QAOA-based Fair Sampling on NISQ Devices

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ABSTRACT: We study the status of fair sampling on Noisy Intermediate Scale Quantum (NISQ) devices, in particular the IBM Q family of backends. Using the recently introduced Grover Mixer-QAOA algorithm for discrete optimization, we generate fair sampling circuits to solve six problems of varying difficulty, each with several optimal solutions, which we then run on ten different backends available on the IBM Q system. For a given circuit evaluated on a specific set of qubits, we evaluate: how frequently the qubits return an optimal solution to the problem, the fairness with which the qubits sample from all optimal solutions, and the reported hardware error rate of the qubits. To quantify fairness, we define a novel metric based on Pearson’s χ² test. We find that fairness is relatively high for circuits with small and large error rates, but drops for circuits with medium error rates. This indicates that structured errors dominate in this regime, while unstructured errors, which are random and thus inherently fair, dominate in noisier qubits and longer circuits. Our results provide a simple, intuitive means of quantifying fairness in quantum circuits, and show that reducing structured errors is necessary to improve fair sampling on NISQ hardware.

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1 Introduction

Combinatorial optimization problems, such as the Minimum Traveling Salesperson problem, the Maximum Satisfiability problem, or the Spin Glass Ising model, are widely viewed to be one of the most promising application domains for quantum computing. Such problems often have multiple optimal solutions, and depending on the algorithm being used to solve the problem, some optima may be much easier to find than others. This is problematic if one is interested not in finding a single solution, but instead determining the overall landscape of optimal solutions. Algorithms which fairly sample from the space of optimal solutions avoid this problem and have practical value in physics and engineering. For instance, it is often difficult in practice to encode all the engineering design goals in the function to be optimized. By allowing an engineer to explore an unbiased assortment of optimal solutions, fair sampling provides an opportunity to apply these other design goals to a more diverse set of options (especially useful when a customer adds one more requirement after the optimization has been performed). It
can also be used to produce an ensemble of predictions from calibrated physical models that can be used to make a forecast including a range of possible outcomes (e.g., in the context of fluid flow in the earth’s subsurface, which can be formulated as a discrete optimization problem [11, 19]).

In this paper, we determine the current status of fair sampling in the context of quantum computing. Specifically, we are interested both in algorithms which theoretically guarantee fair sampling (i.e. generate quantum states where all optimal solutions have the same amplitudes squared and thus are measured with equal probability), as well as actual hardware implementations of such algorithms. Previous studies have shown that quantum annealing cannot be used as a fair sampler for all problems [14]. We therefore focus our work on gate-based quantum computing algorithms and hardware.

The most widely-used quantum optimization framework is the Quantum Alternating Operator Ansatz (QAOA), which alternates between a mixer operator that mixes the amplitudes of all feasible solutions and a phase separator operator that separates the phases of the feasible solutions [10]. Most mixers do not exhibit fair sampling, however, the recently discovered Grover Mixer [2] has the property that all feasible solutions with the same objective value have identical amplitudes. This novel Grover Mixer implementation of QAOA thus solves the theoretical side of fair sampling for gate-based quantum computing.

The majority of this work is dedicated to a practical evaluation of how fair sampling circuits are affected by the errors inherent in Noisy Intermediate Scale Quantum (NISQ) devices. In this study, a paradox quickly becomes apparent: while an error-corrected quantum device could obviously be used as a perfectly fair sampler, so could a quantum device completely dominated by noise. Of course a completely noisy machine would be no different than a random number generator, and would sample from all feasible solutions rather than just the optimal solutions, but it would do so fairly. Therefore, our study seeks to clarify where current NISQ devices lie on the spectrum between these two extremes. Specifically, are the hardware errors predominantly random and unstructured, thus leading to relatively fair sampling of optimal solutions? Or do hardware biases and other structured errors play an important role, thus leading to unfair behavior?

Our methodology for answering these questions consists of the following steps:

1. We define six example problems, which are a slightly expanded set of examples studied in the context of fair sampling in quantum annealing [14].

2. We design quantum circuits for our problems and hand-tune them to minimize circuit depth and gate counts, taking into account different qubit connectivity
topologies as encountered on IBM Q. Our circuits involve two to five qubits and our medium size examples result in circuits with gate counts in the $30 - 60$ range, which is similar to the size of the (random) circuits used to establish the Quantum Volume metric on the IBM Q backends.

3. We execute our circuits in a large number of shots on ten different IBM Q backends that have qubit counts of up to 65 qubits. In addition, we embed our circuits in all possible topologies on the circuits resulting a total of 2482 experiments at 40960 shots each.

4. We define a novel metric for quantum computing based on Pearson’s $\chi^2$ test, a common statistical tool to evaluate how likely it is that a set of observational data came from a null hypothesis distribution. Since all NISQ hardware will necessarily involve some biases and imperfections that inhibit fair sampling, we are interested in how much effort must be expended to prove that a piece of hardware is biased, i.e. reject the null hypothesis of fair sampling. We term this metric ‘number of shots to reject fair sampling,’ and it depends on both a specific set of qubits as well as a fair sampling circuit. This fairness metric is a separate contribution to the main results of the paper.

5. We analyze our experiments using our fairness metric and we calculate the aggregate noise level of each experiment from IBM’s reported gate-specific error rates.

