# 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 parametrized Fourier 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/repos-    | https://github.com/iitis/PyQBench |  |  |
|    | itory used for this code version | 1 110                             |  |  |
| C3 | Code Ocean compute capsule       | https://codeocean.com/capsule/    |  |  |
|    |                                  | 89088992-9a27-4712-8525-          |  |  |
|    |                                  | d92a9b23060f/tree                 |  |  |
| C4 | Legal Code License               | Apache License 2.0                |  |  |
| C5 | Code versioning system used      | git                               |  |  |
| C6 | Software code languages, tools,  | Python, Qiskit, AWS Braket        |  |  |
|    | and services used                |                                   |  |  |
| C7 | Compilation requirements, op-    | Python >= 3.8                     |  |  |
|    | erating environments & depen-    | numpy ~= 1.22.0                   |  |  |
|    | dencies                          | scipy ~= 1.7.0                    |  |  |
|    |                                  | pandas ~= 1.5.0                   |  |  |
|    |                                  | amazon-braket-sdk >= 1.11.1       |  |  |
|    |                                  | pydantic ~= 1.9.1                 |  |  |
|    |                                  | qiskit ~= 0.37.2                  |  |  |
|    |                                  | mthree ~= 1.1.0                   |  |  |
|    |                                  | tqdm ~= 4.64.1                    |  |  |
|    |                                  | pyyaml ~= 6.0                     |  |  |
|    |                                  | qiskit-braket-provider ~= 0.0.3   |  |  |
| C8 | If available Link to developer   | https://pyqbench.readthedocs.io/  |  |  |
|    | documentation/manual             | en/latest/                        |  |  |
| С9 | Support email for questions      | dexter2206@gmail.com              |  |  |

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
- 4 accompanying software solutions. Among hardware providers offering public
- 5 access to their gate—based devices, one could mention Rigetti [2], IBM [3],
- 6 Oxford Quantum Group [4], IonQ [5] or Xanadu [6]. Other vendors offer de-
- <sup>7</sup> vices operating in different paradigms. Notably, one could mention D-Wave
- 8 [7] and their quantum annealers, or QuEra devices [8] based on neural atoms.
- 9 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 or Zapata Computing's Orquestra [14].

It is well known that NISQ devices have their limitations [15]. 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 [16, 17, 18, 19, 20], benchmarks based on the quantum volume [21, 22, 23].

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) [24, 25] or SupermarQ [26, 27] 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 [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.verifica tion.quantum\_volume. Other implementations of Quantum Volume can be found as well, see e.g. [30].

#### 6 3. Preliminaries and discrimination scheme approach

In this section we describe how the benchmarking process in PyQBench works. To do so, we first discuss 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 limitations of the current NISQ devices.

#### 3.1. Mathematical preliminaries

Let us first recall the definition of a von Neumann measurement, which is the only type of measurement used in PyQBench. A von Neumann measurement  $\mathcal{P}$  is a collection of rank-one projectors  $\{|u_0\rangle\langle u_0|,\ldots,|u_{d-1}\rangle\langle u_{d-1}|\}$ , called effects, that sum up to identity, i.e.  $\sum_{i=0}^{d-1}|u_i\rangle\langle u_i|=1$ . 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=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.

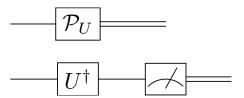


Figure 1: Implementation of a von Neumann measurement using measurement in computational basis. The upper circuit shows a symbolic representation of a von Neumann measurement  $\mathcal{P}_U$ . The bottom, equivalent circuit depicts its decomposition into a change of basis followed by measurement in 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. Note, however, that the discrimination scheme described below can work regardless of dimensionality of the system, see [31] for details.

In general, 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 POVM  $\mathcal{P}_{V_i}$  and perform it on the second qubit, obtaining the output in j. Finally, if j = 0, we say that the performed measurement is  $\mathcal{P}_U$ , otherwise we say that it was  $\mathcal{P}_1$ . Naturally, we need to repeat the same procedure multiple times for both measurements to obtain a reliable estimate of the underlying probability distribution. In PyQBench, we assume that the experiment is repeated the same number of times for both  $\mathcal{P}_U$  and  $\mathcal{P}_1$ .

Unsurprisingly, both the  $|\psi_0\rangle$  and the final measurements  $\mathcal{P}_{V_i}$  have to be chosen specifically for given U to maximize the probability of a correct guess. The detailed description how these choices are made in [32], and for now we will focus only how this scheme can be implemented on the actual devices, assuming that all the components are known.

<sup>&</sup>lt;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 [31] for a in depth explanation.

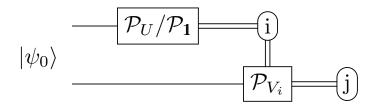


Figure 2: Theoretical scheme of discrimination between von Neumann measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$ .

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

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

#### Scheme 1. (Postselection)

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

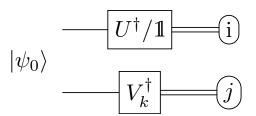


Figure 3: A schematic representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using postselection approach. In postselection scheme, one runs such circuits for both k = 0, 1 and discards results for cases when there is a mismatch between k and i.

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

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

Finally, we count the valid experiments resulting in successful discrimination. If we have chosen  $\mathcal{P}_U$ , then we guess correctly iff j=0. Similarly, for  $P_1$ , we guess correctly iff j=1. If we define

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

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

then the empirical success probability can be computed as

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

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

#### 138 Scheme 2. (Direct sum)

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

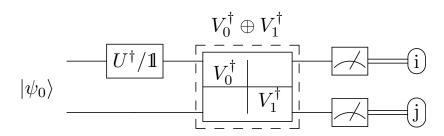


Figure 4: A schematic representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using the  $V_0^{\dagger} \oplus V_1^{\dagger}$  direct sum.

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

$$V_0^{\dagger} \oplus V_1^{\dagger} = |0\rangle\langle 0| \otimes V_0^{\dagger} + |1\rangle\langle 1| \otimes V_1^{\dagger}, \tag{5}$$

we can see that the direct sum in Eq. (5) commutes with the measurement on the first qubit. Thanks to this, we can switch the order of operations to obtain the circuit from Fig. 5. Now, depending on the outcome *i*, one of the

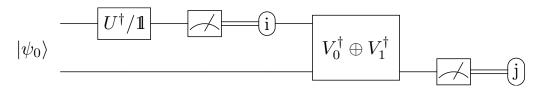


Figure 5: Rewritten representation of the setup for distinguishing measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  using the  $V_0^{\dagger} \oplus V_1^{\dagger}$  direct sum.

summands in Eq. (5) vanishes, and we end up performing exactly the same operations as in the original scheme.

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

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

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

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

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

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

#### 3.2.2. Importance of choosing the optimal discrimination scheme

In principle, the schemes described in the previous section could be used with any choice of  $|\psi_0\rangle$  and final measurements  $\mathcal{P}_{V_i}$ . However, we argue that it is best to choose those components in such a way that they maximize the probability of correct discrimination. To see that, suppose that some choice of  $|\psi_0\rangle$ ,  $\mathcal{P}_{V_0}$ ,  $\mathcal{P}_{V_1}$  yields the theoretical upper bound of discriminating between two measurements of one, i.e. on a perfect quantum computer you will always make a correct guess. Then, on real hardware, we might obtain any empirical value in range  $\left[\frac{1}{2},1\right]$ . On the other hand, if we choose the components of our scheme such that the successful discrimination probability is only  $\frac{3}{5}$ , the possible range of empirically obtainable probabilities is only  $\left[\frac{1}{2},\frac{3}{5}\right]$ . Hence, in the second case, the discrepancy between theoretical and empirical results will be less pronounced.

#### 3.2.3. Constructing optimal discrimination scheme

To construct the optimal discrimination scheme, one starts by calculating the probability of correct discrimination. Using the celebrated result by Helstrom [33], one finds that the optimal probability of correct discrimination between two quantum measurements,  $\mathcal{P}$  and  $\mathcal{Q}$ , is

$$p_{\text{succ}}(\mathcal{P}, \mathcal{Q}) = \frac{1}{2} + \frac{1}{4} \|\mathcal{P} - \mathcal{Q}\|_{\diamond}, \tag{9}$$

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$$\|\mathcal{P} - \mathcal{Q}\|_{\diamond} = \max_{\||\psi\rangle\|_{1}=1} \| ((\mathcal{P} - \mathcal{Q}) \otimes \mathbb{1}) (|\psi\rangle\langle\psi|) \|_{1}. \tag{10}$$

The quantum state  $|\psi_0\rangle$  maximizing the diamond norm above is called the discriminator, and can be computed e.g. using semidefinite programming (SDP) [32, 34]. Furthermore, using the proof of the Holevo-Helstrom theorem, it is possible to construct corresponding unitaries  $V_0$ ,  $V_1$  to create the optimal discrimination strategy. For brevity, we do not describe this procedure here. Instead, we refer the interested reader to [32].

### 4. Discrimination scheme for parameterized Fourier family and implementation

So far, we only discussed how the discrimination is performed assuming that all needed components  $|\psi_0\rangle$ ,  $V_0$ , and  $V_1$  are known. In this section, we provide a concrete example using parametrized Fourier family of measurements.

