

# PyQBench: a Python library for benchmarking gate-based quantum computers

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## Abstract

We introduce PyQBench, an innovative open-source framework for benchmarking gate-based quantum computers. PyQBench can benchmark NISQ devices by verifying their capability of discriminating between two von Neumann measurements. PyQBench offers a simplified, ready-to-use, command line interface (CLI) for running benchmarks using a predefined family of measurements. For more advanced scenarios, PyQBench offers a way of employing user-defined measurements instead of predefined ones.

*Keywords:* Quantum computing, Benchmarking quantum computers, Discrimination of quantum measurements, Discrimination of von Neumann measurements, Open-source, Python programming

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## Current code version

C1	Current code version	0.1.1
C2	Permanent link to code/repository used for this code version	<a href="https://github.com/iitis/PyQBench">https://github.com/iitis/PyQBench</a>
C3	Code Ocean compute capsule	<a href="https://codeocean.com/capsule/89088992-9a27-4712-8525-d92a9b23060f/tree">https://codeocean.com/capsule/89088992-9a27-4712-8525-d92a9b23060f/tree</a>
C4	Legal Code License	Apache License 2.0
C5	Code versioning system used	git
C6	Software code languages, tools, and services used	Python, Qiskit, AWS Braket
C7	Compilation requirements, operating environments & dependencies	<code>Python &gt;= 3.8</code> <code>numpy ~= 1.22.0</code> <code>scipy ~= 1.7.0</code> <code>pandas ~= 1.5.0</code> <code>amazon-braket-sdk &gt;= 1.11.1</code> <code>pydantic ~= 1.9.1</code> <code>qiskit ~= 0.37.2</code> <code>mthree ~= 1.1.0</code> <code>tqdm ~= 4.64.1</code> <code>pyyaml ~= 6.0</code> <code>qiskit-braket-provider ~= 0.0.3</code>
C8	If available Link to developer documentation/manual	<a href="https://pyqbench.readthedocs.io/en/latest/">https://pyqbench.readthedocs.io/en/latest/</a>
C9	Support email for questions	<a href="mailto:dexter2206@gmail.com">dexter2206@gmail.com</a>

Table 1: Code metadata

## 1. Motivation and significance

Noisy Intermediate-Scale Quantum (NISQ) [1] devices are storming the market, with a wide selection of devices based on different architectures and accompanying software solutions. Among hardware providers offering public access to their gate-based devices, one could mention Rigetti [2], IBM [3], Oxford Quantum Group [4], IonQ [5] or Xanadu [6]. Other vendors offer devices operating in different paradigms. Notably, one could mention D-Wave [7] and their quantum annealers, or QuEra devices [8] based on neutral atoms. Most vendors provide their own software stack and application programming interface for accessing their devices. To name a few, Rigetti’s computers are available through their Forest SDK [9] and PyQuil library [10] and IBM Q [3]

12 computers can be accessed through Qiskit [11] or IBM Quantum Experience  
13 web interface [12]. Some cloud services, like Amazon Braket [13], offer ac-  
14 cess to several quantum devices under a unified API. On top of that, several  
15 libraries and frameworks can integrate with multiple hardware vendors. Ex-  
16 amples of such frameworks include IBM Q’s Qiskit or Zapata Computing’s  
17 Orquestra [14].

18 It is well known that NISQ devices have their limitations [15]. The ques-  
19 tion is to what extent those devices can perform meaningful computations?  
20 To answer this question, one has to devise a methodology for benchmarking  
21 them. For gate-based computers, on which this paper focuses, there al-  
22 ready exist several approaches. One could mention randomized benchmark-  
23 ing [16, 17, 18, 19, 20], benchmarks based on the quantum volume [21, 22, 23].

24 In this paper, we introduce a different approach to benchmarking gate-  
25 based devices with a simple operational interpretation. In our method, we  
26 test how well the given device is at guessing which of the two known von  
27 Neumann measurements were performed during the experiment. We imple-  
28 mented our approach in an open-source Python library called PyQBench.  
29 The library supports any device available through the Qiskit library, and  
30 thus can be used with providers such as IBM Q or Amazon Braket. Along  
31 with the library, the PyQBench package contains a command line tool for  
32 running most common benchmarking scenarios.

## 33 2. Existing benchmarking methodologies and software

34 Unsurprisingly, PyQBench is not the only software package for bench-  
35 marking gate-based devices. While we believe that our approach has signif-  
36 icant benefits over other benchmarking techniques, for completeness, in this  
37 section we discuss some of the currently available similar software.

38 Probably the simplest benchmarking method one could devise is simply  
39 running known algorithms and comparing outputs with the expected ones.  
40 Analyzing the frequency of the correct outputs, or the deviation between  
41 actual and expected outputs distribution provides then a metric of the per-  
42 formance of a given device. Libraries such as Munich Quantum Toolkit  
43 (MQT) [24, 25] or SupermarQ [26, 27] contain benchmarks leveraging mul-  
44 tiple algorithms, such as Shor’s algorithm or Grover’s algorithm. Despite  
45 being intuitive and easily interpretable, such benchmarks may have some  
46 problems. Most importantly, they assess the usefulness of a quantum device  
47 only for a very particular algorithm, and it might be hard to extrapolate  
48 their results to other algorithms and applications. For instance, the inability  
49 of a device to consistently find factorizations using Shor’s algorithms does  
50 not tell anything about its usefulness in Variational Quantum Algorithm’s.

