Automated Quantum Algorithm Synthesis

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We present a computational method to automatically design the n-qubit realisations of quantum algorithms. Our approach leverages a domain-specific language (DSL) that enables the construction of quantum circuits via modular building blocks, making it well-suited for evolutionary search. In this DSL quantum circuits are abstracted beyond the usual gate-sequence description and scale automatically to any problem size. This enables us to learn the algorithm structure rather than a specific unitary implementation. We demonstrate our method by automatically designing three known quantum algorithms—the Quantum Fourier Transform, the Deutsch-Jozsa algorithm, and Grover's search. Remarkably, we were able to learn the general implementation of each algorithm by considering examples of circuits containing at most 5-qubits. Our method proves robust, as it maintains performance across increasingly large search spaces. Convergence to the relevant algorithm is achieved with high probability and with moderate computational resources.

I. INTRODUCTION

Quantum computers promise exponential speed-ups, yet there are only a handful of classes of quantum algorithms that realise this. Shor [1] provides us with two possible explanations. Firstly, quantum computers operate so differently from classical computers that our existing techniques for algorithm design and our intuitions about computation may no longer be effective. Secondly, it is possible that only a limited number of such quantum algorithms exist and that many or all of them may have already been discovered.

Given the steadily growing Quantum Algorithm Zoo [2] we might retain some optimism with regards to the latter point. Nevertheless, developing novel protocols—especially those that generate new classes of quantum algorithms, of which Shor's factorising algorithm [3] is an example—is clearly a difficult task. Computational methods could offer a way to bridge the intuition gap and facilitate the discovery process. We propose such a method that uses a bottom-up approach, where a collection of well-constructed examples is translated into an algorithm.

Our approach follows the methodology of neural architecture search (NAS) where the task of automated design is divided into three parts, search space, search strategy and performance estimation strategy [4–7]. Neural architecture search strategies are widely used in machine learning to improve performance in computer vision, natural language processing and time series forecasting [6]. More recently, NAS methods have also been applied in the context of variational quantum algorithms, for a recent survey see [8].

Quantum algorithms, which are associated with highly structured circuits, tend to be modular and to contain repeating patterns. To exploit these facts we use a domain-specific language (DSL)—specific syntax and rules for compactly expressing quantum circuits via modular building blocks, implemented as an open source Python package [9–11]. In this DSL, quantum circuits are abstracted beyond the usual gate-sequence description and scale automatically with problem size. This allows us to optimise the structure of the algorithm, as opposed to the quantum circuit at the level of individual gates. Previous work on automated quantum algorithm design [12–19] was limited to gate-based circuit implementations of algorithms for small circuit sizes, usually 2-8 qubits. In contrast, our learnt algorithms automatically generalise to arbitrary problem size which has not been demonstrated previously. Remarkably, this was achieved by using training examples related to just three small circuit sizes, namely 2, 3 and 4 qubits or 3, 4 and 5 qubits.

Our method is compatible with any gradient-free optimisation procedure, specifically, we use evolutionary search [20–22]. The performance of candidate algorithms is measured by how closely their behaviour matches the examples provided in the training set. In addition, the evaluation takes into account the uniformity of the performance across all examples and the complexity of the candidate algorithm. We demonstrate our methodology by rediscovering three well-known quantum algorithms, the quantum Fourier transform, the Deutsch-Jozsa algorithm and Grover's search. This shows that our method works for oracle-based problems and variational circuits. Our approach also has the necessary functionality for designing both measurement-based algorithms and ansatzes for variational quantum circuits [9, 23].

