BENCHMARKING 16-ELEMENT QUANTUM SEARCH ALGORITHMS ON IBM QUANTUM PROCESSORS

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ABSTRACT. We present experimental results on running 4-qubit unstructured search on IBM quantum processors. Our best attempt attained probability of success around 24.5%. We try several algorithms and use the most recent developments in quantum search to reduce the number of entangling gates that are currently considered the main source of errors in quantum computations. Comparing theoretical expectations of an algorithm performance with the actual data, we explore the hardware limits, showing sharp, phase-transition-like degradation of performance on quantum processors. We conclude that it is extremely important to design hardware-aware algorithms and to include any other low level optimizations on NISQ devices.

1. Preliminaries

In the unstructured search problem we are given a phase oracle and want to find any marked element out of N. The only action of the oracle is negating the amplitude of marked elements. This problem when considered on classical machines and classical oracles cannot be solved faster than in $Ω(\sqrt{N})$ oracle queries, but as showed by Grover in [Gro96] programmable quantum computers allow for an $O(\sqrt{N})$ algorithm.

There is an ongoing effort of implementing algorithms that solve the unstructured search problem on quantum computers. We show how to solve this problem by utilizing small diffusion operators as is described in [Gro02], [ADW15] and most recently in [BGH+20]. We present three successful implementations of unstructured search among 16 elements on IBM quantum computers. To the best of authors’ knowledge, there has been no successful demonstration of quantum search in a space larger than 8 elements.

Preparing efficient circuits for NISQ quantum computers requires acknowledgement of the topology of hardware. We have used hardware-aware circuits to improve previous results on IBM Q processors.

1.1. Prior Work. Since the invention of Grover’s algorithm [Gro96], there were plenty of attempts to run it on actual quantum hardware. So far, the largest search spaces on which the Grover’s algorithm successfully and significantly amplified amplitude of the marked element were 8-element spaces constructed on 3 qubits [FML+17]. Some attempts to search for the marked element in a 16-element space were undertaken, see [MOJ18], [KS18]. The results of [MOJ18] are summarized in Table 1. Back in 2018, as evidenced by the data therein, quantum computers were unable to successfully run unstructured search in a space build on 4 qubits. Analysing these results one has to remember that the probability of randomly finding one marked element among 16 in a classical setting is 6.25%.

| Algorithm (qubits used) | # of gates | Accuracy | Execution time (s) |
|------------------------|------------|----------|--------------------|
| Grover 2-qubit (0,1)   | 18         | 74.05%   | 84.56              |
| Grover 3-qubit (0,1,2) | 33         | 59.69%   | 84.33              |
| Grover 4-qubit (0,1,2,3)| 632        | 6.56%    | 185.13             |

Table 1. [MOJ18] results

We replicate some of previous results in order to understand the scale of hardware improvements achieved since the prior work has been completed.

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4-qubit diffusor, 51-73 2-q gates
-3 RMS Error, 16 × 1024 shots
IBM Q Vigo: 8.2%

4-qubit diffusor, 32 2-qubit gates
-3 RMS Error, 16 × 1024 shots
IBM Q Vigo: 21.0%

Figure 1. Comparison of results from running a single Grover’s iteration on 4 qubits

1.2. Replication of Prior Work on Current Hardware. As the relaxation and dephasing times of real hardware have improved since 2018, we attempted to replicate the results from [KS18] to investigate the improvements of hardware.

A straightforward reimplementation of [MOJ18] of a single Grover’s iteration on IBM Q Vigo yielded the probability of finding the marked element \( p_{\text{succ}} = 8.2\% \) (averaged over all 16 oracles), while the lowest probability was 5.1%, corresponding to the hardest oracle for the processor and the algorithm. The transpiller used between 51 and 73 2-qubit gates, depending on the oracle. These results can be significantly improved. As 2-qubit gate fidelities are noticeably lower than their 1-qubit counterparts, reducing the number of the former was our goal. Throughout this work, whenever we refer to 2-qubit gate count as a measure for the complexity of the circuit.

