

Imposing Constraints on Driver Hamiltonians and Mixing Operators: From Theory to Practical Implementation

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Abstract

We present a general algebraic framework for constructing constraint preserving driver Hamiltonians and mixing operators, a central challenge in constrained quantum optimization. In Ref. [1], we (1) characterize the operators that preserve embedded classical constraints, (2) establish the computational complexity of finding them, and (3) develop practical algorithms for constructing them when locality bounds are known or desired.

We prove that deciding whether constraint preserving operators exist is NP-complete in the general case, while showing that operators with constant locality can be found in worst-case polynomial time. Since many practical optimization problems admit local constraint preserving operators, these results provide an efficient route to ansatz construction despite the intractability of the unrestricted problem.

Building on this framework, we develop algorithmic procedures that transform these algebraic primitives into driver Hamiltonians and mixing operators suitable for Constrained Quantum Annealing (CQA) and the Quantum Alternating Operator Ansatz (QAOA), providing a systematic alternative to handcrafted constructions.

1 Motivation: Ansatz Construction in Quantum Optimization

This extended abstract summarizes the results of Ref. [1]. Variational quantum optimization has become a primary focus for quantum machine learning in the hybrid quantum classical framework. QAOA and related methods rely on parameterized quantum circuit ansätze. In constrained optimization, ansatz construction must either preserve feasibility throughout the evolution or recover it through the introduction of penalty terms in the objective Hamiltonian, among other techniques.

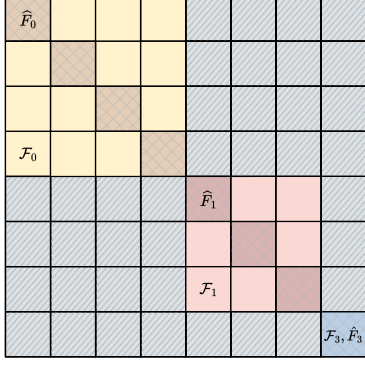
Penalty based encodings are general and widely analyzed, but have several downsides. They can require large energy coefficients, induce long range interactions, and dramatically enlarge the effective search space to include the entire Hilbert space [2–7]. This motivates specialized drivers and mixers that preserve hard constraints natively, such as in constrained quantum annealing and tailored QAOA [3–5, 8–10].

Ansatz construction can aid in improving success probability [9, 11–14], reducing expressibility [15–17], improving learnability [18], and enhancing noise resistance [19].

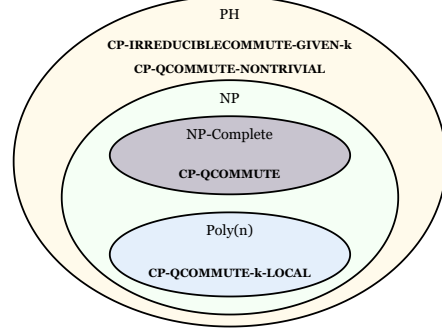
We show that designing constraint preserving mixers is a well-defined computational problem, with existing constructions typically handcrafted for specific problem families. In this work, we provide a complete algebraic framework for reasoning about imposing constraints that allows us to deduce the complexity of the problem and then present an algorithmic pipeline that takes embedded constraints as an input and outputs viable driver or mixer primitives when they exist.

2 Algebraic Characterization, Complexity Classification, and Polynomial-Time Constructions

We develop a unified framework for understanding constraint preserving drivers and mixers. Specifically, these operators commute with the embedded constraint operators. The joint eigenspectrum of these



(a) **Constraint's Feasibility Decomposition and Commutation Space.** An example decomposition, visualizing the embedded constraint operator down the diagonal and the associated commutation space for a constraint $C = x_1x_2 + x_2x_3 + x_1x_3$ leading to $\hat{C} = \sigma_1^1\sigma_2^1 + \sigma_2^1\sigma_3^1 + \sigma_1^1\sigma_3^1 = 0\hat{F}_0 + 1\hat{F}_1 + 3\hat{F}_3$. Then the associated commutation space is $\mathcal{F}_C = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_3$.



(b) **The Complexity of Imposing Constraints on Quantum Operators.** A Venn diagram showing the classification of important problems associated with imposing constraints, under the assumption that $NP \neq P$ and CP-IRREDUCIBLECOMMUTE-GIVEN-k is strictly higher in the polynomial hierarchy (which does not collapse).

operators can be associated with the feasible subspaces of the constraint operators. A valid constraint preserving mixer then lives in the commutation space associated with these operators (Fig. 1a visualizes this for a simple case).

Result 1: We give a necessary and sufficient commutation test based on strings over an overcomplete single qubit basis, where the string locality is controllable. Any Hamiltonian can be written over this overcomplete basis, and it commutes with an embedded constraint operator iff each basis term commutes with that operator, which can be checked via an algebraic condition.

Utilizing this condition, we define the locality hierarchy for constraint preserving mixers, which allows us to characterize important complexity classes.

Result 2: We provide complexity classifications for: finding such mixers (NP-Complete); finding such mixers with a locality bound (polynomial); and recognizing whether a collection of mixers spans the entire feasible subspace (NP-Hard). Fig. 1b summarizes these results.

We then define the Jordan algebra of constraint preserving mixers, which gives us a valuable framework to describe the reachability and separability that any collection of mixers determines for QAOA and CQA.

