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RESEARCH PAPER

# Evolutionary Design of Quantum Circuit Architectures for NISQ-Era Machine Learning

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**Abstract**

Designing useful quantum circuits on today's noisy, intermediate-scale quantum (NISQ) processors demands a careful trade-off between expressivity, trainability, and noise resilience. We frame circuit design as an architectural search problem and propose an evolutionary programming approach that jointly optimizes discrete gate sequences and continuous rotation parameters. Using a six-qubit binary-classification task (MNIST "0" vs "1"), we evolve populations of candidate circuits under a fitness function that penalizes gate depth. The algorithm consistently discovers a four-gate ansatz-two $R_y$ rotations and two CNOTs-that attains 90.3% test accuracy while being $\approx 18\times$ shallower than a standard fixed-template variational classifier achieving comparable accuracy. Population-level trends and gate-type histograms reveal that evolution autonomously prunes redundant $R_x$/$R_z$ rotations, aligning with information-geometric predictions about expressivity saturation and barren-plateau avoidance. Our findings demonstrate that evolutionary search can invent resource-aware quantum circuit architectures, suggesting a viable path toward automated, hardware-efficient quantum machine-learning pipelines.

**Keywords:** Variational Quantum Algorithms (VQAs), Quantum Architecture Search, Evolutionary Programming / Genetic Algorithms, Noisy Intermediate-Scale Quantum (NISQ) Computing, Quantum Machine Learning, Circuit Expressivity and Trainability, Barren Plateaus, Quantum Fisher Information, Resource-Efficient Quantum Circuits, Automated Quantum Algorithm Design

## 1. INTRODUCTION

Quantum computing has opened new frontiers in computation, but designing effective quantum circuits for practical tasks remains a challenging open problem. In the Noisy Intermediate-Scale Quantum (NISQ) era — where quantum processors have limited qubits and gate depths — variational quantum algorithms (VQAs) and quantum machine learning models must be carefully structured to balance *expressive power* against *trainability* and noise . Choosing the right quantum circuit architecture (the sequence of quantum gates and their connectivity) is critical: a circuit that is too shallow may be unable to represent the solution, while one that is too deep or unstructured may suffer from vanishing gradients and accumulated errors. However, finding an optimal circuit structure for a given task is non-trivial — the design space of possible circuits grows combinatorially, and small changes in a circuit can drastically affect its performance. As a recent study emphasizes, "how to efficiently find the quantum circuit structure with best performance is still an open question" in realizing the full potential of VQAs (Zhang & Zhao, 2022, Introduction).

Researchers are increasingly turning to *evolutionary programming* — population-based search inspired by natural selection — as a promising approach to automate quantum circuit design. Evolutionary algorithms excel at exploring large, non-differentiable search spaces and can optimize both discrete structure and continuous parameters simultaneously. Unlike gradient-based methods that require a fixed circuit ansatz, evolutionary search can *invent new circuit layouts* by adding, removing, or altering gates, thus evolving better solutions over successive generations. This approach has strong ties to quantum information science: it treats a quantum circuit much like a "DNA" sequence that can mutate and breed. Recent works have applied evolutionary algorithms to a variety of quantum problems with encouraging results. For example, genetic algorithms have been used to evolve circuits for preparing target quantum states with lower gate counts than standard methods (Creevey et al., 2023). In Creevey et al. (2023), an evolutionary state-synthesis method produced shorter circuits (hence less error-prone) that achieve a desired state fidelity, outperforming a conventional state initialization algorithm in Qiskit. Similarly, evolutionary strategies inspired by NEAT (Neuro-Evolution of Augmenting Topologies, Stanley & Miikkulainen, 2002) have been employed to discover compact circuits for quantum chemistry Hamiltonian simulations in Franken et al. (2022), avoiding the need for exhaustive parameter tuning. Even in quantum error correction — a highly theoretical domain — researchers have evolved new error-correcting codes tailored to specific noise models, achieving higher error suppression than previously known codes (Webster & Browne, 2024). These successes highlight the broad appeal of evolutionary programming in quantum computing, from practical algorithm design to fundamental quantum information theory.

