QuCAT: A Combinatorial Testing Tool for Quantum Software

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Abstract—With the increased developments in quantum computing, the availability of systematic and automatic testing approaches for quantum programs is becoming increasingly essential. To this end, we present the quantum software testing tool `QuCAT` for combinatorial testing of quantum programs. `QuCAT` provides two functionalities of use. With the first functionality, the tool generates a test suite of a given strength (e.g., pairwise). With the second functionality, it generates test suites with increasing strength until a failure is triggered or a maximum strength is reached. `QuCAT` uses two test oracles to check the correctness of test outputs. We assess the cost and effectiveness of `QuCAT` with 3 faulty versions of 5 quantum programs. Results show that combinatorial test suites with a low strength can find faults with limited cost, while a higher strength performs better to trigger some difficult faults with relatively higher cost.
Repository: https://github.com/Simula-COMPLEX/qucat-tool
Video: https://youtu.be/UsqgOudKLio

Index Terms—quantum programs, software testing, combinatorial testing

I. INTRODUCTION

Quantum Software Engineering (QSE) [1], [2] is rapidly growing these years. QSE enables building software engineering solutions to solve complex problems with quantum software that can be executed on quantum computers. Testing quantum software is one area within QSE which presents some challenges due to the unique features of quantum computing, such as its probabilistic nature, destructive measurement, and no-cloning theorem of quantum states. Thus, it is essential to build automated solutions for testing quantum programs [1], [3], [4]. To this end, some approaches have been proposed, employing different techniques such as property-based testing [5], search-based testing [6], mutation testing [7], [8], fuzz testing [9], metamorphic testing [10], in addition to input and output coverage criteria for quantum programs [11]. These approaches are also supported by tools [12]–[15].

However, previous approaches overlook the types of inputs that can trigger a fault. Indeed, in a quantum program, a fault is

often due to a faulty gate of the quantum circuit corresponding to the quantum program. Quantum gates combine the values of one or more qubits; therefore, a specific *combination* of the values for some input qubits should be able to trigger the fault. For classic software, combinatorial testing is a well-known technique which is used to generate test suites to detect faults caused by specific combinations of input parameters (e.g., pair-wise or 3-wise testing) [16]. It has also been successfully applied in many other domains, such as deep neural networks [17] and autonomous driving systems [18].

Motivated by the success of combinatorial testing in different domains, in [19] we proposed an approach for doing combinatorial testing of quantum programs. However, the approach was not implemented in a tool usable by practitioners. To this aim, in this paper, we present how we engineered the approach in the tool `QuCAT`. The tool can generate combinatorial test suites for quantum programs, execute them, and assess the test results automatically. Such quantum programs are written in the Qiskit framework [20]. In Qiskit, a quantum circuit is a computational routine containing quantum wires, quantum gates, initialization, measurements, etc.

`QuCAT` provides two functionalities of use. With functionality `func1`, `QuCAT` can be used to generate a test suite with a specified *strength*, while with functionality `func2`, `QuCAT` can be used to generate test suites with incremental strengths until a fault is detected or the maximum strength is reached. `QuCAT` employs two test oracles to assess test results. We assess the cost and effectiveness of `QuCAT` by experimenting it on 3 faulty versions of 5 different quantum programs.
Paper structure. Sect. II briefly introduces qubits and quantum circuits and provides the definitions of key concepts. We describe the overview and methodology of `QuCAT` in Sect. III. Validation of the approach is presented in Sect. IV. Finally, we conclude our work and discuss the future work in Sect. V.

II. PRELIMINARIES

A. Qubits and Quantum Circuits

Classic computers work on classic bits, which can be either 0 or 1 assigned to each bit. Differently, a quantum computer works on *qubits*, which can be both 0 and 1 simultaneously, i.e., they are in *superposition* until being observed.
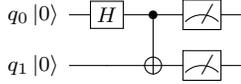
Fig. 1. Entanglement Quantum Circuit

For a qubit, we define its quantum state $|\psi\rangle$ as follows:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$$

where α and β are two complex numbers, each defining the *amplitude* of the qubit in terms of *magnitude* and *phase*. $|\alpha|^2$ and $|\beta|^2$ show the probability for a qubit to be in state $|0\rangle$ or $|1\rangle$, and it holds that $|\alpha|^2 + |\beta|^2 = 1$. An example of quantum circuits is shown in Fig. 1, which is an Entanglement program. First, we can initialize the two qubits to a state. For instance, in this example, we initialize both of them as the $|0\rangle$ state. Then, we apply a Hadamard gate on the first qubit (i.e., q_0) to turn it into superposition and a CX gate on both qubits, i.e., q_0 as the control qubit and q_1 as the target qubit. If q_0 is in state $|1\rangle$, q_1 will be flipped. Otherwise, q_1 won't be flipped. Finally, we measure the two qubits to obtain the outputs. For this circuit, there will be a 50% probability of obtaining output 00 and a 50% probability of obtaining 11.

