Quantum Computing for Binary Optimization and Beyond: Bridging Classical and Quantum Landscapes

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About Me

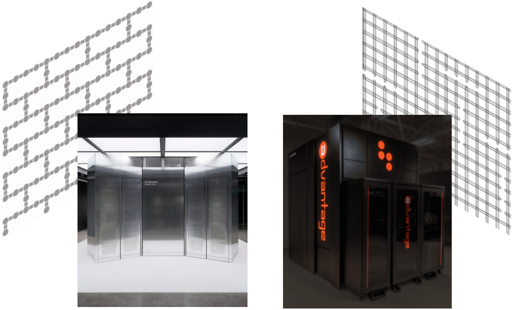
2024-Current: Postdoc
Computer Vision (M. Möller)
Topic: Quantum computing for computer vision
University of Siegen, Germany.

2021-2024: PhD
Computational Life Science (J. Lellmann)
Thesis: Quantum algorithms for image processing
University of Lübeck, Germany.

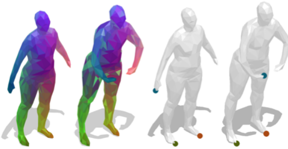
2018-2021: Master
Computational Life Science (J. Lellmann)
Thesis: Trainable detection methods for materials testing
University of Lübeck, Germany.

2012-2015: Bachelor
Mathematics and Computer Sciences (M. Tchoupe)
Thesis: Programming a web application in Java EE
University of Dschang, Cameroon.

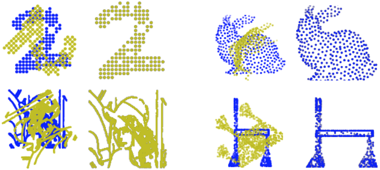
Quantum Computing: What and Why?



Diverse potential applications (e.g., ML, computer vision, ...):



Benker et. al., ICCV, 2021.



Kuete Meli, Mannel, Lellmann. CVPR, 2022.

QC Images: *https://www.ibm.com/quantum/blog/quantum-roadmap-2033*
https://www.dwavesys.com/solutions-and-products/systems

Section 1

Introduction

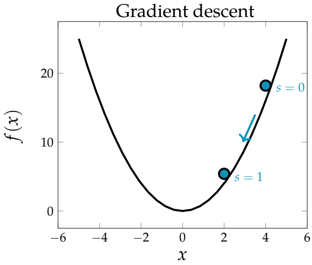
A Quantum View on Optimization

Goal

Find

$$x^\star \in \arg\min_{x \in \mathcal{X}} f(x),$$

for some objective function $f : \mathcal{X} \to \mathbb{R}$.



A Quantum View on Optimization

Goal

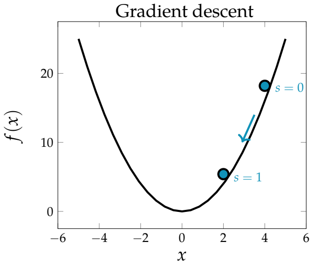
Find

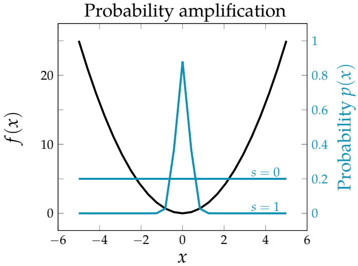
$$x^\star \in \arg\min_{x \in \mathcal{X}} f(x),$$

for some objective function $f : \mathcal{X} \to \mathbb{R}$.

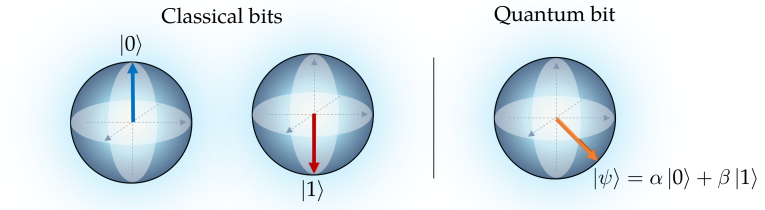
Quantum computing is all about probabilities:

1. Start in a superposition of all states $x \in \mathcal{X}$.
2. Evolve to boost the probability of $x^\star$.
3. Measure and repeat to identify $x^\star$.