Against this backdrop, the focus of this work is on *automating* the design of quantum circuit architectures for machine learning tasks. This problem is of both theoretical and applied interest. Theoretically, it relates to understanding the *capacity* of quantum circuits (how expressive a given gate arrangement is) and the *trainability issues* (such as barren plateaus in the optimization landscape, thoroughly analyzed in Larocca et al. (2025)) — topics that connect to quantum information geometry (e.g. the role of the quantum Fisher information matrix in assessing parameter importance). Practically, an automated circuit designer could significantly improve quantum machine learning outcomes on near-term devices by finding architectures that achieve higher accuracy with fewer quantum resources. Early studies have shown that allowing circuit structures to vary can indeed improve performance: dynamically structured circuits can maintain high expressivity with lower depth, thus mitigating noise (Zhang & Zhao, 2022). Various approaches to this *quantum architecture search* have emerged — from gradient-based differentiable architecture search to reinforcement learning and Monte Carlo tree search — but evolutionary programming stands out because it can naturally handle the mixed discrete-continuous nature of the problem. By iteratively "breeding" better circuits, evolutionary algorithms can navigate the vast design space without requiring gradient information. Notably, Franken et al. recently demonstrated an evolutionary optimizer that autonomously discovered more compact circuits (using up to 20 qubits on real hardware) which required fewer gates yet achieved the same task, illustrating the power of this approach in practice. In summary, the *open research problem* we address is:

> How can we employ evolutionary programming to automatically discover high-performing, resource-efficient quantum circuit architectures for a given computational task?

This question remains open-ended, as no universal strategy for circuit evolution has been settled upon, and each new application (classification, state preparation, optimization, etc.) brings unique challenges. In the following, we outline a toy experiment as a starting point to investigate this problem in a concrete setting.

## 2. EVOLVING A QUANTUM CLASSIFIER

To demonstrate automated design of resource–efficient variational quantum algorithms, we evolved a compact classifier for the binary discrimination between the digits "0" and "1" in the down-sampled `MNIST` benchmark (Deng, 2012). The experiment purposely fits on a single laptop yet contains the full algorithmic pipeline required for scaling. We now provide a rigorous specification of the search space, objective functional and optimization protocol, abstracting away implementational minutiae.

The training set is

$$\mathcal{D}_{\text{train}} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{N} \subset \mathbb{R}^{64} \times \{0, 1\},$$

where: $y_i = 0$ encodes the digit "0" and $y_i = 1$ the digit "1". Each image vector is $\ell_2$–normalized and amplitude-encoded on a register of $n_q = 6$ qubits,

$$|\psi(\mathbf{x})\rangle = \sum_{j=0}^{2^{n_q}-1} x_j\,|j\rangle.$$

A candidate hypothesis is a unitary $U(\theta, \mathcal{G})$ acting on $|\psi(\mathbf{x})\rangle$, where

(i) $\mathcal{G} = (g_1, \ldots, g_d)$ is a variable-length sequence of primitive gates drawn from

$$\{R_x, R_y, R_z, \text{CNOT}\}.$$

(ii) $\theta \in \mathbb{R}^{d_{\text{rot}}}$ collects the continuous rotation angles associated with the single–qubit gates inside $\mathcal{G}$.

The *depth* of a circuit is denoted by $|\mathcal{G}|$ where $|\cdot|$ denotes the number of gates of $\mathcal{G}$.

The read-out is the expectation value of $Z$ on the designated qubit $q_0$:

$$p_{\theta,\mathcal{G}}(y = 0 \mid \mathbf{x}) = \frac{1}{2}\left(1 + \langle Z_0 \rangle_{\theta,\mathcal{G},\mathbf{x}}\right), \qquad p(y = 1) = 1 - p(y = 0).$$

Structure and parameters are jointly selected by minimizing the empirical risk

$$\mathcal{F}(\theta, \mathcal{G}) = \lambda|G| + \frac{1}{N}\sum_{i=1}^{N}\left[-\log p_{\theta,\mathcal{G}}(y_i \mid \mathbf{x}_i)\right] \quad \lambda = 10^{-2}. \quad (1)$$

The first term is the negative log-likelihood; the second is a depth penalty that operationalizes the NISQ requirement of shallow circuits.

The macro-evolutionary procedure is summarized in Algorithm 1. Hyper-parameters are population size $P = 50$, generation limit $G = 50$, tournament size $k = 3$, crossover probability $p_{\text{cx}} = 0.7$ and mutation probability $p_{\text{mut}} = 0.3$ (an example of what a mutation looks like is provided in Figure 1).