B. Definitions

This section provides definitions of key concepts of quantum programs and combinatorial testing.

Definition 1 (Inputs, outputs, and quantum program). Let $Q = \{q_1, q_2, \ldots, q_n\}$ be the set of qubits of a quantum program QP. A subset $I \subseteq Q$ are the *input qubits*, while a subset $O \subseteq Q$ are the *output qubits*. $D_I = \mathcal{B}^{|I|}$ and $D_O = \mathcal{B}^{|O|}$ are the input and output values. A quantum program can be described as a function QP: $D_I \to 2^{D_O}$.

According to the definition, a quantum program can return different outputs with the same input value due to its probabilistic nature. If the expected behaviour of the quantum program is known, we can define it as a program specification.

Definition 2 (Program specification). Given a quantum program QP, PS is identified as the *program specification* which is the expected behaviour of QP. Given an input $i \in D_I$ and a possible output value h, PS states the expected probability of occurrence of output h for input i (i.e., $\text{PS}(i, h) = p_h$).

Due to its non-deterministic nature, for a given input, a quantum program must be executed multiple times to get the distribution of output values.

Definition 3 (Test inputs and test results). A *test input* is defined by the pair $\langle i, n \rangle$, where i is the assignment to input qubits I (i.e., $i \in D_I$), and n represents the number of times that QP needs to be executed with i. *Test results* are defined as $res = [\text{QP}(i), \ldots, \text{QP}(i)] = [o_1, \ldots, o_n]$, where o_j is the output returned by QP at the jth execution.

We define two failure types to assess the test results.
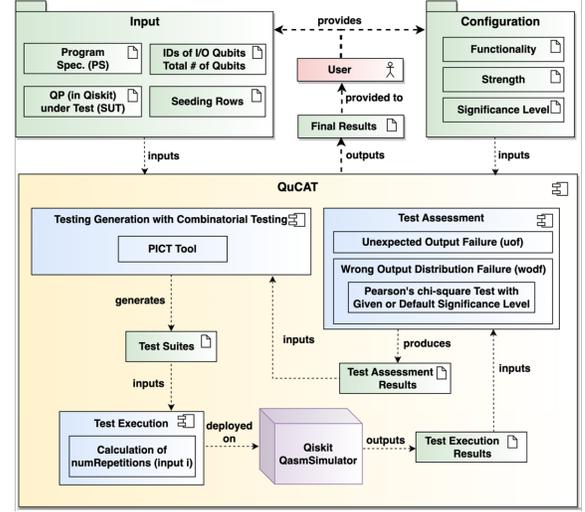
Fig. 2. Architecture of the QuCAT Tool

- *Unexpected Output Failure* (*uof*): for a given input i, it checks whether there exists one output o_j that is unexpected (i.e., $\text{PS}(i, o_j) = 0$).
- *Wrong Output Distribution Failure* (*wodf*): when there is no unexpected output, it checks whether there is a significant difference between the observed distribution of outputs and that defined in the program specification PS. We use *goodness of fit test* with Pearson's chi-square test [21] to assess the difference.

In a quantum program, faults may be caused by the incorrect use of gates, and they could be exposed by some specific values combination of some of the inputs. Combinatorial testing can be applied to find such combinations for testing quantum programs. Value schema [16] specifies a combination of input values that has to be covered in a test.

Definition 4 (Value schema). For a quantum program with input qubits $(q_0, q_2, \ldots, q_{|I|-1})$, a *k-value schema* ($k > 0$ and $k \leq |I|$) is $(\ldots, v_{i_1}, \ldots, v_{i_k}, \ldots)$, where k qubits are assigned with fixed values while the others are not fixed.

Here, we identify with '-' the values of qubits, which are not fixed. For example, given a quantum program with 4 input qubits in which the second and third qubits are fixed with '0' and '1', the *2-value schema* is $(-, 0, 1, -)$.

Definition 5 (Combinatorial test suite). A *combinatorial test suite* T_k of strength k contains, for each *k-value schema*, at least a test covering the schema.

III. QuCAT Tool Description and Methodology

We present how we have engineered the approach proposed in [19] in the tool QuCAT, which automatically generates combinatorial test suites, executes them, and analyzes test results. The overview of QuCAT is shown in Fig. 2.