The parametrized Fourier family of measurements is defined as a set of the measurements  $\{\mathcal{P}_{U_{\phi}} \colon \phi \in [0, 2\pi]\}$ , where

$$U_{\phi} = H \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} H^{\dagger}, \tag{11}$$

and H is the Hadamard matrix of dimension two. For each element of this set, the discriminator is a Bell state:

$$|\psi_0\rangle = \frac{1}{\sqrt{2}} \left( |00\rangle + |11\rangle \right). \tag{12}$$

Observe that  $|\psi_0\rangle$  does not depend on the angle  $\phi$ . However, the unitaries  $V_0, V_1$  depend on  $\phi$  and take the following form:

$$V_0 = \begin{pmatrix} i \sin\left(\frac{\pi - \phi}{4}\right) & -i \cos\left(\frac{\pi - \phi}{4}\right) \\ \cos\left(\frac{\pi - \phi}{4}\right) & \sin\left(\frac{\pi - \phi}{4}\right) \end{pmatrix}, \tag{13}$$

$$V_1 = \begin{pmatrix} -i\cos\left(\frac{\pi-\phi}{4}\right) & i\sin\left(\frac{\pi-\phi}{4}\right) \\ \sin\left(\frac{\pi-\phi}{4}\right) & \cos\left(\frac{\pi-\phi}{4}\right) \end{pmatrix}. \tag{14}$$

Finally, the theoretical probability of correct discrimination between von Neumann measurements  $\mathcal{P}_{U_{\phi}}$  and  $\mathcal{P}_{\mathbf{1}}$  is given by

$$p_{\text{succ}}(\mathcal{P}_{U_{\phi}}, \mathcal{P}_{1}) = \frac{1}{2} + \frac{|1 - e^{i\phi}|}{4}.$$
 (15)

We explore the construction of  $|\psi_0\rangle$ ,  $V_0$  and  $V_1$  for parametrized Fourier family of measurements in Appendix C.

#### 5. Software description

This section is divided into two parts. In Section 5.1 we describe functionalities of PyQBench package. Next, in Section 5.2, we give a general overview of the software architecture.

#### 5.1. Software Functionalities

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

- 1. Assembling circuits for both postselection and direct sum-based discrimination schemes.
- 2. Executing the whole benchmarking scenario on specified backend (either real hardware or software simulator).
- 3. Interpreting the obtained outputs in terms of discrimination probabilities.

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

The PyQBench library also contains a readily available implementation of all necessary components needed to run discrimination experiments for parametrized Fourier family of measurements, defined previously in Section 4. However, if one only wishes to use this particular family of measurements in their benchmarks, then using PyQBench as a command line tool might be more straightforward. PyQBench's command line interface allows running the benchmarking process without writing Python code. The configuration of CLI is done by YAML [35] files describing the benchmark to be performed and the description of the backend on which the benchmark should be run. Notably, the YAML configuration files are reusable. The same benchmark can be used with different backends and vice versa.

The following section describes important architectural decisions taken when creating PyQBench, and how they affect the end-user experience.

#### 5.2. Software Architecture

#### 5.2.1. Overview of the software structure

As already described, PyQBench can be used both as a library and a CLI. Both functionalities are implemented as a part of qbench Python package. The exposed CLI tool is also named qbench. For brevity, we do not discuss the exact structure of the package here, and instead refer an interested reader to the source code available at GitHub [36] or at the reference manual [37].

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

#### 5.2.2. Integration with hardware providers and software simulators

PyQBench is built around the Qiskit [11] ecosystem. Hence, both the CLI tool and the qbench library can use any Qiskit-compatible backend. This includes, IBM Q backends (available by default in Qiskit) and Amazon Braket devices and simulators (available through qiskit-braket-provider package [38, 39]).

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 6, and the detailed description of the expected format can be found at PyQBench's documentation.

#### 5.2.3. 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 structuring the CLI in a hierarchical fashion 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.
- status: query status of experiments submitted for given benchmark. This command is only valid for asynchronous experiments.
- resolve: query the results of asynchronously submitted experiments and write the result YAML file. The output of this command is almost identical to the result obtained from synchronous experiments.
- tabulate: interpret the results of a benchmark and summarize them in the CSV file.

We present usage of each of the above commands later in section 6.

#### 5.2.4. Asynchronous vs. synchronous execution

PyQBench's CLI can be used in synchronous and asynchronous modes. The mode of execution is defined in the YAML file describing the backend (see Section 6 for an example of this configuration). We decided to couple the mode of execution to the backend description because some backends cannot work in asynchronous mode.

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

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

#### 6. Illustrative examples

In this section, we present two examples demonstrating the usage of PyQBench. In the first example, we show how to implement a discrimination scheme for a user-defined measurement and possible ways of using this scheme with qbench library. The second example demonstrates the usage of the CLI. We show how to prepare the input files for the benchmark and how to run it using the qbench tool.

#### 6.1. Using user-defined measurement with qbench package

In this example, we will demonstrate how qbench package can be used with user–defined measurement. For this purpose, we will use U=H (the Hadamard gate). The detailed calculations that lead to the particular form of the discriminator and final measurements can be found in Appendix B. The explicit formula for discriminator in this example reads:

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle),\tag{16}$$

 $_{^{312}}$  with final measurements being equal to

$$V_0 = \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix}, \tag{17}$$

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$$V_1 = \begin{pmatrix} -\beta & \alpha \\ \alpha & \beta \end{pmatrix}, \tag{18}$$

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$$\alpha = \frac{\sqrt{2 - \sqrt{2}}}{2} = \cos\left(\frac{3}{8}\pi\right),\tag{19}$$

 $\beta = \frac{\sqrt{2 + \sqrt{2}}}{2} = \sin\left(\frac{3}{8}\pi\right). \tag{20}$ 

To use the above benchmarking scheme in PyQBench, we first need to construct circuits that can be executed by actual hardware. To this end, we need to represent each of the unitaries as a sequence of standard gates, keeping in mind that quantum circuits start execution from the  $|00\rangle$  state. The circuit taking  $|00\rangle$  to the Bell state  $|\psi_0\rangle$  comprises the Hadamard gate followed by CNOT gate on both qubits (see Fig. 6). For  $V_0$  and  $V_1$  observe that  $V_0 = \text{RY}\left(\frac{3}{4}\pi\right)$ , where RY is rotation gate around the Y axis defined by

$$RY(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}. \tag{21}$$

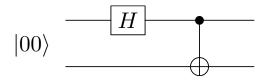


Figure 6: Decomposition of the Bell state  $|\psi_0\rangle$ .

To obtain  $V_1$  we need only to swap the columns, i.e.

$$V_1 = \text{RY}\left(\frac{3}{4}\pi\right) X. \tag{22}$$

Finally, the optimal probability of correct discrimination is equal to

$$p_{\text{succ}}(\mathcal{P}_U, \mathcal{P}_1) = \frac{1}{2} + \frac{\sqrt{2}}{4}.$$
 (23)

We will now demonstrate how to implement this theoretical scheme in PyQBench.
For this example we will use the Qiskit Aer simulator [40]. First, we import
the necessary functions and classes from PyQBench and Qiskit. We also import numpy for the definition of np.pi constant and the exponential function.
The exact purpose of the imported functions will be described at the point of their usage.

Listing 2: Imports needed for running benchmarking example

```
import numpy as np
from qiskit import QuantumCircuit, Aer
from qbench.schemes.postselection import
benchmark_using_postselection
from qbench.schemes.direct_sum import benchmark_using_direct_sum
```

To implement the discrimination scheme in PyQBench, we need to define all the necessary components as Qiskit instructions. We can do so by constructing a circuit object acting on qubits 0 and 1 and then converting them using to\_instruction() method.

Listing 3: Defining components for Hadamard experiment

```
def state_prep():
    def state_prep():
        circuit = QuantumCircuit(2)
        circuit.h(0)
        circuit.cnot(0, 1)
        return circuit.to_instruction()
    def u_dag():
```

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```
circuit = QuantumCircuit(1)
350
       circuit.h(0)
351
      return circuit.to_instruction()
352
353
   def v0_dag():
354
       circuit = QuantumCircuit(1)
355
       circuit.ry(-np.pi * 3 / 4, 0)
356
      return circuit.to_instruction()
357
358
    def v1_dag():
359
       circuit = QuantumCircuit(1)
360
       circuit.ry(-np.pi * 3 / 4, 0)
361
      circuit.x(0)
362
      return circuit.to_instruction()
363
364
    def v0_v1_direct_sum_dag():
365
      circuit = QuantumCircuit(2)
366
      circuit.ry(-np.pi * 3 / 4, 0)
367
      circuit.cnot(0, 1)
368
      return circuit.to_instruction()
369
370
```

We now construct a backend object, which in this case is an instance of Aer simulator.

```
Listing 4: Defining a backend

simulator = Aer.get_backend("aer_simulator")
```

In the simplest scenario, when one does not want to tweak execution details and simply wishes to run the experiment on a given backend, everything that is required is now to run benchmark\_using\_postselection or

benchmark\_using\_direct\_sum function, depending on the user preference.

Listing 5: Simulation benchmark by using postselection

```
380
   postselection_result = benchmark_using_postselection(
381
      backend=simulator,
382
      target=0,
383
      ancilla=1,
      state_preparation=state_prep(),
385
      u_dag=u_dag(),
386
      v0_dag=v0_dag(),
387
      v1_dag=v1_dag(),
388
      num_shots_per_measurement=10000,
   )
390
```

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Listing 6: Simulation benchmark by using direct sum

```
392
   direct_sum_result = benchmark_using_direct_sum(
393
      backend=simulator,
394
      target=1,
395
      ancilla=2,
396
      state_preparation=state_prep(),
397
      u_dag=u_dag(),
      v0_v1_direct_sum_dag=v0_v1_direct_sum_dag(),
399
      num_shots_per_measurement=10000,
400
   )
481
```

The postselection\_result and direct\_sum\_result variables contain now the empirical probabilities of correct discrimination. We can compare them to the theoretical value and compute the absolute error.

Listing 7: Examining the benchmark results

```
p\_succ = (2 + np.sqrt(2)) / 4
407
   print(f"Analytical p_succ = {p_succ}")
408
   f"Postselection: p_succ = {postselection_result}, abs. error =
       {p_succ - postselection_result}"
411
   )
412
   print(f"Direct sum: p_succ = {direct_sum_result}, abs. error =
413
       {p_succ - direct_sum_result}")
414
416
   Analytical p_{succ} = 0.8535533905932737
417
   Postselection: p_succ = 0.8559797193791593, abs. error =
418
       -0.0024263287858855564
419
   Direct sum: p_succ = 0.85605, abs. error = -0.0024966094067262468
439
```

In the example presented above we used functions that automate the whole process – from the circuit assembly, through running the simulations to interpreting the results. But what if we want more control over some parts of this process? One possibility would be to add some additional parameters to benchmark\_using\_xyz functions, but this approach is not scalable. Moreover, anticipating all possible uses cases isimpossible. Therefore, we decided on another approach. PyQBench provides functions performing:

1. Assembly of circuits needed for experiment, provided the components discussed above.

2. Interpretation of the obtained measurements.

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The difference between the two approaches is illustrated on the diagrams in Fig. 7.

For the rest of this example we focus only on the postselection case, as the direct sum case is analogous. We continue by importing two more functions from PyQBench.

#### Listing 8: Assembling circuits