We find that the NISQ devices under evaluation provide noticeably unfair sampling. However, fairness increases as aggregate error approaches both 0 and 1, matching with the theoretical extremes of error-corrected and noise-dominated devices discussed previously. In the case of small aggregate error, this is to be expected, as for 0 error we would retrieve the theoretical guarantees of Grover Mixer QAOA. Likewise, for large aggregate error, one should get samples uniformly at random from all computational basis states. Nonetheless, the result is perhaps counter-intuitive, as one might expect a linear interpolation between these two extremes. For example, the hardware-efficient random circuits in Google’s recent quantum supremacy experiment [1] give a sample distribution consisting of a convex combination of an ideal (error-free) Porter-Thomas distribution and a Uniform distribution (caused by errors). Our differing results indicate that we should not expect errors themselves to be evenly distributed (i.e., in a fair manner) across qubits for highly structured circuits such as ours. Indeed, a previous study found that structured errors (e.g. crosstalk, coherent noise) play a large role in the performance of structured circuits [20]. Our result holds for our selected set of circuits and across the 10 NISQ backends on IBM Q.
In addition to our main result, we thoroughly analyze the state of IBM Q’s back-ends: we see clear improvements in error rates from the lower quantum volume backends to higher quantum volume backends, but we also showcase differences within a single backend, as the mapping of circuits to specific qubits skews results quite dramatically.

We propose that fair sampling in general, perhaps with our proposed fairness metric in particular, be an addition in the emerging set of benchmarks for NISQ devices, which so far have largely focused on circuit correctness, such as the random-circuit-based quantum volume metric. Our work is a step towards understanding fair sampling in general gate-level NISQ devices. As devices improve, our experiments should be repeated to see if the fundamental structure of fairness changes.

2 Review

In this section we describe previous studies of fair sampling in the context of quantum computing. A note on nomenclature: since the optimization problems we study can all be phrased in terms of Ising models, we adopt the more physics-oriented language and refer to ‘optimal solutions’ as ground states. Problems with multiple optimal solutions are thus said to have degenerate ground states.

2.1 Fair sampling in quantum annealing

After quantum annealing was proposed as a possibly useful optimization heuristic [12], it was discovered that naïve approaches to quantum annealing do not always sample degenerate ground states fairly [16]. In fact, certain Hamiltonians feature ground states that are sampled with probability approaching zero as annealing time increases. This effect is inherent to the quantum annealing approaches, and is not the consequence of hardware noise or other technical limitations. This behavior was subsequently verified experimentally [15]. Since unfair sampling (especially when certain ground states are strongly suppressed) can have negative consequences for many applications, techniques were proposed to improve upon the naïve quantum annealing approach [13, 14, 21, 24]. None of these techniques have been tested on quantum annealing hardware, indicating some of the challenges with these approaches. It should also be noted that it has been proposed that there are some advantages of biased samplers, that is, they can be used effectively in an ensemble of samplers each of which has different biases [26].

One technique that has been proposed to improve the fairness of quantum annealing is the introduction of more complex Hamiltonians to drive the annealing process [15]. This generally improves fairness, but is hard to implement and does not resolve the underlying problem. Even for small problems, biases sometimes remain despite using fairly high-order Hamiltonians [14]. In studying these higher-order Hamiltonians, Könz
et al [14] introduced four Ising models that are suitable for our QAOA analyses. The problems are described in Table 1 as Problems (a)–(d). These problems all exhibit biased sampling with quantum annealing, so they present a non-trivial challenge for fair sampling algorithms. Two of them involve 4 qubits, one involves 5 qubits, and another involves 6 qubits. This small number of qubits make it plausible that these problems can be solved with reasonably high fidelity on current NISQ hardware.

2.2 Fair sampling in the Quantum Alternating Operator Ansatz

The Quantum Alternating Operator Ansatz [10] (QAOA) is a promising heuristic quantum algorithm for (combinatorial) optimization problems. In its essence, for a problem instance $I$ with feasible states $F$ and cost Hamiltonian $H_C$ on $n$ qubits, a $p$-round QAOA prepares a parametrized state from which one would like to sample low-energy states with respect to $H_C$:

$$|\beta, \gamma\rangle := U_M(\beta_p)U_P(\gamma_p) \cdots U_M(\beta_1)U_P(\gamma_1)U_S |\uparrow^n\rangle. \quad (2.1)$$

The circuit consists of an initial state preparation unitary operator $U_S$ that creates some superposition of all feasible solutions in $I$, followed by $p$ applications of alternating parametrized phase separating and mixing unitaries $U_P(\gamma_k), U_M(\beta_k)$ with real angle parameters $\gamma = (\gamma_1, \ldots, \gamma_p)^T$ and $\beta = (\beta_1, \ldots, \beta_p)^T$, and a final measurement in the computational basis, see e.g. Fig. 1. The $\beta, \gamma$ angles are traditionally found via a hybrid classical/quantum approach: given some initial parameters, take enough samples to reliably estimate the expectation value $\langle \beta, \gamma | H_C | \beta, \gamma \rangle$, use a classical optimizer to adjust the parameters, and repeat until one has a state with a good (low-energy) expectation value. For further description of, and theoretical justifications for this approach, see [4, 6, 22].

