

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

It is well known that NISQ devices have their limitations [17]. The question is to what extent those devices can perform meaningful computations? To answer this question, one has to devise a methodology for benchmarking them. For gate-based computers, on which this paper focuses, there already exist several approaches. One could mention randomized benchmarking [18, 19, 20, 21, 22], benchmarks based on the quantum volume [23, 24, 25].

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

## 2. Existing benchmarking methodologies and software

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

Probably the simplest benchmarking method one could devise is simply running known algorithms and comparing outputs with the expected ones. Analyzing the frequency of the correct outputs, or the deviation between actual and expected outputs distribution provides then a metric of the performance of a given device. Libraries such as Munich Quantum Toolkit (MQT) [26, 27] or SupermarQ [28, 29] contain benchmarks leveraging multiple algorithms, such as Shor’s algorithm or Grover’s algorithm. Despite being intuitive and easily interpretable, such benchmarks may have some problems. Most importantly, they assess the usefulness of a quantum device only for a very particular algorithm, and it might be hard to extrapolate their results to other algorithms and applications. For instance, the inability of a device to consistently find factorizations using Shor’s algorithms does 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 [30] or PyQuil [31]. Another, equally popular, benchmarking method is quantum tomography [32]. Implementation of quantum tomography for benchmarking NISQ devices can be found in [33].

In [34], the authors evaluated several IBM-Q machines using seven benchmarks taking into account the errors and execution time.

QASMBench [35] is one of the first benchmark suites aiming at evaluating NISQ devices using quantum applications from a broad range of domains, mainly using an approach based on fidelity estimation. The benchmark presented in the paper compares the fidelity of execution among the IBM-Q machines, the IonQ QPU and the Rigetti Aspen M-1 system.

Another quantity used for benchmarking NISQ devices is quantum volume. The quantum volume characterizes the capacity of a device for solving computational problems. It takes into account multiple factors like the number of qubits, connectivity and measurement errors. The Qiskit library allows one to measure the 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. [36].

~~Finally, we should~~ We should also mention cross-entropy benchmarking [37], which was utilized in validation of the Sycamore-53 QPU supremacy experiments [38]. 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.

Finally, it is worth pointing out there is an ongoing effort towards standardization of benchmarking of quantum computers. In [39], the authors present plans for designing a benchmarking suite based on measuring a set of standardized key performance indicators (KPIs).

### 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

90 in a more in-depth discussion of the mathematical foundations behind our  
 91 discrimination scheme to read Section 1 in the supplemental materials.

### 92 3.1. Von Neumann Measurements

93 A von Neumann measurement  $\mathcal{P}$  is a collection of rank-one projectors  
 94  $\{|u_0\rangle\langle u_0|, \dots, |u_{d-1}\rangle\langle u_{d-1}|\}$ , called effects, that sum up to the identity op-  
 95 erator, 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  
 96 construct a von Neumann measurement  $\mathcal{P}_U$  by taking projectors onto its  
 97 columns. In this case we say that  $\mathcal{P}_U$  is described by the matrix  $U$ .

98 Typically, NISQ devices can only perform measurements in computational  
 99  $Z$ -basis, i.e.  $U = \mathbb{1}$ . To implement an arbitrary von Neumann measurement  
 100  $\mathcal{P}_U$ , one has to first apply  $U^\dagger$  to the measured system and then follow with  
 101  $Z$ -basis measurement. This process, depicted in Fig. 1, can be viewed as  
 102 performing a change of basis in which measurement is performed prior to  
 103 measurement in the computational basis.

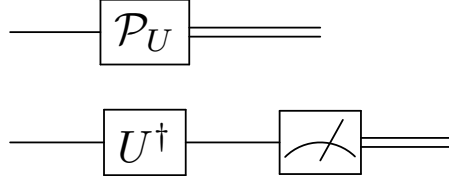


Figure 1: Implementation of a von Neumann measurement using measurement in computational basis. The upper circuit shows a symbolic representation of a von Neumann measurement  $\mathcal{P}_U$ . The bottom, equivalent circuit depicts its decomposition into a change of basis followed by measurement in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

### 104 3.2. Discrimination scheme

105 Benchmarks in PyQBench work by experimentally determining the prob-  
 106 ability of correct discrimination between two von Neumann measurements  
 107 by the device under test and comparing the result with the ideal, theoretical  
 108 predictions.