Another possible approach to benchmarking quantum computers is randomized benchmarking. In this approach, one samples circuits to be run from some predefined set of gates (e.g. from the Clifford group) and tests how much the output distribution obtained from the device running these circuits differs from the ideal one. It is also common to concatenate randomly chosen circuits with their inverses (which should yield the identity circuit) and run those concatenated circuits on the device. Libraries implementing this approach include Qiskit [28] or PyQuil [29].

Another quantity used for benchmarking NISQ devices is quantum volume. The quantum volume characterizes capacity of a device for solving computational problems. It takes into account multiple factors like number of qubits, connectivity and measurement errors. The Qiskit library allows one to measure quantum volume of a device by using its `qiskit.ignis.verification.quantum_volume`. Other implementations of Quantum Volume can be found as well, see e.g. [30].

Finally, we should mention cross-entropy benchmarking [31], which was utilized in validation of the Sycamore-53 QPU supremacy experiments [32]. In this approach, the quality of an algorithm implemented on the QPU is measured by calculating the cross entropy of bit-strings actually sampled from the QPU, compared to ideal bitstrings.

### 3. Preliminaries and discrimination scheme approach

In this section, we describe how the benchmarking process in PyQBench works. We start by discussing necessary mathematical preliminaries. Then, we present the general form of the discrimination scheme used in PyQBench and practical considerations on how to implement it taking into account the limitations of the current NISQ devices. We encourage the readers interested in a more in-depth discussion of the mathematical foundations behind our discrimination scheme to read Section 1 in the supplemental materials.

#### 3.1. Von Neumann Measurements

A von Neumann measurement  $\mathcal{P}$  is a collection of rank-one projectors  $\{|u_0\rangle\langle u_0|, \dots, |u_{d-1}\rangle\langle u_{d-1}|\}$ , called effects, that sum up to the identity operator, i.e.  $\sum_{i=0}^{d-1} |u_i\rangle\langle u_i| = \mathbb{1}$ . If  $U$  is a unitary matrix of size  $d$ , one can construct a von Neumann measurement  $\mathcal{P}_U$  by taking projectors onto its columns. In this case we say that  $\mathcal{P}_U$  is described by the matrix  $U$ .

Typically, NISQ devices can only perform measurements in computational  $Z$ -basis, i.e.  $U = \mathbb{1}$ . To implement an arbitrary von Neumann measurement  $\mathcal{P}_U$ , one has to first apply  $U^\dagger$  to the measured system and then follow with  $Z$ -basis measurement. This process, depicted in Fig. 1, can be viewed as

performing a change of basis in which measurement is performed prior to measurement in the computational basis.

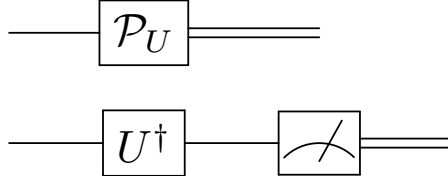


Figure 1: Implementation of a von Neumann measurement using measurement in computational basis. The upper circuit shows a symbolic representation of a von Neumann measurement  $\mathcal{P}_U$ . The bottom, equivalent circuit depicts its decomposition into a change of basis followed by measurement in the  $Z$  basis.

### 3.2. Discrimination scheme

Benchmarks in PyQBench work by experimentally determining the probability of correct discrimination between two von Neumann measurements by the device under test and comparing the result with the ideal, theoretical predictions.

Without loss of generality<sup>1</sup>, we consider discrimination task between single qubit measurements  $\mathcal{P}_1$ , performed in the computational  $Z$ -basis, and an alternative measurement  $\mathcal{P}_U$  performed in the basis  $U$ . The discrimination scheme presented in Fig. 2 requires an auxiliary qubit. First, the joint system is prepared in some state  $|\psi_0\rangle$ . Then, one of the measurements, either  $\mathcal{P}_U$  or  $\mathcal{P}_1$ , is performed on the first part of the system. Based on its outcome  $i$ , we choose another binary measurement  $\mathcal{P}_{V_i}$  and perform it on the second qubit, obtaining the outcome  $j$ . Finally, if  $j = 0$ , we say that the performed measurement is  $\mathcal{P}_U$ , otherwise we say that it was  $\mathcal{P}_1$ .

Note, however, that the discrimination scheme described above can work regardless of dimensionality of the unitary  $U$ . The main difference is the dimension of the auxiliary system, which in general can be larger than two. This dimension depends on the Schmidt rank of the optimal input state. However, for most discrimination schemes, the Schmidt rank equals at most two, and hence the auxiliary system is also a qubit, see [33] for details. Note that the final measurement  $\mathcal{P}_{V_i}$  is always binary, independently of the dimension of auxiliary system.