II. RESULTS

Using our domain-specific language combined with evolutionary search we were able to rediscover three well-known quantum algorithms, the quantum Fourier transform (QFT), the Deutsch-Jozsa algorithm and Grover's search. Figure 1 shows two equivalent n-qubit representations of three automatically designed algorithms, corresponding to each of the learning tasks. On the left-hand
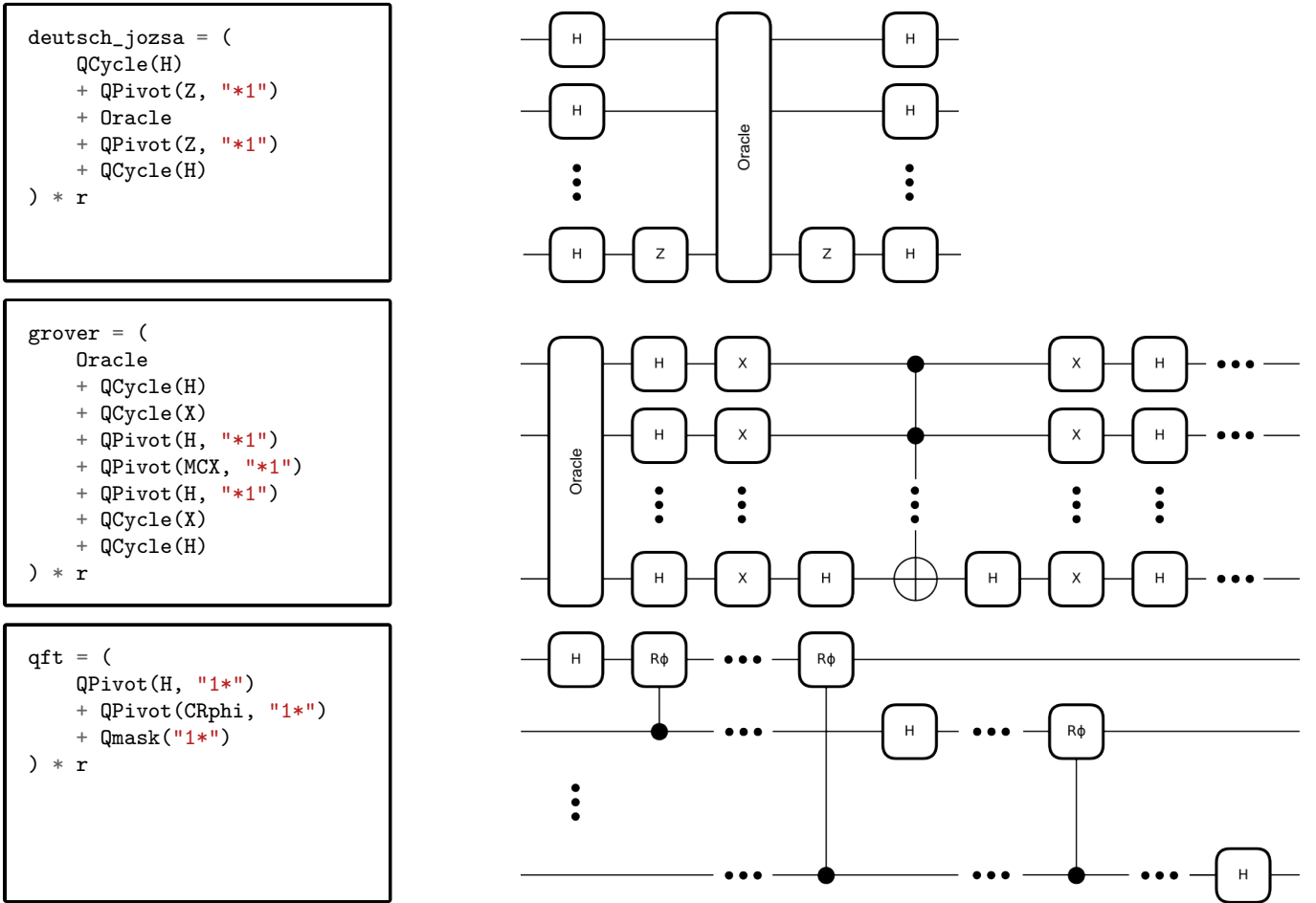
FIG. 1: Two equivalent n-qubit representations of three learnt algorithms, namely the rediscovered implementations of the Deutsch-Jozsa algorithm (top), Grover's search (middle) and the quantum Fourier transform (bottom). Many variations of the algorithms were found in our experiments but one example per task is shown here. Left are DSL descriptions, output by our search method. Right are the corresponding circuit representations that match those typically presented in the literature. The cycle (`QCycle`) and pivot (`QPivot`) motifs encode two different gate placement patterns, as can be seen by comparing the left- and right-hand sides. The mask (`QMask`) motif makes qubits unavailable. The strings `"1*"` and `"*1"` are examples of patterns used to control the behaviour of the mask and pivot motifs, and represent the selection of the first and last qubits, respectively. The parameter `r` controls the number of times the structure is repeated, where the relationship to the circuit size can be inferred from training.

side of Fig. 1 are the leant algorithms expressed in the DSL. On the right-hand side are the corresponding quantum circuit representations, where each circuit matches the common, hardware-agnostic, implementation of each algorithm [24]. Fig. 1 illustrates how the DSL compactly describes the general n-qubit implementation of the algorithms. This allows us to immediately interpret the algorithm structure, as well as identify symmetries and patterns. For example, the symmetric structure of the diffusion term in Grover's search is immediately identifiable.

An evolutionary algorithm is used to explore the search space where new candidate algorithms are generated by changing or combining the fittest candidates from a population of algorithms. Remarkably, we found that to con-

verge to the general algorithm, it was sufficient to evaluate each candidate on three small circuit sizes, namely 2, 3 and 4 qubits for the Deutsch-Jozsa algorithm and QFT, and 3, 4 and 5 qubits for Grover's search. A candidate algorithm has a high fitness if it executes the target algorithm correctly and has low complexity, discussed further in section IV C. Furthermore, we did not tune the hyper-parameters of the evolutionary search. These were kept as consistent as possible across all experiments. That the same hyper-parameters were good enough for all three tasks, indicates that our search strategy is stable and reliable.

