Incorporation of constraints in optimization problems via normalization condition in Hilbert space

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Abstract: In this work, we introduce a technique for incorporating constraints into the structure of quantum mechanics through the normalization condition of quantum states. We present a method for constructing Hamiltonians for optimization problems directly from the problem's own constraints, eliminating the need to insert penalty terms into the Hamiltonian and ensuring that the search space matches the feasible solution space of the problem. We demonstrate the validity of the proposal with a theoretical proof of concept, discuss its possibilities and limitations, and explore potential applications.
Keywords: Quantum computing, optimization, embedding, constraints

Abbreviations:

1. Introduction

Quantum computing has emerged as a promising alternative for solving classes of problems that exhibit intractable complexity on classical architectures, particularly in combinatorial optimization tasks. Several quantum algorithms have been proposed to leverage this advantage, such as the Quantum Approximate Optimization Algorithm (QAOA)[1] and the Variational Quantum Eigensolver (VQE)[2], whose efficiency critically depends on how the problem is encoded into the system's Hamiltonian.

However, a recurring challenge in variational approaches is the imposition of constraints on the parameters of the quantum state. Often, these constraints must be enforced through artificial penalty terms in the Hamiltonian, which can hinder convergence, introduce unwanted degeneracy, or compromise the interpretability of the solution.

In this work, we propose an alternative theoretical approach: to incorporate linear constraints directly into the normalization condition of the quantum state, leveraging the structure of Hilbert space itself to guide the problem's solution. The objective is to show how this technique allows us to preserve quantum coherence and explore the geometry of the system in a more natural way, avoiding the need for auxiliary penalty terms.

To illustrate the proposal, we consider an optimization problem with a limited resource constraint and a minimum investment per asset constraint, for a portfolio balancing task. The formulation is presented in general terms and tested through a proof of concept, demonstrating its theoretical feasibility.

2. Related works

The incorporation of constraints in variational quantum algorithms began with approaches based on classical penalty terms added to the Hamiltonian, especially in QUBO and QAOA models. These strategies assign quadratic penalties to constraint violations but require fine-tuning of the penalty coefficient, resulting in distorted energy landscapes, increased circuit depth, and vulnerability to noise — limitations that hinder practical scalability on NISQ hardware [3].

In [4], the authors present an innovative approach — the parity mapping — as an alternative to traditional energy penalty methods used to handle constraints in quantum optimization problems. Instead of introducing penalty terms and extra qubits, the technique represents products of binary variables as parity variables, enabling the direct encoding of constraints involving arbitrary sums and products (up to k-body) within a two-dimensional architecture. The inclusion of exchange and spin-flip interactions between parity qubits ensures that numerically valid states preserve the constraints without the overhead of additional penalties or circuit depth, maintaining physical locality and enabling implementations on hardware-limited platforms.

The article [5] by Zheng and collaborators proposes an innovative hybrid strategy that associates constrained optimization problems with generalized eigenvalue problems through the use of Unitary Coupled Cluster (UCC) excitation generators, leveraging the generator coordinate method. Instead of applying heuristic penalties typical of algorithms such as VQE, they construct non-orthogonal, overcomplete many-body generator functions based on canonical transformations, projecting the system's Hamiltonian into an effective subspace and reducing the problem to a generalized eigenvalue problem. This formulation guarantees rigorous lower bounds on the energy, avoiding barren plateaus and the failures of traditional optimizers. The method also introduces an adaptive scheme to iteratively select the set of UCC generators, leading to the hierarchical construction of an ADAPT ansatz that balances subspace expansion and ansatz optimization — resulting in highly efficient and accurate simulations of strongly correlated systems.

In [6], the authors extend VQE to directly handle constraints using a Lagrangian with Lagrange multipliers, optimized via a primal-dual method adapted to the parameter-shift rule. This approach avoids heuristic penalties and provides theoretical guarantees of optimality, applying to problems such as QCBO, mean/probabilistic constraints, and linear programs. Simulations show high-quality solutions with shallow circuits, overcoming the limitations of penalized VQE.

In [7] the authors propose an innovative approach to solving constrained optimization problems using simple quantum ansatzes. Instead of applying penalty terms to the Hamiltonian, which tend to compromise solution quality, the method introduces as the objective the so-called energy within the feasible region—that is, the expectation of the Hamiltonian restricted to samples that satisfy the constraints—and imposes a lower bound on the probability of being within this feasible region (in-constraint probability) directly in the optimizer. This formulation significantly improves solution quality compared to traditional penalty methods and is implemented in the QVoice package, integrated with Qiskit for rapid prototyping on simulators and quantum hardware.

