Universität Siegen / 4D and Quantum Vision Group $\langle \cdot | \psi \rangle$

Quantum Binary Optimization

QCVML
In Conjunction with ECCV 2024, Milano

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ECCV

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Binary optimization

Binary optimization

Binary optimization is a classical combinatorial optimization problem. It aims to minimize a real-valued function f, where the decision variables x_i can only take the values ± 1.

Clustering

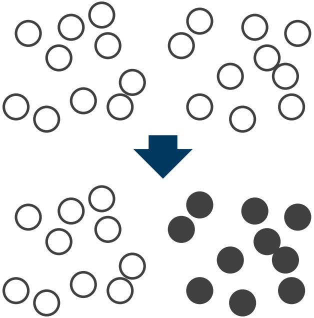
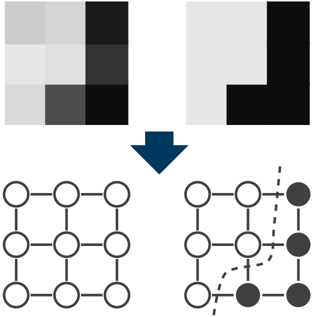
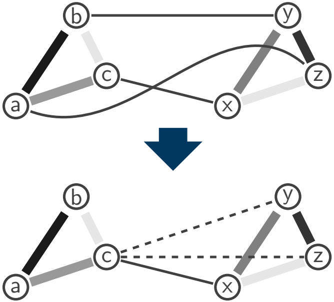


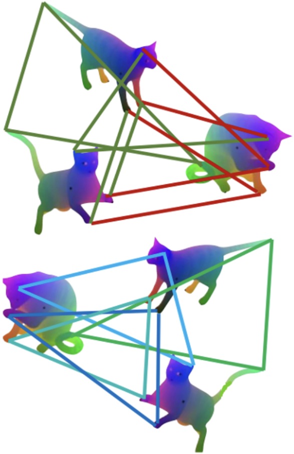
Image segmentation



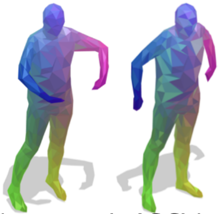
Graph matching



Quantum binary optimization at scale

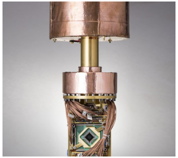


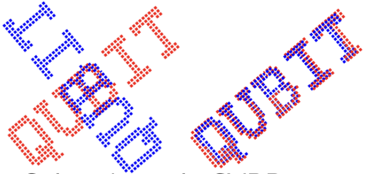
Birdal et al. CVPR 2021



Benkner et al. ICCV 2021

Bhatia et al. CVPR 2023





Golyanik et al. CVPR 2020

Meli et al. CVPR 2022

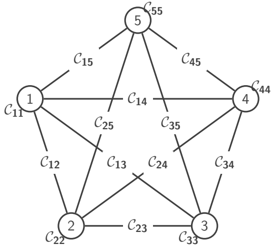
Quadratic unconstrained binary optimization (QUBO/Ising)

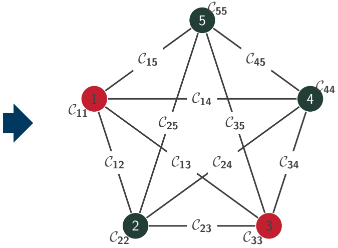
In particular, we are interested in solving QUBO problems of the form

$$\underset{x \in \{-1,1\}^n}{\arg\min}\ f(x),$$

$$f(x) := \sum_{i=1}^{n} \mathcal{C}_{ii} x_i + \sum_{1 \le i < j \le n} \mathcal{C}_{ij} x_i x_j,$$

$$\mathcal{C}_{ii}, \mathcal{C}_{ij} \in \mathbb{R}.$$





Goal

Design efficient QUBO solvers, leverage quantum computing power.

QUBO - Hamiltonian formulation

Quantum computers use qubits (vectors) and manipulate them with matrices. ➡

- Replace binary variables by vectors.
- Find a matrix to describe function value.

