

Invariant-Guided Exploration of the Weyl Chamber for Universal Quantum Gate Discovery

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Two - qubit gates drive the power of quantum circuits, but finding new universal gates remains challenging. In this study, we developed an evolutionary computational framework to systematically discover universal two - qubit gates using Makhlin invariants and Weyl chamber geometry. Candidate gates were generated through iterative mutation and recombination, with universality evaluated based on proximity to canonical coordinates up to local equivalence. The search identified several novel universal gates that are locally equivalent to CNOT. Simulations of these gates show strong entangling power, suggesting they could be applied to optimize quantum circuit design and hardware - aware compilation. Visualizations of the Weyl chamber revealed distinct geometric clusters corresponding to both known and newly realized universal classes, highlighting the structure and diversity of two - qubit gate space.

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