Our implementation of a single iteration of Grover’s algorithm used 32 2-qubit gates, counting native CNOT gates after transpilation. The average \( p_{\text{succ}} \) was 21.0%. Moreover, our implementation had the desirable property of using the same number of CNOT gates independently of the oracle used.

To avoid favouring any oracle in discussing the results, they are presented as the average over possible bitwise symmetric differences between the measured element and the marked one, interpreted as numbers from 0 to 15. Explicitly, for a given oracle marking the element \(|x\rangle\), where \(x \in \{0, \ldots, 15\}\), whenever the measurement yielded \(|y\rangle\), where \(y \in \{0, \ldots, 15\}\) we increment the count of \(y \oplus x\). This aligns the theoretical distributions, thus allowing us to aggregate the counts for different oracles. We are going to use the same approach when describing all our other results, unless clearly stated otherwise. Fig. 1 presents the comparison between two implementations of a single iteration of Grover’s algorithm.

| Algorithm (4 qubit search) | # of 2-qubit gates | \( p_{\text{succ}}, \text{average} \) | \( p_{\text{succ}}, \text{worst} \) |
|---------------------------|-------------------|-----------------|-----------------|
| Grover, 1 iteration, on IBM Q X5 [KS18] | 51-73 | 6.62% (est.) | 3% |
| same as above, on IBM Q Vigo | 51-73 | 8.2% | 5.1% |
| same as above, optimized | 32 | 21.0% | 15.8% |

Table 2. Replication of prior results on modern hardware with and without our improvements; \( p_{\text{succ}} \) denotes probability of success averaged over all oracles

Each run of the algorithm consists of 1024 repetitions, which we sometimes call shots. We performed one run for each of 16 oracles. The left graph in Fig. 1 shows the results obtained using the implementation from [KS18]. The results of our optimized, topology-aware implementation are shown on the right side in the same figure. Both experiments were conducted on the IBM Q Vigo machine. This initial implementation forms a benchmark for future improvements.
Table 2 summarises the best results of running a single Grover’s iteration on IBM Q Vigo, the last entry uses optimizations described in appendix B. Both the original and optimized implementations fail to attain the theoretical frequencies. In an absence of errors, 47.27% of all measurements should yield the pattern corresponding to the oracle. More detailed discussion of the effects the decoherence has on the results is in Appendix C.

2. Our Results

Our aim was to find algorithms and implementation methods for NISQ processors, suitable for demonstration of abilities of these machines to search for a single element in 16-element space. As the candidates, we implement the first iteration of unstructured search algorithms, employing 4-qubit oracles for 16 possible search patterns and 2-, 3- and 4-qubit diffusion operators. Additionally, using an approach similar to [BGH + 20], we perform a fragment of optimal quantum unstructured search algorithm (although using a slightly different pattern of diffusion operators, see Definition I and Appendix A). Implementing oracles and diffusion operators we take care to implement them with accordance to topology of quantum hardware, for more details see Appendix B. To further reduce the number of
2-qubit gates we use the technique of partial uncompute that allows us to not uncompute some ancillae but keep them to expedite the next oracle call; it is described in detail in [BGH+20].

2.1. The Main Result. The main result of this paper, to the best of authors’ knowledge, is the first demonstration of quantum unstructured search in 16-element space, yielding statistically significant outcome on actual quantum computing hardware. Four different algorithms, differing in the size of the diffusion operators and the number of iterations were run on processors from IBM Q family. The results are summarised in Fig. 2. The upper plots show prefixes of $D_2$ circuits for $K = (2, 2)$. The lower left plot shows a single iteration of Grover’s algorithm, and the lower right plot presents a partial search with 3-qubit diffusor. The plots are ordered by their measured probability of success $p_{\text{succ}}$. The range of $p_{\text{succ}}$ is from 18.2% to 24.5%. The numbers of 2-qubit gates of the implementations vary from 12 for a single iteration of search using 2-qubit diffusion operator to 28 for a single iteration of Grover’s algorithm. The only implementation of the algorithm with multiple oracle queries presented shows relatively low $p_{\text{succ}} = 18.2\%$, as it introduces a new source of errors, absent in variants with a single oracle query. Even the best result fails (albeit by a narrow margin) to attain the expected number of oracle queries better that the classical random search.