Fig. 2 and Fig. 3 detail a successful experiment that was able to rediscover Grover's search. Fig. 2 shows an example of the distribution of the population fitness over
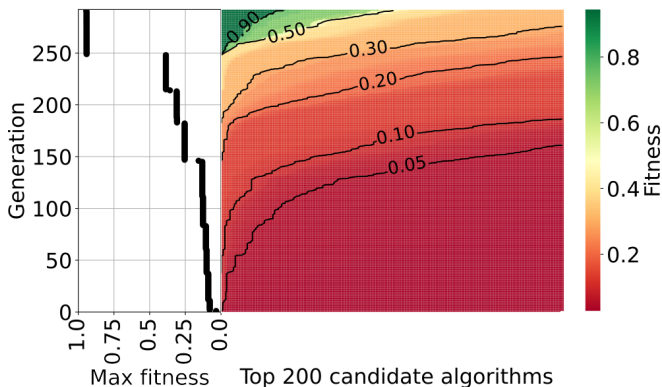
FIG. 2: Evolution of the fitness scores over 292 generations of a successful experiment in which Grover's search was rediscovered. The maximum fitness of the population at each generation of the evolutionary search (left) increases over time with periods of plateau. The heat map and contour plot (right) show the fitness of the best performing 200 candidate algorithms sorted by fitness, decreasing from left to right. Left and right share the same y-axis.

the course of several generations. The left panel of Fig. 2 illustrates the typical step-wise increase of the maximum fitness over time. While fitness initially increases steadily, there is a significant jump in fitness at the 249-th generation. This is owing to the 'dropout' mutation labelled (c) in Fig. 3 and detailed in Fig. 5. Since candidate algorithms are defined by a collection of discrete properties, large jumps in fitness are to be expected for single discrete changes.

The right panel of Fig. 2 shows the changing composition of the population. The slope of the contour lines indicates the rate of displacement of the poorest performing candidates from the top 200 algorithms. The steeper the slope of a contour line, the slower poorer-performing candidates are displaced. The general trend is that the gradient of each contour line decreases over time as the current best algorithm, its duplicates and related variants, propagate rapidly and take up an increasing proportion of the population.

Fig. 3 shows the evolutionary path, represented as a directed graph, that led to Grover's search. The graph contains a roughly equal distribution of mutation types, represented by different edges. This indicates that all four mutation types played an important role in producing the final algorithm, which was the case for all experiments across all three tasks. In the literature, it has been suggested that mutations that combine two candidates, in our case the 'chop-and-join' mutation, do not lead to better-performing architectures [7, 25]. Our results indicate that in the context of algorithm design, this is not the case. A possible explanation is that we break each architecture into two pieces before recombining them, rather than simply appending algorithms head-to-tail. This provides an opportunity for useful sec-
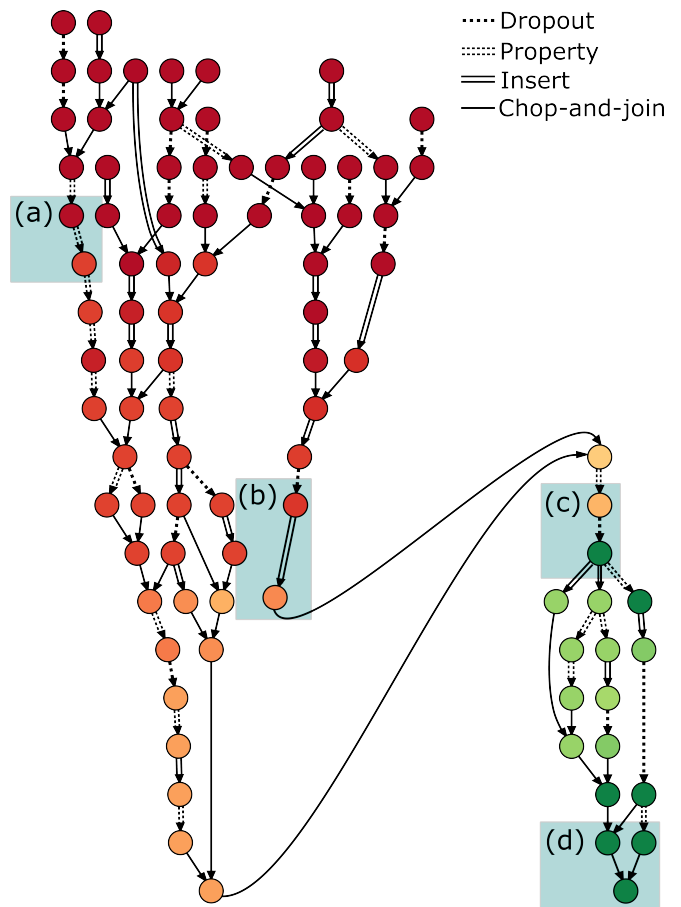

