
DJ_PASS_1	3	2	7	8	5	9
DJ_PASS_2	3	2	7	8	5	8
DJ_INVERT_1	3	2	8	9	6	10
DJ_INVERT_2	3	2	8	9	6	8
DJ_XOR	3	2	8	9	6	10
DJ_XNOR	3	2	9	10	7	11

TABLE II: Results of Toffoli-based DJ quantum circuits

Benchmark	Qubit count		Gate count			Depth		
	tradi.	dyna. 1/2	tradi.	dyna. 1	dyna. 2	tradi.	dyna. 1	dyna. 2
AND	3	2	21	28	33	16	23	26
NAND	3	2	22	29	34	17	24	27
OR	3	2	23	30	35	18	26	29
NOR	3	2	24	31	36	19	27	30
IMPLY_1	3	2	23	30	35	18	26	29
IMPLY_2	3	2	23	30	35	18	25	28
INHIB_1	3	2	22	29	34	17	24	27
INHIB_2	3	2	22	29	34	17	25	28
CARRY	4	2	53	73	82	36	60	68

expected outcomes are shown in Fig. 7. It is clearly evident that the dynamic realization of type 1 (i.e. dynamic-1) significantly reduces the probability of an expected outcome as compared to that of the traditional circuits, while in cases of dynamic realizations of type 2 (i.e. dynamic-2), the probability of expected outcomes remain almost same as that of the traditional quantum circuits. As a result, the transformation based on dynamic-2 provides better computational accuracy as compared to that of dynamic-1. This is achieved using one additional iteration that involves one reset operation and 2 more classically controlled X operation per Toffoli operation.

VI. CONCLUSION

Dynamic Quantum Circuits provides a promising path for executing quantum circuits of many qubits in an architecture of at least two qubits with the support of active reset, mid-circuit measurement and classically controlled operation. In this paper, we have presented two dynamic transformation schemes (dynamic-1 and dynamic-2) for Toffoli gate. The

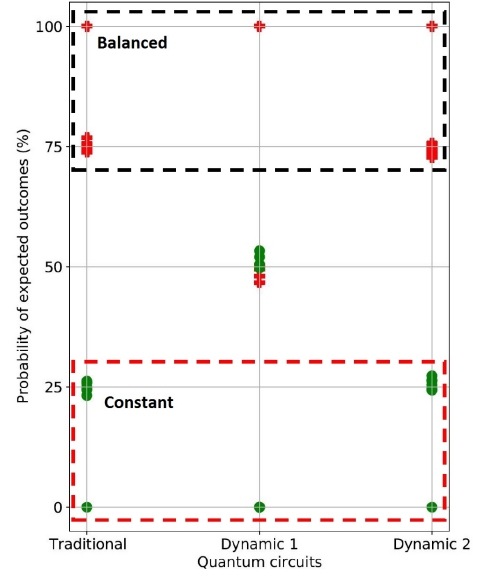


Fig. 7: Performance of Toffoli-based traditional and DQCs

decomposition structure of Toffoli gate affects the number of classically controlled gate operations, which in turn, affects the final outcome of the dynamic quantum circuit. Experiments were conducted for both non-Toffoli and Toffoli based circuits for which we have considered two algorithms: Bernstein–Vazirani and Deutsch–Jozsa. Experimental results reveal that our proposed method provides correct dynamic realization of traditional quantum circuits. We show that the realization based on dynamic-2 with an additional operation overhead (i.e. an active reset and 2 more classically control X operations per Toffoli gate) ensures improved computational accuracy over the dynamic-1. In future, we will consider the dynamic realization of Multiple Control Toffoli gates and their networks.

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