The role of the phase separating unitaries $U_P(\gamma)$ is to add multiplicative phase factors to the amplitudes of feasible computational basis states, with phases proportional to respective energies. We usually have (up to global phases) $U_P(\gamma) \simeq e^{-i\gamma H_C}$. For many problems, such as MaxCut [6] or the problems considered in this paper, $H_C$ is an Ising Hamiltonian with quadratic and sometimes linear terms; but in other problems, $H_C$ can also involve higher-order terms, such as for MaxE3Lin2 [7]. The interplay between the state preparation unitary $U_S$ and the mixing unitary $U_M$ is particularly important, and falls into three categories:

**Original Approach** The original approach by Farhi et.al. [6], termed Quantum Approximate Optimization Algorithm, was inspired by quantum annealing for unconstrained optimization problems, i.e. $U_S = H^{\otimes n}$ (preparing an equal superposition of all states) and $U_M(\beta) = e^{-i\beta \sum X_j}$ (a transverse field of Pauli-X operators acting on individual qubits).
Figure 1. Grover Mixer QAOA: The state preparation unitary $U_S$ for an equal superposition of all feasible states $|F\rangle = \frac{1}{\sqrt{|F|}} \sum_{x \in F} |x\rangle$, its conjugate transpose $U_S^\dagger$, and a multi-controlled phase-shift gate $Z^{-\beta/\pi} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\beta} \end{pmatrix}$ are used to implement the mixer $U_M(\beta) = e^{-i\beta|F\rangle\langle F|}$.

**General Ansatz** The general framework introduced in Eq. 2.1 by Hadfield et.al. [10] is a generalization also suitable for a wide variety of constrained optimization problems. They focus on designing involved mixing unitaries $U_M(\beta)$ and usually split $U_S$ in a layer of Identity and Pauli-X gates preparing some feasible computational basis state, followed by an initial mixing unitary $U_M(\beta_0)$ with new angle $\beta_0$.

**Grover Mixer** If one can design efficient state preparation unitaries $U_S$ preparing an equal superposition of all feasible basis states $|F\rangle = \frac{1}{\sqrt{|F|}} \sum_{x \in F} |x\rangle$, then this gives rise to a mixing unitary resembling Grover’s selective phase-shift operator [9, 18, 25], $U_M(\beta) = e^{-i|F\rangle\langle F|} = Id - (1-e^{-i\beta}) |F\rangle \langle F| = U_S(Id - (1-e^{-i\beta}) |\uparrow\rangle \langle \uparrow|) U_S^\dagger$, see Fig. 1. In some sense, this is the reverse of the method in the general ansatz, and it was shown to be applicable to many relevant optimization problems [2], but there also exists a range of constrained problems where it is ruled out under complexity-theoretic assumptions [3].

Although the Quantum Alternating Operator Ansatz is the most general framework of the three, both the Quantum Approximate Optimization Algorithm as well as Grover Mixer QAOA have their advantages. For example, the original approach by definition can not do worse than a Trotterization of the adiabatic algorithm [8], thus converging to a ground state in the $p \to \infty$ limit [6]. Furthermore its phase separating and mixing operators are periodic, restricting the angles to real values in $[-\pi, \pi)$. Grover Mixer QAOA retrieves these properties for constrained optimization problems with efficient state preparation unitaries $U_S$ [3], but for unconstrained optimization problems the Grover Mixer $e^{-i|F\rangle\langle F|}$ has a larger circuit depth than the Transverse Field Mixer...
\[ e^{-i\beta \sum X_i} \]. In this paper we explore an advantage unique to Grover Mixer QAOA among the three categories: fair sampling.

With Grover Mixer QAOA, all feasible basis states begin with amplitude \(1/\sqrt{|F|}\) (after state preparation with \(U_S\)). The phase separating unitary \(U_P(\gamma) = e^{-i\gamma H_C}\) then phases the amplitude of every basis state proportional to its energy and \(\gamma\), keeping the same phase for basis states of same energy. The mixing unitary \(U_M(\beta) = \text{Id} - (1 - e^{-i\beta}) |F\rangle \langle F|\) then deducts from all amplitudes of their input state \(|\psi\rangle\) the same weighted average of all of its amplitudes, \((1 - e^{-i\beta})/\sqrt{|F|})\langle F | \psi\rangle\). Therefore, basis states with the same energy are sampled with the same amplitude. This property holds for all feasible states (not only ground states) and is independent of the number of QAOA levels or the choice of angles for \(U_M, U_P\). For a complete proof, see [2].

2.3 Description of test circuits

In addition to the four problems from [14], we additionally studied two simpler Ising models with degenerate ground states but only involving two and three qubits. While these models do not feature ground state suppression on quantum annealing hardware, we include them in this study because they represent the simplest non-trivial models with degenerate ground states and thus serve as useful baselines as compared to the more complicated models of [14]. All of the models we studied are depicted in Table 1.

Our general procedure for generating test circuits was to begin with a 1-level Grover Mixer QAOA algorithm with \(q_0\) fixed to \(\uparrow\). We chose a 1-level implementation of Grover-QAOA in order to keep circuit depth low. Following [14], we fix \(q_0 := \uparrow\) as all of the models in Table 1 are \(\uparrow / \downarrow\) symmetric. This allows us to reduce the problems from Ising Hamiltonians \(H_C\) with only quadratic terms acting on qubits \(q_0, \ldots, q_{n-1}\) to new Hamiltonians \(H'_C\) with some linear terms acting only on qubits \(q_1, \ldots, q_{n-1}\). This also transforms \(q_0\) into a classical control bit for the consecutive Grover Mixer, which can be removed. Thus we can embed Ising problems on \(n\) qubits onto circuits with only \(n - 1\) qubits. See Fig. 2 for a visual representation of a generic 1-level Grover Mixer QAOA for an unconstrained optimization problem, along with a description of the simplifications resulting from fixing \(q_0\).

