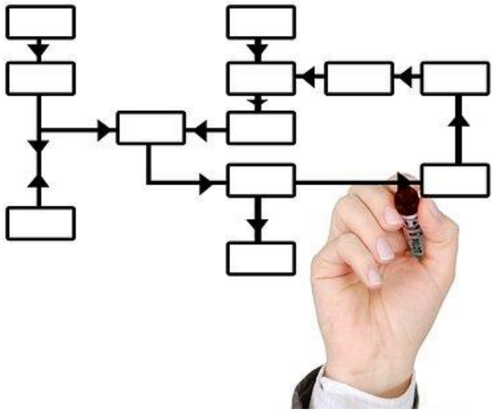
Multiobjective variational quantum optimization for constrained problems

arXiv:2302.04196

ICE-8 QUANTUM INFORMATION IN SPAIN (30/05/2023)

PABLO DÍEZ VALLE (IFF-CSIC)

Outline



I. Motivation.

II. Background.

   I. *Variational Quantum Algorithms.*

   II. *Constrained Combinatorial Optimization.*

   III. *How do we integrate the constraints?*

III. Our proposal: ***MultiObjective Variational Constrained Optimizer (MOVCO).***

IV. Numerical results.

V. Conclusions and outlook.

Motivation

- **Quantum computing** holds the promise of a major impact on science and industry due to its capacity to solve complex problems, such as **Machine Learning** or **Combinatorial Optimization problems** (CO).

- One of the leading quantum paradigms to find approximate solutions to these problems in the near term are the **Variational Quantum Algorithms** (VQA).

- Combinatorial optimization problems are ubiquitous.

Therefore, even if they are potentially only approximations of the global optimum, better CO solutions have **a significant practical value**.

Motivation

- **Real-world combinatorial optimization problems** usually involve not only the minimization of a cost function, but also **a number of equality and inequalities hard constraints** that must be satisfied by the feasible solutions.

- Despite their critical relevance in practical scenarios, few studies have been conducted to explore new possibilities for general constraint encoding in VQAs.

- **In this work, we propose the multiobjective variational constrained optimizer (MOVCO), a method for improving the convergence of variational quantum algorithms to optimal solutions satisfying a set of restrictions.**

Variational Quantum Algorithms (VQA)

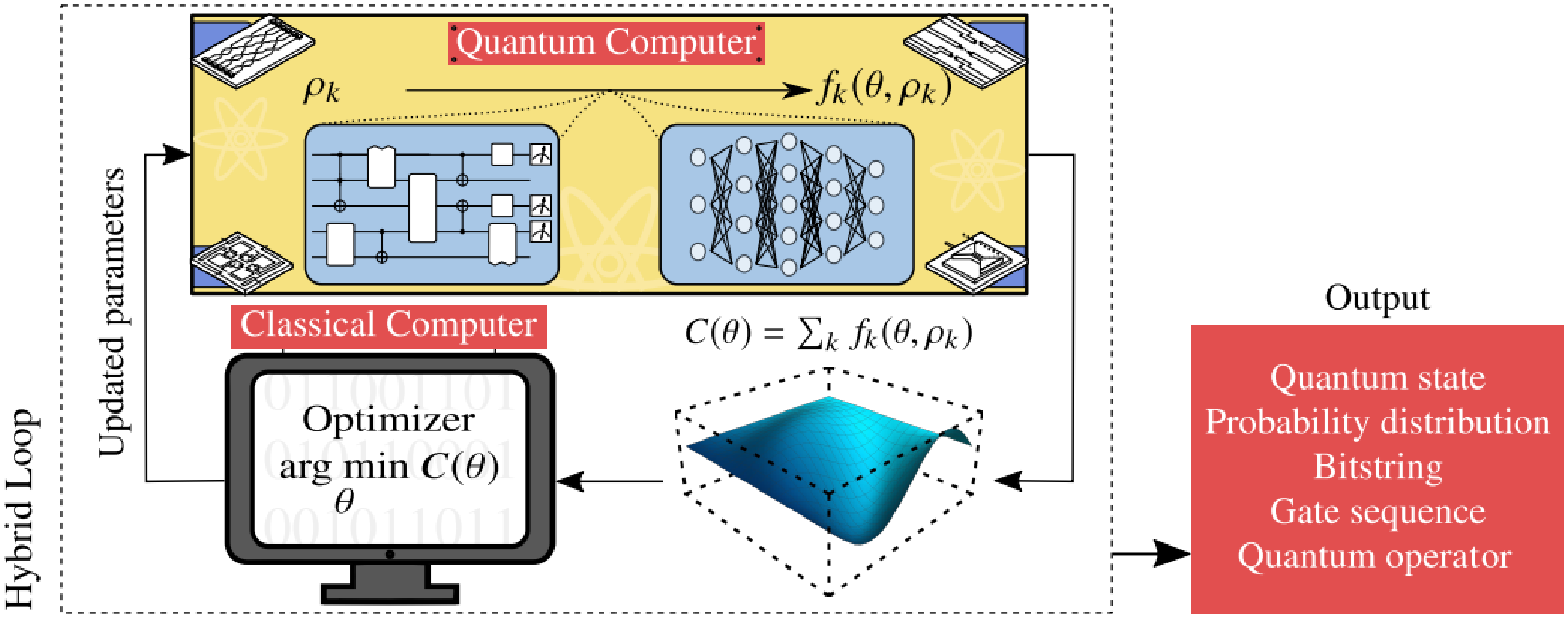


*Image from "Cerezo, M., Arrasmith, A., Babbush, R. et al. Variational quantum algorithms. Nat Rev Phys **3,** 625–644 (2021)"*

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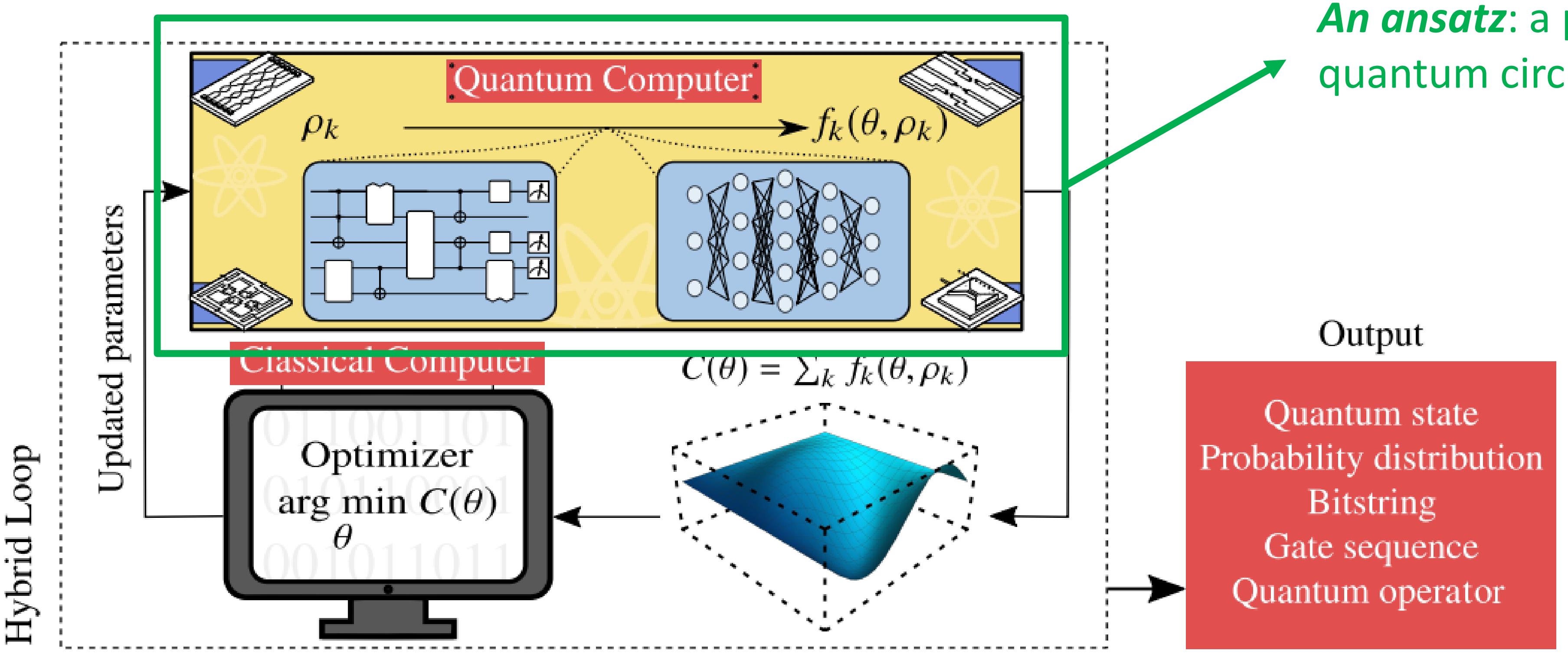