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Hamiltonian formulation: Consider $f(x) = \sum_{i=1}^{n} \mathcal{C}_{ii} x_i + \sum_{1 \leq i < j \leq n} \mathcal{C}_{ij} x_i x_j$.

n=1

$$\text{Defining} \quad \underbrace{\mathbf{Z} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\text{Hamiltonian}}, \quad \underbrace{|0\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{\text{qubits}} \quad \Rightarrow \quad \underbrace{\begin{cases} \langle 0|\mathbf{Z}|0\rangle = 1, \\ \langle 1|\mathbf{Z}|1\rangle = -1. \end{cases}}_{\text{binary variable } x}$$

QUBO - Hamiltonian formulation

Quantum computers use qubits (vectors) and manipulate them with matrices. ➡

- Replace binary variables by vectors.
- Find a matrix to describe function value.

Hamiltonian formulation: Consider $f(x) = \sum_{i=1}^{n} \mathcal{C}_{ii} x_i + \sum_{1 \le i < j \le n} \mathcal{C}_{ij} x_i x_j$.

n=1

Defining $\mathbf{Z} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $|0\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow \begin{cases} \langle 0|\mathbf{Z}|0\rangle = 1, \\ \langle 1|\mathbf{Z}|1\rangle = -1. \end{cases}$

More variables

For

$\mathbf{Z}_i = \mathbf{I} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{Z}}_{\text{pos. } i} \otimes \mathbf{I} \otimes \cdots \otimes \mathbf{I}$, and $|q\rangle = \bigotimes_{i=1}^{n} |q_i\rangle$, $|q_i\rangle \in \{|0\rangle, |1\rangle\}$,

it holds with x such that $x_i = \langle q_i|\mathbf{Z}|q_i\rangle$:

$$\boxed{\langle q|\mathbf{C}|q\rangle = f(x)} \quad \text{where} \quad \mathbf{C} := \sum_{i=1}^{n} \mathcal{C}_{ii} \mathbf{Z}_i + \sum_{1 \le i < j \le n} \mathcal{C}_{ij} \mathbf{Z}_i \mathbf{Z}_j.$$

Quadratic unconstrained binary optimization (QUBO/Ising)

Goal

Solve

$$\underset{q \in \{0,1\}^n}{\arg\min} \langle q | \mathbf{C} | q \rangle ,$$

for

$$\mathbf{C} := \sum_{i=1}^{n} \mathcal{C}_{ii} \mathbf{Z}_i + \sum_{1 \leq i < j \leq n} \mathcal{C}_{ij} \mathbf{Z}_i \mathbf{Z}_j ,$$

given $\mathcal{C}_{ii}, \mathcal{C}_{ij} \in \mathbb{R}$, with $\mathbf{Z}_k$ being the Pauli-Z operator acting on qubit k, $k = 1, \ldots, n$.

Classical challenges

- NP-Hard if non sub-modular
- Combinatorial, not differentiable

Quantum methods

- Quantum annealing (D-Wave)
- Gate-based solvers (QAOA/VQE/Ours)

Quantum QUBO solvers

Adiabatic vs. gate-based QC

At any time $t \in [0, T]$, the evolution of the system's state vector $|\psi(t)\rangle$ obeys Schrödinger's equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \mathbf{H}(t) |\psi(t)\rangle \, ,$$

where **H** is a Hermitian operator known as the system-driven Hamiltonian.

Two computation paradigms

$$\boxed{i\hbar \tfrac{d}{dt} |\psi(t)\rangle = \mathbf{H}(t) |\psi(t)\rangle}$$

$$\boxed{\mathbf{H}(t) = \left(1 - \tfrac{t}{T}\right) \mathbf{H}_I + t\mathbf{H}_C} \qquad \boxed{|\psi(t)\rangle = \mathbf{U}(t) |\psi(0)\rangle}$$

Adiabatic quantum computing

$\mathbf{H}_I$: initial Hamiltonian

$\mathbf{H}_C$: problem Hamiltonian

Gate-based quantum computing

$\mathbf{U}(t)$: unitary operator

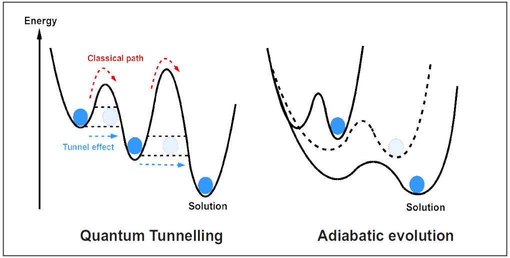
$\mathbf{U}(t)$: depends only on t

Adiabatic vs. gate-based QUBO solvers

$$\mathbf{H}(t) = \left(1 - \tfrac{t}{T}\right) \mathbf{H}_I + t\mathbf{H}_C$$

some Hamiltonian we know the groundstate of.

