Incorporating Inequality Constraints into QAOA

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Constrained Optimization

- Objective function $f : \{0,1\}^N \to \mathbb{R}$
  e.g. QUBO, higher orders possible
- Constraint function $g : \{0,1\}^N \to \mathbb{R}$
- Multiple constraints possible, but we limit to one
- Solution vector $\mathbf{x} \in \{0,1\}^N$
- *Assumption*: $\exp(-if(\mathbf{x}))$ and $\exp(-ig(\mathbf{x}))$ computable on QC

Optimize

$$\mathbf{x}^* = \arg\min_{\mathbf{x}\in\{0,1\}^N} f(\mathbf{x})$$

$$\text{s.t.} \quad g(\mathbf{x}) \leq 0$$

$\downarrow$

Feasible subspace

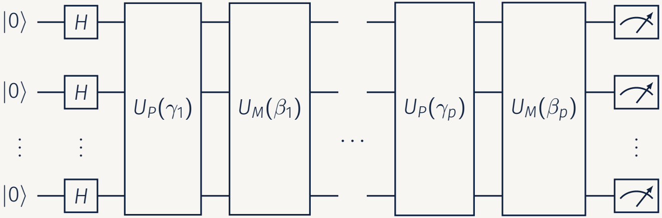
$$\mathcal{F} = \{\mathbf{x} \in \{0,1\}^N \mid g(\mathbf{x}) \leq 0\}$$

$$\mathbf{x}^* = \arg\min_{\mathbf{x}\in\mathcal{F}} f(\mathbf{x})$$

QAOA Brief Introduction

The Quantum Approximate Optimization Ansatz

- Variational circuit for combinatorial optimization, introduced by Farhi et al. [1]
- Trotterization of quantum annealing $H(t) = (1-t)H_M + tH_P$
- Mixer $H_M = -\sum_i \sigma_i^x$, Initial state $|+\rangle = -H_M |+\rangle$
- Problem Hamiltonian, e.g. Ising $H_P = -\sum_{i,j} J_{ij}\sigma_i^z\sigma_j^z - \sum_i h_i\sigma_i^z$



Optimization of Parameters

- State after QAOA iterations $|\beta, \gamma\rangle = \prod_i U_M(\beta_i) U_P(\gamma_i) |+\rangle$
- Initialize parameters β, γ with decreasing βs and increasing γs
- Huge depth $\Rightarrow$ Like QA, $|\beta, \gamma\rangle$ encodes good solution already, otherwise

Classical training of parameters

$$\min_{\beta,\gamma} \langle \beta, \gamma | H_P | \beta, \gamma \rangle$$

The Quantum Alternating Operator Ansatz

- Generalization of the ansatz by Hadfield et al. [2]
  - $U_P(\gamma)$ *phase-separating* unitary that depends on *objective function*
  - $U_M(\beta)$ *mixing* unitary that depends on *domain*

Condition for Mixer

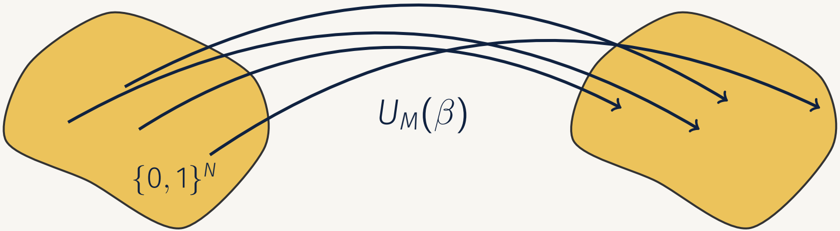
Map between all feasible states

$$\forall \mathbf{x}, \mathbf{y} \in \mathcal{F}, \exists \beta : |\langle \mathbf{x}| U_M(\beta) |\mathbf{y}\rangle|^2 > 0$$

Do not map between feasible to non-feasible state

$$\forall \mathbf{x} \in \mathcal{F}, \mathbf{y} \notin \mathcal{F}, \forall \beta : |\langle \mathbf{x}| U_M(\beta) |\mathbf{y}\rangle|^2 = 0$$