A. Functionalities

QuCAT can be used in two ways:

- `func1`: A user specifies a fixed strength k and the tool generates and assesses a combinatorial test suite T_k.
- `func2`: Test suites are kept on being generated with an incremental strength, beginning from $k = 2$, until a fault is found or the maximum strength K is reached.

B. Input and Configuration

To use `QuCAT`, a user should provide *input* information and the tool *configuration*. The *input* information includes the quantum program under test (SUT), the program specification (PS), the list of input and output qubits, and the total number of qubits. The *configuration* contains parameters of `QuCAT`:

- the functionality to use `QuCAT`, i.e., `func1` or `func2` as described in Sect. II-B.
- a *strength* value. If the user selects `func1`, the strength is the value k for the combinatorial test suite T_k to generate (e.g., $k = 2$ for pairwise testing, $k = 3$ for 3-wise testing). In this case, the default value is $k = 2$. If instead, the user selects functionality `func2`, the value is the maximum strength K until which the tool must generate test suites.
- `QuCAT` employs Pearson's chi-square test to assess failure type *wodf* (see Sect. II-B). The user can specify the significance level for the test. The default value is 0.01.
- Moreover, the user can provide a file of *seeding rows*, which contains test cases required to appear in all generated test suites by combinatorial testing.

Then, `QuCAT` generates tests following the configuration file.

In summary, as shown in Fig. 2, when using `QuCAT`, the user should (i) select one of the two functionalities, (ii) provide input information of the quantum program, (iii) configure parameters for combinatorial testing and test assessment, and (iv) provide a file of seeding rows if needed.

C. Process of Test Generation, Execution, and Assessment

We describe the steps performed by `QuCAT` to generate test suites with combinatorial testing, execute them over the quantum program, get test results, and perform test assessment.

- `QuCAT` employs PICT [22] to generate combinatorial test suites of a given strength (see Def. 5). Dependent on the selected functionality, `QuCAT` works as follows:
  - If the user chooses `func1`, the tool generates a test suite T_k for the strength k defined by the user.
  - If the user chooses `func2`, the tool keeps on generating combinatorial test suites with incremental strengths until a test triggers a failure or the maximum strength value K is reached. Note that `QuCAT` will assess results every time when a new test suite is generated.
- For a test input $\langle i, n \rangle$, the number of executions n is defined according to the program specification. In detail, the number of repetitions is computed as the number of possible outputs for input i multiplied by 100 (i.e., $n = |\{h \in D_O \mid \text{PS}(i, h) \neq 0\}| \times 100$).
- `QuCAT` automatically checks each test case (i.e., test input) according to two failure types *uof* and *wodf*, as defined in Def. 3, by comparing test results with the program specification.

  - `QuCAT` first checks failure type *uof*. For input i, after n executions, if there is any unexpected output value that does not appear in the program specification, the test case fails for *uof*.
  - If there is no unexpected output, `QuCAT` checks *wodf*. After n executions, if the output distribution is significantly different from that of the program specification (checked with the statistical test introduced in Def. 3), the test fails for *wodf*.

- After the generation of all the test suites, their execution, and their assessment, `QuCAT` provides the following files as output: (i) a file containing execution results of all test cases; (ii) a file of assessments of each test case; (iii) unit tests written in the `unittest` framework for the generated test suites that the user can use to rerun the test cases when debugging the quantum program.

IV. Tool Validation

We evaluate `QuCAT` with five quantum programs. For each program, we created three faulty versions (i.e., F_1, F_2 and F_3). F_3 is the most difficult one, followed by F_2 and F_1 based on the number of input values that can trigger the fault. The selected programs are: 1) `BV`: the Bernstein-Vazirani cryptography algorithm; 2) `QR`: quantum random access memory implementation; 3) `IQ`: inverse quantum Fourier transform; 4) `AS`: performing $v1 = v1 + v2 * v2$, where $v1$ and $v2$ are two quantum integers; and 5) `CE`: a conditional addition on a quantum integer. The characteristics of these quantum programs vary in terms of the number of qubits and gates and circuit depth. The gate numbers `BV`, `QR`, `IQ`, `AS`, `CE` are 21, 15, 60, 25, and 25, and the depths are 3, 12, 56, 22, and 26.