$$\sum_{i=1}^{n} \mathcal{C}_{ii}\mathbf{Z}_i + \sum_{1 \le i < j \le n} \mathcal{C}_{ij}\mathbf{Z}_i\mathbf{Z}_j$$



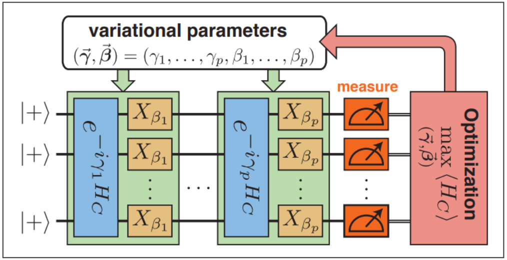
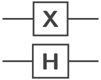
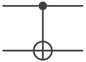
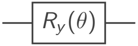


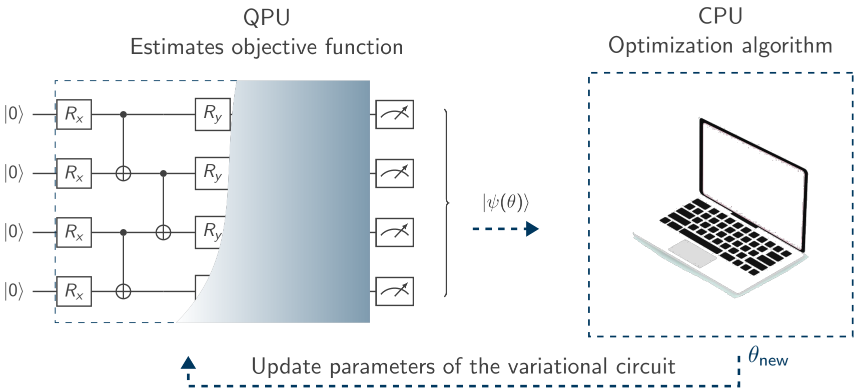
Image sources: https://www.vesselproject.io/life-through-quantum-annealing
https://medium.com/@quantum_wa/quantum-annealing-cdb129e96601
Zhou et al. QAOA: Performance, mechanism, and implementation on near-term devices. Phys. Rev. X, 2020.

Gate-based quantum computing

Gate name	Matrix form	Circuit	Notation
Pauli-X	$\mathbf{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$		$\mathbf{X}\,\lvert 0\rangle = \lvert 1\rangle$
Hadamard	$\mathbf{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$		$\mathbf{H}\,\lvert 0\rangle = \frac{1}{\sqrt{2}}(\lvert 0\rangle + \lvert 1\rangle)$
Multi-qubit gate	$\mathbf{X} \otimes \mathbf{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix}$		$\mathbf{X} \otimes \mathbf{H}\,\lvert 00\rangle = \frac{1}{\sqrt{2}}(\lvert 10\rangle + \lvert 11\rangle)$
Controlled-X on $\lvert q_0 q_1\rangle$	$\mathbf{I} \otimes \mathbf{X}^{q_0} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$		$\mathbf{I} \otimes \mathbf{X}^{q_0}\,\lvert 00\rangle = \lvert 00\rangle$ $\mathbf{I} \otimes \mathbf{X}^{q_0}\,\lvert 10\rangle = \lvert 11\rangle$
Rotation R_y	$R_y(2\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$		$R_y(2\theta)\,\lvert 0\rangle = \cos(\theta)\,\lvert 0\rangle - \sin(\theta)\,\lvert 1\rangle$

Gate-based QC: *Nielsen and Chuang. Quantum Computation and Quantum Information. Cambridge University Press, 2010.*
Sutor. Dancing with Qubits: How quantum computing works and how it can change the world. Packt Publishing Ltd, 2019.

Variational quantum computing (VQC)



VQC: *Cerez et al. Variational quantum algorithms. Nature, 2021.*
Peruzzo et al. A variational eigenvalue solver on a photonic quantum processor. Nature, 2014.
Wang et al. Variational quantum singular value decomposition. Quantum, 2021.