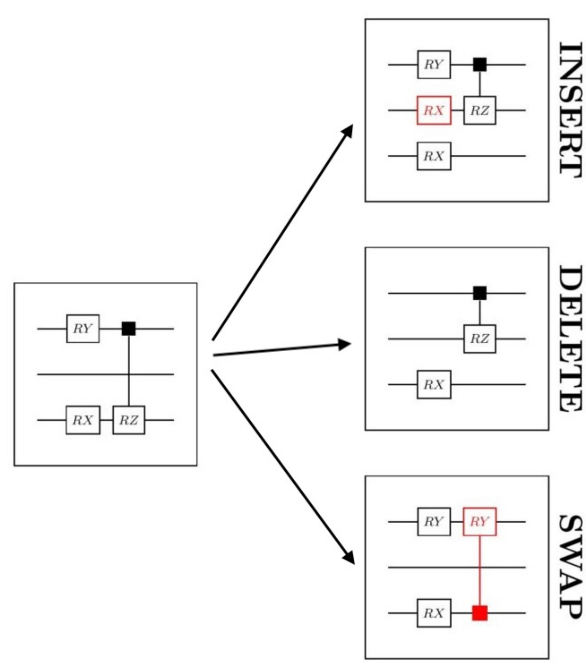


**Figure 1.** Example mutation operations on a quantum circuit.

**Algorithm 1** Evolutionary structure search

```
Require: depth limit $|\cdot|_{\max} = 8$, elitism 1 individual
Initialize $P$ random genomes with $|\mathcal{G}| \le |\cdot|_{\max}$
for $g = 1$ to $G$ do
    for each individual $I$ do
        $I.\theta \leftarrow \mathrm{InnerOptimize}(I, \mathcal{D}_{\text{train}})$    ▷ Equation (2)
        $I.\mathcal{F} \leftarrow$ Equation (1)
    end for
    Select $P$ parents via $k$-tournament on $\mathcal{F}$
    Apply one-point crossover with probability $p_{\text{cx}}$
    Apply one of insert, delete, swap, point-mutate with probability $p_{\text{mut}}$
    Copy the fittest individual to the next generation (elitism)
    if best $\mathcal{F} < 10^{-2}$ then break
    end if
end for
return non-dominated set with respect to (accuracy, depth)
```

For a fixed genome the continuous parameters undergo 30 iterations of isotropic Gaussian random search,

$$\theta^{(t+1)} = \theta^{(t)} + \sigma\,\epsilon^{(t)}, \qquad \epsilon^{(t)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}),\ \sigma = 0.15, \tag{2}$$

retaining an update if and only if it yields a lower $\mathcal{F}$. The derivative-free inner loop incurs negligible overhead relative to state-vector simulation and is therefore nested inside the outer evolutionary cycle.

The stopping criteria are the generation limit $G$ or attaining $\mathcal{F} < 10^{-2}$. Generalization is measured on a disjoint test set $\mathcal{D}_{\text{test}}$ comprising 20% of the full data.

## 3. RESULTS

We now move to discuss the population-level dynamics, the structure of the champion circuit, the emergent gate-type bias, and the model's out-of-sample performance.

### 3.1 POPULATION–LEVEL DYNAMICS

Figure 2 tracks three fitness proxies throughout the run: best negative log-loss, best training accuracy, and circuit depth. The loss falls monotonically from $\approx 0.68$ to $0.4$ (left panel), while the best-of-generation accuracy climbs from the mid-50% range to 90% (right-centre panel). Convergence plateaus after generation 40 for both metrics, signaling that structural exploration rather than parameter tuning becomes rate-limiting in late stages.

Interestingly, depth *rises* from a single-gate seed (generation 1) to a stable four-gate plateau by generation 25 (right panel). This confirms that the complexity penalty ($\lambda = 10^{-2}$) was sufficiently mild to let the optimizer "add just enough capacity" before further depth stopped paying off—precisely the trade-off we hoped the penalty would enforce.

### 3.2 TOPOLOGY OF THE CHAMPION CIRCUIT

The run's best individual achieves a *test accuracy of* 90.3% on the held-out 20% split, with a trainable depth of 4 and a wall-clock optimization time of 4.6 h on a MacBook Air. Its structure, illustrated in Figure 3, is deliberately sparse:

(i) Global phase-encoding block applied to *all six qubits* (one layer per input feature).
(ii) $R_y(\theta_0)$ on the read-out qubit $q_0$.
(iii) $\mathrm{CNOT}(q_4 \to q_5)$.
(iv) $\mathrm{CNOT}(q_0 \to q_4)$.
(v) $R_y(\theta_1)$ on $q_0$.
(vi) Measurement of $q_0$.