109 Without loss of generality<sup>1</sup>, we consider discrimination task between sin-  
 110 gle qubit measurements  $\mathcal{P}_1$ , performed in the computational  $Z$ -basis, and an  
 111 alternative measurement  $\mathcal{P}_U$  performed in the basis  $U$ . The discrimination  
 112 scheme presented in Fig. 2 requires an auxiliary qubit. First, the joint system  
 113 is prepared in some state  $|\psi_0\rangle$ . Then, one of the measurements, either  $\mathcal{P}_U$   
 114 or  $\mathcal{P}_1$ , is performed on the first part of the system. Based on its outcome

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<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 [40] for a in depth explanation.

115  $i$ , we choose another binary measurement  $\mathcal{P}_{V_i}$  and perform it on the second  
 116 qubit, obtaining the outcome  $j$ . Finally, if  $j = 0$ , we say that the performed  
 117 measurement is  $\mathcal{P}_U$ , otherwise we say that it was  $\mathcal{P}_1$ .

118 Note, however, that the discrimination scheme described above can work  
 119 regardless of dimensionality of the unitary  $U$ . The main difference is the  
 120 dimension of the auxiliary system, which in general can be larger than two.  
 121 This dimension depends on the Schmidt rank of the optimal input state.  
 122 However, for most discrimination schemes, the Schmidt rank equals at most  
 123 two, and hence the auxiliary system is also a qubit, see [40] for details.  
 124 Note that the final measurement  $\mathcal{P}_{V_i}$  is always binary, independently of the  
 125 dimension of auxiliary system.

126 Naturally, we need to repeat the same procedure multiple times for both  
 127 measurements to obtain a reliable estimate of the underlying probability  
 128 distribution. In PyQBench, we assume that the experiment is repeated the  
 129 same number of times for both  $\mathcal{P}_U$  and  $\mathcal{P}_1$ .

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

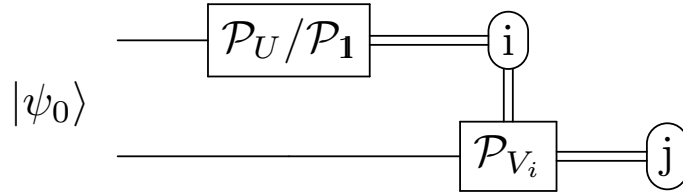


Figure 2: Theoretical scheme of discrimination between von Neumann measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$ .

### 142 3.2.1. Implementation of discrimination scheme on actual NISQ devices

143 Current NISQ devices are unable to perform conditional measurements,  
 144 which is the biggest obstacle to implementing our scheme on real hardware.

145 However, we circumvent this problem by slightly adjusting our scheme so  
 146 that it only uses components available on current devices. For this purpose,  
 147 we use two possible options: using a postselection or a direct sum  $V_0^\dagger \oplus V_1^\dagger$ .

148 **Scheme 1.** (Postselection)

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

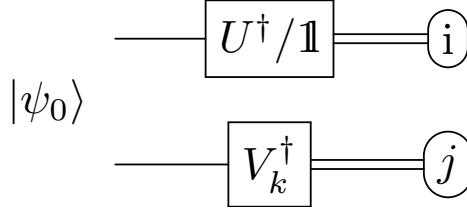


Figure 3: A schematic representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using postselection approach. In postselection scheme, one runs such circuits for both  $k = 0, 1$  and discards results for cases when there is a mismatch between  $k$  and  $i$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