Results for a selection of processors running a single iteration of unstructured search using 2-qubit diffusion operator are presented in Fig. 2 top right plot. We have selected IBM Q Vigo to perform longer circuits. The results of these runs are summarised in the other plots of Fig. 2.

![Figure 2. IBM Q Vigo efficiency](image)

The ratio $R$ of actual and theoretical success frequencies for different algorithms selecting 1 of 16 states vs. 2-qubit gate counts of these algorithms for IBM Q Vigo (errors are 1 RMSE)

2.2. Efficiency of NISQ Hardware. Let us define $R$ as a ratio of actually achieved frequency of counts and the theoretical probability of success $p_{\text{succ}}$ of an algorithm, searching for a single marked element out of 16. Such defined $R$ is presented in Fig. 3 pointing to a sharp degradation of the performance of IBM Q Vigo at 2-qubit gate count of about 30.

The dotted line in Fig. 3 denotes the best fit estimation of degrading performance caused by infidelities of 2-qubit quantum gates as well as setup and measurement errors. It seems not to be enough to explain the behaviour of our algorithms, as the efficiency of those circuits when compared to theoretical results conforms to the red line which is best fit logistic curve. We show that current quantum hardware favours short circuits, as two steps of $D_2$ algorithm that should yield the same probability of measuring the marked element as 3-qubit partial search and higher probability than a single application of 2-qubit diffusor yielded worse results. Besides efficient implementations, many of these results would not be possible if not for consideration of smaller diffusion operators. These were first introduced by Grover in
The concept of benefits arising from the use of local diffusion operators has been studied in other papers, e.g. [ZK20]. Additionally, we demonstrate full search space entanglement. While a single application of a 2-qubit diffusor entangles just $1/4$ of states, 3-qubit diffusor entangles half of the states, applying 4-qubit diffusor or two 2-qubit diffusors entangles all the states in the search space as seen in Fig. 2.3.

Further remarks. This paper shows that it is extremely important to design quantum algorithms on modern NISQ devices with the awareness of their topology to achieve the best performance possible. Further development can be aimed in exploration of better oracle implementation or replacing known algorithms for solving the unstructured search problem with ones more suitable for a given hardware architecture. It can be noted that the placement of diffusion operators in our best circuits is not accidental but carefully chosen among all other possibilities. This is of course possible only due to the fact that we may, most of the time, forgo diffusion operators that act on all qubits.

3. Methodology and Implementation

Firstly, we present $D_n$ circuit that is constructed in similar manner to $W_n$ from [BGH+20], but forces higher amplitude of the marked element then circuit $W_n$ during the first three steps. Circuit $D_n$ also allows for the construction of optimal circuits as stated in Theorem 3 from [BGH+20]. In the following definition we adapt the notation from the aforementioned work.

Definition 1. Let $\vec{k} = (k_1, \ldots, k_m)$ be a sequence of positive integers and let $n := \sum_{j=1}^{m} k_j$. Given a quantum oracle $O$, for $j \in \{0, \ldots, m\}$ we define the circuit $D_j$ recursively as follows:

$$D_j = \begin{cases} 
\text{Id}_n & \text{if } j = 0 \\
D_{j-1} \cdot (\text{Id}_{k_1 + \ldots + k_{j-1}} \otimes G_{k_j} \otimes \text{Id}_{k_{j+1} + \ldots + k_m}) \cdot O \cdot D_{j-1} & \text{if } j \neq 0.
\end{cases}$$

In Appendix A we prove that $D_n$ circuits with Amplitude Amplification [BHMT02] indeed allow us to perform optimal quantum search. The $D_n$ circuits have multiple benefits over Grover’s algorithm. They use smaller diffusion operators which require fewer number of elementary gates to implement. The $D_n$ circuits are quite flexible and can be implemented in a topology-aware and hardware-aware manner. The sparse structure of $D_n$ allows some of the ancillae used in implementation of oracles to stay not uncomputed, as explained in [BGH+20] in section devoted to the partial uncompute technique.