The Action of the Mixer



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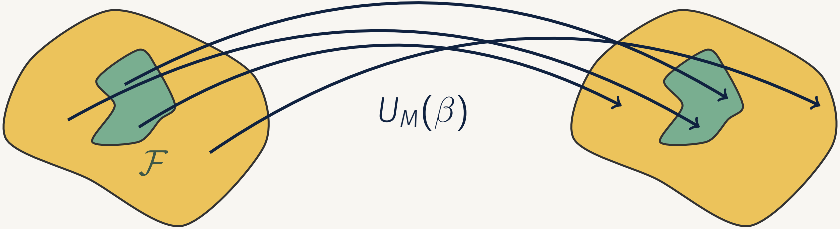

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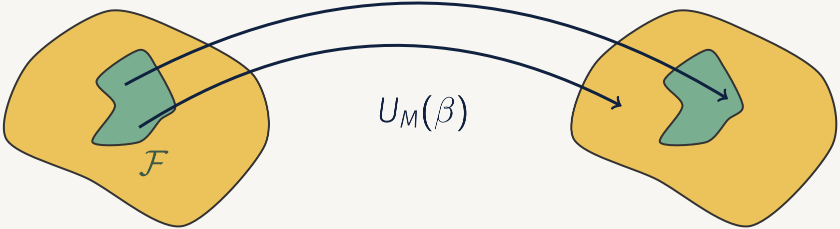

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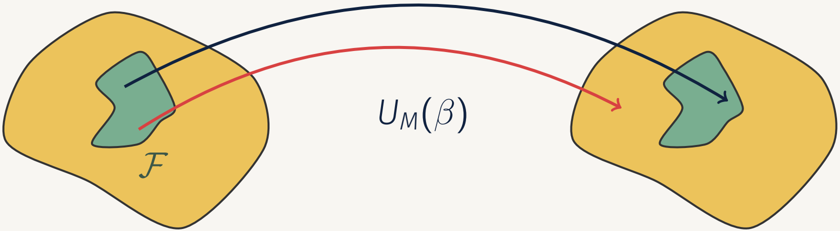

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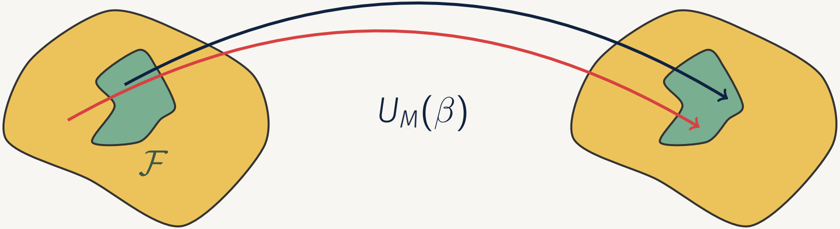
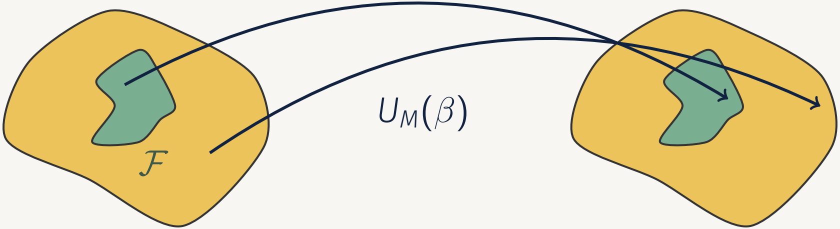


Not possible. For unitary reverse way also possible

The Action of the Mixer



Inequality Constraints so far

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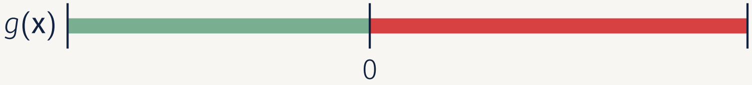
To introduce inequality constraints to binary optimization

- Slack variables $\mathbf{y} \in \{0,1\}^M$ that allow range through integer encoding
- $r_{\mathbf{y}} = \alpha \sum_m 2^m y_m$ with $\alpha = \min_{\mathbf{x} \in \mathcal{F}} g(\mathbf{x})/(2^M - 1)$
- $f(\mathbf{x}) \to f(\mathbf{x}) + \lambda(g(\mathbf{x}) - r_{\mathbf{y}})^2$ assigns large penalties to infeasible states

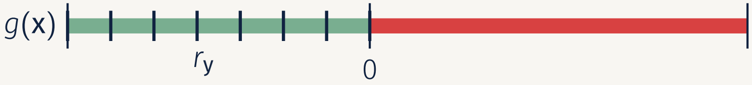
Issues

- Objective function gets distorted for values of $g(\mathbf{x})$ that do not fit the grid spanned by $\mathbf{y}$
- Potentially large penalty-factor diminishes the objective
- Each constraint requires own slack variables
- Infeasible states can still be found