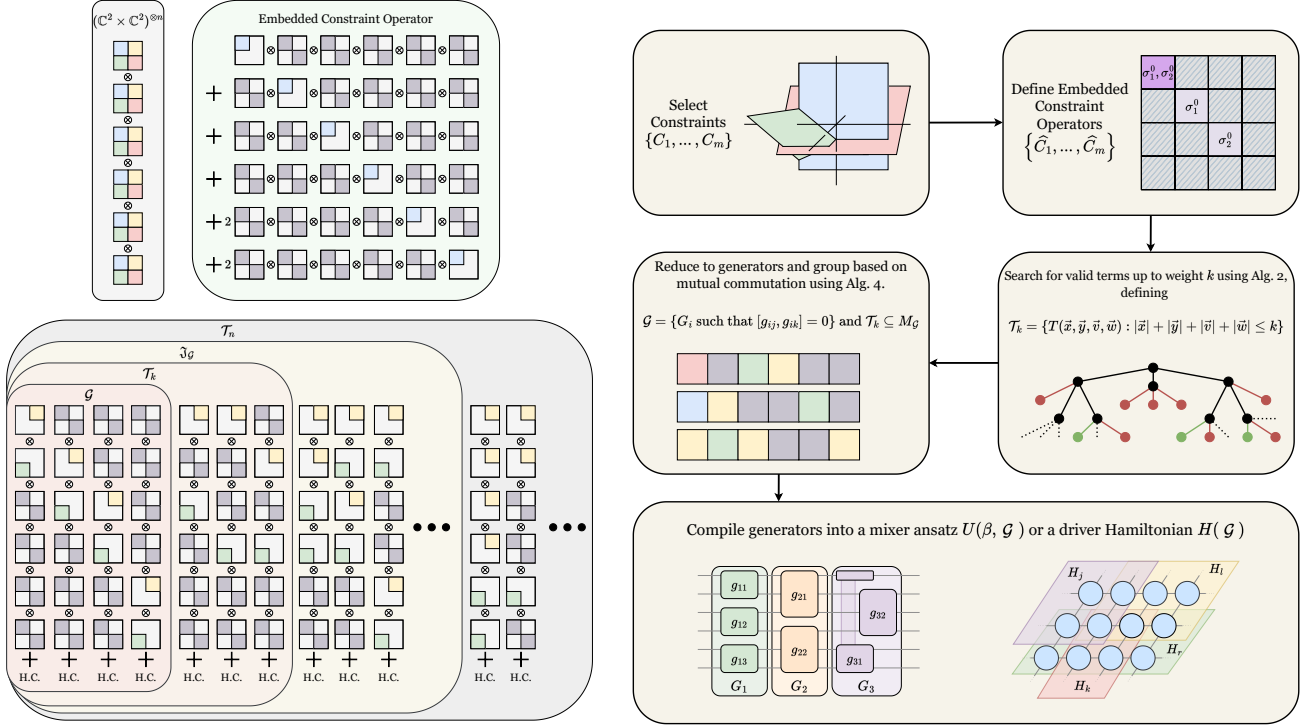
Result 3: Separability: a set of mixing generators commutes with all embedded constraint operators iff its Jordan algebra is contained in their joint commutation space. Reachability: those mixers connect the entire feasible subspace iff their Jordan algebra contains that subspace. Fig. 2a depicts a simple example.

Moreover, we can recognize the equivalence of different sets of mixers on these two axes; that is, two different collections of mixers that have the same reachability and separability.

In many cases of interest local mixers are sufficient to connect the entire feasible subspace, and so we develop efficient polynomial runtime algorithms to find such terms with a given locality bound.

Result 4: Algorithmic primitives to efficiently find local constraint preserving drivers and mixers as well as sequence them into a set of generators.

Almost all mixers and drivers that have been handcrafted for constrained optimization have such a locality bound. Not all such terms may be strictly necessary, since a smaller set of mixers may have an equivalent



(a) **Hierarchy of Constraint Preserving Operators.** An example for a set of generators $\mathcal{G}$ for an embedded constraint operator H , with $\mathcal{T}_k$ contained in its Jordan algebra $\mathfrak{J}_{\mathcal{G}}$.

(b) **Algorithmic Flowchart for Imposing Classical Symmetries.** A flowchart of how commutators for general constraints can be found and then sequenced into an ansatz.

Jordan algebra, and so we also develop primitives for finding low locality weight mixers without losing expressiveness. Fig. 2b summarizes this result, which includes reducing and sequencing such terms into a set of commuting blocks of generators.

3 Conclusion

In this work we provide an algebraic framework for reasoning about constraint preserving mixers and drivers in QAOA and CQA, respectively. Utilizing this framework, we categorize the complexity of finding such mixers (or drivers) and provide efficient algorithmic primitives for doing so when the mixers are constrained to be local. Since most handcrafted ansätze for constrained optimization have been local, they are a strict subset of the mixers that our method is able to find. We show that constraint preserving mixers form a Jordan algebra and that this can be utilized to understand the separability and reachability of a given set of mixers. We find that tailoring the ansatz for 1-in-3 SAT dramatically reduces the time-to-solution of QAOA.

Several important areas for future work stem from our results. It is possible to find sharper classifications for irreducibility and reachability results inside the polynomial hierarchy. Further developing algorithms for finding terms and sequencing the ansatz is an important practical question. Similar machinery can be utilized for ansatz construction in quantum chemistry, practical error suppression, and symmetry aware quantum machine learning.

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