FIG. 3: Directed graph showing the subset of the population that evolved into an implementation of Grover's search. Each node represents a candidate algorithm from the same population shown in Fig. 2. The colour of each node corresponds to the fitness, matching the scale in Fig. 2. Each mutation type is represented by a different edge. Four specific mutations, each of a different type, are highlighted in blue and elaborated on in Fig. 5.

tions of each algorithm to be combined. Dividing each algorithm into two randomly determined pieces before recombination also ensures that the size of candidates does not double with each application of this mutation. Furthermore, random division ensures diversity in the size of candidates.

We demonstrate the robustness of our method by investigating the effect of increasing search space size. The DSL that was used to represent our search space is implemented as an open-source Python package called Hierarqcal [9, 23]. See Section IV A and Fig. 1 for an illustration of the basic functionality of Hierarqcal. In this framework, algorithms are built up of motifs that encode different gate placement patterns. Each motif has several properties, each of which can take on a possibly infinite number of discrete values. Motif properties include mapping, step, stride, offset, boundary condition, global
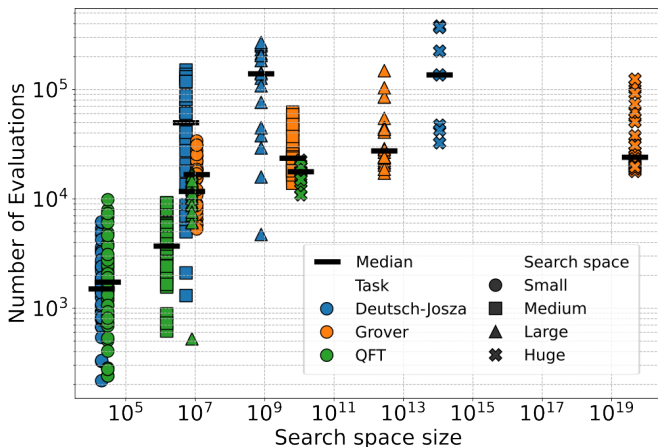
FIG. 4: Number of evaluations required to successfully design three different quantum algorithms. For each task, four search spaces of increasing size were tested. The median number of evaluations is indicated with a horizontal bar.

TABLE I: runtime limit, approximate success rate and median runtime of successful experiments for three different learning tasks and corresponding search spaces. Fifty experiments were run per configuration.

Task	Search space	Limit (CPU hrs)	Success rate	Median (CPU hrs)
Deutsch-Jozsa	Small	28	1.00	0.3
	Medium	56	0.58	15.4
	Large	112	0.34	42.9
	Huge	112	0.14	33.7
Grover	small	28	0.84	10.4
	Medium	56	0.62	13.2
	Large	112	0.44	13.7
	Huge	112	0.60	10.5
QFT	Small	56	0.94	8.8
	Medium	112	0.62	51.8
	Large	168	0.64	116.6
	Huge	168	0.26	129.5

and merge within patterns, weight sharing and edge order. Selecting appropriate sets of discrete values for each of these properties determines the configuration space, which in turn determines the set of possible algorithms that can be constructed, i.e. the search space.

During evolutionary search, no restrictions are placed on the number of Hierarqcal motifs used to construct an algorithm. Consequently, the size of the search space is infinite. For the purposes of analysis, we instead refer to the size of the search space as the number of algorithms that would be evaluated in a worst-case-scenario brute-force search using our DSL. A worst-case-scenario brute-force search would involve evaluating all possible algorithms composed of at most n motifs, where n is the minimum number of motifs known to be required to build the algorithm. This is a useful way to compare experiments and can also be used to compare performance to random search.

In Fig. 4 we see that the number of candidates evaluated in each experiment was a small fraction of the size of the search space, indicating the efficiency of our evolutionary strategy. The number of evaluations required grows with the size of the search space, though favourable at a decreasing rate. A total of 50 experiments were performed for each combination of task and search space size, and successful runs are shown in Fig. 4. An experiment is considered successful if it is completed within a certain runtime limit and if certain stopping conditions are met, which we describe in detail in Section IV C. Table I shows the approximate success rates for each task and notes the runtime limits in core processing unit (CPU) hours. Taking the success rates into account, our method is robust and can plausibly be run on a personal computer – 6-14 CPUs – with a 99% chance of success within a single day in most cases.

When parametrised unitary gates are used, as was the case for the QFT algorithm, runtimes are longer since the parameters of these gates have to be trained during evaluation. We note that, by inspecting the learnt gate parameters it is possible to infer the general relationship between parameters, which may also depend on the circuit sizes. Similarly for all tasks, the relationship between the circuit size and number of repetitions, `r` in Fig. 1, can also be inferred in this way. For example, for QFT we saw that the learnt number of repetitions was equal to the circuit size.