Naturally, we need to repeat the same procedure multiple times for both measurements to obtain a reliable estimate of the underlying probability

<sup>1</sup>Explaining why we can consider only discrimination scheme between  $\mathcal{P}_1$  and  $\mathcal{P}_U$  is beyond the scope of this paper. See [33] for a in depth explanation.

115 distribution. In PyQBench, we assume that the experiment is repeated the  
 116 same number of times for both  $\mathcal{P}_U$  and  $\mathcal{P}_1$ .

117 In principle, our discrimination scheme could be used with any choice of  
 118  $|\psi_0\rangle$  and final measurements  $\mathcal{P}_{V_i}$ . However, we argue that it is best to choose  
 119 those components so that they maximize the probability of correct discrim-  
 120 ination. To see that, suppose that some choice of  $|\psi_0\rangle, \mathcal{P}_{V_0}, \mathcal{P}_{V_1}$  allows for  
 121 correctly discriminating between two measurements with probability equal  
 122 to one, i.e. on a perfect quantum computer you will always make a cor-  
 123 rect guess. Then, on real hardware, we might obtain any empirical value in  
 124 range  $[\frac{1}{2}, 1]$ . On the other hand, if we choose the components of our scheme  
 125 such that the successful discrimination probability is  $\frac{3}{5}$ , the possible range  
 126 of empirically obtainable probabilities is only  $[\frac{1}{2}, \frac{3}{5}]$ . Hence, in the second  
 127 case, the discrepancy between theoretical and empirical results will be less  
 128 pronounced.

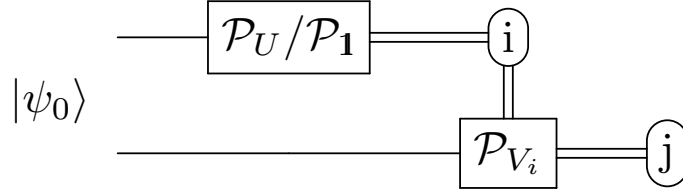


Figure 2: Theoretical scheme of discrimination between von Neumann measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$ .

### 129 3.2.1. Implementation of discrimination scheme on actual NISQ devices

130 Current NISQ devices are unable to perform conditional measurements,  
 131 which is the biggest obstacle to implementing our scheme on real hardware.  
 132 However, we circumvent this problem by slightly adjusting our scheme so  
 133 that it only uses components available on current devices. For this purpose,  
 134 we use two possible options: using a postselection or a direct sum  $V_0^\dagger \oplus V_1^\dagger$ .

#### 135 **Scheme 1.** (Postselection)

136 The first idea uses a postselection scheme. In the original scheme, we  
 137 measure the first qubit and only then determine which measurement should  
 138 be performed on the second one. Instead of doing this choice, we can run two  
 139 circuits, one with  $\mathcal{P}_{V_0}$  and one with  $\mathcal{P}_{V_1}$  and measure both qubits. We then  
 140 discard the results of the circuit for which label  $i$  does not match measurement  
 141 label  $k$ . Hence, the circuit for postselection looks as depicted in Fig. 3.

142 To perform the benchmark, one needs to run multiple copies of the post-  
 143 selection circuit, with both  $\mathcal{P}_U$  and  $\mathcal{P}_1$ . Each circuit has to be run in both



Figure 3: A schematic representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using postselection approach. In postselection scheme, one runs such circuits for both  $k = 0, 1$  and discards results for cases when there is a mismatch between  $k$  and  $i$ .

144 variants, one with final measurement  $\mathcal{P}_{V_0}$  and the second with the final mea-  
 145 surement  $\mathcal{P}_{V_1}$ . The experiments can thus be grouped into classes identified by  
 146 tuples of the form  $(\mathcal{Q}, k, i, j)$ , where  $\mathcal{Q} \in \{\mathcal{P}_U, \mathcal{P}_1\}$  denotes the chosen mea-  
 147 surement,  $k \in \{0, 1\}$  designates the final measurement used, and  $i \in \{0, 1\}$   
 148 and  $j \in \{0, 1\}$  being the labels of outcomes as presented in Fig. 3. We  
 149 then discard all the experiments for which  $i \neq k$ . The total number of valid  
 150 experiments is thus:

$$N_{\text{total}} = \#\{(\mathcal{Q}, k, i, j) : k = i\}. \quad (1)$$

151 Finally, we count the valid experiments resulting in successful discrimi-  
 152 nation. If we have chosen  $\mathcal{P}_U$ , then we guess correctly iff  $j = 0$ . Similarly,  
 153 for  $\mathcal{P}_1$ , we guess correctly iff  $j = 1$ . If we define

$$N_{\mathcal{P}_U} = \#\{(\mathcal{Q}, k, i, j) : \mathcal{Q} = \mathcal{P}_U, k = i, j = 0\}, \quad (2)$$

$$N_{\mathcal{P}_1} = \#\{(\mathcal{Q}, k, i, j) : \mathcal{Q} = \mathcal{P}_1, k = i, j = 1\}, \quad (3)$$

154 then the empirical success probability can be computed as

$$p_{\text{succ}}(\mathcal{P}_U, \mathcal{P}_1) = \frac{N_{\mathcal{P}_U} + N_{\mathcal{P}_1}}{N_{\text{total}}}. \quad (4)$$

155 The  $p_{\text{succ}}$  is the quantity reported to the user as the result of the benchmark.

156 **Scheme 2.** (Direct sum)

157 The second idea uses the direct sum  $V_0^\dagger \oplus V_1^\dagger$  implementation. Here,  
 158 instead of performing a conditional measurement  $\mathcal{P}_{V_k}$ , where  $k \in \{0, 1\}$ , we  
 159 run circuits presented in Fig. 4.