An ansatz: a parameterized quantum circuit.

$$|\Psi(\vec{\theta})\rangle = U(\vec{\theta})\,|0\rangle$$

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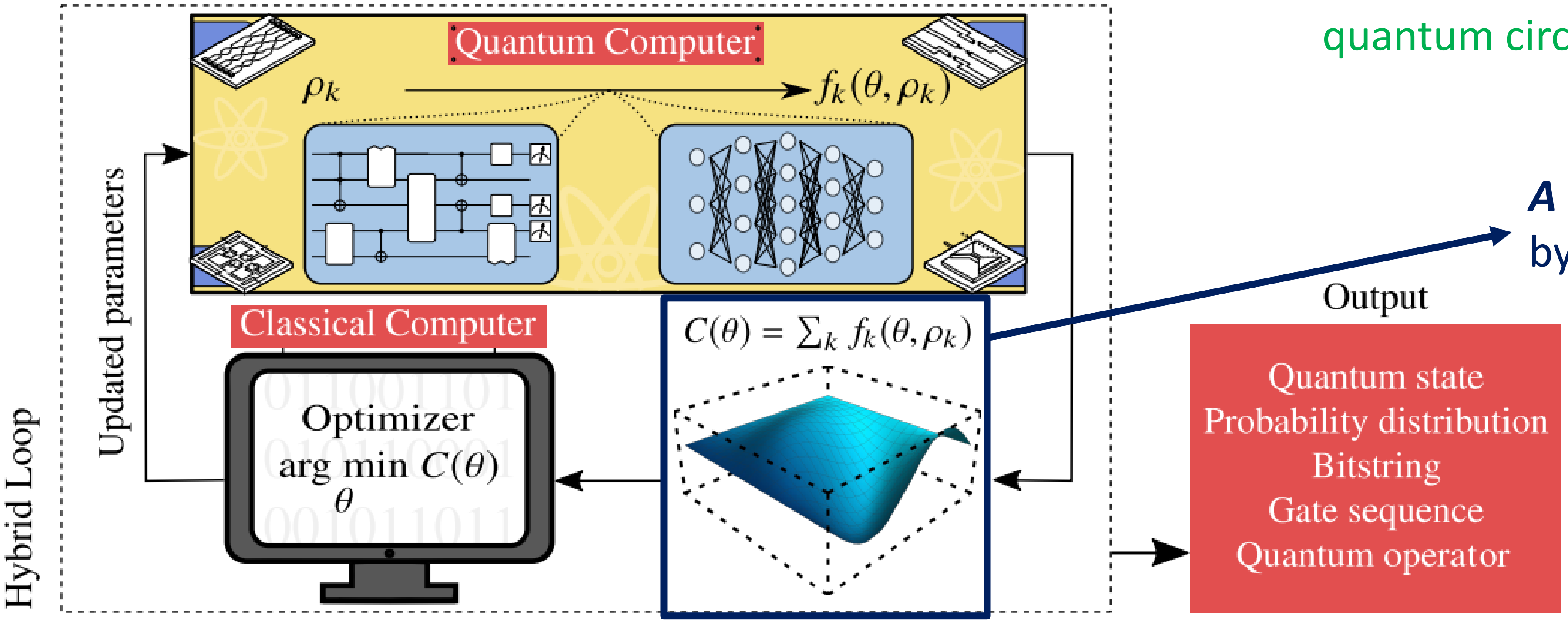

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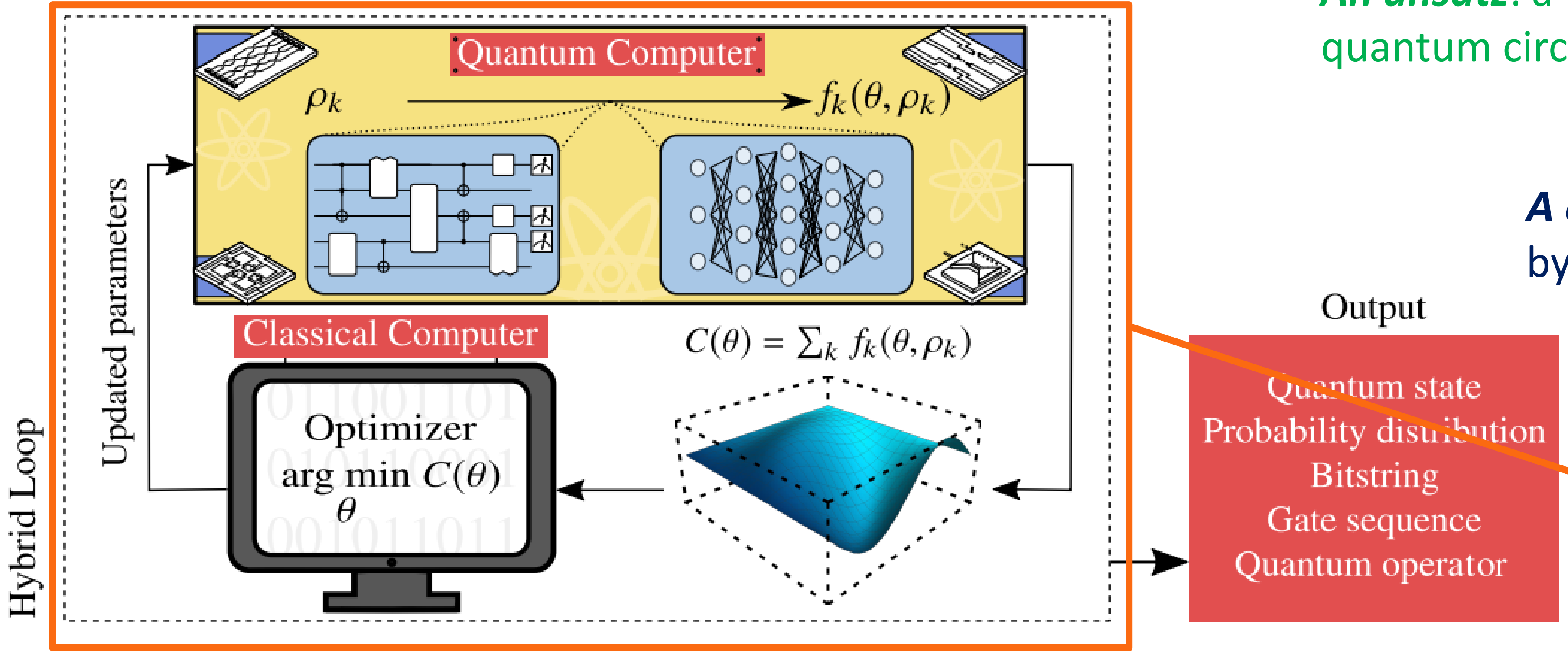

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A cost function: defined by our problem.

A training method: including classical optimization of parameters.