III. DISCUSSION

Our study demonstrates that computational methods can effectively be used to discover quantum algorithms. We successfully rediscover the quantum Fourier transform (QFT), the Deutsch-Jozsa algorithm, and Grover's search validating our approach. Central to our method is a domain-specific language, which captures the inherent scalability of algorithms. Further, the DSL biases the algorithms in the search space to be structured, capturing modularity and repeating patterns. As a result, the learnt algorithms are immediately interpretable and analysable. Notably, convergence to the general algorithm requires evaluation on only three small circuit sizes, containing at most 5 qubits, which significantly reduces the computational cost.

The DSL informs the three aspects of our NAS-inspired design approach. It enables the compact representation of algorithms in the search space. It makes constructing useful mutations for evolutionary search straightforward. And, it allows us to evaluate candidate algorithms on a collection of different circuit sizes.

Furthermore, the DSL contains a small number of building blocks, that in turn depend on a limited number of properties. Therefore, we can greatly reduce the size of the search space compared to using a gate-based cir-

cuit description. Importantly, we are able to reduce the search space size without sacrificing expressivity, since the DSL captures the essential characteristics of algorithms, namely structure and scalability.

Our search strategy is robust and efficiently explores the search space. As the search space size increases, the number of evaluations required grows at a diminishing rate, and the fraction of the space explored decreases rapidly. Good performance was achieved for all tasks, despite maintaining consistent hyper-parameters and without the use of tuning. We found that all mutation types contributed meaningfully to the search, including a mutation that combines two algorithms.

By using a bottom-up approach, we reformulate the task of algorithm design as a task of creating a set of well-constructed training examples. Our performance estimation strategy then evaluates candidate algorithms based on their ability to generalise across these training examples. We prioritize simpler algorithms by incorporating a complexity penalty while simultaneously rewarding algorithms that perform uniformly across training examples. This, combined with the attributes mentioned above, enables us to automatically design the n-qubit realisation of a quantum algorithm.

IV. METHODS

Much of our success is due to the use of a domain-specific language. It allows us to learn the general algorithm structure rather than a specific unitary implementation of the algorithm for some number of qubits. The DSL was adapted from its initial formalism detailed in [9], where many of the core ideas were introduced. For a recent overview, see the blog post [10], and for the associated Python package Hierarqcal, see the GitHub repository [11].

The original inspiration for the DSL came from the field of neural architecture search [26]. In line with NAS we divide our automated algorithm design approach into three components: search space, search strategy, and performance estimation[4–6]. The DSL is used to specify the search space, see Section IV A. Owing to the modular nature of our DSL, evolutionary search is a natural choice for search strategy, detailed in Section IV B. The performance estimation method used to evaluate candidate algorithms is described in Section IV C. Finally, in Section IV D, we provide an overview of each design task, with a particular focus on problem setup.

A. Search space

The DSL provides a way to encode quantum circuits, in fact, it can be used to encode arbitrary compute graphs of which quantum circuits are an example. In place of representing the quantum circuit as a sequence of individual gate placements, we instead work on the abstract level of placement patterns, which we term motifs. Each motif encodes a different pattern of gate placement, see Fig. 1. By design, a motif encodes the gate placements for any circuit size, where scaling happens automatically and in an intuitive way. The definitions of the motifs were heuristically motivated, and capture the regular patterns that we see throughout quantum circuits that perform structured tasks.

The motifs are the building blocks of our DSL and are used to generate hypergraphs associated with a unitary operation. The nodes of the hypergraph correspond to qubit indices and edges represent the input connectivity of the associated unitary. Each motif type corresponds to a different method of edge generation. The cycle iterates through the list of nodes when creating edges, while the pivot connects one or more fixed nodes to all remaining nodes. The mask motif makes nodes unavailable to subsequent motifs, while its counterpart the unmask makes unavailable nodes available again. The mask motif can be associated with non-unitary operations, specifically operations conditioned on measurement outcomes, however, we have not used this functionality in the experiments presented here.

The specific behaviour of each motif is controlled by several properties that influence edge generation. For example, the global pattern property of the pivot is used to control which nodes are fixed in the one-to-many edge generation pattern. Once the number of nodes is fixed, the graph's edges are generated and the associated unitary is repeatedly connected to each edge, resulting in a quantum circuit.

Motifs can be composed to create a sequence of motifs, which can in turn be composed to form higher-level motifs, and so on. When the number of nodes (qubits) is specified, the edges are generated according to the order of the motifs in the composition. For example, in the representation of the Deutsch-Jozsa algorithm in Fig. 1 the cycle of the Hadamard gates is placed before the pivot of the Pauli-Z gates in the circuit representation according to the order of operations in the composition of motifs shown on the left.