We then compiled the circuits to match connectivity graphs and gates available on the IBM Q backend. Instead of employing the tools available in IBM’s qiskit software, we compiled the circuits by hand. This had two benefits. First, this reduced circuit depth by roughly a factor of two as compared to qiskit. Second, it allowed us to generate circuits for architectures that can be found as subgraphs of every hardware connectivity graph among the IBM Q backends, see Fig. 3. Thus, the same exact circuit could be evaluated across many backends, and in many instances across many different qubits on the same backend.
| Problem | Diagram | Ising Hamiltonian \( H_C \) | Ground States \(|(q_0 := \uparrow) \ldots q_{n-1}\)| |
|---------|---------|-----------------|-----------------|
| (a)     | ![Diagram](a) | \(- [Z_0(Z_1 + Z_2 - Z_3) + Z_1(Z_2 - Z_4) + Z_2(Z_3 + Z_4) + Z_3 Z_4] \) | \( |\uparrow\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\downarrow\downarrow\rangle \) |
| (b)     | ![Diagram](b) | \(- [Z_0(2Z_1 + Z_2 + 2Z_3 + Z_4) + Z_1(-2Z_2 - Z_3 + Z_4) + Z_2(Z_3 + 2Z_4 - 2Z_3 Z_4)] \) | \( |\uparrow\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\downarrow\rangle, |\uparrow\uparrow\uparrow\downarrow\rangle, |\uparrow\uparrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\downarrow\rangle | |
| (c)     | ![Diagram](c) | \(- [Z_0Z_2 + Z_1 Z_3 + Z_2(-Z_3 + Z_4 - Z_5) + Z_3(Z_4 - Z_5) + Z_4 Z_5] \) | \( |\uparrow\uparrow\uparrow\uparrow\downarrow\rangle, |\uparrow\uparrow\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\downarrow\downarrow\rangle \) |
| (d)     | ![Diagram](d) | \(- [Z_0Z_1 + Z_1(-Z_2 - Z_3) - Z_2 Z_3] \) | \( |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow \rangle \) |
| (e)     | ![Diagram](e) | \(-[Z_0(-Z_1 - Z_2) - Z_1 Z_2] \) | \( |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle, |\uparrow \rangle \) |
| (f)     | ![Diagram](f) | \(-[-Z_0 Z_1] \) | \( |\uparrow\downarrow\rangle \) |

Table 1. Ising models with degenerate ground states to be studied on NISQ hardware. Problems (a)–(d) are from [14]. All of the Ising models \( H_C = - \sum J_{ij} Z_i Z_j \) have only quadratic terms and no linear terms. The dark red edges indicate a ferromagnetic \( J_{ij} = +2 \) coupling and the light red edges a ferromagnetic \( J_{ij} = +1 \) coupling; the light blue edges represent an antiferromagnetic \( J_{ij} = -1 \) coupling and the dark blue edges an antiferromagnetic \( J_{ij} = -2 \) coupling. Only ground states with \( q_0 = \uparrow \) are listed as all models are symmetric under simultaneous \( \uparrow / \downarrow \)-flips. Note that a symmetry-breaking fixed setting \( q_0 := \uparrow \) results in a Hamiltonian \( H'_C \) on qubits \( q_1, \ldots, q_n \) (without \( q_0 \)) with some linear terms.
Figure 2. (left) A 1-level Grover Mixer QAOA for an unconstrained optimization problem, $U_S |\uparrow^n\rangle = |\rightarrow^n\rangle$, $U_M(\beta) = e^{-i\beta}|\rightarrow^n\rangle\langle\rightarrow^n|$, and the Hamiltonian $|\rightarrow^n\rangle\langle\rightarrow^n| \cong \text{Id} + \sum_i X_i + \sum_{\langle i,j \rangle} X_i X_j + \sum_{\langle i,j,k \rangle} X_i X_j X_k + \ldots$ which has also been proposed to achieve fair sampling in quantum annealing [17], going beyond limited higher-order terms.

(right) For an unconstrained Ising problem with only quadratic terms in the Hamiltonian $H_C$ on $q_0, \ldots, q_{n-1}$, we break symmetries by setting $q_0 = |\uparrow\rangle$ and $U_S |\uparrow^n\rangle = \text{Id} \otimes H^{\otimes n-1} |\uparrow^n\rangle = |\uparrow\rightarrow^{n-1}\rangle$. The quadratic terms of $H_C$ involving $q_0$ turn into linear terms of a Hamiltonian $H'_C$ on $q_1, \ldots, q_{n-1}$, thereby reducing $q_0$ to a classical control bit. The multi-control-$Z^{-\beta/\pi}$ gate is fully symmetric, thus we may swap controls and target.

For Problems (a) and (b), which involve 5 variables (and with $q_0 := \uparrow$ require only 4 qubits) we generated three distinct circuits, each on a different architecture: 4T, 4L, and 5T (see Fig. 3 for notation). The 5T circuits for these problems employ an ancilla qubit, which allows us to discard any sample in which the ancilla was not measured in the $\uparrow$ state. The remaining Problems (c) - (f) each only have a single circuit associated with them. Note that Problem (f), with the Hamiltonian $Z_0 Z_1$ and ground states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, is uniquely simple. In this case we do not fix $q_0 := \uparrow$, nor do we employ Grover-QAOA, as the problem can be “solved” with an almost-trivial circuit of a Hadamard on qubit $q_0$, a $X$-gate on qubit $q_1$, and a consecutive CNOT with control $q_0$ and target $q_1$. Due to the small number of qubits and gates, we use this circuit to explore the highest reaches of accuracy and fairness capable with the hardware.

See Table 2 for a brief description of all of the circuits, including their architectures, gate count, and $\beta$, $\gamma$ parameters. We describe our compilation technique in detail.

