## Extended Abstract: Geodesic Algorithm for Unitary Gate Design with Time-Independent Hamiltonians [\[1\]](#page-0-0)

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## EXTENDED ABSTRACT

The primitive quantum gates of quantum computing platforms usually involve only one or two qubits and simple Hamiltonians. Our aim is to take advantage of the more complex Hamiltonians available in experimental platforms to design larger multi-qubit gates. Finding these restricted Hamiltonians that generate desired quantum gates is numerically challenging. Existing methods of stochastic gradient descent [\[2\]](#page-1-0), differential evolution [\[3\]](#page-1-1), or variational quantum algorithms [\[4\]](#page-1-2) have been attempted, but have limited success for larger gates.

We offer a solution to the problem of generating multi-qubit gates from time-independent Hamiltonians through the lens of differential geometry of the Lie group structure of quantum gates. Some geometric techniques have previously been crucial for understanding quantum circuit complexity [\[5\]](#page-1-3). Our algorithm utilises geodesic information and gradients on the group manifold to rapidly converge to an accurate solution. At each optimisation step, we update the Hamiltonian coupling strengths such that the resulting unitary is closer to the target unitary gate. This can be achieved by updating the couplings such that they follow (as closely as possible) the geodesic curve towards the target. In our paper, we formalise this comparison and demonstrate how the geodesic can be generated by updating Hamiltonian coupling strengths in time-independent Hamiltonians.

We demonstrate the algorithm's efficiency by comparison to gradient descent techniques for the generation of Toffoli and Fredkin gates. Furthermore, we use the algorithm to generate previously unavailable weight- $k$  parity checks with up to 6 qubits, which are necessary for a wide array of quantum error correcting codes. We find that our geodesic algorithm is significantly more efficient than gradient descent algorithms for finding a restricted generating Hamiltonian of a desired unitary gate, see Fig. [1.](#page-0-1) Larger, more complex quantum gates can therefore be implemented directly. Not only could this lead to less noisy gates, but it could also reduce the total time to run a circuit on the hardware. This is crucial for NISQ applications where we have a limited coherence time and gives the significant advantage of increasing the clock



speed for fault-tolerant quantum computation.

<span id="page-0-1"></span>FIG. 1. Comparison of the number of steps required before a solution with infidelity less than  $\varepsilon = 0.001$  is found for: our geodesic algorithm (blue), stochastic gradient descent (SGD) of Ref. [\[6\]](#page-1-4) (green), and a simple gradient descent optimiser that uses gradients computed with JAX (orange). For all methods, we consider 1000 random initialisations of the parameters. Both the geodesic algorithm and SGD algorithm find a solution 100% of the time, whereas the JAX gradient descent algorithm finds a solution 98% of the time.

## ALGORITHM OVERVIEW

The algorithm uses the effective generators of the directional derivatives and geodesic generators. The effective generators,  $\Omega_l$ , of the directional derivatives for each Lie algebra component live in the tangent space of the  $SU(2^n)$  Riemannian manifold. The generator of the geodesic  $\Gamma^{(m)}$  determines the best way to update the parameters. At each optimisation step  $m$ , we want to update the parameters such that the resulting unitary gate is closer to the target unitary,  $V$ . This can be achieved by updating the parameters such that they follow (as closely as possible) the geodesic curve towards the target  $V$ . The paper describes the algorithm formally and shows how the geodesic can be generated by updating interaction strengths in time-independent Hamiltonians by solving a linear least-squares problem.

<span id="page-0-0"></span>[1] D. Lewis, R. Wiersema, J. Carrasquilla, and S. Bose, [Geodesic Algorithm for Unitary Gate Design with](https://doi.org/10.48550/arXiv.2401.05973) [Time-Independent Hamiltonians](https://doi.org/10.48550/arXiv.2401.05973) (2024), arXiv:2401.05973

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- <span id="page-1-1"></span>[3] L. Eloie, L. Banchi, and S. Bose, Quantum arithmetics via computation with minimized external control: The halfadder, [Physical Review A](https://doi.org/10.1103/PhysRevA.97.062321) 97, 062321 (2018), publisher: American Physical Society.
- <span id="page-1-2"></span>[4] A. Majumder, D. Lewis, and S. Bose, [Variational](https://doi.org/10.48550/arXiv.2209.00139) [Quantum Circuits for Multi-Qubit Gate Automata](https://doi.org/10.48550/arXiv.2209.00139) (2022),

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- <span id="page-1-4"></span>[6] L. Innocenti, L. Banchi, A. Ferraro, S. Bose, and M. Paternostro, Supervised learning of time-independent Hamiltonians for gate design [10.1088/1367-2630/ab8aaf](https://doi.org/10.1088/1367-2630/ab8aaf) (2020), iSBN: 82.169.190.85.