```
437
   from qbench.schemes.postselection import (
438
        assemble_postselection_circuits,
439
        compute_probabilities_from_postselection_measurements,
440
    )
441
442
    circuits = assemble_postselection_circuits(
       target=0,
       ancilla=1,
445
       state_preparation=state_prep(),
446
       u_dag=u_dag(),
447
       v0_dag=v0_dag(),
448
       v1_dag=v1_dag(),
449
   )
450
451
```

Recall that for a postselection scheme we have two possible choices of the "unknown" measurement and two possible choices of a final measurement, which gives a total of four circuits needed to run the benchmark. The function assemble\_postselection\_circuits creates all four circuits and places them in a dictionary with keys "id\_v0", "id\_v1", "u\_v0", "u\_v1".

We will now run our circuits using noisy and noiseless simulation. We start by creating a noise model using Qiskit.

#### Listing 9: Adding noise model

```
from qiskit.providers.aer import noise

from qiskit.providers.aer import noise

error = noise.ReadoutError([[0.75, 0.25], [0.8, 0.2]])

from qiskit.providers.aer import noise

error = noise.ReadoutError([[0.75, 0.25], [0.8, 0.2]])

from qiskit.providers.aer import noise

from qiskit.pr
```

Once we have our noise model ready, we can execute the circuits with and without noise. To this end, we will use Qiskit's execute function. One caveat is that we have to keep track which measurements correspond to

### Simplified benchmarking **PyQBench** Backend passes circuit components, backend and number of shots assembles the circuits submits circuits to be executed returns measurements compute probability return probability of success User Backend **PyQBench Execution of circuits controlled by user PyQBench** User passes circuit components and qubit indices returns assembled circuits submits circuits to be executed returns raw measurements passess measurements returns computed probability User Backend PyQBench

Figure 7: Differences between simplified (top) and user–controlled (bottom) execution of benchmarks in PyQBench. Compared to simplified benchmarking, in user-controlled benchmarks the user has direct access to the circuits being run, and hence can alter them (e.g. by adding noise) and/or choose the parameters used for executing them on the backend.

which circuit. We do so by fixing an ordering on the keys in the circuits dictionary.

Listing 10: Running circuits

```
473
   from qiskit import execute
474
475
   keys_ordering = ["id_v0", "id_v1", "u_v0", "u_v1"]
476
   all_circuits = [circuits[key] for key in keys_ordering]
477
478
   counts_noisy = execute(
480
      all_circuits,
      backend=simulator,
481
      noise_model=noise_model,
482
      shots=10000
483
   ).result().get_counts()
484
485
   counts_noiseless = execute(
486
      all_circuits,
487
      backend=simulator,
488
      shots=10000
489
   ).result().get_counts()
489
```

Finally, we use the measurement counts to compute discrimination probabilities using compute\_probabilities\_from\_postselection\_measurements function.

Listing 11: Computation probabilities

```
495
   prob_succ_noiseless =
496
       compute_probabilities_from_postselection_measurements(
497
      id_v0_counts=counts_noiseless[0],
      id_v1_counts=counts_noiseless[1],
499
      u_v0_counts=counts_noiseless[2],
500
      u_v1_counts=counts_noiseless[3],
501
   )
502
503
504
   prob_succ_noisy =
505
       compute_probabilities_from_postselection_measurements(
506
      id_v0_counts=counts_noisy[0],
507
      id_v1_counts=counts_noisy[1],
508
      u_v0_counts=counts_noisy[2],
      u_v1_counts=counts_noisy[3],
510
   )
511
```

We can now examine the results. As an example, in one of our runs, we obtained prob\_succ\_noiseless = 0.8524401115559386 and prob\_succ\_noisy = 0.5017958400693446. As expected, for noisy simulations, the result lies further away from the target value of 0.8535533905932737.

This concludes our example. In the next section, we will show how to use PyQBench's CLI.

#### 6.2. Using qbench CLI

Using PyQBench as a library allows one to conduct a two–qubits benchmark with arbitrary von Neumann measurement. However, as discussed in the previous guide, it requires writing some amount of code. For a Fourier parametrized family of measurements, 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.

#### 6.2.1. 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 12: Defining the experiment

```
type: discrimination-fourier
qubits:
    - target: 0
ancilla: 1
type: discrimination-fourier
qubits:
    - target: 0
ancilla: 2
ancilla: 2
angles:
```

```
start: 0
stop: 2 * pi
stin num_steps: 3
stin gateset: ibmq
stin method: direct_sum
stin num_shots: 100
```

The experiment file contains the following fields:

- type: a string describing the type of the experiment. Currently, the only option of type is discrimination-fourier.
- qubits: a list enumerating pairs of qubits on which the experiment should be run. For configuration in listing 12, the benchmark will run on two pairs of qubits. The first pair is 0 and 1, and the second one is 1 and 2. We decided to describe a pair by using target and ancilla keys rather than using a plain list to emphasize that the role of qubits in the experiment is not symmetric.
- angles: an object describing the range of angles for Fourier parameterized family. The described range is always uniform, starts at the start, ends at stop and contains num\_steps points, including both start and stop. The start and stop can be arithmetic expressions using pi literal. For instance, the range defined in listing 12 contains three points: 0,  $\pi$  and  $2\pi$ .
- gateset: a string describing the set of gates used in the decomposition of circuits in the experiment. The PyQBench contains explicit implementations of circuits The possible options are [ibmq, lucy, rigetti], corresponding to decompositions compatible with IBM Q devices, OQC Lucy device, and Rigetti devices. Alternatively, one might wish to turn off the decomposition by using a special value generic. However, for this to work a backend used for the experiment must natively implement all the gates needed for the experiment, as described in 4.
- method: a string, either postselection or direct\_sum determining which implementation of the conditional measurement is used.
- num\_shots: an integer defines how many shots are performed in the experiment for a particular angle, qubit pair and circuit. Note that if one wishes to compute the total number of shots in the experiment, it is necessary to take into account that the postselection method uses twice as many circuits as the direct\_sum method.

The second configuration file describes the backend. We decided to decouple the experiment and the backend files because it facilitates their reuse. For instance, the same experiment file can be used to run benchmarks on multiple backends, and the same backend description file can be used with multiple experiments.

Different Qiskit backends typically require different data for their initialization. Hence, there are multiple possible formats of the backend configuration files understood by PyQBench. We refer the interested reader to the PyQBench's documentation. Below we describe an example YAML file describing IBM Q backend named Quito.

#### Listing 13: IBMQ backend

```
name: ibmq_quito
see asynchronous: false
provider:
hub: ibm-q
group: open
project: main
```

IBMQ backends typically require an access token to IBM Quantum Experience. Since it would be unsafe to store it in plain text, the token has to be configured separately in IBMQ\_TOKEN environmental variable.

#### 6.2.2. Remarks on using the asynchronous flag

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623 624 For backends supporting asynchronous execution, the **asynchronous** setting can be configured to toggle it. For asynchronous execution to work, the following conditions have to be met:

- Jobs returned by the backend have unique job\_id.
- Jobs are retrievable from the backend using the backend.retrieve\_job method, even from another process (e.g. if the original process running the experiment has finished).

Since PyQBench cannot determine if the job retrieval works for a given backend, it is the user's responsibility to ensure that this is the case before setting asynchronous to true.

#### 6.2.3. Running the experiment and collecting measurements data

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

qbench disc-fourier benchmark experiment\_file.yml backend\_file.yml

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

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

The result of running the above command can be twofold:

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- If backend is asynchronous, the output will contain intermediate data containing, amongst others, job\_ids correlated with the circuit they correspond to.
- If the backend is synchronous, the output will contain measurement outcomes (bitstrings) for each of the circuits run.

For synchronous experiment, the part of output looks similar to the one below. The whole YAML file can be seen in Appendix E.