160 One can see why such a circuit is equivalent to the original discrimination  
 161 scheme. If we rewrite the block-diagonal matrix  $V_0^\dagger \oplus V_1^\dagger$  as follows:

$$V_0^\dagger \oplus V_1^\dagger = |0\rangle\langle 0| \otimes V_0^\dagger + |1\rangle\langle 1| \otimes V_1^\dagger, \quad (5)$$

162 we can see that the direct sum in Eq. (5) commutes with the measurement  
 163 on the first qubit. Thanks to this, we can switch the order of operations to



Figure 4: A schematic representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using the  $V_0^\dagger \oplus V_1^\dagger$  direct sum.

164 obtain the circuit from Fig. 5. Now, depending on the outcome  $i$ , one of the  
 165 summands in Eq. (5) vanishes, and we end up performing exactly the same  
 166 operations as in the original scheme.

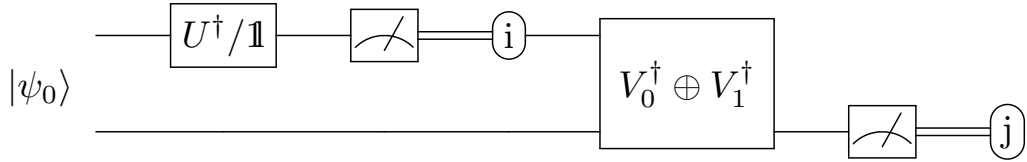


Figure 5: Rewritten representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using the  $V_0^\dagger \oplus V_1^\dagger$  direct sum.

167 In this scheme, the experiment can be characterized by a pair  $(\mathcal{Q}, i, j)$ ,  
 168 where  $\mathcal{Q} = \{\mathcal{P}_U, \mathcal{P}_1\}$  and  $i, j \in \{0, 1\}$  are the output labels. The number of  
 169 successful trials for  $U$  and  $\mathbb{1}$ , respectively, can be written as

$$N_{\mathcal{P}_U} = \#\{(\mathcal{Q}, i, j) : \mathcal{Q} = \mathcal{P}_U, j = 0\}, \quad (6)$$

$$N_{\mathcal{P}_1} = \#\{(\mathcal{Q}, i, j) : \mathcal{Q} = \mathcal{P}_1, j = 1\}. \quad (7)$$

170 Then, the probability of correct discrimination between  $\mathcal{P}_U$  and  $\mathcal{P}_1$  is given  
 171 by

$$p_{\text{succ}} = \frac{N_{\mathcal{P}_U} + N_{\mathcal{P}_1}}{N_{\text{total}}}, \quad (8)$$

172 where  $N_{\text{total}}$  is the number of trials.

173 Compared to these approaches, our approach allows for very simple operational  
 174 interpretation of the scheme and its results. This is especially useful for  
 175 newcomers to the field, who may be put off by more complicated approaches.  
 176 Another benefit is, especially for advanced users, the ability to control resources  
 177 utilized during the benchmarking. We can consider here resources such as  
 178 entanglement or coherence. Finally, the figure of merit we wish calculate



179 and to which we compare are results is fairly simple to obtain. The main  
180 downside of our approach is the exponential number of circuits we need to  
181 consider.

## 182 4. Software description

183 This section is divided into two parts. In Section 4.1 we describe func-  
184 tionalities of PyQBench package. Next, in Section 4.2, we give a general  
185 overview of the software architecture.

### 186 4.1. Software Functionalities

187 The PyQBench can be used in two modes: as a Python library and as a  
188 CLI script. When used as a library, PyQBench allows the customization of  
189 discrimination scheme. The user provides a unitary matrix  $U$  defining the  
190 measurement to be discriminated, the discriminator  $|\psi_0\rangle$ , and unitaries  $V_0$   
191 and  $V_1$  describing the final measurement. The PyQBench library provides  
192 then the following functionalities.

- 193 1. Assembling circuits for both postselection and direct sum-based dis-  
194 crimination schemes.
- 195 2. Executing the whole benchmarking scenario on specified backend (ei-  
196 ther real hardware or software simulator).
- 197 3. Interpreting the obtained outputs in terms of discrimination probab-  
198 ities.

199 Note that the execution of circuits by PyQBench is optional. Instead, the  
200 user might want to opt in for fine-grained control over the execution of the  
201 circuits. For instance, suppose the user wants to simulate the discrimination  
202 experiment on a noisy simulator. In such a case, they can define the necessary  
203 components and assemble the circuits using PyQBench. The circuits can  
204 then be altered, e.g. to add noise to particular gates, and then run using any  
205 Qiskit backend by the user. Finally, PyQBench can be used to interpret the  
206 measurements to obtain discrimination probability.