VQC for QUBO

Recall: We want to solve

$$\underset{q \in \{0,1\}^n}{\arg\min} \langle q|\mathbf{C}|q\rangle ,$$

for

$$\mathbf{C} := \sum_{i=1}^{n} \mathcal{C}_{ii}\mathbf{Z}_i + \sum_{1\leq i<j\leq n} \mathcal{C}_{ij}\mathbf{Z}_i\mathbf{Z}_j .$$

$$|q\rangle = \begin{pmatrix} \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \Rightarrow |\psi(\theta)\rangle = \begin{pmatrix} \vdots \\ \alpha_{k-1}(\theta) \\ \alpha_k(\theta) \\ \alpha_{k+1}(\theta) \\ \vdots \end{pmatrix}$$

Idea

Approximate $|q\rangle = \bigotimes_{i=1}^{n} |q_i\rangle$, $q_i \in \{0, 1\}$ as $|\psi(\theta)\rangle = \sum_q \alpha_q(\theta) |q\rangle$ and solve

$$\underset{\theta\in\Theta}{\arg\min}\ \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \langle \psi(\theta)|\mathbf{C}|\psi(\theta)\rangle .$$

Objective lanscapes of some VQCs for QUBOs

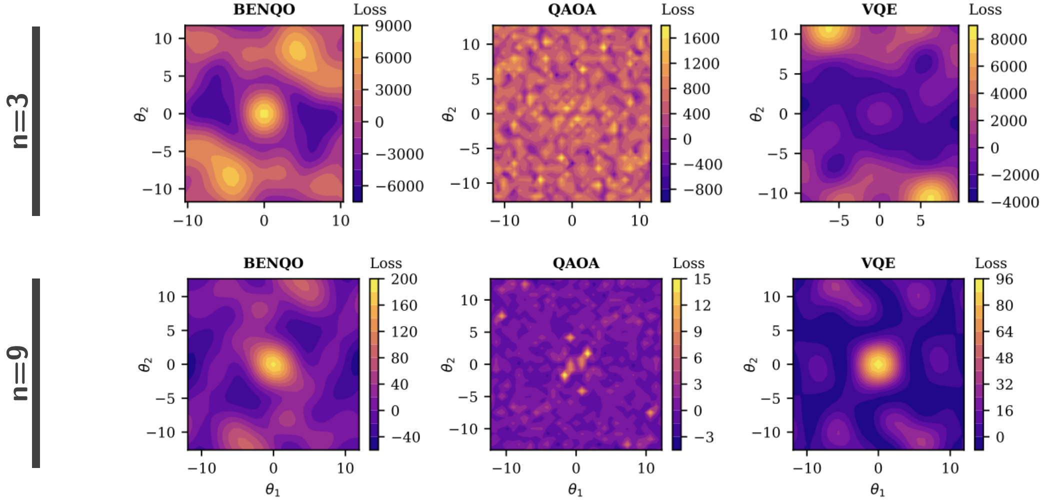


Image source: *Baerligea et al. Solving Combinatorial Optimization Problems with a Block Encoding Quantum Optimizer. arXiv, 2024.*

A block encoding framework of QUBO problems

Block encoding

Idea

Approximate $|q\rangle = \bigotimes_{i=1}^{n} |q_i\rangle\,, q_i \in \{0,1\}$ as $|\psi(\theta)\rangle = \sum_q \alpha_q(\theta)\,|q\rangle$ and solve

$$\arg\min_{\theta\in\Theta}\ \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \langle\psi(\theta)|\mathbf{C}|\psi(\theta)\rangle\,.$$

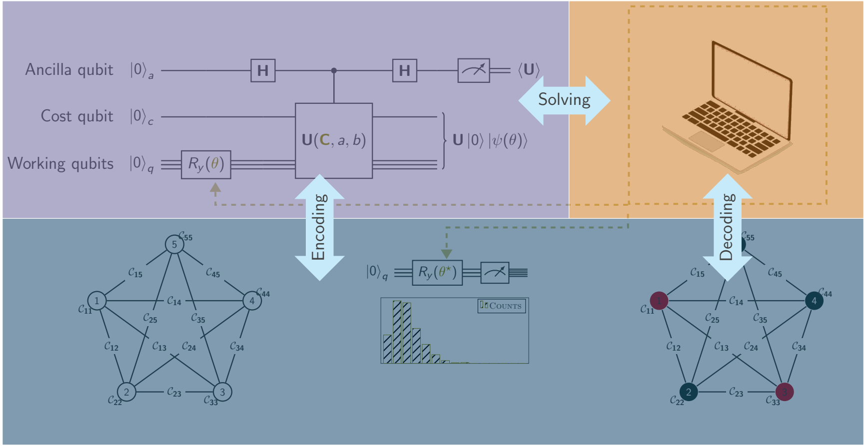
Block encoding: Embed Hamiltonian $\mathbf{C}$ into a unitary operator $\mathbf{U}$ and solve