```
639
   data:
640
   - target: 0
641
     ancilla: 1
642
     phi: 0.0
643
     results_per_circuit:
     - name: id
645
     histogram: {'00': 28, '01': 26, '10': 21, '11': 25}
646
     mitigation_info:
647
      target: {prob_meas0_prep1: 0.05220000000000024,
648
          prob_meas1_prep0: 0.0172}
      ancilla: {prob_meas0_prep1: 0.0590000000000000,
650
          prob_meas1_prep0: 0.0202}
651
     mitigated_histogram: {'00': 0.2637212373658018, '01':
652
         0.25865061319892463, '10': 0.2067279352110304, '11':
653
         0.2709002142242433}
654
655
```

The data includes target, ancilla, phi, and results\_per\_circuit. The first three pieces of information have already been described. The last data results\_per\_circuit gives us the following additional information:

- name: the information which measurement is used during experiment, either string "u" for  $\mathcal{P}_U$  or string "id" for  $\mathcal{P}_1$ . In this example we consider  $\mathcal{P}_1$ .
- histogram: the dictionary with measurements' outcomes. The keys represent possible bitstrings, whereas the values are the number of occurrences.

- mitigation\_info: for some backends (notably for backends corresponding to IBM Q devices), backends.properties().qubits contains information that might be used for error mitigation using the MThree method [41, 42]. If this info is available, it will be stored in the mitigation\_info field, otherwise this field will be absent.
- mitigated\_histogram: the histogram with measurements' outcomes after the error mitigation.

#### 6.2.4. (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.

#### 6.2.5. 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.

#### 6.2.6. Computing probabilities

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

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

A sample CSV file is provided below:

#### 98 7. 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

| 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 [41, 42], if it was applied.

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 [36] under an open source license which will allow users to utilize and extend our package in their specific applications.

#### 718 8. Conclusions

In this study, we develop a Python library 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 parameterized Fourier family of measurements. For

more advanced scenarios, PyQBench offers a way of employing user-defined measurements instead of predefined ones.

#### 9. Conflict of Interest

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its out- come.

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#### 739 References

- John Preskill. Quantum computing in the nisq era and beyond. Quantum, 2:79, 2018.
- [2] Rigetti computing. https://www.rigetti.com/. Accessed on 2023-02-18.
- [3] IBM Quantum. https://www.ibm.com/quantum. Accessed on 2023-02-18.
- 746 [4] Oxford quantum. http://oxfordquantum.org/. Accessed on 2023-02-747 18.
- 748 [5] IonQ. https://ionq.com/. Accessed on 2023-02-18.
- [6] Xanadu. https://www.xanadu.ai/. Accessed on 2023-02-18.
- 750 [7] D-Wave Systems. https://www.dwavesys.com/. Accessed on 2023-02-751 18.
- 752 [8] QuEra. https://www.quera.com/. Accessed on 2023-02-18.
- [9] QCS Documentation. https://docs.rigetti.com/qcs/. Accessed on 2023-02-18.

- 755 [10] PyQuil Documentation. https://pyquil-docs.rigetti.com/en/ 756 stable/. Accessed on 2023-02-18.
- 757 [11] Qiskit. https://qiskit.org/. Accessed on 2023-02-18.
- 758 [12] IBM Quantum Experience. https://quantum-computing.ibm.com/.
  Accessed on 2023-02-18.
- 760 [13] Amazon Braket. https://aws.amazon.com/braket/. Accessed on 2023-02-18.
- 762 [14] Zapata Orquestra Platform. https://www.zapatacomputing.com/ orquestra-platform/. Accessed on 2023-02-18.
- 764 [15] J. Preskill. Quantum computing 40 years later. arXiv preprint arXiv:2106.10522, 2021.
- 766 [16] Y. Liu, M. Otten, R. Bassirianjahromi, L. Jiang, and B. Fefferman.

  Benchmarking near-term quantum computers via random circuit sampling. arXiv preprint arXiv:2105.05232, 2021.
- [17] E. Knill, D. Leibfried, R. Reichle, J. Britton, R. B. Blakestad, J. D.
   Jost, C. Langer, R. Ozeri, S. Seidelin, and D. J. Wineland. Randomized
   benchmarking of quantum gates. *Physical Review A*, 77(1):012307, 2008.
- [18] J. J. Wallman and S. T. Flammia. Randomized benchmarking with confidence. *New Journal of Physics*, 16(10):103032, 2014.
- [19] J. Helsen, I. Roth, E. Onorati, A. H. Werner, and J. Eisert. General framework for randomized benchmarking. PRX Quantum, 3(2):020357, 2022.
- [20] A. Cornelissen, J. Bausch, and A. Gilyén. Scalable benchmarks for gatebased quantum computers. arXiv preprint arXiv:2104.10698, 2021.
- 779 [21] A. W. Cross, L. S. Bishop, S. Sheldon, P. D. Nation, and J. M. Gambetta. Validating quantum computers using randomized model circuits. 781 Physical Review A, 100(3):032328, 2019.
- [22] N. Moll, P. Barkoutsos, L. S. Bishop, J. M. Chow, A. Cross, D. J.
   Egger, S. Filipp, A. Fuhrer, J. M. Gambetta, M. Ganzhorn, A. Kandala,
   A. Mezzacapo, P. Müller, W. Riess, G. Salis, J. Smolin, I. Tavernelli, and
   K. Temme. Quantum optimization using variational algorithms on near term quantum devices. Quantum Science and Technology, 3(3):030503,
   2018.

- <sup>788</sup> [23] E. Pelofske, A. Bärtschi, and S. Eidenbenz. Quantum volume in practice: What users can expect from nisq devices. *IEEE Transactions on Quantum Engineering*, 3:1–19, 2022.
- 791 [24] N. Quetschlich, L. Burgholzer, and R. Wille. Mqt bench: Benchmarking software and design automation tools for quantum computing. arXiv preprint arXiv:2204.13719, 2022.
- 794 [25] MQTBench. https://github.com/cda-tum/MQTBench. Accessed on 2023-02-18.
- [26] T. Tomesh, P. Gokhale, V. Omole, G. S. Ravi, K. N. Smith, J. Viszlai,
   X. Wu, N. Hardavellas, M. R. Martonosi, and F. T. Chong. SupermarQ:
   A scalable quantum benchmark suite. In 2022 IEEE International Symposium on High-Performance Computer Architecture (HPCA), pages
   587–603. IEEE, 2022.
- 801 [27] SupermarQ. https://github.com/SupertechLabs/SupermarQ. Ac-802 cessed on 2023-02-18.
- <sup>803</sup> [28] Qiskit benchmarks. https://github.com/qiskit-community/ qiskit-benchmarks. Accessed on 2023-02-18.
- 805 [29] Forest Benchmarking: QCVV using PyQuil. https://github.com/ 806 rigetti/forest-benchmarking. Accessed on 2023-02-18.
- Quantum volume in practice. https://github.com/lanl/Quantum-Volume-in-Practice. Accessed on 2023-02-18.
- [31] Z. Puchała, Ł. Pawela, A. Krawiec, and R. Kukulski. Strategies for optimal single-shot discrimination of quantum measurements. *Physical Review A*, 98(4):042103, 2018.
- [32] J. Watrous. *The Theory of Quantum Information*. Cambridge University Press, 2018.
- [33] C. W. Helstrom. Quantum detection and estimation theory. *Journal of Statistical Physics*, 1(2):231–252, 1969.
- 816 [34] J. Watrous. Simpler semidefinite programs for completely bounded 817 norms. Chicago Journal of Theoretical Computer Science, 8, 2013.
- <sup>818</sup> [35] YAML Ain't Markup Language (YAML) Version 1.2. https://yaml. org/spec/1.2.2/. Accessed on 2023-02-18.

- 820 [36] PyQBench GitHub Repository. https://github.com/iitis/ 821 PyQBench. Accessed on 2023-02-18.
- <sup>822</sup> [37] PyQBench Documentation. https://pyqbench.readthedocs.io/en/ <sup>823</sup> latest/. Accessed on 2023-02-18.
- 1824 [38] Introducing the Qiskit Provider for Amazon Braket.

  1825 https://aws.amazon.com/blogs/quantum-computing/

  1826 introducing-the-qiskit-provider-for-amazon-braket/. Accessed on 2023-02-18.
- 28 [39] Qiskit Braket Provider GitHub Repository. https://github.com/ qiskit-community/qiskit-braket-provider. Accessed on 2023-02-18.
- 831 [40] Qiskit Aer GitHub Repository. https://github.com/Qiskit/ 832 qiskit-aer. Accessed on 2023-02-18.
- mthree Documentation. https://qiskit.org/documentation/partners/mthree/stubs/mthree.M3Mitigation.html. Accessed on 2023-02-10.
- [42] 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.
- F. D. Murnaghan. On the field of values of a square matrix. *Proceedings* of the National Academy of Sciences, 18(3):246–248, 1932.
- 841 [44] Numerical shadow. https://numericalshadow.org/. Accessed on 2022-10-02.
- [45] P. Lewandowska, A. Krawiec, R. Kukulski, Ł. Pawela, and Z. Puchała.
   On the optimal certification of von Neumann measurements. Scientific Reports, 11(1):3623, 2021.
- <sup>846</sup> [46] F. Hausdorff. Der wertvorrat einer bilinearform. *Mathematische Zeitschrift*, 3(1):314–316, 1919.
- 648 [47] O. Toeplitz. Das algebraische analogon zu einem satze von fejér. Math-649 ematische Zeitschrift, 2(1-2):187–197, 1918.