207 The PyQBench library also contains a readily available implementation  
208 of all necessary components needed to run discrimination experiments for  
209 parametrized Fourier family of measurements (see Section 3 in supplemental  
210 material). However, if one only wishes to use this particular family of mea-  
211 surements in their benchmarks, then using PyQBench as a command line  
212 tool might be more straightforward. PyQBench's command line interface  
213 allows running the benchmarking process without writing Python code. The  
214 configuration of CLI is done by YAML [34] files describing the benchmark

215 to be performed and the description of the backend on which the benchmark  
 216 should be run. The same benchmark can be used with different backends  
 217 and vice versa.

## 218 4.2. Software Architecture

### 219 4.2.1. Overview of the software structure

220 As already described, PyQBench can be used both as a library and a CLI.  
 221 Both functionalities are implemented as a part of **qbench** Python package.  
 222 The exposed CLI tool is also named **qbench**. For brevity, we do not discuss  
 223 the exact structure of the package here, and instead refer an interested reader  
 224 to the source code available at GitHub [35] or at the reference manual [36].

225 PyQBench can be installed from official Python Package Index (PyPI)  
 226 by running `pip install pyqbench`. In a properly configured Python en-  
 227 vironment the installation process should also make the **qbench** command  
 228 available to the user without a need for further configuration.

### 229 4.2.2. Integration with hardware providers and software simulators

230 PyQBench is built around the Qiskit [11] ecosystem. Hence, both the  
 231 CLI tool and the **qbench** library can use any Qiskit-compatible backend.  
 232 This includes, IBM Q backends (available by default in Qiskit) and Amazon  
 233 Braket devices and simulators (available through **qiskit-braket-provider**  
 234 package [37, 38]).

235 When using PyQBench as library, instances of Qiskit backends can be  
 236 passed to functions that expect them as parameters. However, in CLI mode,  
 237 the user has to provide a YAML file describing the backend. An example  
 238 of such file can be found in Section 5, and the detailed description of the  
 239 expected format can be found at PyQBench’s documentation.

### 240 4.2.3. Command Line Interface

241 The Command Line Interface (CLI) of PyQBench has nested structure.  
 242 The general form of the CLI invocation is shown in listing 1.

Listing 1: Invocation of **qbench** script

---

243 **qbench** <benchmark-type> <command> <parameters>

---

246 Currently, PyQBench’s CLI supports only one type of benchmark (discrimi-  
 247 nation of parametrized Fourier family of measurements), but we decided on  
 248 hierarchically structuring the CL to allow for future extensions. Thus, the  
 249 only accepted value of <benchmark-type> is **disc-fourier**. The **qbench**  
 250 **disc-fourier** command has four subcommands:

- 251 • **benchmark**: run benchmarks. This creates either a result YAML file  
252 containing the measurements or an intermediate YAML file for asyn-  
253 chronous experiments.
- 254 • **status**: query status of experiments submitted for given benchmark.  
255 This command is only valid for asynchronous experiments.
- 256 • **resolve**: query the results of asynchronously submitted experiments  
257 and write the result YAML file. The output of this command is almost  
258 identical to the result obtained from synchronous experiments.
- 259 • **tabulate**: interpret the results of a benchmark and summarize them  
260 in the CSV file.

261 We present usage of each of the above commands later in section 5.

#### 262 4.2.4. *Asynchronous vs. synchronous execution*

263 PyQBench’s CLI can be used in synchronous and asynchronous modes.  
264 The mode of execution is defined in the YAML file describing the backend  
265 (see Section 5 for an example of this configuration). We decided to couple  
266 the mode of execution to the backend description because some backends  
267 cannot work in asynchronous mode.

268 When running `qbench disc-fourier benchmark` in asynchronous mode,  
269 the PyQBench submits all the circuits needed to perform a benchmark and  
270 then writes an intermediate YAML file containing metadata of submitted  
271 experiments. In particular, this metadata contains information on correlating  
272 submitted job identifiers with particular circuits. The intermediate file can  
273 be used to query the status of the submitted jobs or to resolve them, i.e. to  
274 wait for their completion and get the measurement outcomes.

275 In synchronous mode, PyQBench first submits all jobs required to run the  
276 benchmark and then immediately waits for their completion. The advantage  
277 of this approach is that no separate invocation of `qbench` command is needed  
278 to actually download the measurement outcomes. The downside, however,  
279 is that if the script is interrupted while the command is running, the inter-  
280 mediate results will be lost. Therefore, we recommend using asynchronous  
281 mode whenever possible.

## 282 5. Illustrative examples

283 In this section, we demonstrate the usage of PyQBench. For brevity, we  
284 decided to present only the usage of the CLI tool, as it is likely to be the  
285 most popular use case. We refer readers interested in implementing their

discrimination schemes using custom measurements to PyQBench’s documentation [36], where we describe the whole process, and to the Section 2 in the supplemental material, where we discuss the relevant mathematical details.