$$\arg\min_{\theta\in\Theta}\ \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \langle 0,\psi(\theta)|\mathbf{U}|0,\psi(\theta)\rangle\,.$$

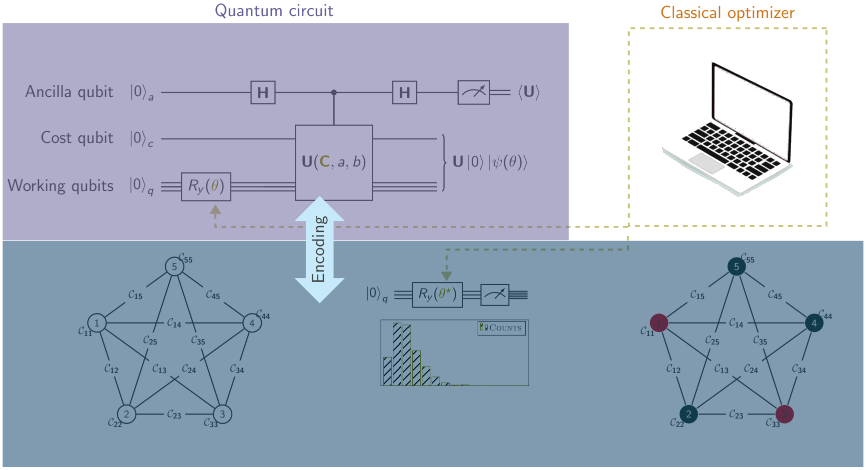
- $\mathbf{U}$ acts directly on as a quantum gate.
- $\mathbf{U}$ encodes the cost of each basis state in its amplitude.
- No need to sample and store $|\psi(\theta)\rangle$ to evaluate $\mathcal{L}(\theta)$.

Block Encoding: Kuete Meli et al. A universal quantum algorithm for weighted maximum cut and Ising problems. Quantum Inf Process, 2023.

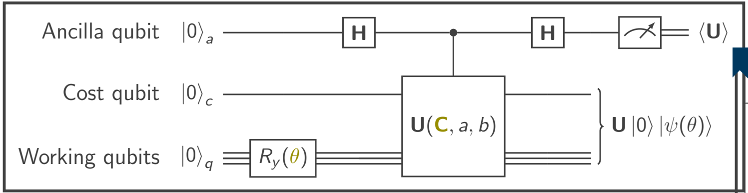
Block encoding: Overview



Block encoding: Overview



Block encoding: Derivations



Hadamard Test

$$
\begin{aligned}
\langle \mathbf{U} \rangle &= p(0) - p(1) \\
&= \sum_q |\alpha_q(\theta)|^2 \cos(\langle q|\hat{\mathbf{C}}|q\rangle)) \\
&= \mathcal{L}(\theta)
\end{aligned}
$$

Embed $\mathbf{C}$ into a $(2^{1+n}) \times (2^{1+n})$ unitary operator

$$
\mathbf{U} := \sum_q \mathbf{U}_{2\times 2}(q) \otimes |q\rangle\langle q|,
$$

$$
\mathbf{U}_{2\times 2}(q) := \begin{pmatrix} \cos(\langle q|\hat{\mathbf{C}}|q\rangle) & -\sin(\langle q|\hat{\mathbf{C}}|q\rangle) \\ \sin(\langle q|\hat{\mathbf{C}}|q\rangle) & \cos(\langle q|\hat{\mathbf{C}}|q\rangle) \end{pmatrix}, \quad \hat{\mathbf{C}} := a\mathbf{C} + b\mathbf{I}, \quad a, b \in \mathbb{R}.
$$

Choose a, b so that $(a\mathbf{C} + b) \in [0, \pi]^{2^n}$, where cos ensures preserving order!