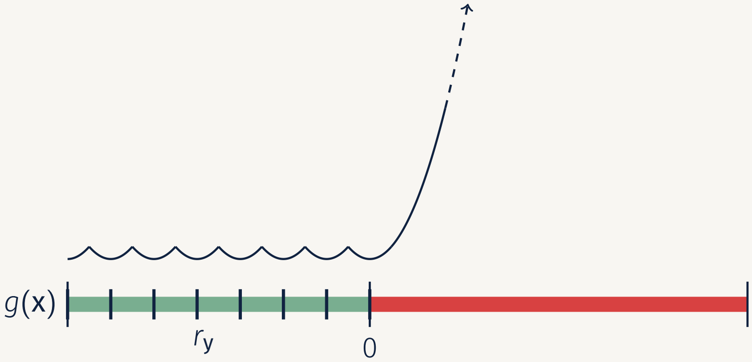
Inequality Constraints so far



Inequality Constraints so far

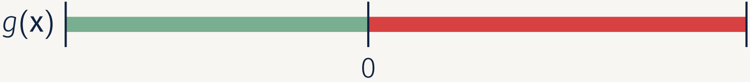


Inequality Constraints so far

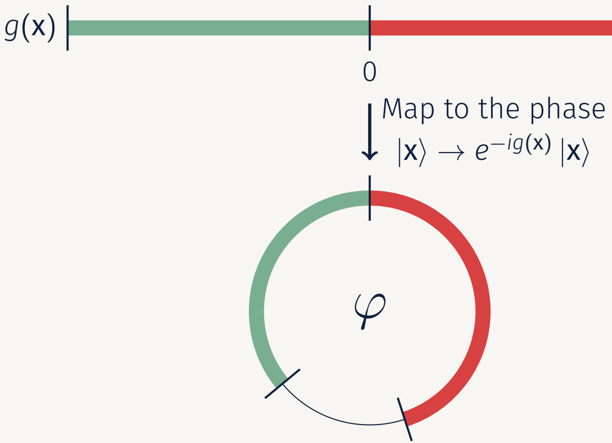


Constrained Mixer for Inequality Constraints

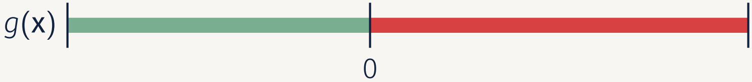
Phase Mapping

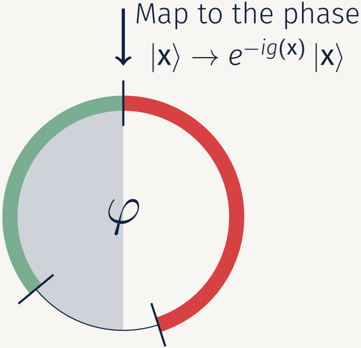


Phase Mapping



Phase Mapping

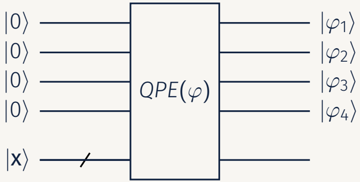




Determine the side of the phase

Quantum Phase Estimation

$\varphi = (-1)^{\varphi_1}\pi 0.\varphi_2\varphi_3\varphi_4$

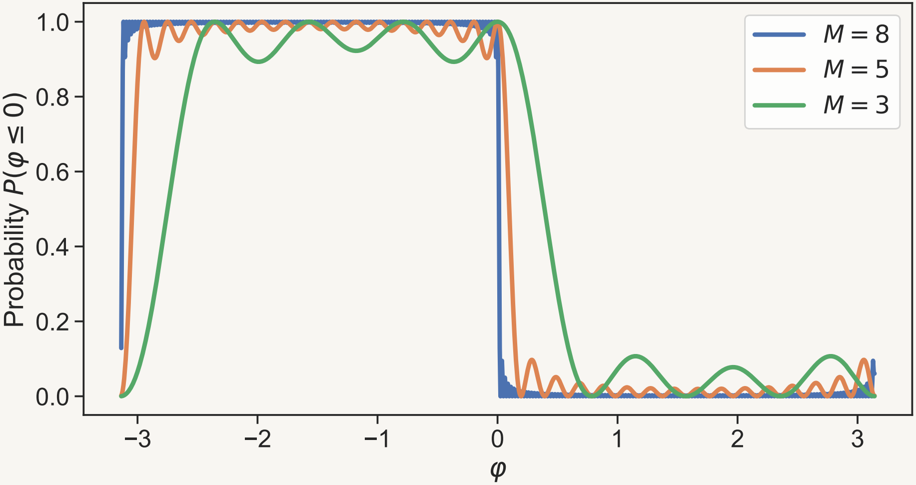


- Rescale the constraint function, such that $-\pi \leq g(\mathbf{x}) \leq \pi$
- Measure φ_1 to determine whether $\varphi = g(\mathbf{x})$ positive or negative.

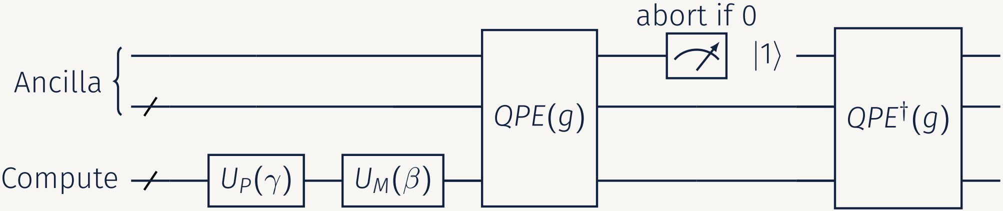
$$P(\varphi \leq 0) = \frac{1}{2^{2M}} \sum_{m=0}^{2^{(M-1)}-1} \left| \frac{\sin(2\pi m + 2^M \varphi)}{\sin(2^{-M+1}\pi m + \varphi)} \right|^2$$