155 To perform the benchmark, one needs to run multiple copies of the post-  
 156 selection circuit, with both  $\mathcal{P}_U$  and  $\mathcal{P}_1$ . Each circuit has to be run in both  
 157 variants, one with final measurement  $\mathcal{P}_{V_0}$  and the second with the final mea-  
 158 surement  $\mathcal{P}_{V_1}$ . The experiments can thus be grouped into classes identified by  
 159 tuples of the form  $(\mathcal{Q}, k, i, j)$ , where  $\mathcal{Q} \in \{\mathcal{P}_U, \mathcal{P}_1\}$  denotes the chosen mea-  
 160 surement,  $k \in \{0, 1\}$  designates the final measurement used, and  $i \in \{0, 1\}$   
 161 and  $j \in \{0, 1\}$  being the labels of outcomes as presented in Fig. 3. We  
 162 then discard all the experiments for which  $i \neq k$ . The total number of valid  
 163 experiments is thus:

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

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

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

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

167 then the empirical success probability can be computed as

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

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

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

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

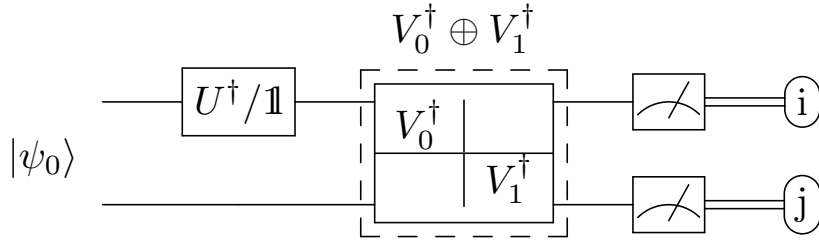


Figure 4: A schematic representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using the  $V_0^\dagger \oplus V_1^\dagger$  direct sum.

172 One can see why such a circuit is equivalent to the original discrimination  
 173 scheme. If we rewrite the block-diagonal matrix  $V_0^\dagger \oplus V_1^\dagger$  as follows:  
 174

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

175 we can see that the direct sum in Eq. (5) commutes with the measurement  
 176 on the first qubit. Thanks to this, we can switch the order of operations to  
 177 obtain the circuit from Fig. 5. Now, depending on the outcome  $i$ , one of the  
 178 summands in Eq. (5) vanishes, and we end up performing exactly the same  
 179 operations as in the original scheme.

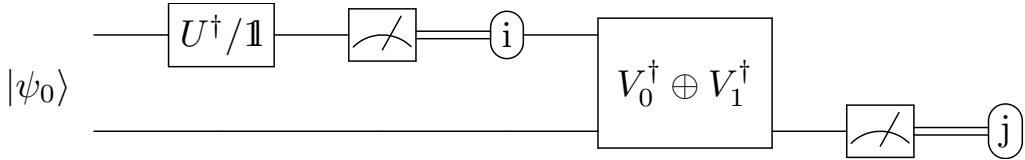


Figure 5: Rewritten representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using the  $V_0^\dagger \oplus V_1^\dagger$  direct sum.

180 In this scheme, the experiment can be characterized by a pair  $(\mathcal{Q}, i, j)$ ,  
 181 where  $\mathcal{Q} = \{\mathcal{P}_U, \mathcal{P}_1\}$  and  $i, j \in \{0, 1\}$  are the output labels. The number of



182 successful trials for  $U$  and  $\mathbb{1}$ , respectively, can be written as

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

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

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

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

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

186 Compared to these approaches, our approach allows for a very simple  
187 operational interpretation of the scheme and its results. This is especially  
188 useful for newcomers to the field, who may be put off by more complicated  
189 approaches. Another benefit is, especially for advanced users, the ability to  
190 control resources utilized during the benchmarking. We can consider here  
191 resources such as entanglement or coherence. Finally, the figure of merit we  
192 wish to calculate and to which we compare the results is fairly simple to  
193 obtain. The main downside of our approach is the exponential number of  
194 circuits we need to consider.

## 195 4. Software description

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

### 199 4.1. Software Functionalities

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

- 206 1. Assembling circuits for both postselection and direct sum-based dis-  
207 crimination schemes.
- 208 2. Executing the whole benchmarking scenario on specified backend (ei-  
209 ther real hardware or software simulator).
- 210 3. Interpreting the obtained outputs in terms of discrimination probab-  
211 ities.