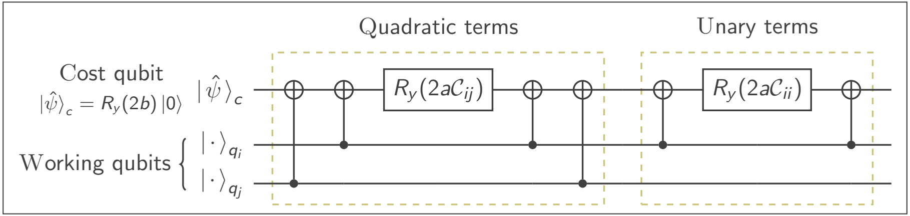
Block encoding: Circuit implementation

Using that

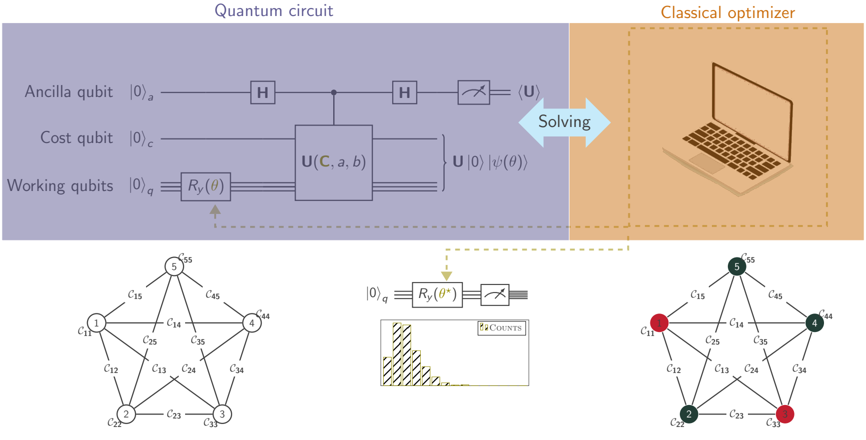
$$\langle q|\hat{\mathbf{C}}|q\rangle = a\,\langle q|\mathbf{C}|q\rangle + b, \quad \langle q|\mathbf{C}|q\rangle = \sum_{i=1}^{n}(-1)^{q_i}\mathcal{C}_{ii} + \sum_{1\le i<j\le n}(-1)^{q_i+q_j}\mathcal{C}_{ij},$$

we can implement $\mathbf{U}_{2\times 2}(q)$ as

$$\mathbf{U}_{2\times 2}(q) = R_y(\langle q|\hat{\mathbf{C}}|q\rangle) = \prod_{i=1}^{n} \mathbf{X}^{q_i}\cdot R_y(2a\mathcal{C}_{ii})\cdot \mathbf{X}^{q_i}\cdot \prod_{1\le i<j\le n} \mathbf{X}^{q_i+q_j}\cdot R_y(2a\mathcal{C}_{ij})\cdot \mathbf{X}^{q_i+q_j}\cdot R_y(2b).$$



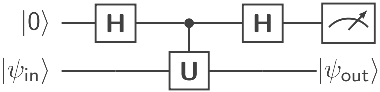
Block encoding: Overview



Problem model

Block encoding: Hadamard test

Consider the Hadamard test circuit and define operators $\mathbf{P}_{\pm} := \frac{1}{2}(\mathbf{I} \pm \mathbf{U})$.



Measurement with operators $\mathbf{P}_0 = |0\rangle\langle 0| \otimes \mathbf{I}$ and $\mathbf{P}_1 = |1\rangle\langle 1| \otimes \mathbf{I}$ yields

$$p(0) = \left\langle \psi_{\text{in}} \middle| \mathbf{P}_+^\dagger \mathbf{P}_+ \middle| \psi_{\text{in}} \right\rangle \qquad \text{and} \qquad p(1) = \left\langle \psi_{\text{in}} \middle| \mathbf{P}_-^\dagger \mathbf{P}_- \middle| \psi_{\text{in}} \right\rangle,$$

so that it holds $\mathrm{Re}\left(\langle \psi_{\text{in}} \,|\, \mathbf{U} \,|\, \psi_{\text{in}} \rangle\right) = p(0) - p(1)$.