For each of the tasks we tested, we imposed a fixed macro-architecture template at the highest level of the structural hierarchy. This may not be applicable in all scenarios and can easily be modified or removed. Specifically, we assume that the algorithm is made up of a composition of motifs repeated r times. The number of repetitions r may depend on the problem size and is a trainable parameter. We also point out that any single gate placement can be achieved using the pivot motif with an appropriate global pattern. This ensures that it is always possible to map a gate-based circuit representation into the DSL.

A quantum circuit is itself a unitary operation and can therefore be associated with a motif. This allows larger structures to be built from sub-substructures, for example building multiplication from addition. While it was not necessary to exploit this functionality in the current

work, it allows structurally complex algorithms to be represented compactly. For instance, Shor's factorisation algorithm lends itself well to this. It is straightforward to allow an algorithm from the population to be associated with a motif, thereby building larger complex structures. However, we speculate that for the search to remain robust and efficient, it would be necessary to implement a more sophisticated search strategy.

A hierarchical representation of a large architecture is an effective way to reduce search complexity and leads to better search efficiency [26–28]. By limiting the search space to a small number of motifs, that in turn depend on a limited number of properties, we can significantly reduce the size of the search space compared to a gate-sequence circuit encoding. Importantly, we are able to reduce the search space complexity without sacrificing expressivity. Algorithms are inherently scalable and our DSL captures this property. Further, our DSL biases the search space toward structured circuits which are likely to include the structured operations necessary to build algorithms. In this way, we were able to automatically design large circuit structures in reasonable times, as demonstrated in Fig. 4 and Table I.

Our DSL simplifies the search strategy compared to approaches that use a gate-based circuit representation. Using the DSL, it is no longer necessary to construct a set of rules to govern gate placements within the circuit during search [25]. Instead, we define a configuration space, that is a set of available discrete values for each property of the motifs. This in turn determines the set of possible algorithms that can be constructed.

For a given task, heuristically motivated constraints can be applied to the property values in the configuration space. For example, the global pattern can be restricted to values that reflect information about qubits that have a special significance. In our implementation, the oracle for the Deutsch-Jozsa algorithm performs a multi-controlled bit flip on the last qubit. This makes the global pattern that encodes a pivot on the last qubit relevant to the algorithm structure. While a pivot on a middle qubit is unlikely to be relevant since the middle qubit has no special significance. Similarly, if we interleave ancillary qubits into our circuit then we are justified in assuming that the patterns "10" and "01" are relevant.

B. Search strategy

Evolutionary search is a gradient-free optimisation technique inspired by the process of natural selection. It remains a popular optimisation method due to its flexibility, conceptual simplicity, and competitive results [7]. Beginning with a collection of randomly generated candidate algorithms, the fittest candidates are selected and used to produce the next generation, growing the population over time. New algorithms are produced by combining two algorithms or by changing a property of a single algorithm. These operations are referred to as mutations.

The pseudo-code that summarises our optimisation procedure is given in Algorithm 1.

Algorithm1 Evolutionary algorithm: An iterative optimization process that maintains a population of candidate algorithms, refining them through selection, mutation, and evaluation. The search continues until a predefined stopping condition is met. Arrows indicate assignment and plus operations indicate appendage.

1: **procedure** EVOLUTIONARYSEARCH
2:     $population \leftarrow InitialisePopulation()$
3:     $flag \leftarrow StoppingCondition(population)$
4:     **while** $\neg flag$ **do**
5:         $children \leftarrow []$
6:         **for** $i \leftarrow 1, n_{batch}$ **do**
7:             $m_1, m_2 \leftarrow$ SELECTION$(population)$
8:             $children \leftarrow children +$ MUTATE(m_1, m_2)
9:         **end for**
10:         $population \leftarrow population +$ EVALUATE$(children)$
11:         $flag \leftarrow StoppingCondition(population)$
12:     **end while**
13:     **return** $population$
14: **end procedure**

We initialise our population by selecting a random sample of algorithms from the set of algorithms composed of a small number of motifs. The properties of these motifs are determined by the configuration space. In particular, we start with a sample of 200 algorithms composed of 2 or 3 motifs, depending on the size of the configuration space. These algorithms are then evaluated to form the initial population of algorithms, see Alg. 1 line 2.

In the selection step, we choose two candidate algorithms to mutate, line 7 of Alg. 1. Here we balance exploration and exploitation, that is trying new algorithms versus further optimising ones that already have a high fitness score compared to the rest of the population. This is done by randomly deciding between two selection methods, namely random selection or tournament selection (i.e. selection according to fitness ranking) which emphasise exploration and exploitation, respectively. Tournament selection depends on selection pressure which determines the percentage of the population considered. A higher selection pressure corresponds to greater exploitation since each candidate competes against a larger subset of the total population. The probability of performing random or tournament selection and the selection pressure are hyper-parameters of the search strategy. These can be changed over the course of an experiment. We begin in a highly exploratory phase followed by an exploitative phase, with the transition between these phases scheduled according to a sine function. By using a periodic function we can alternate between phases of exploration and exploitation during long experiments.