Figure 3. The hardware architectures we transpile our circuits to: Linear Nearest Neighbor connectivities on 2,3,4 qubits (2L,3L,4L), as well as T-shaped connectivities on 4,5 qubits (4T,5T). These architectures form connectivity subgraphs of all IBM Q devices. By fixing $q_0 := \uparrow$, each $n$-qubit problem in Table 1 can be mapped to a $(n - 1)$-qubit architecture.
Table 2. Details for 1-round Grover-QAOA fair sampling circuits studied on NISQ hardware. For each circuit, we list the problem from Table 1 being solved, the qubit connectivity from Fig. 3 employed, the total number of single-qubit (i.e. rotation) gates, the total number of CNOT gates, the $\beta, \gamma$ parameters used, the expectation value $\langle \beta, \gamma | H_{C} | \beta, \gamma \rangle$, and the probability of selecting a ground state (GSP).

3 Methodology

We evaluated the previously described set of circuits across a wide swath of current hardware on the IBM Q platform. Since our interest was not in identifying the best performing qubits, but rather observing trends in circuit correctness vs. fairness, we evaluated the same circuit many times per chip, each time using a different subset of qubits. For example, testing the circuit for Problem (e), which has only two qubits, on a chip with 5 qubits in an LNN architecture would involve 4 separate evaluations (on the pairs of qubits $\{q_{i}, q_{i+1}\}$ for $i = 1 \ldots 4$). The machines we tested, along with the number of qubit subsets for each architecture, are listed in Table 3. It is important to emphasize that there was no additional transpilation or optimization of these circuits beyond that discussed in the previous section.

We collected 40960 shots for each circuit on each set of applicable qubits, which gave us sufficient data to achieve repeatable statistics. None of the hardware consistently reported fair results, i.e. hardware noise introduced significant biases for even the simplest circuits. In order to characterize how fair a given set of qubits performed with a given circuit, we adopted the metric: how many shots does one need of a given
Table 3. Details of IBM Q backends to be studied. The name of the backend, the Quantum Volume (QV), the number of qubits, and the number of subsets of qubits on each device matching the relevant circuit architectures (2L, 3L, 4L, 4T, and 5T) are listed.

| Backend     | QV | Qubits | 2L  | 3L  | 4L  | 4T  | 5T  |
|-------------|----|--------|-----|-----|-----|-----|-----|
| manhattan   | 32 | 65     | 72  | 190 | 232 | 96  | 92  |
| montreal    | 32 | 27     | 28  | 74  | 80  | 48  | 36  |
| toronto     | 32 | 27     | 28  | 74  | 80  | 48  | 36  |
| rome        | 32 | 5      | 4   | 6   | 4   | 0   | 0   |
| santiago    | 32 | 5      | 4   | 6   | 4   | 0   | 0   |
| bogota      | 32 | 5      | 4   | 6   | 4   | 0   | 0   |
| valencia    | 16 | 5      | 4   | 8   | 4   | 6   | 2   |
| vigo        | 16 | 5      | 4   | 8   | 4   | 6   | 2   |
| melbourne   | 8  | 15     | 20  | 72  | 130 | 66  | 120 |
| ourense     | 8  | 5      | 4   | 8   | 4   | 6   | 2   |

To calculate the number of shots to reject fair sampling, we utilized Pearson’s $\chi^2$ test, which evaluates how likely a set of observations $\{O_i\}$ is given some expected null hypothesis values $\{E_i\}$. If a given circuit has $d$ degenerate ground states, and $n_{g.s.}$ is the number of ground state observations (out of the 40960 total shots), our null hypothesis is that

$$E_i = E = \frac{n_{g.s.}}{d}. \quad (3.1)$$

The $\chi^2$ value is determined via

$$\chi^2 = \sum_i \frac{(O_i - E)^2}{E}. \quad (3.2)$$

The null hypothesis is rejected at a significance level based on the value of $\chi^2$ as compared against the upper-tail critical values of the $\chi^2$ distribution

$$f(x, k) = \frac{x^{k/2-1}e^{-x/2}}{2^{k/2}\Gamma(k/2)}, \quad (3.3)$$

where $k$ is the number of degrees of freedom in the observed data. For example, with five degrees of freedom a $\chi^2$ value of 11.070 indicates a rejection of the null hypothesis with 95% significance level.
In principle, the value of $\chi^2$ is itself a measure of fairness for a set of observational data, however we found it a poor metric for our application. This is because the actual significance of a given $\chi^2$ value is dependent on the size of the data set as well as the number of degrees of freedom. Since our circuits reported widely varying numbers of ground state observations, and had different numbers of degenerate ground states, comparing $\chi^2$ values across circuits did not compare apples to apples. One could instead report the significance level at which the observational data rejects the fair sampling hypothesis, as that takes sample size and degrees of freedom into account. However, current hardware rejects the fair sampling hypothesis at significance levels so close to 100% that numerical differences between rejection levels were difficult to meaningfully interpret. Instead, determining how many samples from a distribution are necessary (on average) to reject fair sampling at 95% significance can be done with observational data of any size and degrees of freedom, and provides an intuitive measure of the fairness of the underlying qubits.