#### Appendix A. Mathematical preliminaries

Let  $\mathcal{M}_{d_1,d_2}$  be the set of all matrices of dimension  $d_1 \times d_2$  over the field  $\mathbb{C}$ . For simplicity, square matrices will be denoted by  $\mathcal{M}_d$ . By  $\Omega_d$ , we will denote the set of quantum states, that is positive semidefinite operators having trace equal to one. The subset of  $\mathcal{M}_d$  consisting of unitary matrices will be denoted by  $\mathcal{U}_d$ , while its subgroup of diagonal unitary operators will be denoted by  $\mathcal{D}\mathcal{U}_d$ .

We will also need a linear mapping transforming  $\mathcal{M}_{d_1}$  into  $\mathcal{M}_{d_2}$ , which will be denoted

$$\Phi: \mathcal{M}_{d_1} \to \mathcal{M}_{d_2}. \tag{A.1}$$

There exists a bijection between the set of linear mappings  $\Phi$  and the set of matrices  $\mathcal{M}_{d_1d_2}$ , known as the Choi-Jamiołkowski isomorphism. For a given linear mapping  $\Phi$  the corresponding Choi operator  $J(\Phi)$  is explicitly written as

$$J(\Phi) := \sum_{i,j=0}^{d-1} \Phi(|i\rangle\langle j|) \otimes |i\rangle\langle j|. \tag{A.2}$$

We also introduce a special subset of all mappings  $\Phi$ , called quantum channels, which are completely positive and trace preserving (CPTP). In this work we will consider a special class of quantum channels, called unitary channels. A quantum channel  $\Phi_U$  is said to be a unitary channel if it has the following form  $\Phi_U(\cdot) = U \cdot U^{\dagger}$  for any  $U \in \mathcal{U}_d$ .

Let us recall a general form of a quantum measurement, so called Positive Operator Valued Measure (POVM). A POVM  $\mathcal{P}$  is a collection of positive semidefinite operators  $\{E_1,\ldots,E_m\}$ , called effects, that sum up to the identity operator, i.e.  $\sum_{i=1}^m E_i = 1$ . In PyQBench, we are interested only in von Neumann measurements, that is measurements for which all the effects are rank-one projectors. Every such measurement can be parameterized by a unitary matrix  $U \in \mathcal{U}_d$  with effects  $\{|u_0\rangle\langle u_0|,\ldots,|u_{d-1}\rangle\langle u_{d-1}|\}$ , are created by taking  $|u_i\rangle$  as (i+1)-th column of the unitary matrix U. We will denote von Neumann measurements described by the matrix U by  $\mathcal{P}_U$ . The action of von Neumann measurement  $\mathcal{P}_U$  on some state  $\rho \in \Omega_d$  can be seen as a measure-and-prepare quantum channel as follows

$$\mathcal{P}_U: \rho \to \sum_{i=0}^{d-1} \langle u_i | \rho | u_i \rangle | i \rangle \langle i |. \tag{A.3}$$

Moreover, observe that each von Neumann measurement  $\mathcal{P}_U$  poses a composition of a unitary channel  $\Phi_{U^{\dagger}}$  and the maximally dephasing channel  $\Delta$ , that means  $\mathcal{P}_U = \Delta \circ \Phi_{U^{\dagger}}$ .

We need to also briefly discuss about the distance between quantum operations. From [31, Theorem 1], the distance between measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  can be expressed in the notion of diamond norm, that is

$$\|\mathcal{P}_U - \mathcal{P}_1\|_{\diamond} = \min_{E \in \mathcal{D}\mathcal{U}_d} \|\Phi_{UE} - \Phi_1\|_{\diamond}. \tag{A.4}$$

To express the distance between unitary channels, we need to introduce the definition of numerical range [43]. The set

$$W(A) = \{ \langle x | A | x \rangle : | x \rangle \in \mathbb{C}^d, \ \langle x | x \rangle = 1 \}$$
 (A.5)

is called the numerical range of a given matrix  $A \in \mathcal{M}_d$ . The detailed properties of the numerical range and its generalizations we can read on the website [44].

Due to the definition of W(A), the distance between two unitary channels  $\Phi_U$  and  $\Phi_1$  can be written as

$$\|\Phi_U - \Phi_1\|_{\diamond} = 2\sqrt{1 - \nu^2},$$
 (A.6)

where  $\nu = \min_{x \in W(U^{\dagger})} |x|$ .

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#### Appendix B. Discrimination task for Hadamard gate

For the discrimination task between von Neumann measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$ , where U = H (the Hadamard gate), the key is to calculate the diamond norm  $\|\mathcal{P}_H - \mathcal{P}_1\|_{\diamond}$  and determine the discriminator  $|\psi_0\rangle$ . Using semidefinite programming [34], we obtain

$$\|\mathcal{P}_H - \mathcal{P}_1\|_{\diamond} = \sqrt{2}.\tag{B.1}$$

From [45] we have

$$\|\mathcal{P}_H - \mathcal{P}_1\|_{\diamond} = \|\Phi_{HE_0} - \Phi_1\|_{\diamond}, \tag{B.2}$$

where  $\Phi_U$  is a unitary channel and  $E_0$  is of the form

$$E_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1+i & 0\\ 0 & -1-i \end{pmatrix}.$$
 (B.3)

Next, in order to construct the discriminator  $|\psi_0\rangle$  we use Lemma 5 and the proof of Theorem 1 in [31]. We show that there exist states  $\rho_1$  and  $\rho_2$  of the form  $\rho_1 = \frac{1}{2} \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$  and  $\rho_2 = \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$ , respectively. Thus, we construct the quantum state  $\rho_0$  as follows:

$$\rho_0 = \frac{1}{2}\rho_1 + \frac{1}{2}\rho_2 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$
 (B.4)

 $_{904}$  According to the Lemma 5 and the proof of Theorem 1 in [31] we assume  $_{905}$  that

$$|\psi_0\rangle = \left|\sqrt{\rho_0^{\top}}\right\rangle. \tag{B.5}$$

906 It directly implies that

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle). \tag{B.6}$$

Next, from Holevo-Helstrom theorem [32], we determine the final measurement  $\mathcal{P}_{V_i}$ . Let us consider

$$X = (\mathcal{P}_H \otimes \mathbb{1}) (|\psi_0\rangle\langle\psi_0|) - (\mathcal{P}_1 \otimes \mathbb{1}) (|\psi_0\rangle\langle\psi_0|). \tag{B.7}$$

909 From the Hahn-Jordan decomposition [32], let us note

$$X = P - Q, (B.8)$$

where  $P,Q \geq 0$ . Let us define projectors  $\Pi_P$  and  $\Pi_Q$  onto  $\operatorname{im}(P)$  and  $\operatorname{im}(Q)$ , respectively. Observe, that P and Q are block-diagonal. Then,  $\Pi_P$  and  $\Pi_Q$  have the following forms

$$\Pi_P = \begin{pmatrix} |x_p\rangle\langle x_p| & 0\\ 0 & |y_p\rangle\langle y_p| \end{pmatrix}, \tag{B.9}$$

913 and

$$\Pi_Q = \begin{pmatrix} |x_q\rangle\langle x_q| & 0\\ 0 & |y_q\rangle\langle y_q| \end{pmatrix}.$$
 (B.10)

Hence, we define  $V_0$  as

$$\begin{cases} |x_p\rangle = V_0|0\rangle \\ |x_q\rangle = V_0|1\rangle \end{cases}$$
 (B.11)

ond  $V_1$  as

$$\begin{cases} |y_p\rangle = V_1|0\rangle \\ |y_q\rangle = V_1|1\rangle \end{cases}$$
 (B.12)

For the discrimination task between  $\mathcal{P}_H$  and  $\mathcal{P}_1$  the explicit form of  $V_0$  and  $V_1$  is given as follows (see also mathematics/optimal\_final\_measurement\_ discrimination.nb in the source code repository):

$$V_0 = \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix}, \tag{B.13}$$

919 and

$$V_1 = \begin{pmatrix} -\beta & \alpha \\ \alpha & \beta \end{pmatrix}, \tag{B.14}$$

920 where

$$\alpha = \frac{\sqrt{2 - \sqrt{2}}}{2} = \cos\left(\frac{3}{8}\pi\right),\tag{B.15}$$

921 and

$$\beta = \frac{\sqrt{2 + \sqrt{2}}}{2} = \sin\left(\frac{3}{8}\pi\right). \tag{B.16}$$

#### Appendix C. Optimal probability for parameterized Fourier family

Let us focus on single-qubit von Neumann measurements  $\mathcal{P}_1$  and  $\mathcal{P}_U$ .

Assume that the unitary matrix U is of the form

$$U = H \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} H^{\dagger} \tag{C.1}$$

where H is the Hadamard matrix of dimension two and  $\phi \in [0, 2\pi)$ . In this section we present theoretical probability of correct discrimination between these measurements. To do that, we will present an auxiliary lemma.

Lemma 1. Let  $U = H \operatorname{diag}(1, e^{i\phi}) H^{\dagger}$ ,  $\phi \in [0, 2\pi)$  and let  $\Phi_U$  and  $\Phi_1$  be two unitary channels. Then, the following equation holds

$$\min_{E \in \mathcal{D}U_2} \|\Phi_{UE} - \Phi_1\|_{\diamond} = \|\Phi_U - \Phi_1\|_{\diamond}, \tag{C.2}$$

Proof. Recall that the distance between two unitary channels is given by  $\|\Phi_U - \Phi_1\|_{\diamond} = 2\sqrt{1-\nu^2}$ , where  $\nu = \min_{x \in W(U^{\dagger})} |x|$  for any  $U \in \mathcal{U}_d$ . For  $U = H \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} H^{\dagger}$  the readers briefly observe that  $\nu^2 = 1 - \frac{|1-e^{-i\phi}|^2}{4} = 1 - \frac{|1-e^{i\phi}|^2}{4}$ . So,

$$\|\Phi_U - \Phi_1\|_{\diamond} = |1 - e^{i\phi}|.$$
 (C.3)

935 It implies that it is enough to prove

$$\min_{E \in \mathcal{D}\mathcal{U}_2} \|\Phi_{UE} - \Phi_1\|_{\diamond} = |1 - e^{i\phi}|. \tag{C.4}$$

This condition is equivalent to show that for every  $E \in \mathcal{DU}_2$ 

$$\nu_E \le \frac{|1 + e^{i\phi}|}{2},\tag{C.5}$$

where  $\nu_E = \min_{x \in W(U^{\dagger}E)} |x|$ . 937

The celebrated Hausdorf-Töplitz theorem [46, 47] states that W(A) of 938 any matrix  $A \in \mathcal{M}_d$  is a convex set, and therefore we have

$$W(A) = \{ \operatorname{tr}(A\rho) : \rho \in \Omega_d \}. \tag{C.6}$$

So, we can assume that 940

$$\min_{|x\rangle \in \mathbb{C}^2: |x\rangle\langle x|=1} |\langle x|U^{\dagger}|x\rangle| = \min_{\rho \in \Omega_2} |\operatorname{tr}(U^{\dagger}\rho)|. \tag{C.7}$$