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

220 The PyQBench library also contains a readily available implementation  
 221 of all necessary components needed to run discrimination experiments for  
 222 parametrized Fourier family of measurements (see Section 3 in supplemental  
 223 material). However, if one only wishes to use this particular family of mea-  
 224 surements in their benchmarks, then using PyQBench as a command line  
 225 tool might be more straightforward. PyQBench’s command line interface  
 226 allows running the benchmarking process without writing Python code. The  
 227 configuration of CLI is done by YAML [41] files describing the benchmark  
 228 to be performed and the description of the backend on which the benchmark  
 229 should be run. The same benchmark can be used with different backends  
 230 and vice versa.

## 231 *4.2. Software Architecture*

### 232 *4.2.1. Overview of the software structure*

233 As already described, PyQBench can be used both as a library and a CLI.  
 234 Both functionalities are implemented as a part of `qbench` Python package.  
 235 The exposed CLI tool is also named `qbench`. For brevity, we do not discuss  
 236 the exact structure of the package here, and instead limit ourselves to sum-  
 237 marizing the architecture on the diagram in Fig. 6. For further details, we  
 238 refer an interested reader to the source code available at GitHub [42] or at  
 239 the reference manual [43].

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

### 244 *4.2.2. Integration with hardware providers and software simulators*

245 PyQBench is built around the Qiskit [11] ecosystem. Hence, both the  
 246 CLI tool and the `qbench` library can use any Qiskit-compatible backend.  
 247 This includes, IBM Q backends (available by default in Qiskit) and Amazon  
 248 Braket devices and simulators (available through `qiskit-braket-provider`  
 249 package [44, 45]).

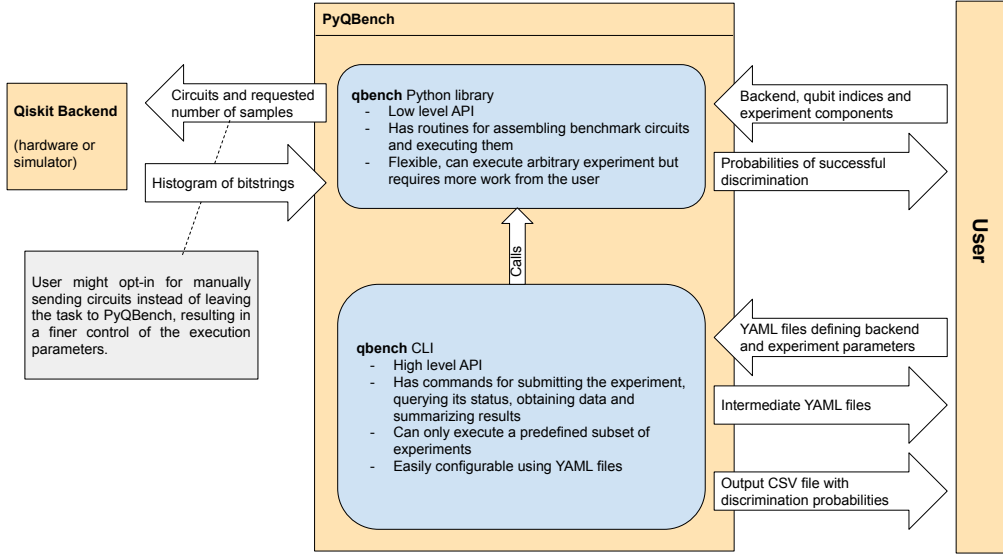


Figure 6: Overview of PyQBench's architecture.

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

#### 4.2.3. Command Line Interface

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

Listing 1: Invocation of `qbench` script

```
qbench <benchmark-type> <command> <parameters>
```

Currently, PyQBench's CLI supports only one type of benchmark (discrimination of parametrized Fourier family of measurements), but we decided on hierarchically structuring the CL to allow for future extensions. Thus, the only accepted value of `<benchmark-type>` is `disc-fourier`. The `qbench disc-fourier` command has four subcommands:

- **benchmark:** run benchmarks. This creates either a result YAML file containing the measurements or an intermediate YAML file for asynchronous experiments.