- The more ancilla qubits the more $P(\varphi \leq 0)$ resembles Heaviside theta $\theta(-\varphi)$

Quantum Phase Estimation



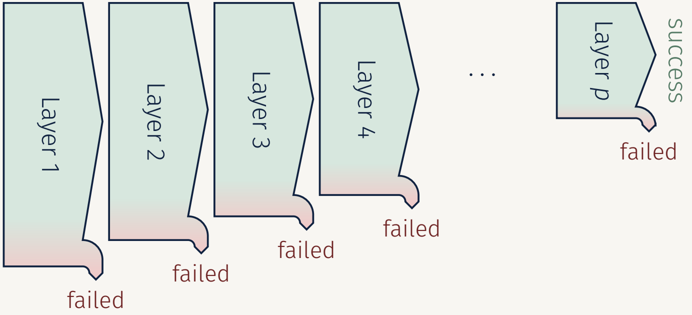
The new QAOA Layer



New Mixer operator (not unitary) $\tilde{U}_M(\beta) = \hat{P}_{g\leq 0}\,\mathbf{exp}\left(-i\beta\sum_i \sigma_i^x\right)$

$$\forall \mathbf{x} \in \mathcal{F}, \mathbf{y} \notin \mathcal{F}: \quad |\langle \mathbf{y}|\,\hat{P}_{g\leq 0} U_M(\beta)\,|\mathbf{x}\rangle\,|^2 \leq P[g(\mathbf{y}) \leq 0] \xrightarrow{M\to\infty} 0$$

A note on success probability



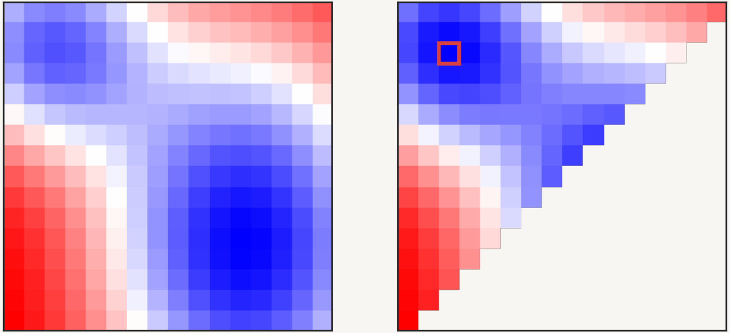
Each layer has the chance of succeeding $p_i \Rightarrow$ All layers together $p_{\text{success}} = \prod_i p_i$.

$$p_i = \sum_{\mathbf{x}} |\psi_{\mathbf{x}}|^2 P[g(\mathbf{x}) \leq 0]$$

Experiments

Simple Example

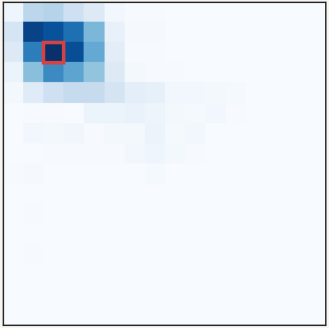
Function $f(x, y)$ of two 4-bit integers. Simple linear inequality constraint.