Image from "Cerezo, M., Arrasmith, A., Babbush, R. et al. Variational quantum algorithms. Nat Rev Phys ***3****, 625–644 (2021)"*

Variational Quantum Eigensolver (VQE)

Peruzzo, A. et al. Nature Communications, 5:4213 (2014)

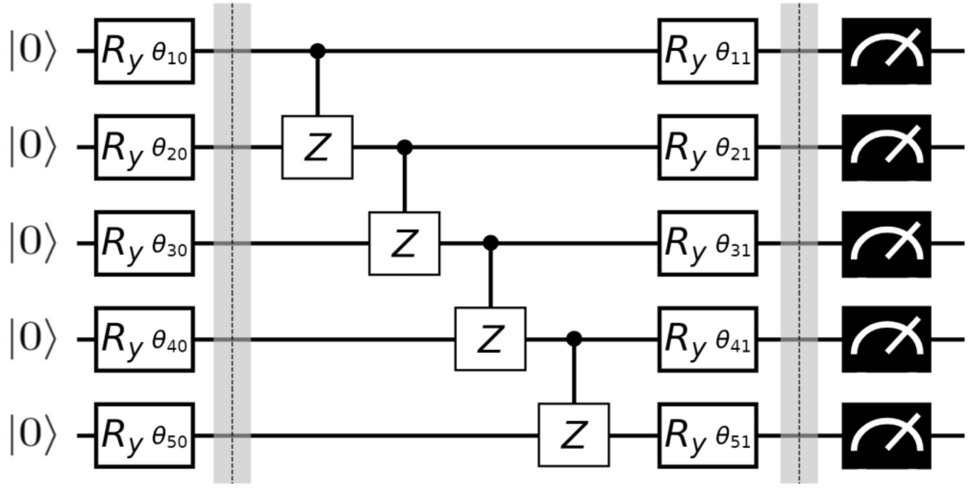
- Originally proposed as a variational algorithm for finding the ground state energy of a chemical molecule.

ansatz

variational parameters

$$|\Psi(\vec{\theta})\rangle = U(\vec{\theta})\,|0\rangle$$

Hardware-efficient ansatz



- The parameters of an ansatz are trained by the minimization of the expectation value of the Hamiltonian.

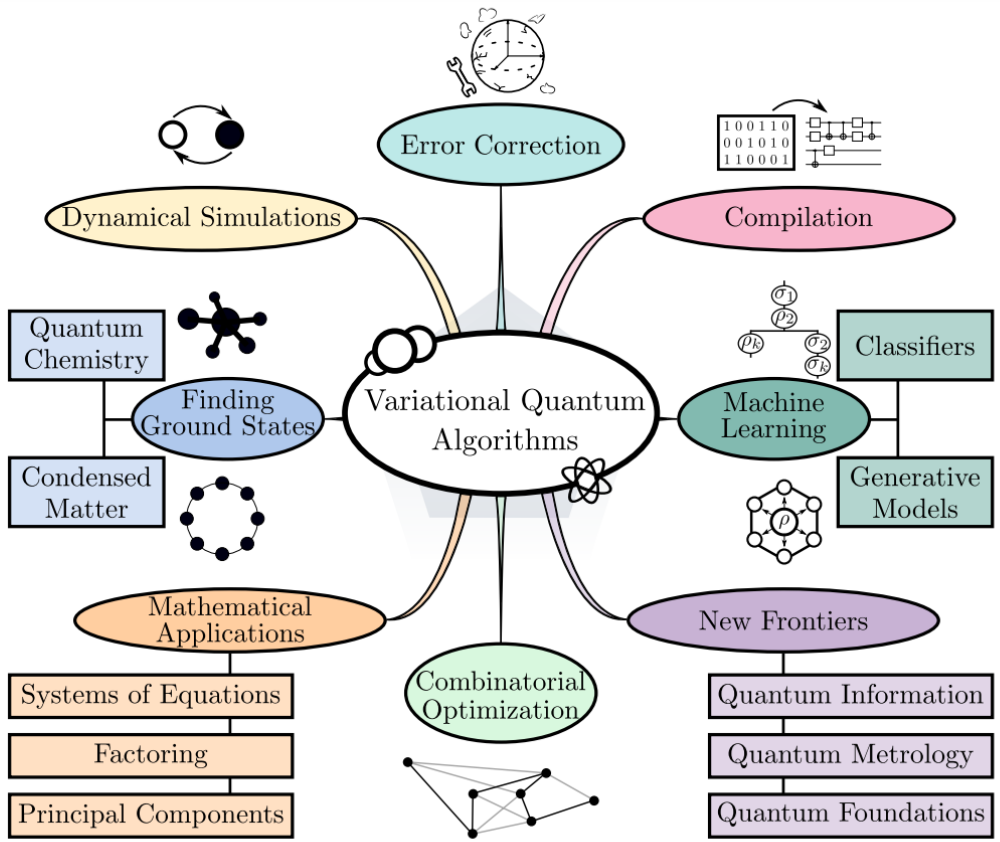
$$\langle\Psi(\vec{\theta})|\,\hat{H}\,|\Psi(\vec{\theta})\rangle$$

Encodes our problem

- With the optimal parameters, the state matches or approximates the global minimum of the problem.

Variational Quantum Algorithms (VQA)

- Many applications envisioned for VQAs: Quantum Chemistry, Dynamical Simulations, Numerical Analysis, Machine Learning, Optimization etc…



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- Strengths:
  - Suitability for NISQ devices: limited number of qubits, limited qubit connectivity, limited quantum circuit depth.
  - High versatility.
  - Quantum analog of highly succesful classical machine-learning methods, such as neural networks.

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  - Existence of many local minima.
  - Barren plateau phenomenon: induced by deep random circuits, global cost functions, too expresibility and entanglement.
  - Effect of hardware noise.
  - Trainability in realistic problems which involve hard constraints.

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Talk "Variational waveguide QED simulators"
Wednesday 31, 11:40-12:00
Cristian Tabares

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  - **Trainability in realistic problems which involve hard constraints.**

Constrained combinatorial optimization

Definition of the problem

$$\min C(z) \;\; \text{with} \;\; z \in \{-1,+1\}^N \,,$$

such that the solution z must fulfill a number of inequality and equality constraints:

$$b_i(z) = 0 \;,\;\; g_j(z) \leq 0$$

→ Find an optimal solution among a finite set of elements.

→ Hard constraints that must be satisfied by the feasible solutions

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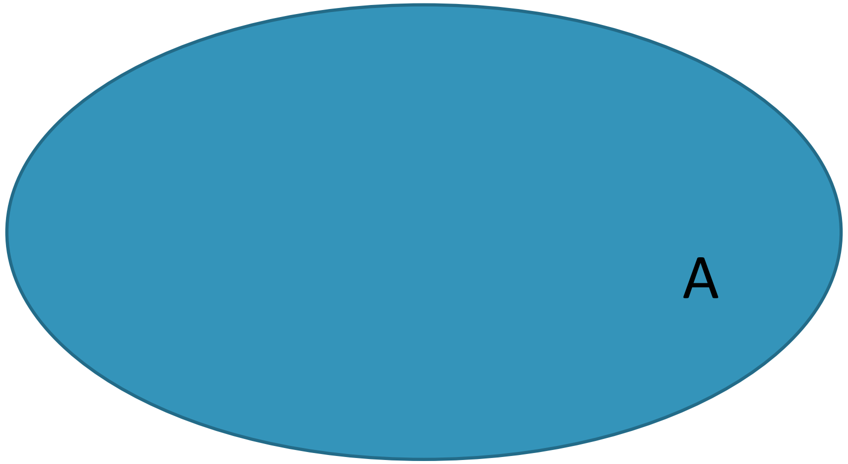

A : total space of possible solutions. (2^N states)

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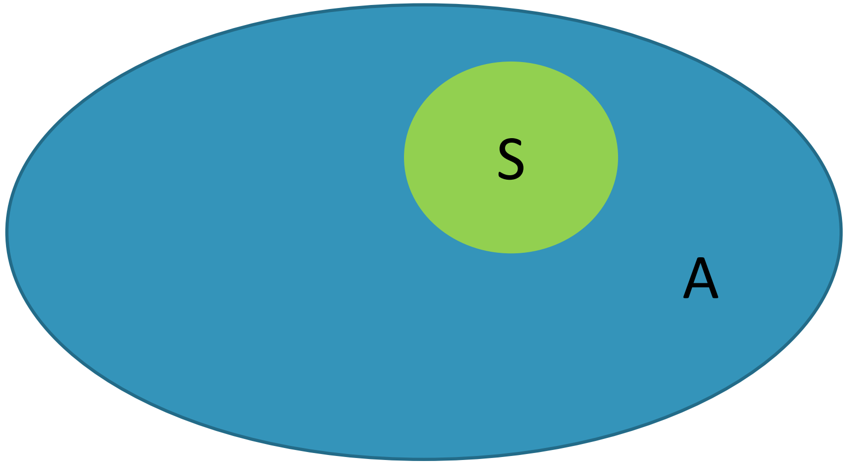