A formal description of our algorithm for determining the number of shots to reject fair sampling can be found in Appendix A, here we describe the method in general terms. Based on our observational data of a given circuit $C$ on a set of qubits $Q$, we determined the relative frequency of observing each ground state. We then generated 1000 synthetic samples, each containing $n$ ground state observations matching the relative frequency in the observed data. For each sample we calculated $\chi^2$, then took the median value for the set of 1000 samples. We repeated for increasing values of $n$ until we arrived at a median value of $\chi^2$ matching the level necessary to reject the fair sampling hypothesis with 95% statistical significance given the number of degenerate ground states. As an example, with this methodology a coin biased 60/40 requires an average of 95 flips to reject fair sampling.

4 Results

As mentioned in the introduction, none of the qubits or circuits consistently reported fair sampling. Instead, we sought to understand the correlation between qubit fidelity and fair sampling. Our method for quantifying the degree of fair sampling for a circuit on a piece of hardware was described in the previous section. We used two complementary methods of quantifying qubit fidelity. The first is simply the frequency with which a given set of qubits accurately identify an optimal solution for the problem at hand. In this context, higher fidelity qubits are those that obtain a ground state more

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1We found that taking fewer than 1000 samples resulted in inconsistent median values, and more then 1000 samples resulted in slow performance.
frequently. The benefit of this method is that it relies on direct observation of qubits solving a real problem, while the downside is that it can’t be used to directly compare results from different problems. Our second method for quantifying qubit fidelity is to use the hardware error rates as reported by qiskit. This method, which we will discuss in more detail later in this section, has the benefit of more accurately comparing results from different circuits. However, the practical relevance of this reported error data for our application is unclear.

A broad issue for experimental tests of existing NISQ hardware is the highly stochastic nature of the results. We observed significant variance in all of our observed data, and therefore used a very large experiment count (with 2482 distinct evaluations of the IBM Q hardware) to observe consistent trends. To be precise, each data point in the following plots is generated by specifying: a circuit to be evaluated, an IBM Q backend, and a subset of qubits on the backend which match the connectivity of the given circuit. We then collected 40960 shots of the circuit on those specific qubits, and the results of those shots correspond to a single data point in the plots below. This large number of data points allowed us to identify repeatable positive or negative correlations, and we include lines of best fit to indicate these trends.

4.1 Ground state probability vs. fairness

With that proviso out of the way, let us now discuss the results of directly comparing quantity (as measured by the number of ground state observations) vs. quality (as measured by the number of shots to reject fair sampling). We observed a positive correlation between ground state probability and fair sampling for three circuits, those solving the “easy” problems: (d), (e), (f), see Fig. 4. Note that these circuits all have \( \leq 3 \) qubits and circuit depths 40, 20, and 3 respectively. We call this “soft” unfairness, in that improving ground state probability and fairness of sampling are both accomplished by evaluating the circuit on the highest performing qubits possible.

However, with the remaining circuits we observed the opposite: qubits that more frequently obtained ground states did so with increasing bias, see Fig. 5. Note that these circuits all have \( \geq 4 \) qubits and depths ranging from 72 to 152. We call this “hard” unfairness, as improving ground state probability results in less fair results, and vice versa.

We believe this “hard” unfairness comes from the fact that long circuits on noisy qubits produce increasingly random results. This means that the likelihood of selecting a ground state decreases, but the distribution across ground states is fairly even. To test this conjecture, we compared the fairness and ground state probabilities of both a “soft” and “hard” circuit as functions of the error rate of the qubits.
Figure 4. Each data point represents 40960 shots of the specified circuit on a fixed set of qubits on an IBM Q backend. The Quantum Volume (QV) of the backend is indicated by blue for QV32, green for QV16, and red for QV8. In these shorter circuits we observe a positive correlation (as indicated by the black lines of best fit) between ground state probability and number of shots to reject fair sampling.

4.2 Aggregate error rate vs. fairness

The IBM Q hardware reports the latest calibration data for a given chip at the time of evaluating a circuit. Specifically, qiskit reports the error rates for a $U_2$ rotation on all individual gate and a CX operation on each pair of connected qubits. We used this data to generate what we call an aggregate error of the chip and circuit in combination. For a circuit $C$ composed of a sequence of gates $g_1, \ldots, g_n$ evaluated on a chip $H$, this aggregate error $E_{C,H}$ is calculated via

$$E_{C,H} = 1 - \prod_{i=1}^{n} (1 - e_i), \quad (4.1)$$

where $e_i$ is the error for gate $g_i$ as reported by qiskit at the time of evaluation. We believe this aggregate error metric evaluates roughly the likelihood of success of a given circuit on a specific piece of hardware. However, the usefulness of the error rates as reported by qiskit has been drawn in to question [20, 23]. These experiments therefore serve as a test of the relevance of this reported error value in the context of fair sampling.

In Fig. 6 we see that both the soft and hard circuits report lower ground state probabilities as aggregate error rates increase, as expected$^2$. For Problem (d), we see that increased error rates results in less fair results. In other words, the errors result
Figure 5. In these “hard” circuits, involving four or five qubits and between 72 and 152 gates, we observe a negative correlation between ground state probability and number of shots to reject fair sampling.

in systemic bias in favor of some ground states over others. For Problem (a), we see the opposite behavior: increased error rates result in fairer solutions. We can see in Fig. 6 that the likelihood of obtaining a ground state is $\approx 0.18$ in the high error rate case. There are 3 degenerate ground states for this problem, out of 16 total states. Therefore a circuit that selected a state at random would select a ground state with
Figure 6. Results for a hard circuit, Problem (a) on the 4T architecture, as compared to results for a soft circuit, Problem (d). All circuits studied featured a negative correlation between ground state probability and aggregate error, as pictured here for these two circuits in the leftmost plots. For hard circuits, increase in aggregate error leads to behavior reminiscent of a random number generator, decreasing ground state probability but increasing fairness, as indicated in the top right plot.