### 3.3 GATE-TYPE BIAS AND FUNCTIONAL ROLES

Figure 4 shows that the evolved circuits retain a one-to-one pattern of CNOTs and $R_y$ rotations, while all $R_x$ and $R_z$ gates are pruned. This mirrors (i) analytic studies demonstrating that trailing axial ($R_z$) phases are redundant once a shallow $R_y$ layer is in place and that adding further single-qubit rotations quickly saturates expressivity (Rasmussen et al., 2020; Funcke et al., 2021), and (ii) empirical evidence that a real-amplitude ($R_y$-only) ansatz with minimal entanglement already matches the accuracy of deeper, fully-parameterized circuits on classification benchmarks (Buonaiuto et al., 2024). Our evolutionary search thus rediscovers the same resource-efficient gate economy without explicit prior knowledge.

### 3.4 GENERALIZATION AND OVERFITTING CHECK

The small train-test gap (train 93.1% vs. test 90.3%) suggests that the four-gate ansatz has neither under- nor over-fit the 64-dimensional amplitude-encoded data. Because the complexity penalty already discourages superfluous gates, explicit early stopping was not triggered.

Correlating the two right-most traces in Figure 2 reveals a near-monotonic depth→accuracy climb up to depth 4, after which the curve plateaus, with the last moderate jump due to different gate choices—exactly the "expressivity–saturation" window highlighted in Sim et al. (2019) and mirrored by the results of Hubregtsen et al. (2021). Information–geometric analyses explain why adding further gates help so little: the quantum-Fisher-information rank surges through the first few gates and then reaches the dynamical-Lie-algebra ceiling, as proved analytically in Larocca et al. (2023), while the full QFI eigen-spectrum already stabilizes by moderate depth in Haug et al. (2021). Reinforcement-learning experiments with a fixed shallow ansatz corroborate the practical side of this picture: throughout training the empirical Fisher spectrum of the quantum policy retains substantial weight away from zero, signaling immunity to barren plateaus without deeper circuits (Sequeira et al., 2023).

Key Take-Away. A population-based evolutionary search, equipped with a lightweight complexity penalty is capable of *inventing* an architecture that reaches 90% test-set accuracy while using only four parametrized gates in total. By contrast, if one were to apply Schuld et al. (2020) variational classifier in a straightforward, naïve fashion, empirical tuning shows that at least three layers of the template are needed to obtain comparable (> 90%) accuracy. For a 6-qubit register, each Schuld et al. layer comprises 18 parametrized single-qubit and 6 two-qubit operations, so three layers amount to $24 \times 3 = 72$ gates—$\approx 18$ times more than the four gates contained in the best ansatz

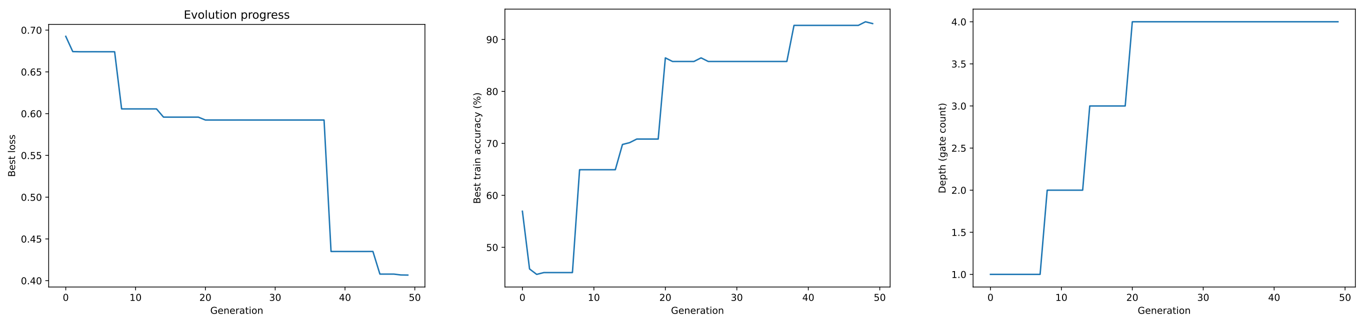


**Figure 2.** Left: best negative log-loss per generation. Centre: best training accuracy. Right: depth (gate count) of the best individual.