A : total space of possible solutions. (2^N states)

S : subspace of solutions that satisfy all constraints.

feasible subspace

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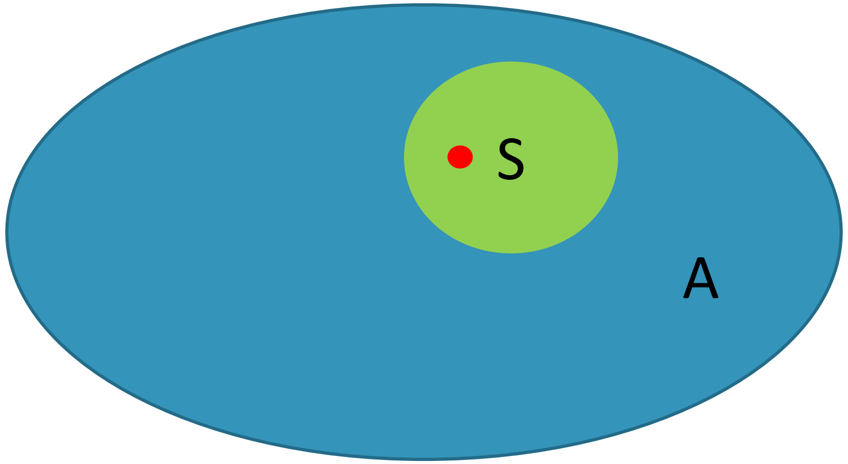

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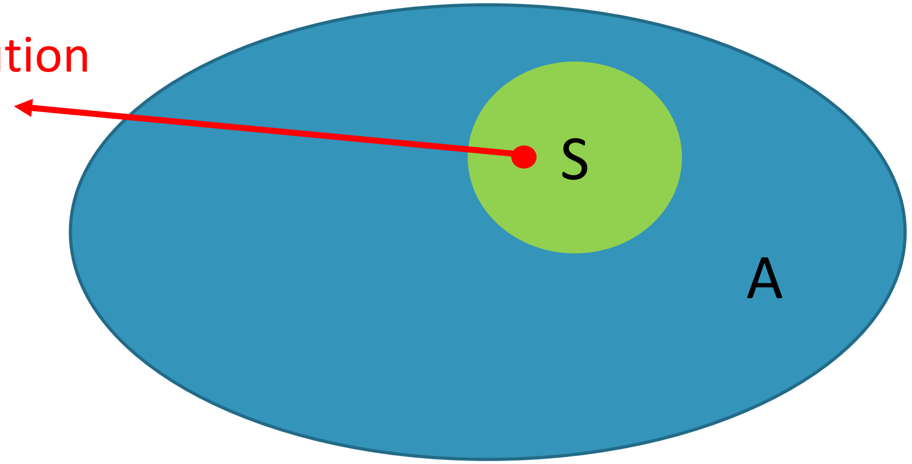
Hard constraints that must be satisfied by the feasible solutions

Best global solution or solutions



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Constrained combinatorial optimization

Regarding variational algorithms

Binary variable — Pauli Z operator — Hamiltonian

$$z_i \rightarrow \hat{Z}_i \qquad C(z) \rightarrow \hat{C}(\hat{Z})$$

$$b_i(z) \rightarrow \hat{B}_i(\hat{Z})$$

$$g_j(z) \rightarrow \hat{G}_j(\hat{Z})$$

Measuring K times the quantum processor, the sample mean is the estimator that we actually minimize:

$$\langle \Psi(\vec{\theta}) | \hat{C}(\hat{Z}) | \Psi(\vec{\theta}) \rangle \approx \min_{\vec{\theta}} \left[\frac{1}{K} \sum_{k=1}^{K} \hat{C}_k(\vec{\theta}) \right]$$

$$|\Psi_k\rangle = \{-1, +1\}^N$$

$$C_k = \langle \Psi_k | \hat{C} | \Psi_k \rangle$$

Constrained variational quantum optimization aims to **approximate a wavefunction able to sample classical states with low cost C_k such that**

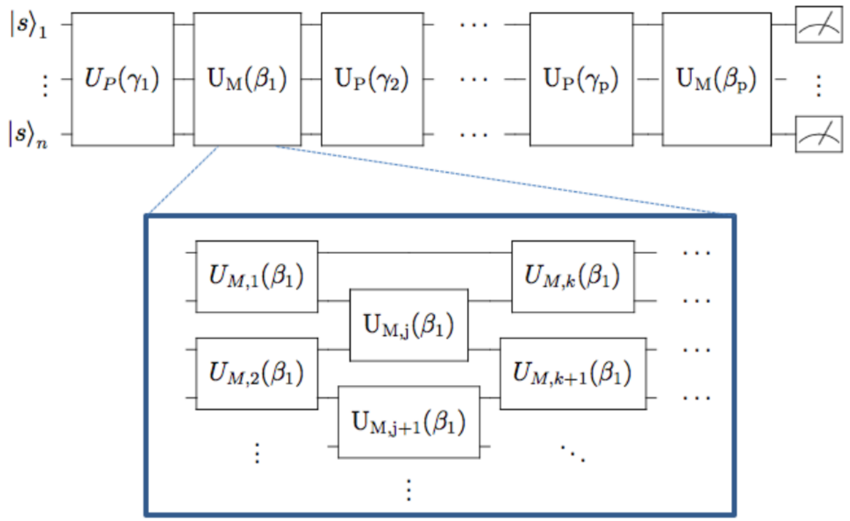
$$\langle \Psi_k | \hat{B}_i(\hat{Z}) | \Psi_k \rangle = 0 \qquad \langle \Psi_k | \hat{G}_j(\hat{Z}) | \Psi_k \rangle \leq 0$$

How do we integrate the constraints?

- Strategy 1: Quantum circuits capable of natively preserve the constraints.

Quantum Alternating Operator Ansatz

Hadfield, S. et al. Algorithms, 12(2):34 (2019)



Constrained quantum optimization for extractive summarization on a trapped-ion quantum computer

Pradeep Niroula, Ruslan Shaydulin, Romina Yalovetzky, Pierre Minssen, Dylan Herman, Shaohan Hu & Marco Pistoia

Scientific Reports **12**, Article number: 17171 (2022) | Cite this article

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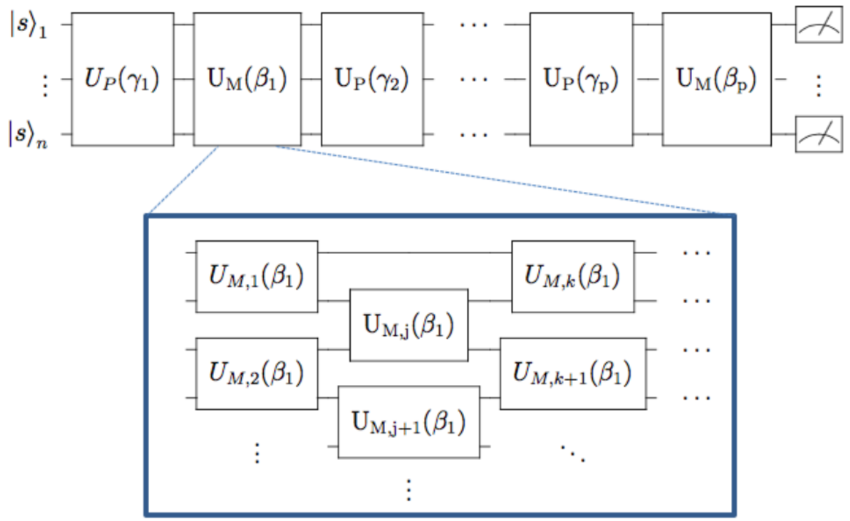

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- Strategy 2: Transform the original cost function by penalty terms and/or extra *slack* variables.