\[ \frac{3}{16} = 0.1875 \text{ probability.} \]

By combining all of the data in to a single plot we can get a bigger picture view of how structured vs. unstructured errors impact our results. In Fig. 7 we see that fairness is highest for low aggregate error, decreases as the error approaches approximately 0.42, and then begins increasing again. This suggests that structured, i.e. biased, errors dominate in the middle of our error spectrum. As the overall error rate increases, either due to longer circuits or worse performing qubits, the net result is more unstructured
Figure 7. Fairness as a function of aggregate error rate across all experiments. Fairness is highest for small and large error rates, with a decrease in the middle. This indicates that structured errors dominate in the middle regime, while unstructured errors play an increasingly important role as error increases. The log-quadratic line of best fit (in black) is included to graphically indicate these overall trends.

Finally, we believe these results constitute a serious evaluation broadly of the current status of the IBM Q system. We found that the IBM metric of Quantum Volume [5] did broadly correlate with decreased aggregate error, which led to improved fairness in short circuits (see Fig. 6). However, the Quantum Volume metric is only based off of the highly tuned performance of the best performing qubits available on a machine, instead of the overall hardware performance. This study, which ranges over all available qubits on a wide range of available chips, gives a more comprehensive view of performance. For example, we have plotted the results for Problem (d) evaluated on all 190 connected 3-qubit subsets on the manhattan backend (which has QV32 and 65
Figure 8. Detailed results for Problem (d) evaluated on all 3-qubit subsets of the manhattan backend. Each plot represents the same underlying data, and the set of qubits with the maximum ground state probability (max GSP), maximum number of shots to reject fair sampling (max NSRFS), and minimum aggregate error (min AR) have been highlighted. This plot shows the high variance in results from a single backend.

qubits), see Fig. 8. In these plots one can see a wide range of results, and the best performing qubits for a single metric (ground state probability, number of samples to reject fair sampling, and aggregate error rate) can perform quite poorly when evaluated by a different metric. Thus, this study emphasizes the need for more comprehensive benchmarking that does not only focus on random circuits evaluated on a small subset of qubits, as also discussed in [20].

5 Conclusion

We have studied the extent to which today’s gate-based quantum computing hardware can fairly sample from the space of optimal solutions for discrete optimization problems. First, we introduced a novel metric for evaluating the fairness of current hardware: the number of shots to reject fair sampling. Using this metric, we found that hardware errors had a significant impact on fairness. For short circuits with $\leq 3$ qubits, higher fidelity qubits resulted in increased fairness. We call these circuits “soft.” However, for longer circuits with $\geq 4$ qubits, higher fidelity qubits actually resulted decreased fairness. We call these circuits “hard.” This is because low fidelity hardware begins behaving like a random number generator for long circuits, which contains no information but is relatively fair.

It would be interesting to test multiple quantum computing hardware technologies (e.g. optical, trapped ions, etc...) to see if they have different fairness profiles. Our studies show that individual machines on the IBM Q backend can have dramatically
different fairness and ground state probabilities when different qubits are used. As quantum computing hardware improves, we hope and expect to see an increase in qubit fairness and consistency.

In this study we have avoided exploring the exact nature by which errors in the hardware produce the biases which inhibit fairness. The reported error rates used in Fig. 6 are known to present an incomplete picture of how ordered circuits will perform [20]. This can be slightly improved upon by employing just-in-time noise data [23]. However, a broader theory of how different types of errors (read-out, crosstalk, etc.) affect not only ground state probability but also fairness is worth future study.
A Algorithm for Number of Shots to Reject Fair Sampling

Algorithm 1 Number of Shots to Reject Fair Sampling

**Input:** Qubits $Q$, quantum circuit $C$ for a problem $P$ with $k$ degenerate ground states labeled $s_1, \ldots, s_k$; $n_s$ number of shots, $n_i$ number of inner loops

**Output:** Number $N$ of shots to reject fair sampling for $C$ on $Q$.

1. Execute $n_s$ shots of circuit $C$ on qubits $Q$
2. $o_i :=$ the number of times ground state $s_i$ observed
3. $w_i := o_i / \sum_{i=1}^{k} o_i$ \quad $\triangleright$ relative frequency of ground state $s_i$
4. chiSqToReject := the $\chi^2$ value necessary to reject the fair sampling hypothesis with 95% statistical significance for $k − 1$ degrees of freedom
5. \textbf{function} medianChiSq($N$)
6. chiSqArray := {} 
7. \textbf{while} length(chiSqArray) $< n_i$ \textbf{do}
8. testSamples := $N$ samples drawn from the set $\{s_i\}$ with weights $\{w_i\}$
9. testChiSq := $\chi^2$ for testSamples
10. append(chiSqArray, testChiSq)
11. \textbf{end while}
12. \textbf{return} median(chiSqArray)
13. \textbf{end function}
14. $N := 2$ \quad $\triangleright$ $\chi^2$ ill-defined on sets of length 1
15. \textbf{while} medianChiSq($N$) $< \text{chiSqToReject}$ \textbf{do}
16. $N := 2N$
17. \textbf{end while}
18. upperBound := $N$
19. lowerBound := $N/2$
20. \textbf{while} upperBound-lowerBound $> 2$ \textbf{do}
21. $N := \lfloor(\text{upperBound} + \text{lowerBound})/2\rfloor$
22. \textbf{if} medianChiSq($N$) $< \text{chiSqToReject}$ \textbf{then}
23. lowerBound := $N$
24. \textbf{else}
25. upperBound := $N$
26. \textbf{end if}
27. \textbf{end while}
28. \textbf{return} $N$

For the calculations in this paper we used $n_s = 40960$ and $n_i = 1000$. As explained in the main text, these values were chosen via a ‘goldilocks’ principle: much smaller,
and the stochastic nature of the experiments resulted in inconsistent results, much larger and the computational burden was considerable. It is also worth noting that this algorithm becomes less useful as the samples become more evenly distributed, e.g. calculating the number of shots to reject fair sampling on a coin biased 50.001/49.999 takes $O(1\text{hr})$.