The composability of motifs makes it intuitive to construct methods for generating new algorithms from a pair of parent algorithms. In particular, we used a 'chop-and-

```
algorithm = (
 QPivot(H, "1*")
 + QPivot(H, "*1") # -
 + QPivot(H, "1*") # +
 + QCycle(X)
 + QPivot(MCX, "*1")
 + QPivot(MCX, "*1")
 + QPivot(MCX, "*1")
 + Oracle
 + QCycle(H)
) * r
```

(a) Property mutation: A motif and a property thereof are randomly selected. Here, the global pattern of the selected pivot is changed from *1 to 1*.

```
algorithm = (
 Oracle
 + QCycle(H)
 + QCycle(X)
 + QPivot(H, "*1") # +
 + QPivot(MCX, "*1")
 + QCycle(x)
) * r
```

(b) Insert motif: A random motif is inserted at a random position in the larger composition.

```
algorithm = (
 Oracle
 + QCycle(H)
 + QCycle(x)
 + QPivot(H, "*1")
 + QPivot(MCX, "*1")
 + QPivot(MCX, "*1")
 + QPivot(MCX, "*1")
 + QCycle(H)
 + Oracle # -
 + Oracle
 + Oracle
 + QCycle(H)
 + QPivot(H, "*1")
 + QCycle(x)
 + QCycle(H)
) * r
```

(c) Dropout: A randomly selected motif is removed.

```
algorithm = (
 # head
 Oracle
 + QCycle(H)
 + QCycle(x)
 + QPivot(H, "*1")
 + QPivot(MCX, "*1")
 # tail
 + QPivot(H, "*1")
 + QCycle(x)
 + QCycle(H)
) * r
```

(d) Chop and join: Two pieces, each from a different algorithm, are combined to produce a new algorithm.

FIG. 5: Examples of mutations, written in the DSL. Mutations (a), (b), (c) and (d) correspond to those highlighted in Fig. 3.

join' mutation which separates each of a pair of algorithms into two pieces, where the division is made at a random point in the sequence of motifs. The first pieces of each algorithm are exchanged to produce two new algorithms. In addition, three types of mutations were used that operate on a single algorithm. The 'property' mutation selects a motif at random from the composition of motifs and either modifies a randomly chosen property or replaces the selected motif with a randomly generated one. The 'dropout' and 'insert' mutations work by removing and inserting a randomly generated motif, respectively. The probability of using a mask, unmask, cycle, or pivot when randomly generating a motif is an another hyper-parameter of the search. If the task uses an oracle then it is treated as a motif and is also assigned a probability of being used. Fig. 5 shows an example of

each of these four mutations. Each example corresponds to a mutation that occurred during the experiment discussed in Fig. 3. If the chop-and-join mutation was omitted then such an evolutionary tree could only be a linear sequence of algorithms.

The process of selection and mutation is repeated according to the batch size hyper-parameter n_{batch}, as shown in Alg. 1 lines 6-8. The number of new algorithms created in each generation is $8n_{batch}$ since two algorithms are selected and we apply four mutations. The new candidate algorithms are evaluated in parallel and the batch size is chosen according to available hardware. Consequently, the rate of growth of the population is determined by the batch size and this should be taken into account when scheduling the probability of performing random or tournament selection. Once evaluated, the new algorithms are added to the population, see line 10 in Alg. 1.

Since the learning tasks that we tested were known algorithms, we implemented early stopping in line 3 Alg. 1. This is not a requirement of the method and line 3 can be replaced with a tautology, creating an infinite loop. In our implementation, the primary stopping condition is met when the overlap between the state output by the algorithm and the target state is greater than a chosen threshold for all training examples. In addition, for problems that employ an oracle, we require that the composition of motifs contains at most one oracle call. Finally, we set a maximum runtime for an experiment. In general, it is useful to strike a balance between allowing an experiment to run for sufficient time and running multiple experiments. Performing multiple experiments is useful since the search strategy depends on several random processes which affect convergence.

C. Performance estimation

The fitness function associates a numerical value to the performance of a candidate algorithm. The fitness is then used to generate a relative ranking of the algorithms in the population. Designing a fitness function is important as it governs how the search space is navigated. We determine the fitness of a candidate algorithm by analysing its performance with respect to a set of training examples and by considering its complexity.