Quantum Bit



Quantum bit [Nielsen & Chuang. '2010]

A quantum bit, or qubit, is a one-particle quantum system whose state is expressed as a superposition of two basis states $|0\rangle$ and $|1\rangle$,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad \text{with} \quad |0\rangle := \begin{pmatrix}1\\0\end{pmatrix}, \quad |1\rangle := \begin{pmatrix}0\\1\end{pmatrix},$$

and where $|\alpha|^2 + |\beta|^2 = 1,\ \alpha, \beta \in \mathbb{C}$.

Measuring $|\psi\rangle$ gives $|0\rangle$ with probability $|\alpha|^2$, or $|1\rangle$ with probability $|\beta|^2$.

State Vector: one Qubit, more Qubits

The state vector of an n-particle quantum system, $n \in \mathbb{N}$, is the tensor product of the n single state vectors $|\psi^{(i)}\rangle$, $i = 1, \dots, n$:

$$|\psi\rangle = \otimes_{i=1}^{n} |\psi^{(i)}\rangle = \sum_{q \in \{0,1\}^n} \alpha_q |q\rangle, \qquad \sum_{q \in \{0,1\}^n} |\alpha_q|^2 = 1.$$

- The set $\{|q\rangle, q \in \{0,1\}^n\}$ form the new computational basis. Example for $n = 2$ qubits:

$$|00\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad |01\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \quad |10\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad |11\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

- Notation either in binary or decimal representation, i.e., $|1\rangle \otimes |1\rangle = |11\rangle = |3\rangle$.

Evolution

At any time $t \in [0, T]$, rescaled $s = t/T \in [0, 1]$, the evolution of the state vector $|\psi(s)\rangle$ obeys Schrödinger's equation

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

where $\mathbf{H}$ is a Hermitian operator known as the system-driven Hamiltonian.

Two computation paradigms

$$i\hbar \tfrac{d}{Tds} |\psi(s)\rangle = \mathbf{H}(s) |\psi(s)\rangle$$

$$\mathbf{H}(s) = \mathcal{A}(s)\mathbf{H}(0) + \mathcal{B}(s)\mathbf{H}(1)$$

Adiabatic quantum computing
$\mathbf{H}(0)$: initial Hamiltonian
$\mathbf{H}(1)$: problem Hamiltonian

$$|\psi(s)\rangle = \mathbf{U}(s) |\psi(0)\rangle$$

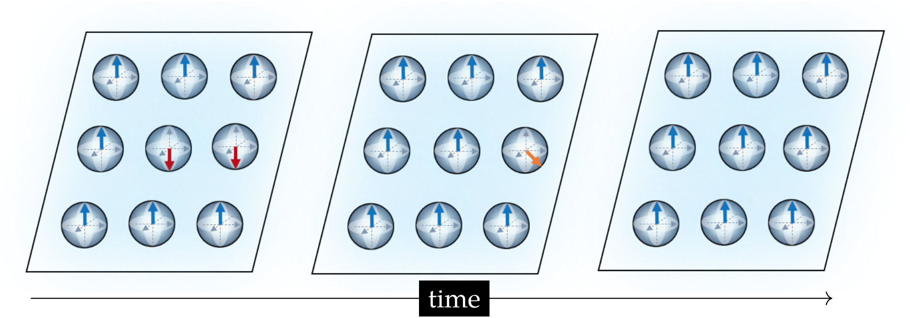
Universal quantum computing
$\mathbf{U}(s)$: unitary operator
$\mathbf{U}(s)$: depends lonely on s

Section 2

Adiabatic Quantum Computing

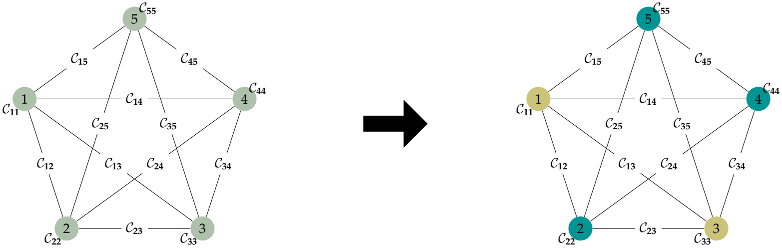
$$\mathbf{H}(s) = \mathcal{A}(s)\mathbf{H}(0) + \mathcal{B}(s)\mathbf{H}(1)$$

Ising Ferromagnetism



Magnetism of n spin systems $s_i \in \{-1, 1\}, i = 1, \ldots, n$:
$\rightarrow$ the final state is the ground state, it minimizes the overall energy of the system.

