

Dynamical Lie algebra and CNOT gates

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Abstract

Parameterized Quantum Circuits (PQCs) have emerged as a central framework for variational algorithms in the NISQ regime, with major applications in quantum simulation, combinatorial optimization, and, more recently, quantum machine learning (QML). By developing a new approach for computing dynamical Lie algebras associated with quantum circuits combining parametrized gates and non-parametrized entangling gates, we aim to extend the applicability of recent algebraic results to architectures that are actually used in quantum machine learning.

Parameterized Quantum Circuits (PQCs) have emerged as a central framework for variational algorithms in the NISQ regime, with major applications in quantum simulation, combinatorial optimization, and, more recently, quantum machine learning (QML) models [13] [3] [2] [16]. In these models, in general hybrid quantum-classical, an initial quantum state is transformed by a parameter-dependent circuit and subsequently measured in order to evaluate a cost function, which is then optimized using classical routines. Several works have shown that the trainability of such architectures strongly depends on the circuit structure and its expressivity [11] [9] [14] [6]; this is strongly related to the so-called dynamical Lie algebra (DLA).

Indeed, results in the literature consistently define the DLA $\mathfrak{g}$ of an L-layer ansatz of the form

$$V(\boldsymbol{\theta}) = \prod_{\ell=1}^L V_{\ell}(\theta_{\ell}), \quad V_{\ell}(\theta_{\ell}) = \prod_{k=1}^K e^{-i\theta_{\ell,k} H_{\ell,k}}, \quad (1)$$

as a subalgebra of the d -dimensional special unitary algebra $\mathfrak{su}(d)$, spanned by [10] [9] [14]

$$\mathfrak{g} = \langle i\mathcal{G} \rangle_{\text{Lie}} = \langle iH_1, \dots, iH_K \rangle_{\text{Lie}}. \quad (2)$$

The set of generators $\mathcal{G} = \{H_k\}_{k=1}^K$ consist of traceless Hermitian operators that span the unitary transformations realizable within a single layer and $\langle i\mathcal{G} \rangle_{\text{Lie}}$ denotes the associated Lie closure, namely the set obtained by repeatedly taking the nested commutators between the elements in $\mathcal{G}$.

The importance of the DLA $\mathfrak{g}$ in variational quantum algorithms is such that, the dimension and structure of $\mathfrak{g}$ encode the controllability and expressivity of the circuit [5] [9]: a larger algebra typically corresponds to a richer reachable set of unitaries. We recall that by expressiveness we mean the breadth of unitaries that the circuit can generate as the parameters are varied.

In contrast, many architectures relevant for QML and near-term hardware usually have ansatzes with one parameterized part and one unparameterized part, such as CNOT or CZ gates, such that:

$$V(\boldsymbol{\theta}) = \prod_{\ell=1}^L U_{\ell} W_{\ell}(\boldsymbol{\theta}_{\ell}) = \prod_{\ell=1}^L U_{\ell} \prod_{k=1}^K e^{-i\boldsymbol{\theta}_{\ell,k} H_{\ell,k}}. \quad (3)$$

In such cases, the identification of the effective generators and the computation of the associated DLA become significantly more subtle, and remain open problems, since the unparameterized part U_{ℓ} is not generated by continuous parameters [1] [7] [8] [12] [17]. The blocks U_{ℓ} contain no trainable parameters, and the central idea is that one can move the parametrized gates of latter before the unparameterized gates, recursively using conjugation. This viewpoint is standard in quantum control theory, where controllability is characterized by the Lie algebra generated by drift and control Hamiltonians [4] [15]. More precisely, the fixed part of the circuit (such as the CNOT layers) plays the role of a *drift Hamiltonian*, while the parameterized single-qubit rotations correspond to *control Hamiltonians*.

Each parameterized quantum gate $e^{-i\theta_{\ell j} H_{\ell j}}$ applied to the qubit j , can be moved across the fixed block $U^{(\ell-1)}$ by conjugation, as

$$U e^{-i\theta_j H_j} = U e^{-i\theta_j H_j} U^{\dagger} U. \quad (4)$$

To calculate $U e^{-i\theta_j H_j} U^{\dagger}$, we use that if A is a real or complex $n \times n$ matrix, and B is a unitary matrix, then $e^{BAB^{\dagger}} = B e^A B^{\dagger}$. Therefore,

$$U e^{-i\theta_j H_j} = e^{-i\theta_j U H_j U^{\dagger}} U. \quad (5)$$

Applying this last identity successively across the circuit shows that the trainable directions of the depth- L ansatz are not only the original generators H_j , but also all their conjugates by powers of the fixed entangling block,

i.e

$$H_j, \quad UH_jU^\dagger, \quad U^2H_j(U^\dagger)^2, \quad \dots, \quad U^{L-1}H_j(U^\dagger)^{L-1}. \quad (6)$$

The structure described above suggests that, in this architecture of finite orbit, one should not focus on the generators of a single layer, but rather on the sequence of sets that appears as layers are added. Indeed computing only the commutators between the generators of the first layer is obviously not enough, and one has to deal with those coming from the generators modified by the action of conjugation, in order to capture all the Lie algebra. This is because at each new layer, new conjugated Pauli strings may be added, and these new strings may in turn create new directions through commutators.

As a result, a sufficient number of layers is needed to generate the whole Lie algebra of a quantum circuit. Note that orbit closure and Lie-algebra saturation are not the same notion. Indeed, orbit closure only indicates when the action of conjugation starts repeating itself, ending the possibility of finding new generators. On the other hand, Lie-algebra saturation indicates the point where these generators no longer produce new independent direction after the Lie closure, the dimension of the Lie algebra thus becoming maximal. This saturation phenomenon usually happens before the conjugation orbit is fully completed, so that we do not have to compute all this orbit to calculate the Lie closure.

In our work, we prove that after a finite number of layers one can find the maximal dynamical Lie algebra generated by the circuit. By identifying the group of Pauli matrices with the finite field $\mathbb{F}_2^2$, we give an upper bound for the number of needed layers which is closely related the order of X in the quotient field $\mathbb{F}_2[X]/\chi_U$ where χ_U is the characteristic polynomial of a certain matrix linked to the action of conjugation by U_ℓ in (3). By doing so we give a relatively simple method to compute the Lie algebra of a quantum circuit written as in (3), without having to calculate all the orbit of the conjugation action. This allows to have a better understanding of the expressiveness of a quantum circuit, especially when dealing with ansatzes using unparameterized gates such as CNOT gates.

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