- 269 • **status**: query status of experiments submitted for given benchmark.  
270 This command is only valid for asynchronous experiments.
- 271 • **resolve**: query the results of asynchronously submitted experiments  
272 and write the result YAML file. The output of this command is almost  
273 identical to the result obtained from synchronous experiments.
- 274 • **tabulate**: interpret the results of a benchmark and summarize them  
275 in the CSV file.

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

#### 277 4.2.4. *Asynchronous vs. synchronous execution*

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

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

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

## 297 5. Illustrative examples

298 In this section, we demonstrate the usage of PyQBench. For brevity, we  
299 decided to present only the usage of the CLI tool, as it is likely to be the  
300 most popular use case. We refer readers interested in implementing their  
301 discrimination schemes using custom measurements to PyQBench’s docu-  
302 mentation [43], where we describe the whole process, and to the Section 2  
303 in the supplemental material, where we discuss the relevant mathematical  
304 details.

### 305 5.1. Using *qbench* CLI

306 PyQBench offers a simplified way of conducting benchmarks using a Com-  
307 mand Line Interface (CLI). The workflow with PyQBench’s CLI can be sum-  
308 marized as the following list of steps:

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

#### 317 5.1.1. Preparing configuration files

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

Listing 2: Defining the experiment

```
324 

---


325 type: discrimination-fourier
326 qubits:
327   - target: 0
328     ancilla: 1
329   - target: 1
330     ancilla: 2
331 angles:
332   start: 0
333   stop: 2 * pi
334   num_steps: 3
335 gateset: ibmq
336 method: direct_sum
337 num_shots: 100
338 

---


```

339 The second configuration file describes the backend. We decided to de-  
340 couple the experiment and the backend files because it facilitates their reuse.  
341 For instance, the same experiment file can be used to run benchmarks on  
342 multiple backends, and the same backend description file can be used with  
343 multiple experiments.

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

Listing 3: IBMQ backend

---

```
349
350 name: ibmq_quito
351 asynchronous: false
352 provider:
353   hub: ibm-q
354   group: open
355   project: main
```

---

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

#### 360 5.1.2. Running the experiment and collecting measurements data

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

---

```
363 qbench disc-fourier benchmark experiment_file.yml backend_file.yml
```

---

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

---

```
368 qbench disc-fourier benchmark experiment_file.yml backend_file.yml
369 --output async_results.yml
```

---

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

- 373 • If the backend is asynchronous, the output will contain intermediate  
 374 data containing, amongst others, `job_ids` correlated with the circuit  
 375 they correspond to.
- 376 • If the backend is synchronous, the output will contain measurement  
 377 outcomes (bitstrings) for each of the circuits run.

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

---

```
381 data:
```

---

```

383 - target: 0
384   ancilla: 1
385   phi: 0.0
386   results_per_circuit:
387     - name: id
388     histogram: {'00': 28, '01': 26, '10': 21, '11': 25}
389     mitigation_info:
390       target: {prob_meas0_prep1: 0.052200000000000024,
391               prob_meas1_prep0: 0.0172}
392       ancilla: {prob_meas0_prep1: 0.059000000000000005,
393                prob_meas1_prep0: 0.0202}
394     mitigated_histogram: {'00': 0.2637212373658018, '01':
395                           0.25865061319892463, '10': 0.2067279352110304, '11':
396                           0.2709002142242433}
397

```

---

### 398 5.1.3. (Optional) Getting status of asynchronous jobs

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

```

401
402 qbench disc-fourier status async_results.yml
403

```

---

404 and it will display dictionary with histogram of statuses.

### 405 5.1.4. Resolving asynchronous jobs

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

```

409
410 qbench disc-fourier resolve async-results.yml resolved.yml
411

```

---

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

### 417 5.1.5. Computing probabilities

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

```

420
421 qbench disc-fourier tabulate results.yml results.csv
422

```

---

423 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 [46, 47], if it was applied.

## 6. Impact

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

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

Finally, we provide the source code of PyQBench on GitHub [42] under an open source license which will allow users to utilize and extend our package in their specific applications.



## 444 7. Conclusions

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

## 453 8. Conflict of Interest

454 We wish to confirm that there are no known conflicts of interest associated  
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