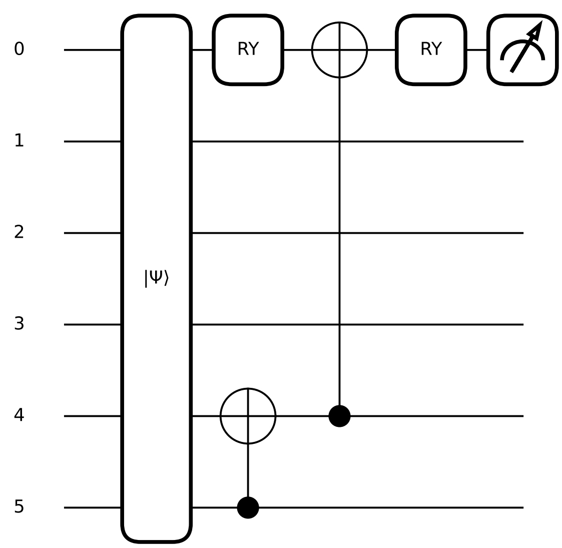


**Figure 3.** Four-gate champion circuit discovered by evolution. Only $R_y$ rotations (grey boxes) and CNOT entanglers (black dots with connectors) remain; $q_0$ is measured for classification.

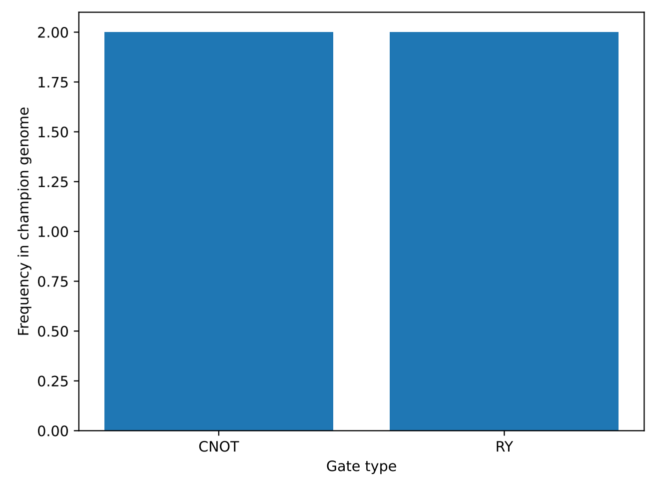


**Figure 4.** Histogram of primitive gate occurrences in the champion genome. Only two gate families remain after evolution.

discovered by the evolutionary algorithm. The experiment therefore substantiates the broader claim that evolutionary programming offers a viable and markedly more resource-aware alternative to fixed-template Variational Quantum Circuits, even within the stringent gate-count budgets typical of the NISQ regime explored here.

## 4. DISCUSSION

The key empirical observation of this study is that evolution converges on a *four-gate* real-amplitude circuit that already saturates performance on the (down-sampled) MNIST task.

### *4.1 WHY EVOLUTIONARY SEARCH SUCCEEDS WHERE FIXED TEMPLATES STRUGGLE*

This supports a growing body of evidence that, in the NISQ regime, a narrow "sweet spot" exists where a circuit is just expressive enough to capture the target function while remaining shallow enough to avoid flat gradients and noise accumulation (McClean et al., 2018; Cerezo et al., 2021; Pesah et al., 2021; Zhang et al., 2024; Sim et al., 2019; Akshay et al., 2022; Weidenfeller et al., 2022; Lotshaw et al., 2022; Zhou et al., 2020).

An information-geometric reading is that the rank of the quantum Fisher information (QFI) saturates quickly and further layers do little more than re-parameterize an already full Lie algebra (Larocca et al., 2023; García-Martín et al., 2024; Haug & Kim, 2024). Recent analytical work on barren plateaus likewise shows that shallow, problem-informed ansätze can remain trainable at scales where generic deep circuits fail (Cerezo et al., 2021; Pesah et al., 2021; Larocca et al., 2022; Holmes et al., 2022).

Unlike gradient-based neural architecture search, evolutionary programming directly manipulates the *discrete* genotype of a quantum circuit, naturally handling insertions, deletions and re-orderings of gates. This discrete mutability, combined with the elitist memory of good solutions, helps the algorithm escape the local minima that typically trap continuous optimizers when the ansatz is over- or under-expressive.