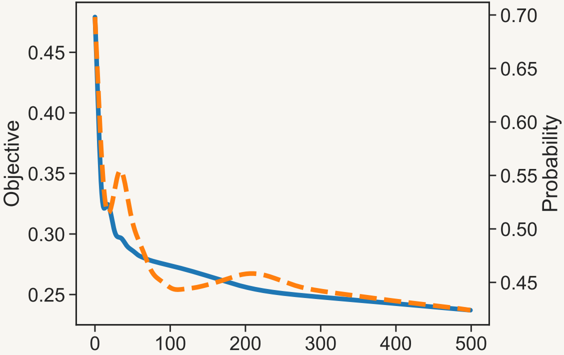


Simple Example

QPE Method. 500 iterations of Gradient Descent with ADAM.

Measuring minimum: 3.56% Non-feasible outcomes: 0.09%

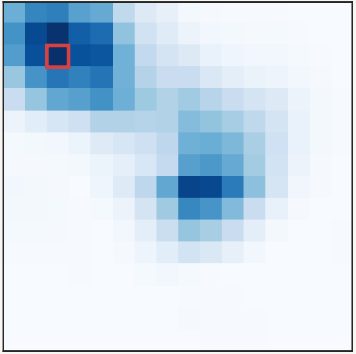


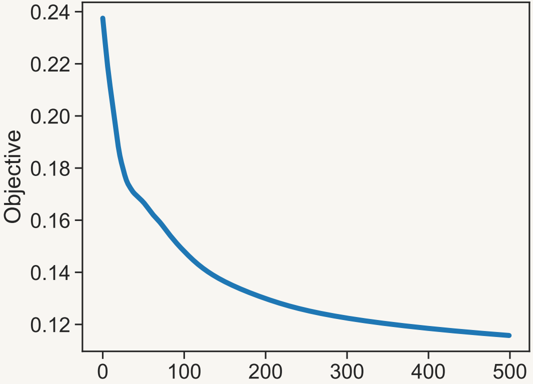


Simple Example

Penalty Method. 500 iterations of Gradient Descent with ADAM.

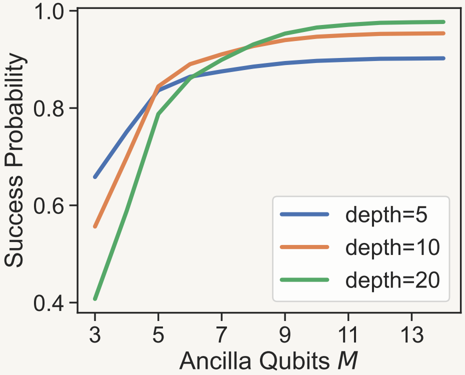
Measuring minimum: 2.39% Non-feasible outcomes: 27.10%