  Lucas, A. Frontiers in physics, 2, 5 (2014)

$$C_{pen} = C + \sum_i \lambda_i b_i^2 + \sum_j \lambda'_j f(g_j)$$

Penalty hyperparameters

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  Penalty hyperparameters

  Not guarantee the convergence of the algorithm to a feasible solution.
  Huge overhead produced by the need of optimally tuning the penalty terms, so as to impose the constraints without disturbing the optimization process.

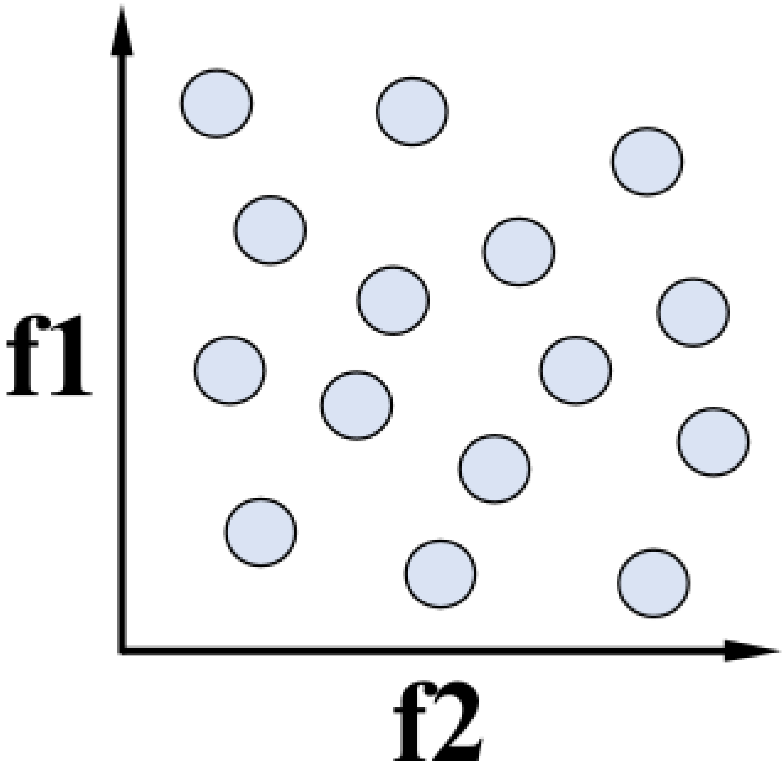
MOVCO

MULTIOBJECTIVE VARIATIONAL CONSTRAINED OPTIMIZER

Multiobjective Genetic Algorithm

- The Non-dominated Sorting Genetic Algorithm (**NGSA-II**) is an evolutionary algorithm (meta-heuristic optimization techniques) to perform multiobjective optimization.

K. Deb et al., IEEE Trans. Evol. Comput, 6, 2,182-197 (2002)



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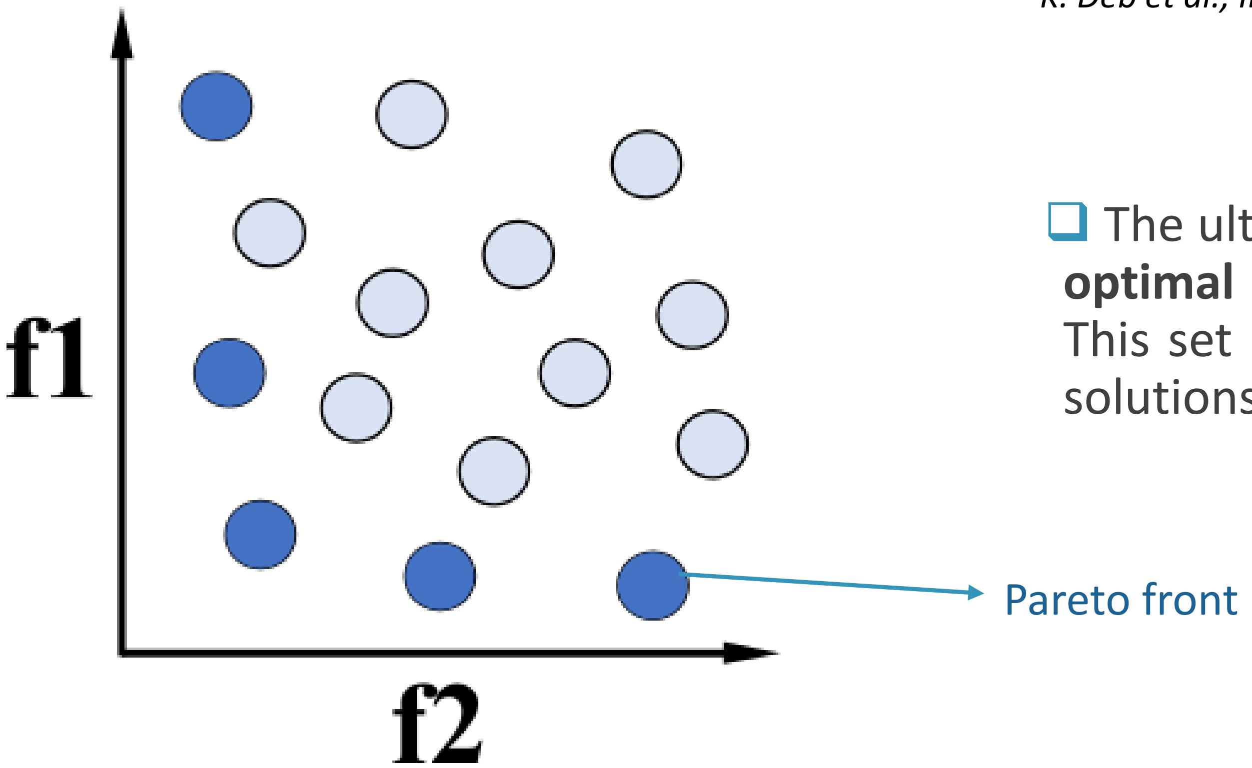

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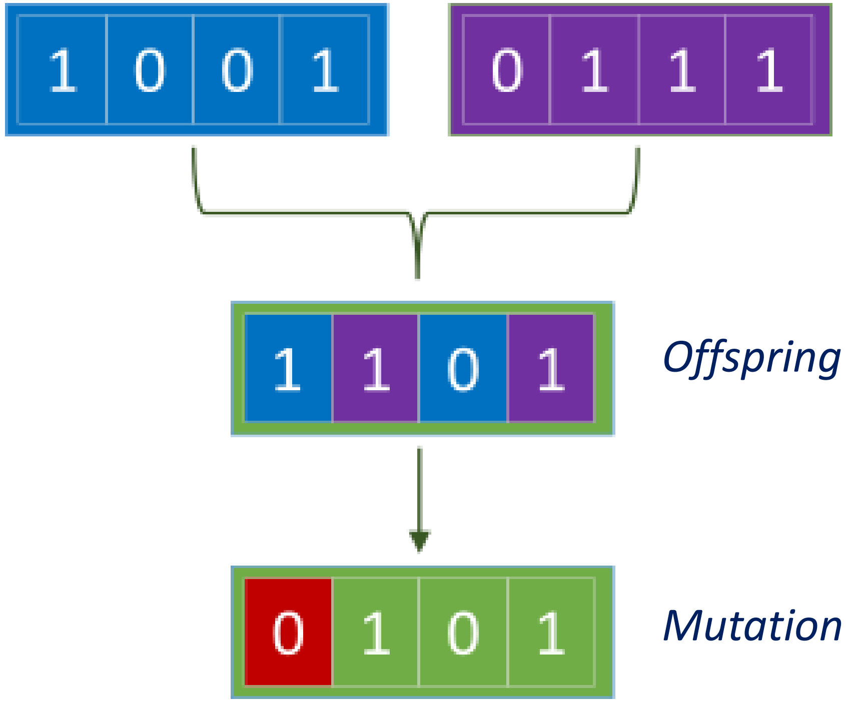
Multiobjective Genetic Algorithm

- The Non-dominated Sorting Genetic Algorithm (**NGSA-II**). *K. Deb et al., IEEE Trans. Evol. Comput, 6, 2,182-197 (2002)*

- The optimization process is carried out by iteratively **evolving a population** (a set of solutions) to obtain better individuals (better solutions) **using the concept of survival of the fittest** and biological-inspired operators.