In our application

$$\mathcal{L}(\theta) = \langle \psi_{\text{in}} \,|\, \mathbf{U} \,|\, \psi_{\text{in}} \rangle = \langle 0, \psi(\theta) \,|\, \mathbf{U} \,|\, 0, \psi(\theta) \rangle = \langle \psi(\theta) | \cos(\hat{\mathbf{C}}) | \psi(\theta) \rangle \in \mathbb{R}.$$

Block encoding: Optimization

In an iterative process, we solve

$$\underset{\theta \in \Theta}{\arg\min}\ \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \langle 0, \psi(\theta) | \mathbf{U} | 0, \psi(\theta) \rangle \,,$$

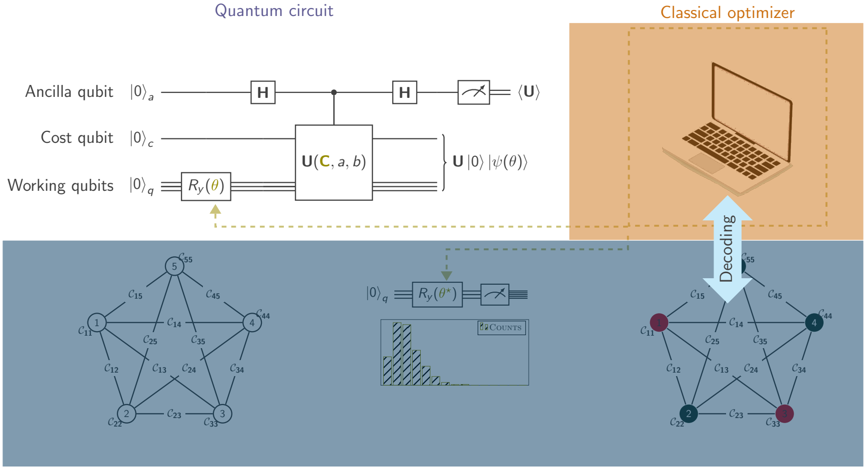
where we evaluate $\mathcal{L}(\theta)$ with Hadamard test.
Optimization with normalized gradient descent and decreasing step size:

$$\theta^{(k+1)} = \theta^{(k)} - \alpha_k \cdot \frac{\nabla_\theta \mathcal{L}(\theta^{(k)})}{\|\nabla_\theta \mathcal{L}(\theta^{(k)})\|_2^2}.$$

Parameter shift rule [Mitara et al. '2018]

$$\frac{\partial}{\partial \theta_i} \mathcal{L}(\theta) = \frac{1}{2} \left(\mathcal{L}\left(\theta + \frac{\pi}{2} e_i\right) - \mathcal{L}\left(\theta - \frac{\pi}{2} e_i\right) \right).$$

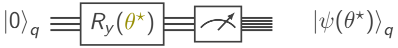
Block encoding: Overview



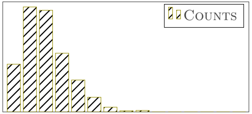
Block encoding: Decoding

Once optimal parameter vector $\theta^\star$ is found:

- Prepare and measure ansatz



- Measure and get count histogram

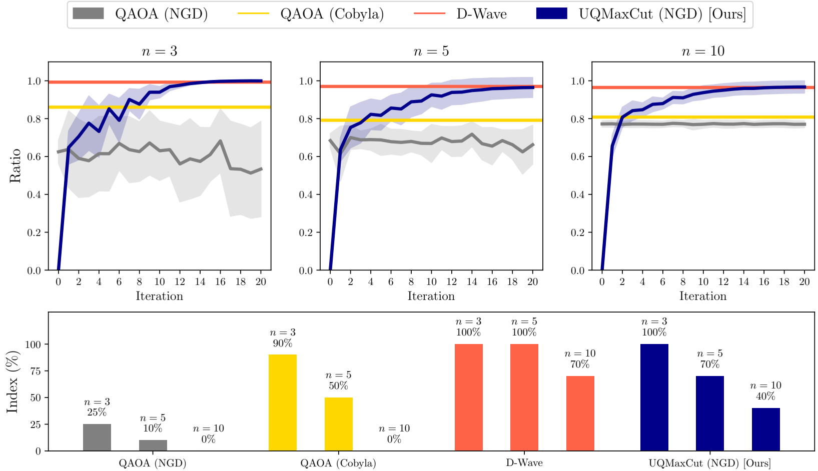


- Select solution (without loss of generality)

$$|\psi(\theta^\star)\rangle = \alpha_0 |0\rangle + \ldots + \alpha_{q^\star} |q^\star\rangle + \ldots + \alpha_{\max} |q_{\max}\rangle + \ldots + \alpha_{2^n-1} |2^n - 1\rangle$$