Secondly, we also try to implement the oracle as efficiently as possible. Notice that if we have an ancilla qubit we can decompose standard CCCX gate into two CCX and one CCZ gates. The second CCX is basically needed solely to uncompute the byproduct on the ancilla qubit. We notice that it is possible to apply partial uncompute technique [BGH+20], so sometimes we can spare the second CCX. Additionally, we can replace the first CCX with Margolus gate [SK03]. The implementation can be seen in Fig. 5 the implementation of the first step of Grover’s algorithm can be seen in Fig. 6.

Thirdly, it is crucial to be topology-aware and hardware-aware when implementing the circuits. This way it is possible to achieve drastic improvement of performance on NISQ devices. As it was mentioned in Section 1 it is possible to achieve major improvement on IBM Q Vigo by being hardware-aware.

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The first step

The implementation with uncomputing

The implementation without uncomputing

Figure 5. The first step of D_2 for \( k = (2, 2) \) with one ancilla qubit

Figure 6. Implementation of the first step of Grover’s algorithm on qubits (0,2,3,4) on IBM Q Vigo quantum processor

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Appendix A. Analysis of the Tree circuit

For the sake of completeness we include here a proof that the circuits $D_n$ together with amplitude amplification [BHMT02] allow us to solve the unstructured search problem optimally. The notation we will work with here is analogous to the one used in section 3 of [BGH’14].

Lemma 2. Let $m \in \mathbb{N}_+$ and $\mathbf{k} \in \mathbb{N}_n^m$ be fixed, and let $n = \sum_{j=1}^m k_j$. Assume we are given a phase oracle $O$ that operates on $n$ qubits and marks a single vector of the standard computational basis, which we then use in the circuits $D_j$. Then for any $j \in \{0, \ldots, m\}$ we have

$$D_jO \mathbf{D}_j = O.$$

Proof. We proceed by induction on $j$. For $j = 0$ the claim is trivial. For $j > 0$ we expand $D_j$ according to the recursive definition as follows

$$D_jO \mathbf{D}_j = D_{j-1}(I_{d_{-k_1}} \otimes G_{k_1} \otimes I_{d_n-\mathbf{s}})O D_{j-1}O D_{j-1}(I_{d_{-k_1}} \otimes G_{k_1} \otimes I_{d_n-\mathbf{s}})O D_{j-1}$$

(1)

$$= D_{j-1}(I_{d_{-k_1}} \otimes G_{k_1} \otimes I_{d_n-\mathbf{s}})O (I_{d_{-k_1}} \otimes G_{k_1} \otimes I_{d_n-\mathbf{s}})O D_{j-1}$$

$$= D_{j-1}(I_{d_{-k_1}} \otimes G_{k_1} \otimes I_{d_n-\mathbf{s}})(I_{d_{-k_1}} \otimes G_{k_1} \otimes I_{d_n-\mathbf{s}})O D_{j-1}$$

$$= D_{j-1}O \mathbf{D}_{j-1}$$

(2)

$$= O$$

where in eqs. (1) and (2) we used the inductive hypothesis. \qed

Lemma 3. Let $m \in \mathbb{N}_+$ and $\mathbf{k} \in \mathbb{N}_n^m$ be fixed, and let $n = \sum_{j=1}^m k_j$. Assume we are given a phase oracle $O$ that operates on $n$ qubits and marks a single vector of the standard computational basis denoted target. Define the numbers

$$\beta_j = \langle \text{target} | \{D_j|u_1^j\} | \text{target}_{j+1}^m \rangle$$

for $j \in \{0, \ldots, m\}$. Then $\beta_j$ satisfy the recurrence

$$\beta_j = \begin{cases} 1, & \text{if } j = 0 \\ \frac{1}{2^{k_1/2}} \left(1 - \frac{2}{2^{k_1}}\right) + \frac{1}{2^{k_1}} \left(2 - \frac{2}{2^{k_1}}\right) \beta_{j-1}, & \text{if } j > 0. \end{cases}$$