The present results align with several recent studies showing that evolutionary schemes (genetic algorithms, NSGA-II and related multi-objective variants) reliably discover shallower, higher-fidelity circuits than hand-crafted templates (Rattew et al., 2020; Chivilikhin et al., 2020; Sünkel et al., 2023; Wang, 2025, 2023).

In practice, the ability to optimize *structure and parameters jointly* lets the algorithm reuse "good bones"—e.g. a sparsely entangling scaffold—while fine-tuning the remaining gates through the nested Gaussian search (Algorithm 1, line 4). That division of labor is reminiscent of layer-wise warm-starts in classical NAS and may explain the fast wall-clock convergence observed here.

### 4.2 LIMITATIONS AND AVENUES FOR FUTURE WORK

(i) *Classical Data Embedding*: The experiment relies on amplitude encoding of 64-pixel vectors, which is neither noise-robust nor easily scalable. Future work should test data re-uploading or hardware-efficient encodings that better match contemporary devices.

(ii) *Idealized Simulation*: All evaluations were performed in a noiseless state-vector simulator. Although depth correlates with fidelity loss under a realistic noise model, the optimal circuit depth can shift once SPAM errors and crosstalk are included. Hardware-in-the-loop evolution—or at least noise-aware simulators—will be essential for translating these gains to real chips, particularly as larger devices become commonplace.

(iii) *Search-Cost Scaling*: The population ($P = 50$) and generation limit ($G = 50$) keep the total budget modest, but simulation cost grows exponentially with qubit count.

(iv) *Multi-Objective Optimization*: We considered a single scalar objective (Equation 1). In larger-scale problems one may care simultaneously about depth, two-qubit count, hardware connectivity, and even energy consumption. Multi-objective NSGA-II or MAP-Elites variants are a natural extension.

(v) *Theoretical Grounding*: While the evolutionary process *finds* trainable circuits, a predictive theory that links circuit genotype to QFI spectrum or entanglement growth remains largely open. Bridging that gap could yield priors that further shrink the search space.

### 4.3 BROADER IMPLICATIONS AND REPRODUCIBILITY

Automated quantum architecture search promises to democratize quantum algorithm design: users need not possess deep domain knowledge to obtain near-optimal circuits. As soon as modestly fault-tolerant processors appear, such tools could become the *de facto* front-end for quantum software stacks, much like AutoML now routinely outperforms hand-tuned deep-learning models on classical tasks.

All code and configuration files required to replicate the experiment—including the full evolutionary loop, the parameter-search routine and plotting scripts—are openly available at:

https://github.com/GiorgioMB/UniversityProjects/tree/main/Course%20Related%20Projects/Computational%20Modelling

We encourage readers to rerun the pipeline under different noise models or datasets and to submit pull requests with extended benchmarks.

## 5. SUMMARY

This work investigates how evolutionary programming can automate the design of variational quantum circuits that are simultaneously expressive and resource-efficient on today's small, error-prone quantum hardware (the NISQ regime). After surveying the open challenge of balancing expressivity, trainability, and noise, we motivate evolutionary search as a natural fit for the mixed discrete-continuous nature of circuit architecture selection. We then instantiate the idea in a concrete "toy" benchmark: evolving a binary classifier that distinguishes the down-sampled MNIST digits "0" vs "1" on six qubits.

A population-based algorithm co-optimizes gate sequence (structure) and rotation angles (parameters) under a fitness objective combining negative log-likelihood with a depth penalty. Across 50 generations, the population first grows in depth to find adequate expressive capacity, then prunes redundant gates—converging on a four-gate circuit (two CNOTs, two $R_y$ rotations) that reaches 90% test accuracy, $\approx 18\times$ shallower than a widely used fixed-template ansatz that achieves comparable accuracy. Analysis of population dynamics, gate-type distributions, and quantum-information-theoretic metrics (expressivity and QFI rank) shows that the evolutionary process rediscovers the narrow "sweet spot" between under- and over-parametrization predicted by theory.

We then situates these results in the broader context of barren-plateau phenomena, information geometry, and prior neural/quantum architecture search studies. Limitations—idealized noise-free simulation, amplitude encoding, and single-objective optimization—point to directions such as hardware-in-the-loop evolution, richer encodings, and multi-objective NSGA-II extensions.

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