The first contribution to our fitness function is constructed using state overlap. The training set, $T = \cup_{q \in Q} \{(x_i^{(q)}, y_i^{(q)})\}_{i \in I}$, is a collection of input-target pairs, $(x_i^{(q)}, y_i^{(q)})$, which are grouped by $q \in Q$, where Q is a set of circuit sizes. We define the fitness function as follows

$$f(m) := \min_{q \in Q} f_q(m) := \min_{q \in Q} \left\{ \sum_{i \in I} |\langle y_i^{(q)} | U_{(m)}^{(q)} | x_i^{(q)} \rangle|^2 \right\},$$
(1)

where $U_{(m)}^{(q)}$ is the quantum circuit (unitary operation) associated with the candidate algorithm m instantiated

for the relevant circuit size implied by q. Here we take the minimum fitness across the set of circuit sizes, but taking the mean is also valid. It turns out that it is sufficient to evaluate an algorithm on a small number of circuit sizes for the general structure to be learnt. In particular, circuits of size 2, 3 and 4 qubits were sufficient for the Deutsch-Jozsa algorithm and QFT, and circuits of size 3, 4 and 5 qubits were sufficient for Grover's search.

The fitness can be improved by adding penalties to $f_q(m)$ that depend on the complexity of $U_{(m)}^{(q)}$. To favour smaller simpler structures, a penalty is added in terms of the number of unitary gates in the circuit $U_i^{(m)}$. A penalty is also added for the number of oracle calls and the number of gate parameters, where applicable. Lastly, we add a penalty based on the Jensen–Shannon divergence [29] which penalises circuits that perform non-uniformly across the elements of the training set. The relative weights of these penalties are a hyper-parameter of the search.

When an algorithm contains parametrised gates, these are trained numerically using gradient decent [30, 31] to maximise the fitness of the candidate. In order to speed up evaluation, we allow parameter training to run for only a few seconds, which further penalises highly parametrised circuits. Parameters are later trained more carefully during post-processing.

During evaluation, the repetition parameter is increased incrementally from 1 until the fitness no longer increases, or until the number of repetitions is equal to the circuit size. This upper limit on the number of repetitions is motivated by the fact that we would like the size of our learnt algorithm to scale at most linearly in the number of qubits. During post-processing, the relationship between the circuit size and the number of repetitions can be inferred by evaluating the algorithm on a larger number of circuit sizes.

D. Tasks

In our approach, setting up the problem is the primary task of the user, while the task of designing the algorithm is delegated to the computer. As we use a bottom-up approach, the user needs to carefully construct training examples that capture the desired behaviour of the algorithm. If required, the user should also define an appropriate oracle. Here we simply used the known oracles. However, many formulations of the problem may need

to be tested to arrive at the final algorithm, which is straightforward to do using our method. Below we discuss the problem setup for each task.

The quantum Fourier transform (QFT) [3] maps an input state to an output state whose amplitudes are related by the discrete Fourier transform. The training examples are constructed using the computational basis states and their corresponding Fourier-transformed counterparts. An additional training pair is added where the input state is given by an equal superposition of all computational basis states. This penalises erroneous relative phase shifts between all other output states.

The Deutsch-Jozsa algorithm [32] distinguishes between a constant and a balanced function, $f : \mathbb{R} \to \{0, 1\}$, in a single function evaluation. An oracle is provided that performs the transformation $|x\rangle |0\rangle \to |x\rangle |f(x)\rangle$. Since we would like the learnt algorithm to use as few oracle calls as possible, i.e. only one, we assume at most a single repetition of the learnt algorithm. The training set contains a training pair for each possible balanced function for the given circuit size. For each of these training pairs, we add another pair for the constant function, which makes the training set balanced. We distinguish between the training pairs associated with balanced and constant functions by specifying that the expected fidelity with respect to the zero state, $| \langle y_i^{(q)} = 0 | U_{(m)}^{(q)} | x_i^{(q)} \rangle |^2$, should be zero and one, respectively.

Grover's search [33] provides an optimal method for searching an unstructured database. The oracle marks the state associated with the sought database entry with a phase, namely $\exp(i\pi) = -1$. A training pair is constructed for each of the possible sought entries (computational basis states) for the given problem size 2^q, where q is the number of qubits. A fixed input state of $(\frac{|0\rangle + |1\rangle}{\sqrt{2}})^{\otimes q}$ is used, which encodes the assumption that each database entry has an equal probability being the sought entry.

Oracles are implemented as Python lambda functions so that relevant parameters can be passed at the time of evaluation. Namely the target state, in the case of Grover's search algorithm, and the function f in the case of the Deutsch-Jozsa algorithm.

V. DATA AVAILABILITY

The dataset generated and analysed during the current study is not publicly available due to its size but is available from the corresponding author upon reasonable request.

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VII. AUTHOR CONTRIBUTIONS

AR and ML conceived and designed the study. AR implemented the search strategy, performed the numerical experiments and analysed the results. AR prepared the manuscript with input from ML. FP supervised the research. All authors read and approved the final manuscript.

VIII. COMPETING INTERESTS

All authors declare no financial or non-financial competing interests.