B Details on Circuit Compilation

In this appendix we provide supplementary information detailing the specifics of our compilation techniques. Full details of every hand compilation procedure would be too lengthy, instead we illustrate the compilation of Problem (d) as an example. Before we delve into details, we mention some broad ideas which aided in the compilation.

- **Circuit parameters:** The values for $\beta$ and $\gamma$ in Table 2 were found by conducting a grid search over the angles $(\beta, \gamma) \in [-\pi, 0) \times [-\pi, \pi)$ with a resolution of $\pi/60$ and calculating the expectation value $\langle \beta, \gamma | H_C | \beta, \gamma \rangle$ classically (where the search space for $\beta$ was cut in half due to a $(\beta, \gamma) \approx (-\beta, -\gamma)$ symmetry of the expectation value). This was efficient due to the relatively low circuit depths involved; for more complex circuits the hybrid approach detailed in Sec. 2.2 is more appropriate.

- **Multi-controlled phase-shifts:** First, we note that since terms in an Ising Hamiltonian pairwise commute, implementing the phase separating unitary can be done for each term individually, with 2 CNOTs and one phase-shift gate $Z^{\pm 2\gamma/\pi}$. Care has to be taken, however, to address the connectivity constraints in the architectures. More difficult is the compilation of the multi-control phase-shift gate at the heart of the Grover Mixer. Fig. 9 gives two recursive compilations into gates with fewer controls, one without ancillas, and one with a $|\uparrow\rangle$-initialized ancilla.
We note that careful recursive calls to these compilations and using symmetries can result in some of the smaller multi-control gates to cancel each other.

- **SWAP operations:** We allow SWAP operations for qubits to change location in the circuit without having to go back to the original location. This is possible because the Grover Mixer is fully symmetric, i.e. we can arbitrarily exchange controls with the phase-shift gate, thus the input order to the Grover Mixer does not matter.

We track qubit SWAPs with a permutation array from which in the end we read a read-out map for the measurements. This gives us a significant advantage over transpilation tools which are not aware of such symmetries. Introducing SWAPs (which usually cost 3 CNOTs) at the right place in a circuit (next to a CNOT) will cost only 1 CNOT. Similarly, moving SWAPs through to the beginning or end of the circuit results in complete removal of the SWAP cost, as the SWAP gate can be replaced with a change in the permutation array and corresponding readout.

**Example: Problem (d)**

Let us now describe in detail the compilation of Problem (d) to the 3L architecture. Starting with the general form of the 1-level Grover Mixer QAOA with fixed qubit \( q_0 := \uparrow \), we implement each quadratic term of the Ising Hamiltonian with 2 CNOTs and a single-qubit phase-shift gate \( Z^{\mp 2\gamma/\pi} = \begin{pmatrix} 1 & 0 \\ 0 & e^{\mp i\gamma} \end{pmatrix} \).

The CNOTs with control \( q_0 \) can be removed, leaving \( q_0 \) in the role of a classical bit, see Fig. 10. We notice that the other three quadratic terms form a triangle in the
problem graph, hence we cannot map them to a 3L Linear Nearest Neighbor architecture, but rather need at least one SWAP. Inserting the SWAP as 3 CNOTs right to an existing CNOT of the phase separating unitary $e^{-i\gamma(Z_2Z_3)}$ gives a cancellation of 2 CNOTs, thus the addition of the SWAP results in only 1 additional CNOT. Rather than reversing this SWAP at the end of $U_P(\gamma)$, we keep track of the permutation of the qubits ($q_2$ and $q_3$ have swapped places).

This end configuration (swapped qubits) now builds the start of the Grover Mixer unitary. The X-gates and the control on qubit $q_0$ can be dropped, as explained in Fig. 2 (right). Using the recursive decomposition from Fig. 9, we again see that we need to add a SWAP, see Fig. 11. The remaining single-controlled phase-shift gate between the middle two circuit wires can be implemented with 2 CNOTs and 3 phase-shift gates as shown. Keeping track of the SWAP throughout the end of the circuit, we see that qubits $q_2$ and $q_3$ end up back in their original position – in general, this need not be the case.

**Comment on 5-qubit Ising Problems on 5T Using an Ancilla**

Since an ancilla offers no benefit for the implementation of the phase separating unitary, and due to limited connectivity in the considered architectures, we found that decomposing multi-controlled phase-shift gates using an ancilla as shown in Fig. 9 (right) can only be used advantageously for the 5-qubit Ising Problems (a) and (b).

Following the approach outlined for Problem (d), both Problems (a) and (b) result in a multi-controlled phase-shift gate acting on 4 qubits. Using a remaining qubit on the 5T architecture as a $|\uparrow\rangle$-initialized ancilla (which has to be swapped around), we can implement the mentioned decomposition, which should return the ancilla to the $|\uparrow\rangle$-state. As mentioned in the primary text, we discarded all samples where the ancilla qubit was not measured in the $|\uparrow\rangle$ state.
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