### 5.1. Using *qbench* CLI

PyQBench offers a simplified way of conducting benchmarks using a Command Line Interface (CLI). The workflow with PyQBench’s CLI can be summarized as the following list of steps:

1. Preparing configuration files describing the backend and the experiment scenario.
2. Submitting/running experiments. Depending on the experiment scenario, execution can be synchronous, or asynchronous.
3. (optional) Checking the status of the submitted jobs if the execution is asynchronous.
4. Resolving asynchronous jobs into the actual measurement outcomes.
5. Converting obtained measurement outcomes into tabulated form.

#### 5.1.1. Preparing configuration files

The configuration of PyQBench CLI is driven by YAML files. The first configuration file describes the experiment scenario to be executed. The second file describes the backend. Typically, this backend will correspond to the physical device to be benchmarked, but for testing purposes, one might as well use any other Qiskit-compatible backend including simulators. Let us first describe the experiment configuration file, which might look as follow.

Listing 2: Defining the experiment

---

```

type: discrimination-fourier
qubits:
  - target: 0
    ancilla: 1
  - target: 1
    ancilla: 2
angles:
  start: 0
  stop: 2 * pi
  num_steps: 3
gateset: ibmq
method: direct_sum
num_shots: 100

```

---

324 The second configuration file describes the backend. We decided to de-  
 325 couple the experiment and the backend files because it facilitates their reuse.  
 326 For instance, the same experiment file can be used to run benchmarks on  
 327 multiple backends, and the same backend description file can be used with  
 328 multiple experiments.

329 Different Qiskit backends typically require different data for their initial-  
 330 ization. Hence, there are multiple possible formats of the backend config-  
 331 uration files understood by PyQBench. We refer the interested reader to  
 332 the PyQBench’s documentation. Below we describe an example YAML file  
 333 describing IBM Q backend named Quito.

Listing 3: IBMQ backend

---

```
334 name: ibmq_quito
335 asynchronous: false
336 provider:
337   hub: ibm-q
338   group: open
339   project: main
```

---

342 IBMQ backends typically require an access token to IBM Quantum Experi-  
 343 ence. Since it would be unsafe to store it in plain text, the token has to be  
 344 configured separately in `IBMQ_TOKEN` environmental variable.

#### 345 5.1.2. Running the experiment and collecting measurements data

346 After preparing YAML files defining experiment and backend, running the  
 347 benchmark can be launched by using the following command line invocation:

---

```
348 qbench disc-fourier benchmark experiment_file.yml backend_file.yml
349
350
```

---

351 The output file will be printed to stdout. Optionally, the `--output OUTPUT`  
 352 parameter might be provided to write the output to the `OUTPUT` file instead.

---

```
353 qbench disc-fourier benchmark experiment_file.yml backend_file.yml
354 --output async_results.yml
355
356
```

---

357 The result of running the above command can be twofold:

- 358 • If the backend is asynchronous, the output will contain intermediate  
 359 data containing, amongst others, `job_ids` correlated with the circuit  
 360 they correspond to.
- 361 • If the backend is synchronous, the output will contain measurement  
 362 outcomes (bitstrings) for each of the circuits run.

For the synchronous experiment, the part of the output looks similar to the one below. The whole YAML file can be seen in Section ?? in the supplemental material.

---

```

data:
- target: 0
  ancilla: 1
  phi: 0.0
  results_per_circuit:
  - name: id
    histogram: {'00': 28, '01': 26, '10': 21, '11': 25}
    mitigation_info:
      target: {prob_meas0_prep1: 0.052200000000000024,
        prob_meas1_prep0: 0.0172}
      ancilla: {prob_meas0_prep1: 0.059000000000000005,
        prob_meas1_prep0: 0.0202}
    mitigated_histogram: {'00': 0.2637212373658018, '01':
      0.25865061319892463, '10': 0.2067279352110304, '11':
      0.2709002142242433}

```

---

### 5.1.3. (Optional) Getting status of asynchronous jobs

PyQBench provides also a helper command that will fetch the statuses of asynchronous jobs. The command is:

---

```

qbench disc-fourier status async_results.yml

```

---

and it will display dictionary with histogram of statuses.

### 5.1.4. Resolving asynchronous jobs

For asynchronous experiments, the stored intermediate data has to be resolved in actual measurements' outcomes. The following command will wait until all jobs are completed and then write a result file.

---

```

qbench disc-fourier resolve async-results.yml resolved.yml

```

---

The resolved results, stored in `resolved.yml`, would look just like if the experiment was run synchronously. Therefore, the final results will look the same no matter in which mode the benchmark was run, and hence in both cases the final output file is suitable for being an input for the command computing the discrimination probabilities.