Tournament selection

MultiObjective Variational Constrained Optimizer (MOVCO)

- The parameters of a variational wavefunction are iteratively updated through the **simultaneous optimization of two fitness functions**, using the genetic algorithm NGSA-II.

Fitness function to **maximize the constraints satisfaction**.

$$P(\vec{\theta}) = \frac{1}{K}\sum_{k=1}^{K} P_k(\vec{\theta})$$

Percentage of constraints satisfied

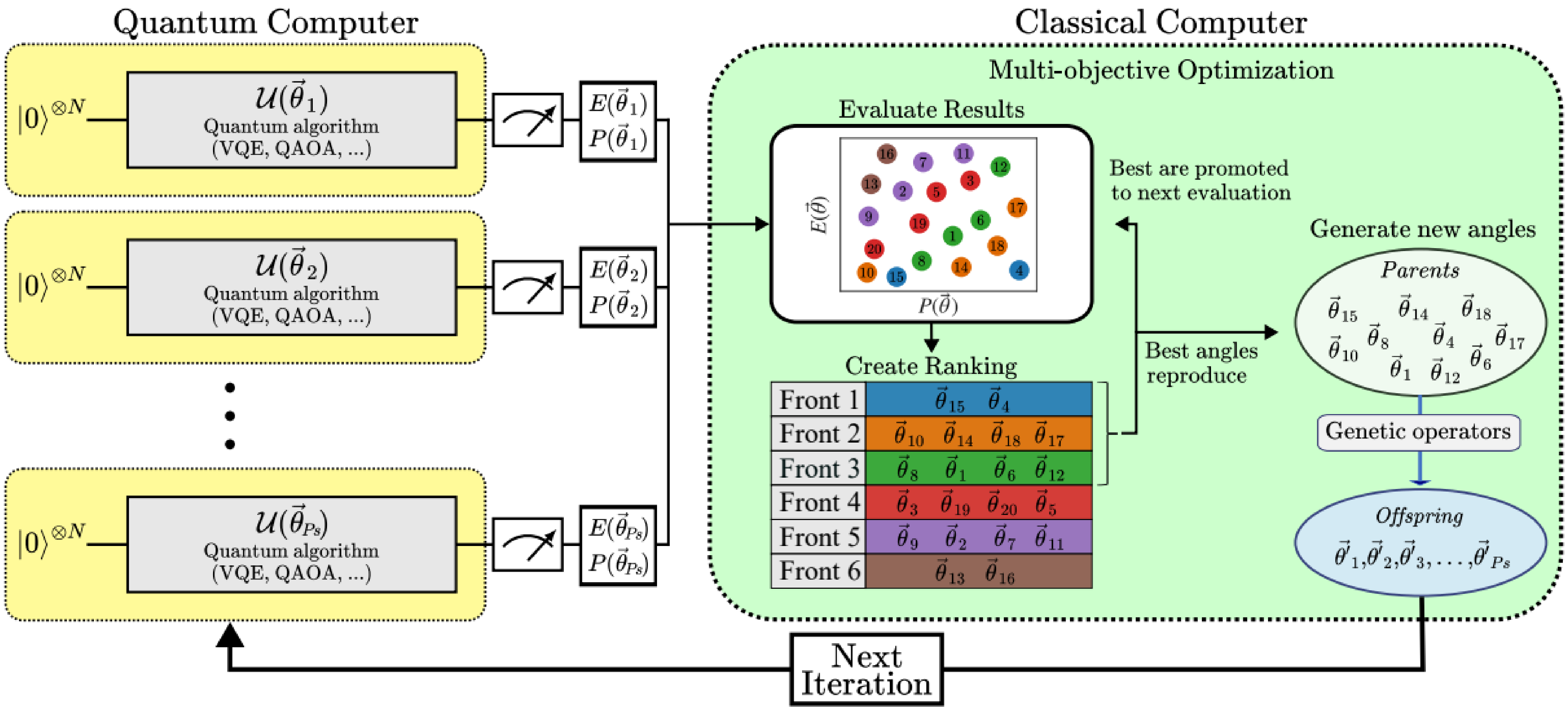
Fitness function to **minimize the energy of feasible solutions**

$$E(\vec{\theta}) = \sum_{k\in\mathcal{S}} \left(C_k(\vec{\theta}) - \max\left[C\right]\right)/K$$

Feasible subspace

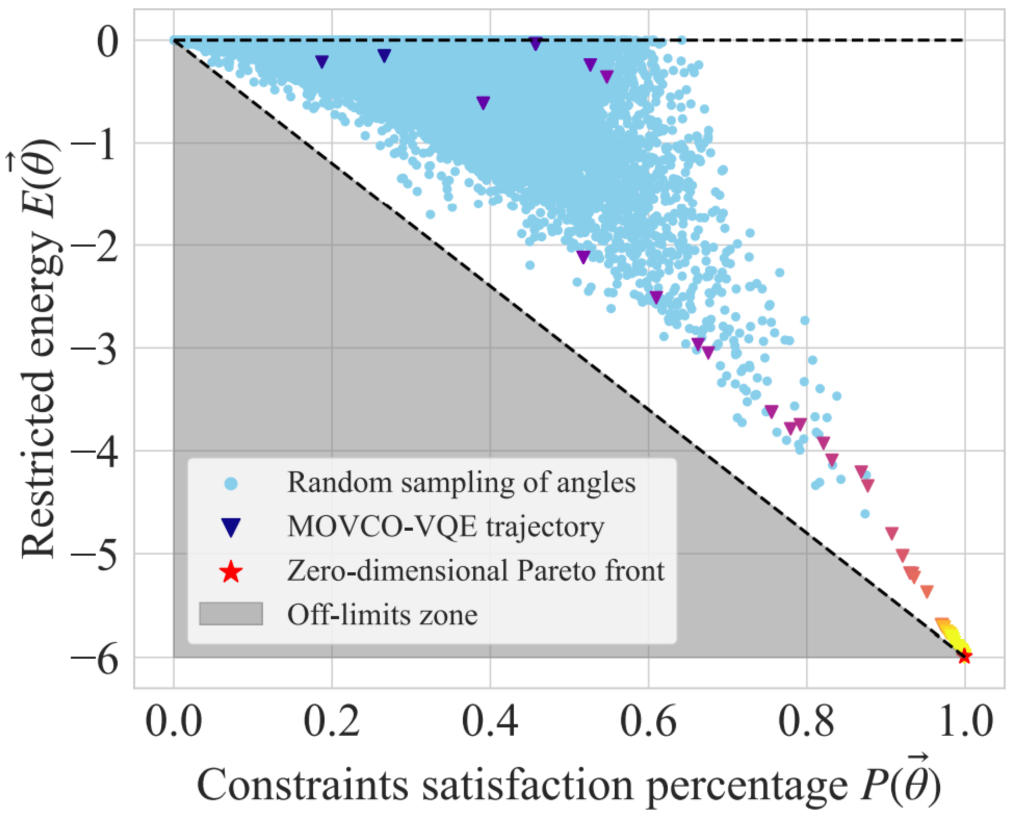
These functions are commuting observables, so that they can be simultaneously measured in the quantum processor.