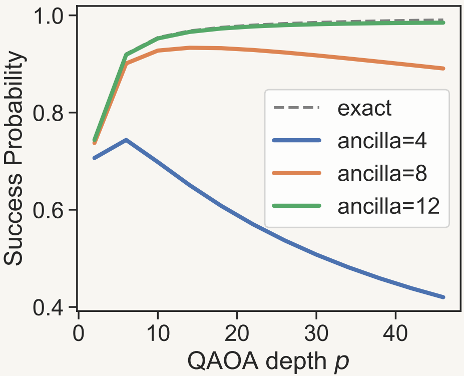




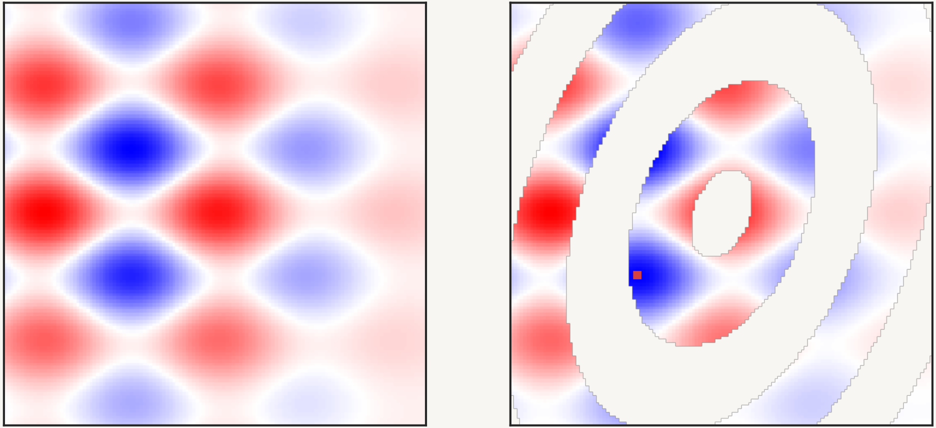
What about the success probability?

Quantum Annealing parametrization.



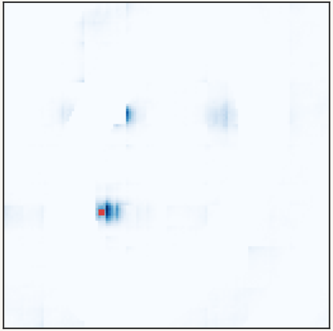


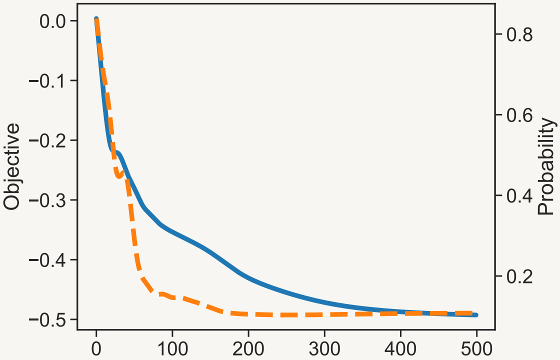
A little more complex example



A little more complex example

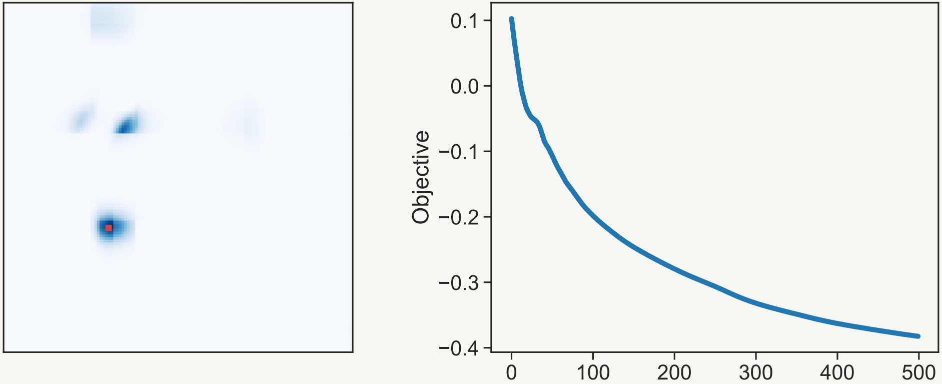
Measuring minimum: 0.04% Non-feasible outcomes: 0.00%





A little more complex example

Measuring minimum: 0.54% Non-feasible outcomes: 28.59%



Conclusion and future directions

Conclusion and future directions

- Promising first results, but more in depth research needs to be conducted
- Shrinking success probability is the main caveat
- Deeper comparison between the penalty and the QPU based ansätze. May have advantage for some kinds of constraints.
- Similar ansatz based on Quantum Zeno Dynamics provided advantage on real hardware tests [3].

[1] Edward Farhi et al. *A Quantum Approximate Optimization Algorithm*. 2014. arXiv: 1411.4028 [quant-ph].

[2] Stuart Hadfield et al. “From the Quantum Approximate Optimization Algorithm to a Quantum Alternating Operator Ansatz”. In: *Algorithms* 12.2 (Feb. 2019), p. 34. ISSN: 1999-4893. DOI: 10.3390/a12020034.

[3] Dylan Herman et al. *Portfolio Optimization via Quantum Zeno Dynamics on a Quantum Processor*. 2023. arXiv: 2209.15024 [quant-ph].