Proof. By definition of $D_j$ we have $\beta_0 = 1$ giving the base case. For $j > 0$, we proceed to compute $\beta_j$ by expanding the circuit $D_j$ according to the recursive definition. We split the computation into stages as follows

$$|w_1\rangle = D_{j-1}(|u_1^j\rangle | \text{target}_{j+1}^m \rangle)$$

$$|w_2\rangle = O|w_1\rangle$$

$$|w_3\rangle = (I_{d_{-k_1}} \otimes G_{k_1} \otimes I_{d_n-\mathbf{s}})|w_2\rangle$$

$$|w_4\rangle = D_{j-1}|w_3\rangle$$

where $s = k_1 + \cdots + k_j$.

$$|w_1\rangle = D_{j-1} \left( \frac{1}{2^{k_1/2}} |u_1^{j-1}\rangle | \text{target}_{j+1}^m \rangle + |u_1^{j-1}\rangle | \text{target}_{j}^m \rangle | \text{target}_{j+1}^m \rangle \right)$$

$$= \frac{1}{2^{k_1/2}} D_{j-1} |u_1^{j-1}\rangle | \text{target}_{j+1}^m \rangle + |u_1^{j-1}\rangle | \text{target}_{j}^m \rangle | \text{target}_{j+1}^m \rangle$$

$$|w_2\rangle = O \left( \frac{1}{2^{k_1/2}} D_{j-1} |u_1^{j-1}\rangle | \text{target}_{j+1}^m \rangle + |u_1^{j-1}\rangle | \text{target}_{j}^m \rangle | \text{target}_{j+1}^m \rangle \right)$$

$$= \frac{1}{2^{k_1/2}} OD_{j-1} |u_1^{j-1}\rangle | \text{target}_{j+1}^m \rangle + |u_1^{j-1}\rangle | \text{target}_{j}^m \rangle | \text{target}_{j+1}^m \rangle$$

$$= \frac{1}{2^{k_1/2}} |n\rangle | \text{target}_{j+1}^m \rangle + |u_1^{j-1}\rangle | \text{target}_{j}^m \rangle | \text{target}_{j+1}^m \rangle$$
Where $|n\rangle$ is some state in $(\mathbb{C}^2)^{\otimes(k_1 + \cdots + k_{j-1})}$. We can write so, as all diffusors within $D_{j-1}$ operate only on the prefix consisting of first $k_1 + \cdots + k_{j-1}$ qubits, while $O$ only changes relative phases.

$|w_3\rangle = \text{Id}_{s-k_j} \otimes G_{k_j} \otimes \text{Id}_{n-s} \left( \frac{1}{2^{k_j/2}} |n\rangle |\text{target}_j^{m}\rangle + |u_1^{i-1}\rangle |\text{target}_j^{m}\rangle \right)$

$= \frac{1}{2^{k_j/2}} |n\rangle \left( \frac{2}{2^{k_j/2}} |u_j\rangle - |\text{target}_j^{m}\rangle \right) |\text{target}_j^{m}\rangle + |u_1^{i-1}\rangle \left( \left( 1 - \frac{2}{2^{k_j}} \right) |u_j\rangle + \frac{1}{2^{k_j/2}} |\text{target}_j^{m}\rangle \right) |\text{target}_j^{m}\rangle$

$= \frac{1}{2^{k_j/2}} \left( \frac{2}{2^{k_j}} - 1 \right) |n\rangle + \left( 2 - \frac{2}{2^{k_j}} \right) |u_1^{i-1}\rangle \left( \left( 1 - \frac{2}{2^{k_j}} \right) |u_j\rangle + \frac{1}{2^{k_j/2}} |\text{target}_j^{m}\rangle \right) |\text{target}_j^{m}\rangle$

$= \frac{1}{2^{k_j/2}} \left( \frac{2}{2^{k_j}} - 1 \right) O |u_1^{i-1}\rangle |\text{target}_j^{m}\rangle + \left( 2 - \frac{2}{2^{k_j}} \right) D_{j-1} |u_1^{i-1}\rangle |\text{target}_j^{m}\rangle$