MultiObjective Variational Constrained Optimizer (MOVCO)



MultiObjective Variational Constrained Optimizer (MOVCO)

Optimization in the space of fitness functions



$$P(\vec{\theta}) = \frac{1}{K}\sum_{k=1}^{K} P_k(\vec{\theta})$$

$$E(\vec{\theta}) = \sum_{k\in\mathcal{S}} \left(C_k(\vec{\theta}) - \max[C]\right)/K$$

$$0 \geq E(\vec{\theta}) \geq \sum_{k\in\mathcal{S}} \frac{1}{K}(\min[C] - \max[C])$$

$$1 \geq P(\vec{\theta}) \geq \sum_{k\in\mathcal{S}} \frac{1}{K}$$

- The Pareto front is zero-dimensional in the space of the functions.

$$(P, E)_{PF} \;=\; (1, \min E) \quad \textit{Pareto front}$$

$$\min\left[E(\vec{\theta})\right] = \min[C] - \max[C]$$

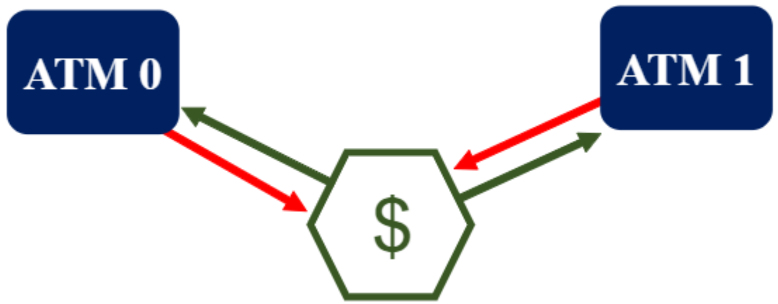
Numerical results

Application to a real-world problem
Cash Management

- The Cash Management problem consists in finding the **optimal scheduling of cash delivery to a network of branches and ATMs** in a given geography in a way that the cost of the transactions performed is minimized, while satisfying some requirements.

- It is a **scheduling problem** similar to the Nurse Scheduling Problem, where a series of tasks have to be scheduled over a time interval so that they meet certain constraints.

(a)

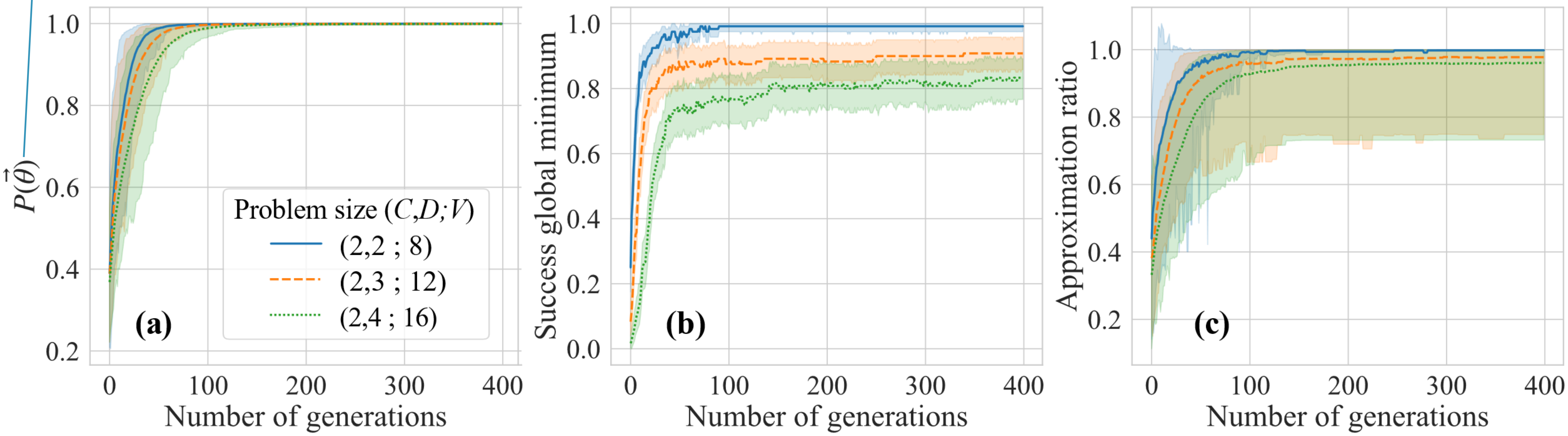


(b)

		DAY 1	DAY 2	DAY 3	DAY 4
ATM 0	Send/Withdraw				-1k
	Initial prediction	8k	8k	9k	7k
	Final cash	8k	8k	9k	6k
ATM 1	Send/Withdraw	+3k	-6k		
	Initial prediction	4k	10k	9k	10k
	Final cash	7k	7k	6k	7k

Average of the the percentage of constraints satisfied by each sampled solution

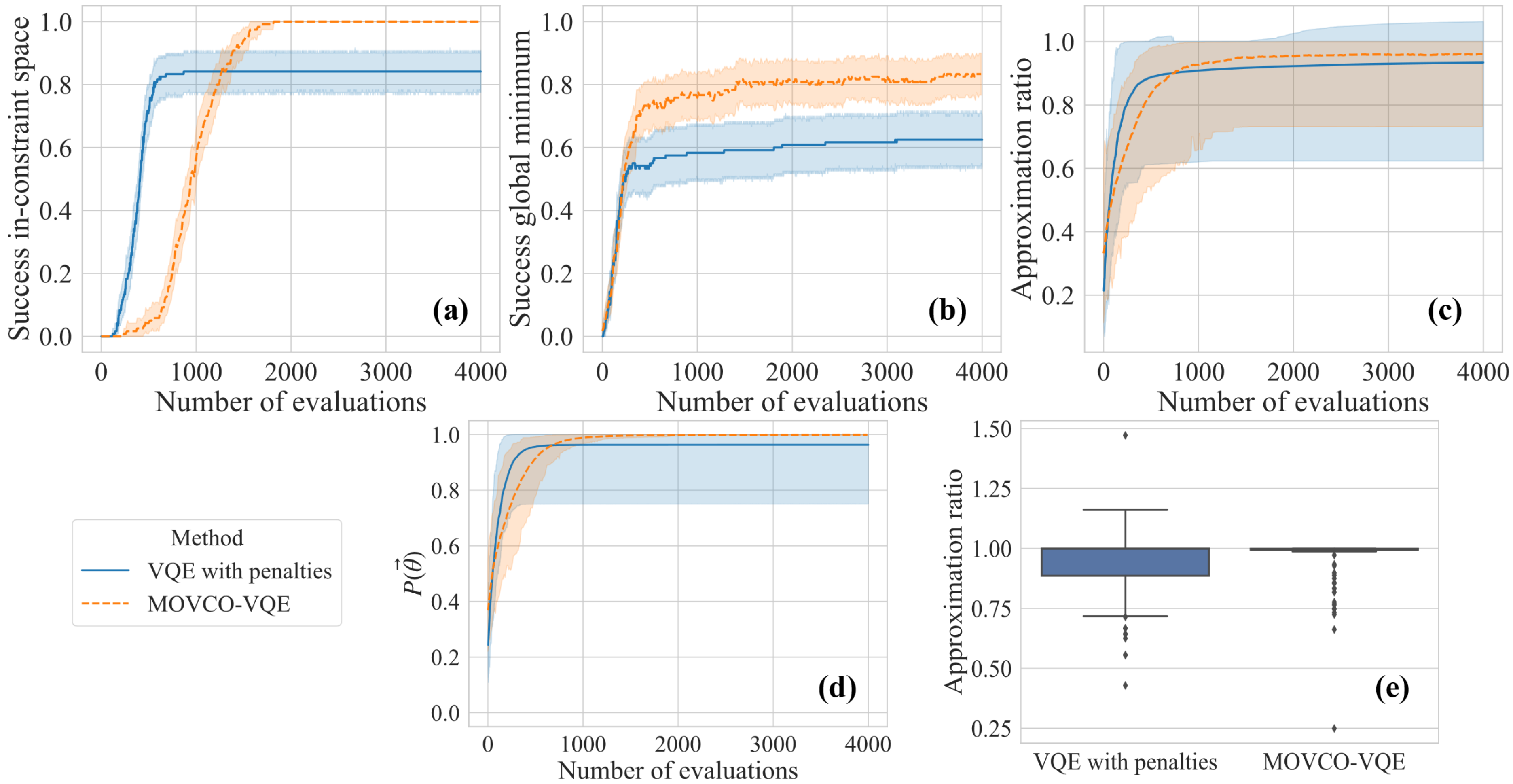
$$\epsilon(\vec{\theta}) = \frac{C_{max} - \langle \Psi(\vec{\theta})|\, \hat{C}\, |\Psi(\vec{\theta})\rangle}{C_{max} - C_{min}}$$ *Approximation ratio*