Then, we have

$$\nu_E = \min_{\rho \in \Omega_2} |\operatorname{tr}(\rho U E)|. \tag{C.8}$$

For that, our task is reduced to show that for every  $E \in \mathcal{DU}_2$  there exists  $\rho \in \Omega_2$  such that

$$|\operatorname{tr}(\rho UE)| \le \frac{|1 + e^{i\phi}|}{2}.$$
 (C.9)

Let us define  $E = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}$  and take  $\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$ . From spectral theorem, let us decompose U as 945

$$U = \lambda_0 |x_0\rangle \langle x_0| + \lambda_1 |x_1\rangle \langle x_1|, \tag{C.10}$$

where for eigenvalue  $\lambda_0 = 1$ , the corresponding eigenvector is of the form  $|x_0\rangle = \begin{vmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{vmatrix}$ , whereas for  $\lambda_1 = e^{i\phi}$  we have  $|x_1\rangle = \begin{vmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{vmatrix}$ . Then, for every  $E \in \mathcal{D}\mathcal{U}_2$  we have

$$|\operatorname{tr}(\rho U E)| = \frac{1}{2} \left| \operatorname{tr} \left( H \operatorname{diag}(1, e^{i\phi}) H^{\dagger} E \right) \right| = \frac{1}{2} \left| \operatorname{tr} \left( (|x_0\rangle \langle x_0| + e^{i\phi} |x_1\rangle \langle x_1|) E \right) \right|$$

$$= \frac{1}{2} \left| \langle x_0 | E | x_0 \rangle + e^{i\phi} \langle x_1 | E | x_1 \rangle \right| = \frac{1}{2} \left| \frac{E_0 + E_1}{2} + e^{i\phi} \frac{E_0 + E_1}{2} \right|$$

$$= \frac{\left| 1 + e^{i\phi} \right|}{2} \left| \frac{E_0 + E_1}{2} \right| \le \frac{\left| 1 + e^{i\phi} \right|}{2},$$
(C.11)

which completes the proof. 949

**Theorem 1.** The optimal probability of correct discrimination between von 950 Neumann measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$  for  $U = H \operatorname{diag}(1, e^{i\phi}) H^{\dagger}$ , where  $\phi \in$ 951  $[0,2\pi)$  is given by

$$p_{succ}(\mathcal{P}_U, \mathcal{P}_1) = \frac{1}{2} + \frac{|1 - e^{i\phi}|}{4}.$$
 (C.12)

953 *Proof.* From Holevo-Helstrom theorem, we obtain

$$p_{\text{succ}}(\mathcal{P}_U, \mathcal{P}_1) = \frac{1}{2} + \frac{1}{4} \|\mathcal{P}_U - \mathcal{P}_1\|_{\diamond}. \tag{C.13}$$

From [31, Theorem 1], we have

$$\|\mathcal{P}_U - \mathcal{P}_1\|_{\diamond} = \min_{E \in \mathcal{D}\mathcal{U}_d} \|\Phi_{UE} - \Phi_1\|_{\diamond}. \tag{C.14}$$

From Lemma 1, we know that for  $U = H \operatorname{diag}(1, e^{i\phi}) H^{\dagger}$ , it also holds that

$$\min_{E \in \mathcal{D}U_2} \|\Phi_{UE} - \Phi_1\|_{\diamond} = \|\Phi_U - \Phi_1\|_{\diamond}, \tag{C.15}$$

which is exactly equal to

$$\|\Phi_U - \Phi_1\|_{\diamond} = 2\sqrt{1 - \nu^2} = |1 - e^{i\phi}|.$$
 (C.16)

957 It implies that

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$$p_{\text{succ}}(\mathcal{P}_U, \mathcal{P}_1) = \frac{1}{2} + \frac{|1 - e^{i\phi}|}{4},$$
 (C.17)

which completes the proof.

## Appendix D. Optimal discrimination strategy for parameterized Fourier family

In this Appendix we create the optimal theoretical strategy of discrimination between  $\mathcal{P}_U$  and  $\mathcal{P}_1$ . To indicate the optimal strategy, we will present two propositions. The first one is concentrated around the discriminator as the optimal input state of discrimination strategy, whereas the second one describes the optimal final measurement.

Proposition 1. Consider the problem of discrimination between von Neumann measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$ ,  $U = H \operatorname{diag}(1, e^{i\phi}) H^{\dagger}$  and  $\phi \in [0, 2\pi)$ . The discriminator has the form

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}|\mathbb{1}_2\rangle\rangle.$$
 (D.1)

Proof. Let  $U = H \operatorname{diag}(1, e^{i\phi}) H^{\dagger}, \phi \in [0, 2\pi)$  be decomposed as

$$U = \lambda_0 |x_0\rangle \langle x_0| + \lambda_1 |x_1\rangle \langle x_1|, \qquad (D.2)$$

where for eigenvalue  $\lambda_0=1$ , the corresponding eigenvector is of the form  $|x_0\rangle=\begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$ , whereas for  $\lambda_1=e^{i\phi}$  we have  $|x_1\rangle=\begin{bmatrix}\frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}}\end{bmatrix}$ . For Hermitian-preserving maps [32] the diamond norm may be expressed as

$$\|\Phi\|_{\diamond} = \max_{\rho \in \Omega_d} \| (\mathbb{1} \otimes \sqrt{\rho}) J(\Phi) (\mathbb{1} \otimes \sqrt{\rho}) \|_1.$$
 (D.3)

973 Hence, we obtain

$$\|\mathcal{P}_{U} - \mathcal{P}_{1}\|_{\diamond} = \max_{\rho \in \Omega_{2}} \|(\mathbb{1} \otimes \sqrt{\rho}) J(\mathcal{P}_{U} - \mathcal{P}_{1}) (\mathbb{1} \otimes \sqrt{\rho})\|_{1}$$

$$= \max_{\rho \in \Omega_{2}} \|(\mathbb{1} \otimes \sqrt{\rho}) \sum_{i=0}^{1} |i\rangle\langle i| \otimes (|u_{i}\rangle\langle u_{i}| - |i\rangle\langle i|)^{\top} (\mathbb{1} \otimes \sqrt{\rho})\|_{1}$$

$$= \max_{\rho \in \Omega_{2}} \|\sum_{i=0}^{1} |i\rangle\langle i| \otimes \sqrt{\rho} (|u_{i}\rangle\langle u_{i}| - |i\rangle\langle i|)^{\top} \sqrt{\rho}\|_{1}$$

$$= \max_{\rho \in \Omega_{2}} \sum_{i=0}^{1} \|\sqrt{\rho} (|u_{i}\rangle\langle u_{i}| - |i\rangle\langle i|)^{\top} \sqrt{\rho}\|_{1}.$$
(D.4)

One can prove that for all  $\alpha, \beta \geq 0$ , and unit vectors  $|x\rangle, |y\rangle$  the following equation holds [32]

$$\|\alpha|x\rangle\langle x| - \beta|y\rangle\langle y|\|_1 = \sqrt{(\alpha+\beta)^2 - 4\alpha\beta|\langle x|y\rangle|^2}.$$
 (D.5)

976 By taking  $|x\rangle = \frac{\sqrt{\rho}|\bar{u_i}\rangle}{\|\sqrt{\rho}|\bar{u_i}\rangle\|}$  and  $|y\rangle = \frac{\sqrt{\rho}|i\rangle}{\|\sqrt{\rho}|i\rangle\|}$  we have

$$\|\mathcal{P}_{U} - \mathcal{P}_{1}\|_{\diamond} = \max_{\rho \in \Omega_{2}} \sum_{i=0}^{1} \sqrt{\left(\langle \bar{u}_{i} | \rho | \bar{u}_{i} \rangle + \langle i | \rho | i \rangle\right)^{2} - 4|\langle \bar{u}_{i} | \rho | i \rangle|^{2}}.$$
 (D.6)

Let us take  $\rho_0 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ , we obtain

$$||\mathcal{P}_{U} - \mathcal{P}_{1}||_{\diamond} \geq \sum_{i=0}^{1} \sqrt{(\langle \bar{u}_{i} | \rho_{0} | \bar{u}_{i} \rangle + \langle i | \rho_{0} | i \rangle)^{2} - 4|\langle i | \rho_{0} | \bar{u}_{i} \rangle|^{2}}$$

$$= \sum_{i=0}^{1} \sqrt{1 - |\langle i | U | i \rangle|^{2}}$$

$$= \sum_{i=0}^{1} \sqrt{1 - |1 \cdot \langle i | u_{0} \rangle \langle u_{0} | i \rangle + e^{i\phi} \cdot \langle i | u_{1} \rangle \langle u_{1} | i \rangle|^{2}}$$

$$= \sum_{i=0}^{1} \sqrt{1 - \left| \frac{1 + e^{i\phi}}{2} \right|^{2}} = 2\sqrt{1 - \left| \frac{1 + e^{i\phi}}{2} \right|^{2}}$$

$$= |1 - e^{i\phi}|.$$
(D.7)

Due to Theorem 1 and the following equality

$$\| (\mathbb{1} \otimes \sqrt{\rho}) J(\mathcal{P}_U - \mathcal{P}_1) (\mathbb{1} \otimes \sqrt{\rho}) \|_1 = \| ((\mathcal{P}_U - \mathcal{P}_1) \otimes \mathbb{1}) (|\sqrt{\rho}^\top\rangle) \langle \langle \sqrt{\rho}^\top | \rangle \|_1,$$
(D.8)

the discriminator  $|\psi_0\rangle$  is equal to

$$|\psi_0\rangle = |\sqrt{\rho_0}^{\top}\rangle\rangle = \frac{1}{\sqrt{2}}|\mathbb{1}_2\rangle\rangle,$$
 (D.9)

980 which completes the proof.

Proposition 2. Consider the problem of discrimination between von Neumann measurements  $\mathcal{P}_U$  and  $\mathcal{P}_1$ ,  $U = H \operatorname{diag}(1, e^{i\phi}) H^{\dagger}$  and  $\phi \in [0, 2\pi)$ . The controlled unitaries  $V_0$  and  $V_1$  have the form

$$V_0 = \begin{pmatrix} i \sin\left(\frac{\pi - \phi}{4}\right) & -i \cos\left(\frac{\pi - \phi}{4}\right) \\ \cos\left(\frac{\pi - \phi}{4}\right) & \sin\left(\frac{\pi - \phi}{4}\right) \end{pmatrix}, \tag{D.10}$$

984 and

$$V_1 = \begin{pmatrix} -i\cos\left(\frac{\pi-\phi}{4}\right) & i\sin\left(\frac{\pi-\phi}{4}\right) \\ \sin\left(\frac{\pi-\phi}{4}\right) & \cos\left(\frac{\pi-\phi}{4}\right) \end{pmatrix}. \tag{D.11}$$

Proof. From Proposition 1 we obtain the exact form of discriminator givenby

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}|\mathbb{1}_2\rangle\rangle.$$
 (D.12)

Repeating the procedure used to distinguish the von Neumann measurements in the Hadamard basis (see Appendix B), we use the Hahn-Jordan decomposition and then we create the projective operators into the positive and negative part of X matrix. Hence, the explicit form of  $V_0$  and  $V_1$  is given as follows:

$$V_0 = \begin{pmatrix} i \sin\left(\frac{\pi - \phi}{4}\right) & -i \cos\left(\frac{\pi - \phi}{4}\right) \\ \cos\left(\frac{\pi - \phi}{4}\right) & \sin\left(\frac{\pi - \phi}{4}\right) \end{pmatrix}, \tag{D.13}$$

992 and

$$V_1 = \begin{pmatrix} -i\cos\left(\frac{\pi-\phi}{4}\right) & i\sin\left(\frac{\pi-\phi}{4}\right) \\ \sin\left(\frac{\pi-\phi}{4}\right) & \cos\left(\frac{\pi-\phi}{4}\right) \end{pmatrix}, \tag{D.14}$$

993 where  $\phi \in [0, 2\pi)$ .

## 994 Appendix E. Output YAML files

In this appendix we present examples of YAML's files obtained from synchronous ans asynchronous experiments. We will start at synchronous case.

Listing 14: Defining experiment file