Note that we used Lemma 2 when applying $D_{j-1}$ in the first summand. Now we can plug $|w_3\rangle$ into the expression defining $\beta_j$. Observe that the second summand in final expression is orthogonal to $|\text{target}\rangle$, thus can be safely discarded. We obtain

$\beta_j = \langle \text{target} | \left( \frac{2}{2^{k_j}} - 1 \right) O |u_1^{i-1}\rangle |\text{target}_j^{m}\rangle + \left( 2 - \frac{2}{2^{k_j}} \right) D_{j-1} |u_1^{i-1}\rangle |\text{target}_j^{m}\rangle \rangle$

$= \frac{1}{2^{k_j/2}} \left( \frac{2}{2^{k_j}} - 1 \right) \left[ \frac{1}{2^{s-k_j}/2} + \left( 2 - \frac{2}{2^{k_j}} \right) \beta_{j-1} \right]$

$= \frac{1}{2^{k_j + \cdots + k_{j-1}/2}} \left( 1 - \frac{2}{2^{k_j}} \right) + \frac{1}{2^{k_j/2}} \left( 2 - \frac{2}{2^{k_j/2}} \right) \beta_{j-1}$

concluding the proof.

**Theorem 4.** Fix any $\epsilon > 0$, and any $N \in \mathbb{N}$ of the form $N = 2^n$. Suppose we are given a quantum oracle $O$ operating on $n$ qubits that marks exactly one element. Then there exists a quantum circuit $A$ which uses the oracle $O$ at most $(1 + \epsilon) \frac{2}{\sqrt{N}}$ times and uses at most $O \left( \log(1/\epsilon) \sqrt{N} \right)$ non-oracle basic gates, which finds the element marked by $O$ with certainty.

**Proof.** We first begin by choosing a particular sequence of sizes for diffusors in the circuit $D_m$ – namely $k_j = (x + 1) \cdot j$ where $x \in \mathbb{N}_+$. Is some parameter, and let us assume that the number of qubits we work with is precisely $(x + 1) + (x + 1) \cdot 2 + \cdots + (x + 1) \cdot m = (x + 1) \cdot m(m + 1)/2$. From Lemma 3 we get that the amplitude the circuit $D_m$ in the marked state is given by the following recurrence

$\beta_j = \begin{cases} 
1, & \text{if } j = 0 \\
\frac{1}{2^{x+1}+\cdots+x+1} \frac{1}{2^{s-k_j}/2} + \frac{1}{2^{x+1}+\cdots+x+1} \frac{1}{2^{s-k_j}/2} \beta_{j-1}, & \text{if } j > 0.
\end{cases}$

To simplify the analysis of this recurrence, let us begin by substituting $\gamma_j = \beta_j \cdot 2^{(x+1)(j+1)/4} \cdot 2^{-j}$, which yields

$\gamma_j = \begin{cases} 
1, & \text{if } j = 0 \\
1 - 2^{-x(j+1)} \gamma_{j-1}, & \text{if } j > 0.
\end{cases}$

We easily obtain the following inequality for $j > 0$

$\gamma_j \geq (1 - 2^{-x}) (2^{-j} + \gamma_{j-1})$.

We may thus set

$\delta_j = \begin{cases} 
1, & \text{if } j = 0 \\
(1 - 2^{-x}) (2^{-j} + \delta_{j-1}), & \text{if } j > 0
\end{cases}$

and we easily obtain the inequality $\gamma_j \geq \delta_j$. We can express the solution to this recurrence as a sum

$\delta_m = \sum_{j=0}^{m-1} 2^{j-m} \cdot \prod_{k=m-j}^{m} (1 - q^k) + \prod_{k=1}^{m} (1 - q^k)$

where $q = 2^{-x}$. 