Performance of MOVCO

We observe how the method prevents the variational wave function from being trapped in local minima outside the feasible space. Besides in the percentage of constraints satisfied, we get a good performance in the probability of sampling the global minimum, as well as in the cost of the solutions obtained.

arXiv:2302.04196



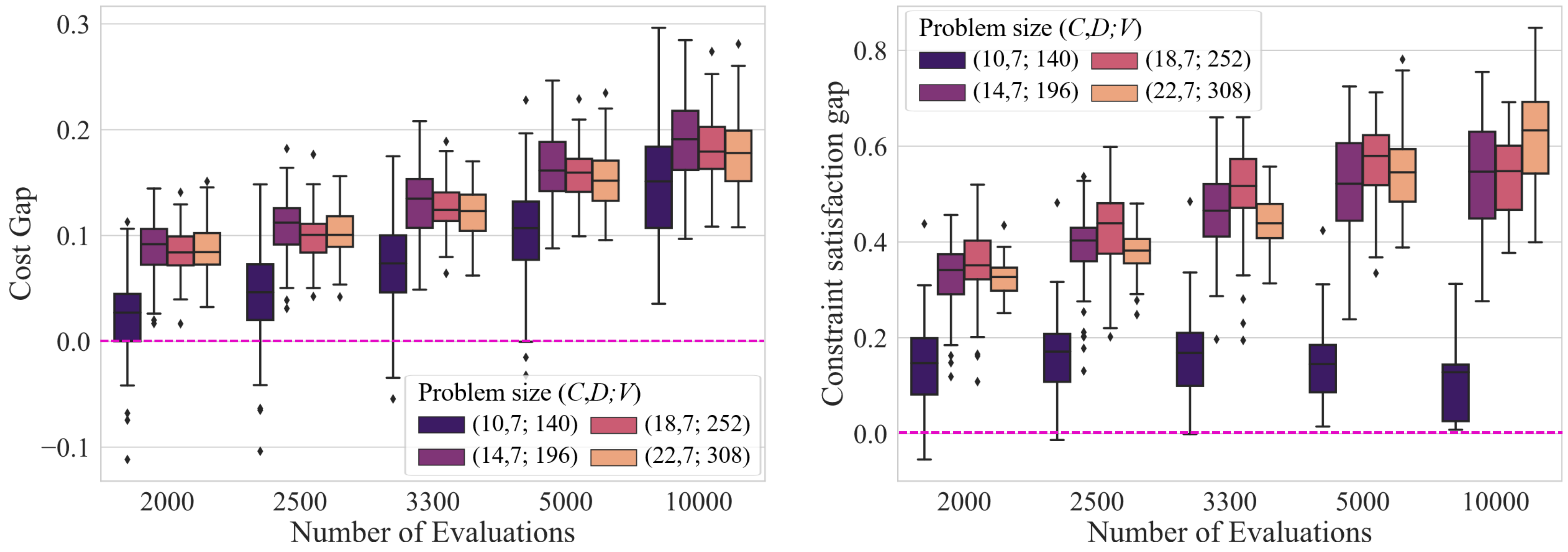
Comparison with the penalties approach

MOVCO overcomes the algorithm with penalties in every considered metric.

arXiv:2302.04196

$$C_{gap} = \frac{C_{VQEpen} - C_{MOVCO}}{C_{VQEpen}}$$

$$P_{gap} = P(\vec{\theta}_{MOVCO}) - P(\vec{\theta}_{VQEpen})$$



Benchmarking for larger systems by product states

The improvement is noticeable in both constraint satisfaction and transaction cost of the sampled solutions and becomes more pronounced as we increase the iterations of the algorithms.

$$|\Psi_{sp}(\vec{\theta})\rangle = \prod_{n}^{N} e^{i\theta_n \hat{Y}_n} |0\rangle = \bigotimes_{n=1}^{N} |\psi(\theta_n)\rangle$$

with $|\psi(\theta_n)\rangle = \cos\theta_n |0\rangle + \sin\theta_n |1\rangle$

arXiv:2302.04196

Team

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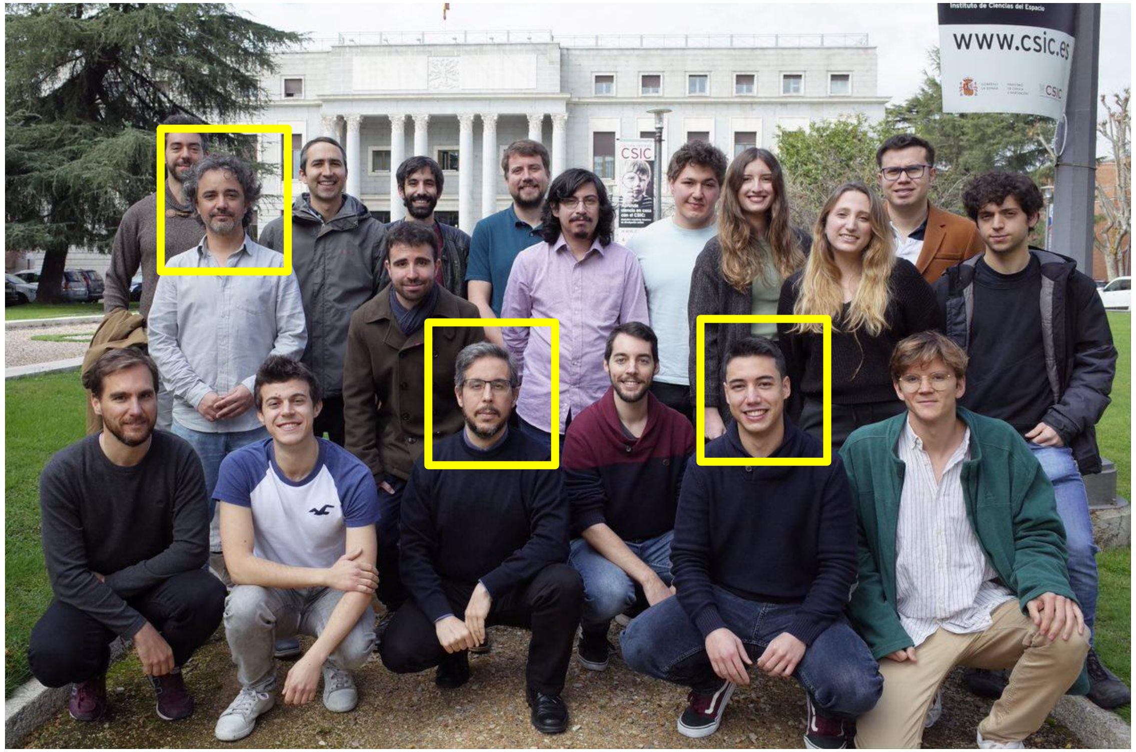
Jorge Luis-Hita, Senaida Hernández-Santana, Álvaro Díaz-Fernández, Eva Andrés, Escolástico Sánchez-Martínez



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Conclusions

I. We introduce the Multi-Objective Variational Constrained Optimizer (MOVCO), a variational quantum method to solve problems with hard constraints.

II. This method allows improving the performance of Variational Quantum Algorithms. It provides benefits in avoiding unfeasible minima while enhancing convergence to lower energy solutions.

III. We provide empirical evidence of the robust performance of MOVCO on a very relevant industrial problem, the Cash Management problem.

IV. This work provides further insight into the application of variational algorithms to real-world problems of practical interest, where it is essential to include a large number of constraints.

V. These ideas on multiobjective optimization can be extended to a broad range of quantum algorithms, for example in Quantum Machine Learning.

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