Table I shows the results of testing the faulty versions of the five quantum programs with functionality `func1` using values 2, 3, and 4 for strength k. $|I|$ is the number of input qubits and $|T_k|$ is the test suite size. Column *failure* tells whether a failure is triggered by the test suite (i.e., a fault is detected). Higher numbers of qubits and strength k (e.g., $k = 4$) result in a higher test suite size, i.e., the higher cost in terms of test suite size (e.g., `CE` and `IQ`). One observation is that even with the lower strength (i.e., pairwise testing), `QuCAT` can still find the easiest faults (i.e., F_1) in all the programs. All the faults, including the most difficult one (i.e., F_3), are triggered by the test suites generated with strength 4.

Table II reports the results of running `QuCAT` with functionality `func2` using 4 as maximum strength K. k_{end} refers to the strength of the generated test suite containing the test case which triggered the fault; $|T^c|$ reports the number of executed tests, i.e., all the tests in the generated test suites $T_2, \ldots, T_{k_{end}-1}$ and the tests in $T_{k_{end}}$ that have been executed before triggering the fault (including the failing test). F_1 faults for all the programs and F_2 faults of three programs are triggered by test suites with strength 2. Test suites with strength 3 have been necessary to detect faults of two programs with F_2 faults and two programs with F_3 faults. For the rest of F_3 faulty programs, `QuCAT` had to generate till the test suites with the maximum strength 4, which were able to detect these faults.

TABLE I
RESULTS FOR FUNCTIONALITY `FUNC1`

QP	$\lvert I\rvert$	$k=2$ F$_1$ failure	$\lvert T_2\rvert$	$k=2$ F$_2$ failure	$\lvert T_2\rvert$	$k=2$ F$_3$ failure	$\lvert T_2\rvert$	$k=3$ F$_1$ failure	$\lvert T_3\rvert$	$k=3$ F$_2$ failure	$\lvert T_3\rvert$	$k=3$ F$_3$ failure	$\lvert T_3\rvert$	$k=4$ F$_1$ failure	$\lvert T_4\rvert$	$k=4$ F$_2$ failure	$\lvert T_4\rvert$	$k=4$ F$_3$ failure	$\lvert T_4\rvert$
AS	6	✓	6	✓	6	✗	6	✓	14	✓	13	✗	13	✓	26	✓	27	✓	24
BV	7	✓	7	✗	6	✗	7	✓	15	✓	14	✓	14	✓	31	✓	30	✓	32
CE	11	✓	8	✗	9	✗	8	✓	19	✓	19	✓	19	✓	47	✓	43	✓	46
IQ	10	✓	8	✓	9	✗	8	✓	18	✓	18	✓	18	✓	43	✓	44	✓	44
QR	9	✓	8	✓	8	✗	8	✓	14	✓	17	✗	16	✓	38	✓	38	✓	38

TABLE II
RESULTS FOR FUNCTIONALITY `FUNC2`

QP	F$_1$ $\lvert T^c\rvert$	F$_1$ k_{end}	F$_2$ $\lvert T^c\rvert$	F$_2$ k_{end}	F$_3$ $\lvert T^c\rvert$	F$_3$ k_{end}
AS	5	2	8	3	32	4
BV	4	2	6	2	39	4
CE	2	2	6	2	13	3
IQ	1	2	15	3	25	3
QR	2	2	6	2	26	4

V. CONCLUSIONS AND FUTURE WORK

We presented `QuCAT`– an automated tool for combinatorial testing of quantum programs. `QuCAT` uses two test oracles to assess test results and two functionalities to generate tests. We also presented the architecture of the tool. Finally, we validated the tool by testing three faulty versions of five quantum programs to assess the cost and effectiveness of `QuCAT` followed by discussing the results. In the future, we plan to extend the tool further to provide features such as pinpointing the location where the program failed (i.e., fault localisation) and porting the tool for real quantum computers.

REFERENCES

[1] J. Zhao, "Quantum software engineering: Landscapes and horizons," *CoRR*, vol. abs/2007.07047, 2020.

[2] M. A. Serrano, R. Pérez-Castillo, and M. Piattini, Eds., *Quantum Software Engineering*. Springer International Publishing, 2022.

[3] A. Miranskyy and L. Zhang, "On testing quantum programs," in *Proceedings of the 41st International Conference on Software Engineering: New Ideas and Emerging Results*, ser. ICSE-NIER '19. IEEE Press, 2019, pp. 57–60.

[4] A. Miranskyy, L. Zhang, and J. Doliskani, "Is your quantum program bug-free?" in *Proceedings of the ACM/IEEE 42nd International Conference on Software Engineering: New Ideas and Emerging Results*, ser. ICSE-NIER '20. New York, NY, USA: Association for Computing Machinery, 2020, pp. 29–32.