For \( a \in \mathbb{N} \cup \{\infty\} \), let
\[ \mathcal{P}(a) = \prod_{k=1}^{a} (1 - q^k). \]
In terms of \( \mathcal{P}(a) \), we can lower bound \( \delta_m \), as each term in our product is strictly less than 1, thus
\[ \delta_m \geq \sum_{j=0}^{m-1} 2^{-m+j} \mathcal{P}(m) = \sum_{j=0}^{m} 2^{-j} \mathcal{P}(m) = (2 - 2^{-m}) \mathcal{P}(m) \geq (2 - 2^{-m}) \mathcal{P}(\infty). \]

We now need a lower bound on \( \mathcal{P}(\infty) \), which we can obtain via Euler’s Pentagonal Number Theorem \([Eul83]\), which states that
\[ \mathcal{P}(\infty) = \prod_{k=1}^{\infty} (1 - q^k) = 1 + \sum_{k=1}^{\infty} (-1)^k \left(q^{(5k-1)/2} + q^{(5k+1)/2}\right) \]
from which, one can easily derive the inequality
\[ \mathcal{P}(\infty) \geq 1 - q - q^2. \]

Combining these inequalities we get
\[ \beta_m \geq (2 - 2^{-m}) \left(1 - 2^{-x} - 2^{-2x}\right) \cdot 2^m \cdot 2^{-n/2}. \]
By Amplitude Amplification \([BHMT02]\), we need
\[ \left\lfloor \frac{\pi}{4 \beta_m} \right\rfloor \]
iterations of the \( D_m \) circuit and its conjugate, where \( \theta_m = \arcsin \beta_m \)
Consider the standard inequality for \( z \in (0, 1] \)
\[ \sin z \leq z \]
which we can restate to
\[ \frac{1}{\arcsin z} \leq \frac{1}{z}. \]
Inequalities \([\text{3}]\) and \([\text{4}]\) together allow us to bound the number of iterations by
\[ \frac{\pi}{4} \cdot \frac{1}{2 - 2^{-m}} \cdot \frac{1}{1 - q - q^2} \cdot 2^m \cdot 2^{-n/2}. \]
Each \( D_m \) has exactly \( 2^m - 1 \) oracle calls, so one iteration has \( 2^{m+1} - 1 \) oracle calls (tree, its conjugate and 1 extra call). Thus the number of oracle calls is at most
\[ \frac{\pi}{4} \cdot \frac{1}{2 - 2^{-m}} \cdot \frac{1}{1 - q - q^2} \cdot 2^m \cdot 2^{n/2} \cdot (2^{m+1} - 1) = \frac{\pi}{4} \cdot \frac{1}{1 - q - q^2} \cdot 2^{n/2} \]
so we are only a factor of \( \frac{1}{1 - 2^{-x} - 2^{-2x}} \) away from optimal number of oracle calls.
\( D_m \) can be implemented with \( O\left(\sum_{k=1}^{m} kx \cdot 2^{m-k}\right) \) gates. So we get at most
\[ O \left( \left( \sum_{k=1}^{m} kx \cdot 2^{m-k}\right) \cdot 2^m \cdot 2^{n/2} \right) = O \left( \left( \sum_{k=1}^{m} kx2^{-k}\right) 2^{n/2} \right) \]
on-oracle gates used by our algorithm. We use the following simple observation
\[ \sum_{k=1}^{m} kx2^{-k} \leq \sum_{k=1}^{\infty} kx2^{-k} = 2x \]
to get that the total number of nonoracle gates used by our algorithm is bounded by \( O \left( x \cdot 2^{n/2} \right) \). Thus, for any \( \epsilon > 0 \) that is sufficiently small, we obtain an algorithm that makes at most
\[ (1 + \epsilon) \frac{\pi}{4} \cdot 2^{n/2} \]
oracle calls, and uses at most
\[ O \left( \log \left( \epsilon^{-1} \right) \cdot 2^{n/2} \right) \]
non-oracle gates by setting \( x \in \Theta \left( \log \left( \epsilon^{-1} \right) \right) \). \( \square \)
Appendix B. Topology-Aware Implementation

Most of decoherence in hardware comes from CNOT gates, so the hardware-aware optimizations performed by us were focused mostly on reducing their number. IBM software transpiles any quantum circuit to an equivalent one that consists of arbitrary 1-qubit and CNOT gates. Moreover, there are restrictions on which pairs of qubits a CNOT gate can be applied to, in this case SWAP gates are used to transport the relevant qubits to the suitable pair of qubits adjacent in the underlying topology. Each of the SWAP gates requires 3 CNOT gates to be implemented. These restrictions vary from one quantum computer to another. For example, IBM Q Vigo has these restrictions as in Fig. 7. By careful analysis of architecture of IBM quantum computers we reduce the number of CNOT gates in our circuits noticeably.