### 402 5.1.5. Computing probabilities

403 As a last step in the processing workflow, the results file has to be passed  
404 to `tabulate` command:

---

```
405 qbench disc-fourier tabulate results.yml results.csv
```

---

A sample CSV file is provided in Table 2.

target	ancilla	phi	ideal_prob	disc_prob	mit_disc_prob
0	1	0	0.5	0.46	0.45
0	1	3.14	1	0.95	0.98
0	1	6.28	0.5	0.57	0.58
1	2	0	0.5	0.57	0.57
1	2	3.14	1	0.88	0.94
1	2	6.28	0.5	0.55	0.56

Table 2: The resulting CSV file contains table with columns `target`, `ancilla`, `phi`, `ideal_prob`, `disc_prob` and, optionally, `mit_disc_prob`. Each row in the table describes results for a tuple of (`target`, `ancilla`, `phi`). The reference optimal value of discrimination probability is present in `ideal_prob` column, whereas the obtained, empirical discrimination probability can be found in the `disc_prob` column. The `mit_disc_prob` column contains empirical discrimination probability after applying the `Mthree` error mitigation [39, 40], if it was applied.

408

## 409 6. Impact

410 With the surge of availability of quantum computing architectures in  
411 recent years it becomes increasingly difficult to keep track of their relative  
412 performance. To make this case even more difficult, various providers give  
413 access to different figures of merit for their architectures. Our package allows  
414 the user to test various architectures, available through `qiskit` and Amazon  
415 BraKet using problems with simple operational interpretation. We provide  
416 one example built-in in the package. Furthermore, we provide a powerful  
417 tool for the users to extend the range of available problems in a way that  
418 suits their needs.

419 Due to this possibility of extension, the users are able to test specific  
420 aspects of their architecture of interest. For example, if their problem is  
421 related to the amount of coherence (the sum of absolute value of off-diagonal  
422 elements) of the states present during computation, they are able to quickly  
423 prepare a custom experiment, launch it on desired architectures, gather the

424 result, based on which they can decide which specific architecture they should  
425 use.

426 Finally, we provide the source code of PyQBench on GitHub [35] under an  
427 open source license which will allow users to utilize and extend our package  
428 in their specific applications.

## 429 7. Conclusions

430 In this paper, we presented a Python library PyQBench, an innovative  
431 open-source framework for benchmarking gate-based quantum computers.  
432 PyQBench can benchmark NISQ devices by verifying their capability of dis-  
433 criminating between two von Neumann measurements. PyQBench offers a  
434 simplified, ready-to-use, command line interface (CLI) for running bench-  
435 marks using a predefined parameterized Fourier family of measurements. For  
436 more advanced scenarios, PyQBench offers a way of employing user-defined  
437 measurements instead of predefined ones.

## 438 8. Conflict of Interest

439 We wish to confirm that there are no known conflicts of interest associated  
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## 450 References

- 451 [1] John Preskill. Quantum computing in the nisc era and beyond. *Quan-*  
452 *tum*, 2:79, 2018.
- 453 [2] Rigetti computing. <https://www.rigetti.com/>. Accessed on 2023-02-  
454 18.
- 455 [3] IBM Quantum. <https://www.ibm.com/quantum>. Accessed on 2023-02-  
456 18.



- 457 [4] Oxford quantum. <http://oxfordquantum.org/>. Accessed on 2023-02-  
458 18.
- 459 [5] IonQ. <https://ionq.com/>. Accessed on 2023-02-18.
- 460 [6] Xanadu. <https://www.xanadu.ai/>. Accessed on 2023-02-18.
- 461 [7] D-Wave Systems. <https://www.dwavesys.com/>. Accessed on 2023-02-  
462 18.
- 463 [8] QuEra. <https://www.quera.com/>. Accessed on 2023-02-18.
- 464 [9] QCS Documentation. <https://docs.rigetti.com/qcs/>. Accessed on  
465 2023-02-18.
- 466 [10] PyQuil Documentation. [https://pyquil-docs.rigetti.com/en/  
467 stable/](https://pyquil-docs.rigetti.com/en/stable/). Accessed on 2023-02-18.
- 468 [11] Qiskit. <https://qiskit.org/>. Accessed on 2023-02-18.
- 469 [12] IBM Quantum Experience. <https://quantum-computing.ibm.com/>.  
470 Accessed on 2023-02-18.
- 471 [13] Amazon Braket. <https://aws.amazon.com/braket/>. Accessed on  
472 2023-02-18.
- 473 [14] Zapata Orchestra Platform. [https://www.zapatacomputing.com/  
474 orchestra-platform/](https://www.zapatacomputing.com/orchestra-platform/). Accessed on 2023-02-18.
- 475 [15] J. Preskill. Quantum computing 40 years later. *arXiv preprint*  
476 *arXiv:2106.10522*, 2021.
- 477 [16] Y. Liu, M. Otten, R. Bassirianjahromi, L. Jiang, and B. Fefferman.  
478 Benchmarking near-term quantum computers via random circuit sam-  
479 pling. *arXiv preprint arXiv:2105.05232*, 2021.
- 480 [17] E. Knill, D. Leibfried, R. Reichle, J. Britton, R. B. Blakestad, J. D.  
481 Jost, C. Langer, R. Ozeri, S. Seidelin, and D. J. Wineland. Randomized  
482 benchmarking of quantum gates. *Physical Review A*, 77(1):012307, 2008.
- 483 [18] J. J. Wallman and S. T. Flammia. Randomized benchmarking with  
484 confidence. *New Journal of Physics*, 16(10):103032, 2014.
- 485 [19] J. Helsen, I. Roth, E. Onorati, A. H. Werner, and J. Eisert. General  
486 framework for randomized benchmarking. *PRX Quantum*, 3(2):020357,  
487 2022.