```
998
    type: discrimination-fourier
999
    qubits:
1000
        - target: 0
1001
          ancilla: 1
1002
        - target: 1
1003
          ancilla: 2
1004
1005
    angles:
        start: 0
1006
        stop: 2 * pi
1007
       num_steps: 3
1008
1009
    gateset: ibmq
    method: direct_sum
1010
    num_shots: 100
1811
```

Listing 15: Defining backend file

```
name: ibmq_quito
name: ibmq_quito
asynchronous: false
provider:
hub: ibm-q
group: open
project: main
```

```
1021
    metadata:
1022
       experiments:
1023
          type: discrimination-fourier
1024
          qubits:
1025
          - {target: 0, ancilla: 1}
1026
          - {target: 1, ancilla: 2}
1027
          angles: {start: 0.0, stop: 6.283185307179586, num_steps: 3}
1028
          gateset: ibmq
1029
          method: direct_sum
1030
1031
          num_shots: 100
       backend_description:
1032
          name: ibmq_quito
1033
          asynchronous: false
1034
          provider: {group: open, hub: ibm-q, project: main}
1035
    data:
1036
    - target: 0
1037
      ancilla: 1
1038
      phi: 0.0
1039
      results_per_circuit:
1040
      - name: id
1041
       histogram: {'00': 28, '01': 26, '10': 21, '11': 25}
       mitigation_info:
1043
          target: {prob_meas0_prep1: 0.05220000000000024,
1044
              prob_meas1_prep0: 0.0172}
1045
          ancilla: {prob_meas0_prep1: 0.0590000000000000,
1046
              prob_meas1_prep0: 0.0202}
1047
       mitigated_histogram: {'00': 0.2637212373658018, '01':
1048
           0.25865061319892463, '10': 0.2067279352110304, '11':
1049
           0.2709002142242433}
1050
      - name: u
1051
       histogram: {'00': 30, '01': 16, '10': 28, '11': 26}
1052
       mitigation_info:
1053
          target: {prob_meas0_prep1: 0.05220000000000024,
1054
              prob_meas1_prep0: 0.0172}
1055
          ancilla: {prob_meas0_prep1: 0.0590000000000005,
1056
              prob_meas1_prep0: 0.0202}
1057
       mitigated_histogram: {'00': 0.2857378991684036, '01':
1058
           0.14975297832942433, '10': 0.28142307224788693, '11':
1059
           0.2830860502542851}
1060
    - target: 0
1061
      ancilla: 1
1062
      phi: 3.141592653589793
1063
```

```
results_per_circuit:
1064
      - name: id
1065
       histogram: {'00': 4, '01': 5, '10': 45, '11': 46}
1066
       mitigation_info:
          target: {prob_meas0_prep1: 0.05220000000000024,
1068
             prob_meas1_prep0: 0.0172}
1069
          ancilla: {prob_meas0_prep1: 0.0590000000000000,
1070
             prob_meas1_prep0: 0.0202}
1071
       mitigated_histogram: {'00': 0.011053610583159325, '01':
1072
          0.02261276648026373, '10': 0.4593955619936729, '11':
1073
          0.5069380609429042}
1074
      - name: u
1075
       histogram: {'00': 56, '01': 43, '10': 1}
1076
       mitigation_info:
1077
          target: {prob_meas0_prep1: 0.05220000000000024,
1078
             prob_meas1_prep0: 0.0172}
1079
          ancilla: {prob_meas0_prep1: 0.0590000000000000,
1080
             prob_meas1_prep0: 0.0202}
1081
       mitigated_histogram: {'00': 0.5573987337172156, '01':
1082
          0.44424718645642625, '10': -0.0016459201736417181}
1083
    - target: 0
1084
      ancilla: 1
1085
      phi: 6.283185307179586
1086
      results_per_circuit:
1087
      - name: id
1088
       histogram: {'00': 36, '01': 18, '10': 25, '11': 21}
1089
       mitigation_info:
1090
          target: {prob_meas0_prep1: 0.05220000000000024,
1091
             prob_meas1_prep0: 0.0172}
1092
          ancilla: {prob_meas0_prep1: 0.0590000000000000,
1093
             prob_meas1_prep0: 0.0202}
1094
       mitigated_histogram: {'00': 0.3488190312089973, '01':
1095
           0.17355281935572894, '10': 0.2505792064871127, '11':
          0.22704894294816103}
1097
      - name: u
1098
       histogram: {'00': 32, '01': 27, '10': 24, '11': 17}
1099
       mitigation_info:
1100
          target: {prob_meas0_prep1: 0.05220000000000024,
1101
             prob_meas1_prep0: 0.0172}
1102
          ancilla: {prob_meas0_prep1: 0.0590000000000000,
1103
             prob_meas1_prep0: 0.0202}
1104
       mitigated_histogram: {'00': 0.3025357275361897, '01':
1105
          0.27413673119534815, '10': 0.24313373302688793, '11':
1106
```

```
0.18019380824157433}
1107
    - target: 1
1108
      ancilla: 2
1109
      phi: 0.0
1110
      results_per_circuit:
1111
      - name: id
1112
       histogram: {'00': 27, '01': 20, '10': 24, '11': 29}
1113
       mitigation_info:
1114
          target: {prob_meas0_prep1: 0.0590000000000000,
1115
              prob_meas1_prep0: 0.0202}
1116
          ancilla: {prob_meas0_prep1: 0.0754000000000000,
1117
              prob_meas1_prep0: 0.0528}
1118
       mitigated_histogram: {'00': 0.2594378169217188, '01':
1119
           0.19318893233269735, '10': 0.23035366874292057, '11':
1120
           0.3170195820026633}
1121
      - name: u
1122
       histogram: {'00': 31, '01': 24, '10': 23, '11': 22}
1123
       mitigation_info:
1124
          target: {prob_meas0_prep1: 0.0590000000000000,
1125
              prob_meas1_prep0: 0.0202}
1126
          ancilla: {prob_meas0_prep1: 0.07540000000000000,
1127
              prob_meas1_prep0: 0.0528}
1128
       mitigated_histogram: {'00': 0.30056875246775644, '01':
1129
           0.2438221628798003, '10': 0.22180309809696985, '11':
1130
           0.23380598655547338}
1131
    - target: 1
1132
      ancilla: 2
1133
      phi: 3.141592653589793
1134
      results_per_circuit:
1135
      - name: id
1136
       histogram: {'00': 5, '01': 4, '10': 50, '11': 41}
1137
       mitigation_info:
1138
          target: {prob_meas0_prep1: 0.0590000000000000,
1139
              prob_meas1_prep0: 0.0202}
1140
          ancilla: {prob_meas0_prep1: 0.0754000000000000,
1141
              prob_meas1_prep0: 0.0528}
1142
       mitigated_histogram: {'00': 0.009552870928837118, '01':
1143
           0.007194089383161034, '10': 0.5236791012692514, '11':
1144
           0.4595739384187503}
1145
      - name: u
1146
       histogram: {'00': 41, '01': 51, '10': 3, '11': 5}
1147
       mitigation_info:
1148
          target: {prob_meas0_prep1: 0.0590000000000000,
1149
```

```
prob_meas1_prep0: 0.0202}
1150
          ancilla: {prob_meas0_prep1: 0.07540000000000000,
1151
              prob_meas1_prep0: 0.0528}
1152
       mitigated_histogram: {'00': 0.4073387714165384, '01':
1153
           0.5614614121117936, '10': 0.006431862814564833, '11':
1154
           0.024767953657102992}
1155
      target: 1
1156
      ancilla: 2
1157
      phi: 6.283185307179586
1158
      results_per_circuit:
1159
      - name: id
1160
       histogram: {'00': 30, '01': 28, '10': 23, '11': 19}
1161
       mitigation_info:
1162
          target: {prob_meas0_prep1: 0.0590000000000000,
1163
              prob_meas1_prep0: 0.0202}
1164
          ancilla: {prob_meas0_prep1: 0.0754000000000000,
1165
              prob_meas1_prep0: 0.0528}
1166
       mitigated_histogram: {'00': 0.2868459834940102, '01':
1167
           0.2919564941384742, '10': 0.22466574543735374, '11':
1168
           0.19653177693016174}
1169
      - name: u
1170
       histogram: {'00': 15, '01': 20, '10': 36, '11': 29}
1171
       mitigation_info:
1172
          target: {prob_meas0_prep1: 0.0590000000000000,
1173
              prob_meas1_prep0: 0.0202}
1174
          ancilla: {prob_meas0_prep1: 0.07540000000000002,
1175
              prob_meas1_prep0: 0.0528}
1176
       mitigated_histogram: {'00': 0.1187719606657805, '01':
1177
           0.1962085394489247, '10': 0.3710195249988589, '11':
1178
           0.31399997488643583}
<del>11</del>78
    For the same experiment file, we use the flag asynchronous:
                                                                 true to define
```

asynchronous experiment. 1182

Listing 17: Backend file

```
1183
    name: ibmq_quito
1184
    asynchronous: true
1185
    provider:
1186
       hub: ibm-q
1187
        group: open
1188
       project: main
1188
```

If the backend is asynchronous, the output will contain intermediate data

containing, amongst others, job ids correlated with the circuit they correspond to.

Listing 18: Resolved results