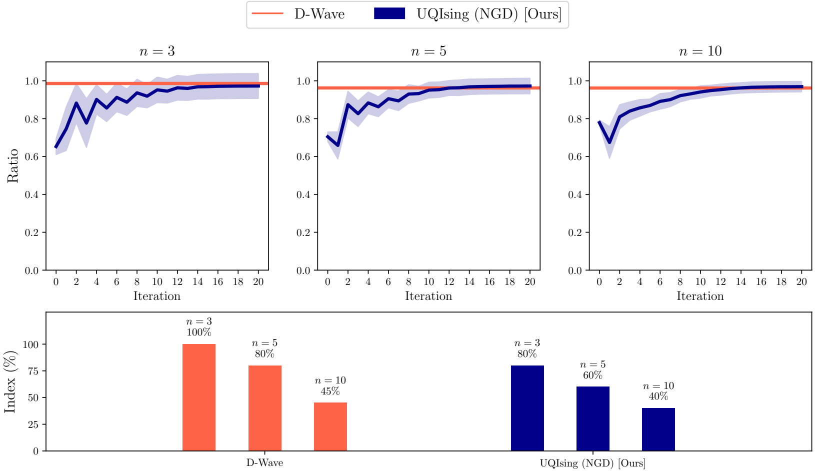
$$|\psi^\star\rangle = |q_{\max}\rangle$$

Results on Maxcut



Kuete Meli, Mannel, and Lellmann. A universal quantum algorithm for weighted maximum cut and Ising problems. Springer, 2023.

Results on full QUBOs



Kuete Meli, Mannel, and Lellmann. A universal quantum algorithm for weighted maximum cut and Ising problems. Springer, 2023.

Take-home message

Take-home message

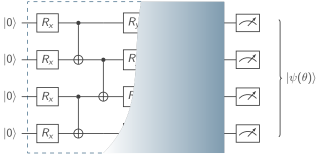
1. QUBOs can be solved by adiabatic quantum computing:

$$\underset{x \in \{-1,1\}^n}{\arg\min}\; f(x), \qquad f(x) := \sum_{i=1}^{n} \mathcal{C}_{ii} x_i + \sum_{1 \le i < j \le n} \mathcal{C}_{ij} x_i x_j .$$

2. Gate-based quantum computing allows flexibility:
   - Allows variational forms as

$$\underset{\theta \in \Theta}{\arg\min}\; \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \langle \psi(\theta) | \mathbf{C} | \psi(\theta) \rangle .$$

   - Gradient computable via parameter shift rule.



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Thank You!

Block encoding: Derivations

Embed $\mathbf{C}$ into a $(2^{1+n}) \times (2^{1+n})$ unitary operator

$$\mathbf{U} := \mathbf{U}(\mathbf{C}, a, b) := \sum_q \mathbf{U}_{2\times 2}(q) \otimes |q\rangle\langle q|,$$

$$\mathbf{U}_{2\times 2}(q) := \begin{pmatrix} \cos(\langle q|\hat{\mathbf{C}}|q\rangle) & -\sin(\langle q|\hat{\mathbf{C}}|q\rangle) \\ \sin(\langle q|\hat{\mathbf{C}}|q\rangle) & \cos(\langle q|\hat{\mathbf{C}}|q\rangle) \end{pmatrix}, \quad \hat{\mathbf{C}} := a\mathbf{C} + b\mathbf{I}, \quad a, b \in \mathbb{R}.$$

Measuring $\mathbf{U}$ on $|0, \psi(\theta)\rangle = \sum_q \alpha_q(\theta)\,|0, q\rangle$ yields

$$\begin{aligned} \langle 0, \psi(\theta)\,|\,\mathbf{U}\,|\,0, \psi(\theta)\rangle &= \sum_q |\alpha_q(\theta)|^2 \langle 0|\mathbf{U}_{2\times 2}(q)|0\rangle \otimes \langle q|q\rangle \\ &= \sum_q |\alpha_q(\theta)|^2 \cos(\langle q|\hat{\mathbf{C}}|q\rangle) \end{aligned}$$

Choose a, b so that $(a\mathbf{C} + b) \in [0, \pi]^{2^n}$, where cos ensures preserving order!