- 488 [20] A. Cornelissen, J. Bausch, and A. Gilyén. Scalable benchmarks for gate-  
489 based quantum computers. *arXiv preprint arXiv:2104.10698*, 2021.
- 490 [21] A. W. Cross, L. S. Bishop, S. Sheldon, P. D. Nation, and J. M. Gam-  
491 betta. Validating quantum computers using randomized model circuits.  
492 *Physical Review A*, 100(3):032328, 2019.
- 493 [22] N. Moll, P. Barkoutsos, L. S. Bishop, J. M. Chow, A. Cross, D. J.  
494 Egger, S. Filipp, A. Fuhrer, J. M. Gambetta, M. Ganzhorn, A. Kandala,  
495 A. Mezzacapo, P. Müller, W. Riess, G. Salis, J. Smolin, I. Tavernelli, and  
496 K. Temme. Quantum optimization using variational algorithms on near-  
497 term quantum devices. *Quantum Science and Technology*, 3(3):030503,  
498 2018.
- 499 [23] E. Pelofske, A. Bäertschi, and S. Eidenbenz. Quantum volume in prac-  
500 tice: What users can expect from nisq devices. *IEEE Transactions on*  
501 *Quantum Engineering*, 3:1–19, 2022.
- 502 [24] N. Quetschlich, L. Burgholzer, and R. Wille. Mqt bench: Benchmarking  
503 software and design automation tools for quantum computing. *arXiv*  
504 *preprint arXiv:2204.13719*, 2022.
- 505 [25] MQTBench. <https://github.com/cda-tum/MQTBench>. Accessed on  
506 2023-02-18.
- 507 [26] T. Tomesh, P. Gokhale, V. Omole, G. S. Ravi, K. N. Smith, J. Visslai,  
508 X. Wu, N. Hardavellas, M. R. Martonosi, and F. T. Chong. SupermarQ:  
509 A scalable quantum benchmark suite. In *2022 IEEE International Sym-*  
510 *posium on High-Performance Computer Architecture (HPCA)*, pages  
511 587–603. IEEE, 2022.
- 512 [27] SupermarQ. <https://github.com/SupertechLabs/SupermarQ>. Ac-  
513 cessed on 2023-02-18.
- 514 [28] Qiskit benchmarks. [https://github.com/qiskit-community/](https://github.com/qiskit-community/qiskit-benchmarks)  
515 [qiskit-benchmarks](https://github.com/qiskit-community/qiskit-benchmarks). Accessed on 2023-02-18.
- 516 [29] Forest Benchmarking: QCVV using PyQuil. [https://github.com/](https://github.com/rigetti/forest-benchmarking)  
517 [rigetti/forest-benchmarking](https://github.com/rigetti/forest-benchmarking). Accessed on 2023-02-18.
- 518 [30] Quantum volume in practice. [https://github.com/lanl/](https://github.com/lanl/Quantum-Volume-in-Practice)  
519 [Quantum-Volume-in-Practice](https://github.com/lanl/Quantum-Volume-in-Practice). Accessed on 2023-02-18.

- [31] Sergio Boixo, Sergei V Isakov, Vadim N Smelyanskiy, Ryan Babbush, Nan Ding, Zhang Jiang, Michael J Bremner, John M Martinis, and Hartmut Neven. Characterizing quantum supremacy in near-term devices. *Nature Physics*, 14(6):595–600, 2018.
- [32] Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando GSL Brandao, David A Buell, et al. Quantum supremacy using a programmable superconducting processor. *Nature*, 574(7779):505–510, 2019.
- [33] Z. Puchała, Ł. Paweł, A. Krawiec, and R. Kukulski. Strategies for optimal single-shot discrimination of quantum measurements. *Physical Review A*, 98(4):042103, 2018.
- [34] YAML Ain’t Markup Language (YAML) Version 1.2. <https://yaml.org/spec/1.2.2/>. Accessed on 2023-02-18.
- [35] PyQBench GitHub Repository. <https://github.com/iitis/PyQBench>. Accessed on 2023-02-18.
- [36] PyQBench Documentation. <https://pyqbench.readthedocs.io/en/latest/>. Accessed on 2023-02-18.
- [37] Introducing the Qiskit Provider for Amazon Braket. <https://aws.amazon.com/blogs/quantum-computing/introducing-the-qiskit-provider-for-amazon-braket/>. Accessed on 2023-02-18.
- [38] Qiskit Braket Provider GitHub Repository. <https://github.com/qiskit-community/qiskit-braket-provider>. Accessed on 2023-02-18.
- [39] mthree Documentation. <https://qiskit.org/documentation/partners/mthree/stubs/mthree.M3Mitigation.html>. Accessed on 2023-02-10.
- [40] P. D. Nation, H. Kang, N. Sundaresan, and J. M. Gambetta. Scalable mitigation of measurement errors on quantum computers. *PRX Quantum*, 2(4):040326, 2021.