```
1194
    metadata:
1195
       experiments:
1196
          type: discrimination-fourier
1197
          qubits:
1198
          - {target: 0, ancilla: 1}
1199
          - {target: 1, ancilla: 2}
          angles: {start: 0.0, stop: 6.283185307179586, num_steps: 3}
1201
          gateset: ibmq
1202
          method: direct_sum
1203
          num_shots: 100
1204
       backend_description:
1205
1206
          name: ibmq_quito
          asynchronous: true
1207
          provider: {group: open, hub: ibm-q, project: main}
1208
    data:
1209
    - job_id: 63e7f17a17b7ed49ca24e05b
1210
      keys:
1211
      -[0, 1, id, 0.0]
1212
      - [0, 1, u, 0.0]
1213
      - [0, 1, id, 3.141592653589793]
1214
      - [0, 1, u, 3.141592653589793]
1215
      - [0, 1, id, 6.283185307179586]
1216
      - [0, 1, u, 6.283185307179586]
      -[1, 2, id, 0.0]
1218
      - [1, 2, u, 0.0]
1219
      - [1, 2, id, 3.141592653589793]
1220
      - [1, 2, u, 3.141592653589793]
1221
      - [1, 2, id, 6.283185307179586]
      - [1, 2, u, 6.283185307179586]
1223
```

Finally, if the status of jobs is DONE, we resolve the measurements from the submitted jobs obtaining the following file.

Listing 19: Results (asynchronous)

```
1227
1228 metadata:
1229 experiments:
1230 type: discrimination-fourier
1231 qubits:
1232 - target: 0
```

```
ancilla: 1
1233
       - target: 1
1234
          ancilla: 2
1235
       angles:
1236
          start: 0.0
1237
          stop: 6.283185307179586
1238
         num_steps: 3
1239
       gateset: ibmq
1240
       method: direct_sum
1241
       num_shots: 100
1242
       backend_description:
1243
       name: ibmq_quito
1244
       asynchronous: true
1245
       provider:
1246
           group: open
1247
           hub: ibm-q
1248
           project: main
1249
    data:
1250
1251
    - target: 0
      ancilla: 1
1252
      phi: 0.0
1253
      results_per_circuit:
1254
       - name: id
1255
       histogram:
1256
           '00': 27
1257
           '01': 28
1258
           '10': 18
1259
           111: 27
1260
       mitigation_info:
1261
          target:
1262
           prob_meas0_prep1: 0.05220000000000024
1263
           prob_meas1_prep0: 0.0172
1264
          ancilla:
1265
           prob_meas0_prep1: 0.0590000000000005
1266
           prob_meas1_prep0: 0.0202
1267
       mitigated_histogram:
1268
           '00': 0.254196166145997
1269
           '01': 0.2790358060520916
1270
           '10': 0.1732699847244092
1271
           '11': 0.29349804307750227
1272
       - name: u
1273
       histogram:
1274
           ,00,: 29
1275
```

```
'01': 17
1276
          '10': 30
1277
          111: 24
1278
       mitigation_info:
1279
         target:
1280
          prob_meas0_prep1: 0.05220000000000024
1281
          prob_meas1_prep0: 0.0172
1282
         ancilla:
1283
          prob_meas0_prep1: 0.0590000000000005
1284
          prob_meas1_prep0: 0.0202
1285
       mitigated_histogram:
1286
          '00': 0.2733793468261183
1287
          '01': 0.1621115306717096
1288
          '10': 0.3045273800167787
1289
          '11': 0.2599817424853933
1290
    - target: 0
1291
      ancilla: 1
1292
      phi: 3.141592653589793
1293
      results_per_circuit:
1294
      - name: id
1295
       histogram:
1296
          ,00,: 3
1297
          '01': 5
1298
          '10': 37
1299
          111: 55
1300
       mitigation_info:
1301
1302
         target:
          prob_meas0_prep1: 0.05220000000000024
1303
          prob_meas1_prep0: 0.0172
1304
1305
          prob_meas0_prep1: 0.0590000000000005
1306
          prob_meas1_prep0: 0.0202
1307
       mitigated_histogram:
1308
          '00': 0.006189545789708441
1309
          '01': 0.016616709640352317
1310
          '10': 0.3675478279476653
1311
          '11': 0.6096459166222741
1312
      - name: u
1313
       histogram:
1314
          '00': 56
1315
          '01': 42
1316
          '10': 2
1317
       mitigation_info:
1318
```

```
1319
         target:
          prob_meas0_prep1: 0.05220000000000024
1320
          prob_meas1_prep0: 0.0172
1321
1322
         ancilla:
          prob_meas0_prep1: 0.0590000000000005
1323
          prob_meas1_prep0: 0.0202
1324
       mitigated_histogram:
1325
          '00': 0.55731929321128
1326
          '01': 0.43367489257574243
1327
          '10': 0.009005814212977551
1328
    - target: 0
1329
      ancilla: 1
1330
      phi: 6.283185307179586
1331
      results_per_circuit:
1332
      - name: id
1333
       histogram:
1334
          '00': 18
1335
          '01': 28
1336
          10:30
1337
          111: 24
1338
       mitigation_info:
1339
         target:
1340
          prob_meas0_prep1: 0.05220000000000024
1341
          prob_meas1_prep0: 0.0172
1342
1343
          prob_meas0_prep1: 0.0590000000000005
1344
          prob_meas1_prep0: 0.0202
1345
       mitigated_histogram:
1346
          '00': 0.15258295844557557
1347
          '01': 0.2829079190522524
1348
          '10': 0.3071204587046501
1349
          '11': 0.25738866379752195
1350
      - name: u
1351
       histogram:
1352
          ,00,: 32
1353
          '01': 28
1354
          '10': 23
1355
          111: 17
1356
       mitigation_info:
1357
         target:
1358
          prob_meas0_prep1: 0.05220000000000024
1359
          prob_meas1_prep0: 0.0172
1360
         ancilla:
1361
```

```
prob_meas0_prep1: 0.0590000000000005
1362
          prob_meas1_prep0: 0.0202
1363
       mitigated_histogram:
1364
          '00': 0.3026150836796529
1365
          '01': 0.28491749668524724
1366
          '10': 0.23230862145681827
1367
          '11': 0.18015879817828173
1368
    - target: 1
1369
      ancilla: 2
1370
      phi: 0.0
1371
      results_per_circuit:
1372
      - name: id
1373
       histogram:
1374
          '00': 27
1375
          '01': 16
1376
          '10': 30
1377
          111: 27
1378
       mitigation_info:
1379
         target:
1380
          prob_meas0_prep1: 0.0590000000000005
1381
          prob_meas1_prep0: 0.0202
1382
         ancilla:
1383
          prob_meas0_prep1: 0.0754000000000002
1384
          prob_meas1_prep0: 0.0528
1385
       mitigated_histogram:
1386
          '00': 0.256742095057232
1387
          '01': 0.15000257115061383
1388
          '10': 0.29821012040758116
1389
          '11': 0.29504521338457296
1390
      - name: u
1391
       histogram:
1392
          ,00;: 34
1393
          '01': 22
1394
          '10': 25
1395
          '11': 19
1396
       mitigation_info:
1397
        target:
1398
          prob_meas0_prep1: 0.0590000000000005
1399
          prob_meas1_prep0: 0.0202
1400
         ancilla:
1401
          prob_meas0_prep1: 0.0754000000000002
1402
          prob_meas1_prep0: 0.0528
1403
       mitigated_histogram:
1404
```

```
'00': 0.3325088211394024
1405
          '01': 0.22335261496979697
1406
          '10': 0.2441636375921354
1407
          '11': 0.19997492629866526
1408
    - target: 1
1409
      ancilla: 2
1410
      phi: 3.141592653589793
1411
      results_per_circuit:
1412
1413
      - name: id
       histogram:
1414
          '00': 3
1415
          '01': 9
1416
          '10': 51
1417
          111: 37
1418
       mitigation_info:
1419
         target:
          prob_meas0_prep1: 0.0590000000000005
1421
          prob_meas1_prep0: 0.0202
1422
         ancilla:
1423
          prob_meas0_prep1: 0.0754000000000000
1424
          prob_meas1_prep0: 0.0528
1425
       mitigated_histogram:
1426
          '00': -0.016627023111853642
1427
          '01': 0.06778554570877951
1428
          '10': 0.53899887367658
1429
          '11': 0.40984260372649417
1430
1431
      - name: u
       histogram:
1432
          '00': 43
1433
          '01': 45
1434
          10:7
1435
          111: 5
1436
       mitigation_info:
1437
         target:
1438
          prob_meas0_prep1: 0.0590000000000005
1439
          prob_meas1_prep0: 0.0202
1440
         ancilla:
1441
          prob_meas0_prep1: 0.0754000000000000
1442
          prob_meas1_prep0: 0.0528
1443
       mitigated_histogram:
1444
          '00': 0.42955729968594086
1445
          '01': 0.49336080079582095
1446
          '10': 0.04937406434533623
1447
```

```
'11': 0.02770783517290191
1448
    - target: 1
1449
      ancilla: 2
1450
      phi: 6.283185307179586
1451
      results_per_circuit:
1452
      - name: id
1453
       histogram:
1454
          '00': 22
1455
          '01': 19
1456
          '10': 35
1457
          111: 24
1458
       mitigation_info:
1459
         target:
1460
          prob_meas0_prep1: 0.05900000000000005
1461
          prob_meas1_prep0: 0.0202
1462
         ancilla:
1463
          prob_meas0_prep1: 0.0754000000000000
1464
          prob_meas1_prep0: 0.0528
1465
       mitigated_histogram:
1466
          '00': 0.19592641048040849
1467
          '01': 0.18787721420415215
1468
          '10': 0.3590258049844047
1469
          '11': 0.25717057033103463
1470
      - name: u
1471
          histogram:
1472
          '00': 27
1473
          '01': 24
1474
          10: 25
1475
          111: 24
1476
       mitigation_info:
1477
         target:
1478
          prob_meas0_prep1: 0.05900000000000005
1479
          prob_meas1_prep0: 0.0202
1480
         ancilla:
1481
          prob_meas0_prep1: 0.0754000000000000
1482
          prob_meas1_prep0: 0.0528
1483
       mitigated_histogram:
1484
          '00': 0.25555866817587225
1485
          '01': 0.2429501641251142
1486
          '10': 0.24509293912212946
1487
          '11': 0.2563982285768841
1488
1489
```