[5] S. Honarvar, M. R. Mousavi, and R. Nagarajan, "Property-based testing of quantum programs in Q#," in *Proceedings of the IEEE/ACM 42nd International Conference on Software Engineering Workshops*, ser. ICSEW'20. New York, NY, USA: Association for Computing Machinery, 2020, pp. 430–435.

[6] X. Wang, P. Arcaini, T. Yue, and S. Ali, "Generating failing test suites for quantum programs with search," in *Search-Based Software Engineering*. Cham: Springer International Publishing, 2021, pp. 9–25.

[7] D. Fortunato, J. Campos, and R. Abreu, "Mutation testing of quantum programs: A case study with Qiskit," *IEEE Transactions on Quantum Engineering*, vol. 3, pp. 1–17, 2022.

[8] X. Wang, T. Yu, P. Arcaini, T. Yue, and S. Ali, "Mutation-based test generation for quantum programs with multi-objective search," in *Proceedings of the Genetic and Evolutionary Computation Conference*, ser. GECCO '22. New York, NY, USA: Association for Computing Machinery, 2022, pp. 1345–1353.

[9] J. Wang, F. Ma, and Y. Jiang, "Poster: Fuzz testing of quantum program," in *2021 14th IEEE Conference on Software Testing, Verification and Validation (ICST)*, 2021, pp. 466–469.

[10] R. Abreu, J. Fernandes, L. Llana, and G. Tavares, "Metamorphic testing of oracle quantum programs," in *Proceedings of the 3rd International Workshop on Quantum Software Engineering*, ser. Q-SE '22. New York, NY, USA: Association for Computing Machinery, 2023, pp. 16–23.

[11] S. Ali, P. Arcaini, X. Wang, and T. Yue, "Assessing the effectiveness of input and output coverage criteria for testing quantum programs," in *2021 14th IEEE Conference on Software Testing, Verification and Validation (ICST)*, 2021, pp. 13–23.

[12] E. Mendiluze, S. Ali, P. Arcaini, and T. Yue, "Muskit: A mutation analysis tool for quantum software testing," in *2021 36th IEEE/ACM International Conference on Automated Software Engineering (ASE)*, 2021, pp. 1266–1270.

[13] X. Wang, P. Arcaini, T. Yue, and S. Ali, "Quito: a coverage-guided test generator for quantum programs," in *2021 36th IEEE/ACM International Conference on Automated Software Engineering (ASE)*, 2021, pp. 1237–1241.

[14] ——, "QuSBT: Search-based testing of quantum programs," in *Proceedings of the ACM/IEEE 44th International Conference on Software Engineering: Companion Proceedings*, ser. ICSE '22. New York, NY, USA: Association for Computing Machinery, 2022, pp. 173–177.

[15] D. Fortunato, J. Campos, and R. Abreu, "QMutPy: A mutation testing tool for quantum algorithms and applications in Qiskit," in *Proceedings of the 31st ACM SIGSOFT International Symposium on Software Testing and Analysis*, ser. ISSTA 2022. New York, NY, USA: Association for Computing Machinery, 2022, pp. 797–800.

[16] C. Nie and H. Leung, "A survey of combinatorial testing," *ACM Comput. Surv.*, vol. 43, no. 2, Feb. 2011.

[17] J. Tao, Y. Li, F. Wotawa, H. Felbinger, and M. Nica, "On the industrial application of combinatorial testing for autonomous driving functions," in *2019 IEEE International Conference on Software Testing, Verification and Validation Workshops (ICSTW)*, 2019, pp. 234–240.

[18] L. Ma, F. Juefei-Xu, M. Xue, B. Li, L. Li, Y. Liu, and J. Zhao, "DeepCT: Tomographic combinatorial testing for deep learning systems," in *2019 IEEE 26th International Conference on Software Analysis, Evolution and Reengineering (SANER)*, 2019, pp. 614–618.

[19] X. Wang, P. Arcaini, T. Yue, and S. Ali, "Application of combinatorial testing to quantum programs," in *2021 IEEE 21st International Conference on Software Quality, Reliability and Security (QRS)*, 2021, pp. 179–188.

[20] R. Wille, R. Van Meter, and Y. Naveh, "IBM's Qiskit tool chain: Working with and developing for real quantum computers," in *2019 Design, Automation Test in Europe Conference Exhibition (DATE)*, 2019, pp. 1234–1240.

[21] A. Agresti, *An introduction to categorical data analysis*, 3rd ed. Wiley-Blackwell, 2019.

[22] PICT, "Pairwise independent combinatorial testing," https://github.com/microsoft/pict, 2021.