Let us note that restrictions from Fig. 7 apply also to Valencia, Ourense and Essex quantum processors.

Let us restrict ourselves to the IBM Q Vigo topology and try to implement a quantum circuit from Appendix A as close to optimal as possible. First, let us try to optimize the total number of CNOT gates in oracle (see Fig. 5). We can use qubit $q_1$ as a target so that all 2-qubit gates needed to perform Margolus gate can be run on the neighboring qubits, see Fig. 8. Margolus gate is a substitute for a standard Toffoli gate whenever we only aggregate result of logical AND operation between two input qubits (in our case $q_0$, $q_2$) in ancilla qubit (i.e. $q_1$). Furthermore, it is usually required to uncompute this operation before proceeding with further computations that involve input qubits.

To implement a CCZ gate on qubits $q_1$, $q_3$, $q_4$ with standard approach we would need to perform two SWAPs to let qubits $q_1$ and $q_4$ interact, see Fig. 9.

It can be circumvented with a more efficient circuit that requires only 8 CNOTs, see Fig. 10.

We also reduce the total number of CNOT gates in implementations of diffusors. Implementation of a diffusor on qubits $q_3$, $q_4$ is straightforward and costs only 1 entangling gate. To implement a diffusor on qubits $q_0$, $q_2$ we would need to use two SWAP gates that would result in a circuit with 7 entangling gates. To reduce the amount of entangling gates we note that there exists an equivalent circuit that requires only three 2-qubit gates, see Fig. 11.
Figure 10. Simplified implementation of CCZ on qubits $q_1$, $q_3$, $q_4$ in line topology

Figure 11. Diffusor on qubits $q_0$, $q_2$ that are topologically separated by qubit $q_1$ that is in state $|0\rangle$
APPENDIX C. Error Mitigation

The performance of different quantum processors in IBM Q family varies significantly. In Fig. 12 we compare IBM Q Melbourne against IBM Q Vigo, running a single iteration of unstructured search in 16-element space using 2-qubit diffusion operators, implemented with a 2-qubit gate count of 16, as an example. We run 1024 shots of this algorithm for each of 16 possible oracles.

While IBM Q Melbourne failed to find the marked element, IBM Q Vigo attained $p_{\text{succ}} = 15\%$. We investigated the difference in performance with the following approach.

In the main body of this work, we used the method described in Section 1.1 which allowed for superimposing the distributions for different oracles. Contrary, in this Appendix, we add the counts for each measured pattern, effectively measuring the quantum processor’s preference for each measured pattern, while not affecting the 2-qubit circuit depths of experiments.

The biggest effect is related to decoherence, bringing qubits to their ground state. This results in patterns containing more 0’s to be observed more often, as presented in Fig. 12 where the colours code the distance from the expected average value of counts, marked in dashed line.

The same effect becomes evident for IBM Q Vigo for larger circuits, for example for a single iteration of the 3-qubit diffusor as illustrated in Fig. 13, the left hand side plot. The right side plot shows dependence on the state of Lowest Significant Qubit of the pattern. We have attempted mitigating these errors, by computing a $16 \times 16$ correction matrix, using counts we measured for all the patterns for all the oracles. Subsequently, we have applied the corrections to raw counts, reshuffled as in Fig. 2 so the theoretical distributions overlap. After the correction, the average $p_{\text{succ}}$ changed marginally from 24.5\% to 24.8\% (still not enough to better a classical search in an expected number of oracle calls), however the result for the worst performing oracle improved from 20.6\% to 22.7\%.

Figure 12. Melbourne vs. Vigo decoherence for circuits with 16 2-qubit gates

Figure 13. IBM Q Vigo, 24 2-qubit gates