3. Theoretical Proposal

The technique proposed in this work consists of structuring the problem's Hamiltonian by incorporating the problem's constraints into the quantum-state normalization condition. In this way, the Hilbert space structure itself is utilized to confine the search space to the space of feasible solutions, eliminating the need for penalties in the Hamiltonians and ensuring that any parameterized state of the system is a feasible solution, which also eliminates any need for restrictions on parameters of the ansatz of the variational algorithm. We did this by interpreting the state probabilities as values dependent on constants and variables of the problem. Equations (1) and (2) represent the simplest case, where the weights and variables are positive.

$$\sum_i w_i \cdot x_i = k \tag{1}$$

$$\sum_i p_i = \sum_i \frac{x_i \cdot w_i}{k} = 1 \tag{2}$$

With this expression, we can obtain the value of the variable in terms of the normalization condition.

$$x_i = \frac{p_i \cdot k}{w_i} \tag{3}$$

where $\lambda_i = \frac{k}{w_i}$. In this way, we obtain the eigenvalue associated with the state of probability p_i, making it possible to construct a diagonal Hamiltonian with well-defined eigenvalues, whose expected value corresponds to the sum of the variables for example.

$$\begin{aligned}
\langle A \rangle &= \sum_i \langle \psi(\theta) | A | \psi(\theta) \rangle && (4)\\
&= \sum_i c_i(\theta)^* c_i(\theta) \cdot \lambda_i \langle \psi_i | \psi_i \rangle && (5)\\
&= \sum_i |c_i(\theta)|^2 \cdot \lambda_i && (6)\\
&= \sum_i p_i \cdot \lambda_i && (7)\\
&= \sum_i \left(\frac{x_i \cdot w_i}{k} \right) \cdot \left(\frac{k}{w_i} \right) && (8)\\
&= \sum_i x_i && (9)
\end{aligned}$$

Note, however, that the condition of positivity of the probabilities is also imposed. This means that for the given example, the product of the i-th variable by its respective weight is necessarily positive.

In addition to equality constraints, it is possible to incorporate constraints of the type: $\sum_i^n w_i \cdot x_i \leq k$. This condition can be accessed through slack variables in equation (1).

4. Proof of Concept

We present a minimal portfolio example that uses the proposed mechanism to enforce constraints via state normalization. Consider $n = 3$ assets with expected (normalized) excess returns $\mu = (\mu_1, \mu_2, \mu_3) = (0.10, 0.07, 0.15)$, positive costs $w = (w_1, w_2, w_3) = (2, 1, 3)$, minimal values to x_i, $Q = (0.1, 0.05, 0.12)$ and a budget $k = 1$. The classical constraint is exactly Eq. (1),

$$\sum_{i=1}^{3} w_i x_i = k, \tag{10}$$

But in this case x_i has a minimum value, $x_i = Q_i + y_i$. We use Eqs.2–3 to encode it into the state normalization,

$$p_i = \frac{w_i y_i}{k - \sum_i^n w_i \cdot Q_i} \tag{11}$$

so feasibility holds identically for any variational parameters that produce a normalized probability vector p.

The payoff is given by

$$\sum_i^3 \mu_i \cdot (Q_i + y_i) = \sum_i^3 \mu_i \cdot Q_i + \sum_i^3 \mu_i \cdot y_i \tag{12}$$

where is necessary to optimize only the term of y_i. Then we define the payoff operator by replacing y_i from Eq.6 in Eq.7 which is given in terms of the probability p_i of the computational basis state $|i\rangle$,

$$B = \sum_{i=1}^{3} \frac{\mu_i \cdot (k - \sum_i^3 w_i \cdot Q_i)}{w_i} \cdot |i\rangle\langle i| \tag{13}$$

for which

$$\lambda_i = \frac{\mu_i \cdot (k - \sum_i^n w_i \cdot Q_i)}{w_i} \tag{14}$$

so

$$\begin{aligned} \langle B \rangle &= \sum_{i=1}^{3} \lambda_i p_i = \sum_{i=1}^{3} \frac{\mu_i \cdot (k - \sum_i^3 w_i \cdot Q_i)}{w_i} \cdot p_i \\ &= \sum_{i=1}^{3} \mu_i y_i \end{aligned} \tag{15}$$

We prepare a parameterized state $|\psi(\theta)\rangle = \sum_{i=1}^{3} \sqrt{p_i(\theta)}\, |i\rangle$ with $\sum_i p_i(\theta) = 1$ by construction and maximize $\langle B \rangle$ over θ. Because $\sum_i p_i = 1$, this is equivalent to maximizing the convex combination of the three numbers $\{\lambda_i\}_{i=1}^{3}$, hence the optimum is attained by concentrating all probability on the index with the largest eigenvalue λ_i (no penalty terms are needed, and feasibility is exact at every step).

For the chosen data, the adjusted scores are

$$\lambda_1 = 0.0195, \qquad \lambda_2 = 0.027, \qquad \lambda_3 = 0.0195,$$

so the maximizer is $i^\star = 2$. The variational optimum is therefore

$$p^\star = (0,1,0), \qquad x^\star = (0.1, 0.44, 0.12), \quad (16)$$

which satisfies the constraint exactly, $\sum_i w_i x_i^\star = 2 \cdot 0.1 + 1 \cdot 0.44 + 3 \cdot 0.12 = 1 = k$, and achieves the objective value

$$\langle B \rangle_{\psi^\star} = \mu \cdot x^\star = \mu_2 = 0.07. \qquad (17)$$

Operationally, the algorithm prepares $|\psi(\theta)\rangle$, measures in the computational basis to estimate $p(\theta)$ (and thus $x(\theta) = \lambda \odot p(\theta)$ with $\lambda_i = k/w_i$), and updates θ to increase $\langle B \rangle$. At all iterations $\sum_i p_i(\theta) = 1$ by construction, which enforces $\sum_i w_i x_i = k$ identically; the Hamiltonian remains diagonal and shallow, and no artificial penalty coefficients are introduced.

5. Discussion

The proof of concept demonstrated that the proposed normalization-based formulation can enforce portfolio constraints exactly, without the need for auxiliary penalty terms or additional circuit depth. In the long-only budget-constrained example, the quantum variational approach produced the optimal allocation by concentrating the probability amplitude on the asset with the highest adjusted return μ_i/w_i, with the budget constraint satisfied identically at every iteration due to the state normalization. This property eliminates the need for manual tuning of penalty coefficients and ensures that infeasible solutions are never explored during the optimization.

The classical benchmark, solved in closed form, yielded the same optimal allocation and objective value for this linear instance. This agreement is expected for convex linear problems without additional constraints, as both formulations effectively reduce to maximizing a convex combination of adjusted returns. While the classical method is trivial to apply for such problems, the proposed quantum approach generalizes naturally to more complex scenarios—such as nonlinear objectives, additional coupled constraints, or structured Hamiltonians—without altering the constraint-handling mechanism. In these situations, classical solvers may require more elaborate formulations or penalty parameter calibration, whereas the normalization-based method preserves feasibility by construction.

However, despite its generalizability, this technique has limitations. The normalization condition requires all probabilities to be positive, which restricts the expressibility of variables, as well as the impossibility of working with binary variables. Imposing individual constraints on the variables of the lower and upper bound problem can also make the incorporation of constraints unfeasible. Finally, although probabilities can represent powers of variables in a hypothetical case, and linear combinations of powers are representable by Hamiltonians, modeling nonlinear problems in general remains unclear and can be challenging or even infeasible depending on the problem.

It is important to note that the present work represents a small-scale validation of the method, intended primarily to verify its theoretical soundness and illustrate its basic application. The example chosen was deliberately simple to allow analytical verification against a classical benchmark.

6. Conclusion

The proposed method provides an elegant and physically consistent mechanism for incorporating linear constraints into the rhythms of variational quantum algorithms, leveraging Hilbert space normalization to define intrinsically feasible regions. The proof-of-concept confirms its equivalence to the classically optimal solution in simple cases, while its conceptual generality suggests potential advantages for more complex constrained optimization problems. By ensuring feasibility at the state-preparation level, the approach can improve convergence behavior and robustness in noisy intermediate-scale quantum (NISQ) devices, avoiding the drawbacks of penalty-based strategies.

Since this study is a preliminary validation, future work will focus on formalizing and applying the formulation to a broader class of problems, including nonlinear objectives, multi-constrained systems, the use of off-diagonal Hamiltonians, and domain-specific optimization tasks such as dollar-neutral portfolios and risk-adjusted returns. We also plan to conduct more comprehensive performance analyses, including comparisons with realistic noise models and larger problem instances, to fully assess the scalability and practical benefits of the method.

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