QUBO: Quadratic Unconstrained Binary Optimization



With couplings and biases $\mathcal{C}_{ij}, \mathcal{C}_{ii} \in \mathbb{R}$, the ground state solves QUBO/Ising problem:

$$\arg \min_{s \in \{-1,1\}^n} \mathcal{J}(s), \qquad \mathcal{J}(s) := \sum_{i=1}^{n} \mathcal{C}_{ii} s_i + \sum_{1 \leq i < j \leq n} \mathcal{C}_{ij} s_i s_j .$$

Adiabatic quantum computing

Careful initialization $\Rightarrow$ Ground state $\Rightarrow$ Solution of QUBO!

WHY?

QUBO: Hamiltonian Formulation

Define Pauli-I, X, Y, Z operators

$$\mathbf{I} := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{X} := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{Y} := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbf{Z} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\mathbf{M}_i := \mathbf{I} \otimes \cdots \otimes \mathbf{I} \otimes \underbrace{\mathbf{M}}_{i\text{th pos}} \otimes \mathbf{I} \otimes \cdots \otimes \mathbf{I} \qquad \text{for} \qquad \mathbf{M} \in \{\mathbf{I}, \mathbf{X}, \mathbf{Y}, \mathbf{Z}\}.$$

Hamiltonian formulation

Let

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

Let $|q\rangle := \bigotimes_{i=1}^{n} |q_i\rangle$ for $q_i \in \{0, 1\}$ so that $\mathbf{Z}\,|q_i\rangle = s_i\,|q_i\rangle, \forall i = 1, \ldots, n$. It holds

$$\mathcal{J}(s) = \langle q|\mathbf{C}|q\rangle$$

and

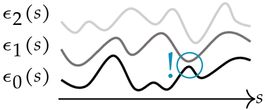
$$\arg \min_{s \in \{-1,1\}^n} \mathcal{J}(s) \quad \Leftrightarrow \quad \arg \min_{q \in \{0,1\}^n} \langle q|\mathbf{C}|q\rangle.$$

Adiabatic Quantum Theorem

D-Wave initial and problem Hamiltonians:

$$\mathbf{H}(0) = \mathbf{B}, \quad \mathbf{B} := \sum_{i=1}^{n} \mathbf{X}_i,$$

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



Adiabatic theorem (roughly) [Albash et al. '2018]

Let $\mathbf{H}(s) := (1-s)\mathbf{H}(0) + s\mathbf{H}(1)$ for $s \in [0,1]$ be an Hamiltonian with eigenstates $|\epsilon_j(s)\rangle$ to the eigenvalues $\epsilon_j(s)$, and so that $\epsilon_j(s) < \epsilon_{j+1}(s)$, $\forall s \in [0,1], j \in \{0,1,\cdots\}$. If the system is initialized in the state $|\epsilon_j(0)\rangle$, then Schrödinger's equation $i\hbar\frac{d}{Tds}|\psi(s)\rangle = \mathbf{H}(s)|\psi(s)\rangle$ instantly keeps $|\psi(s)\rangle$ in $|\epsilon_j(s)\rangle$, provided that $\mathbf{H}(s)$ varies slowly enough.

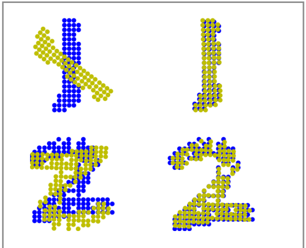
Start in ground state $|+\rangle^{\otimes n}$ of $\mathbf{B}$ and end up in any ground state $|q^\star\rangle$ of $\mathbf{C}$!!!

Application (Notebook)

Goal

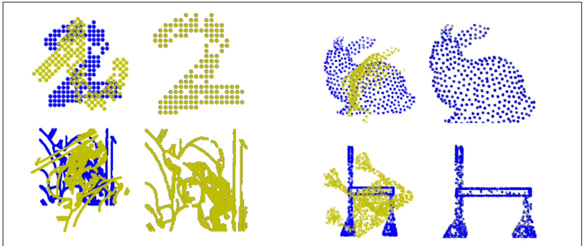
Given N pairs of points $(x_i, y_i) \in \mathbb{R}^d$, solve $\min_{R \in SO(d)} \sum_{i=1}^{N} \|x_i - Ry_i\|^2$.

QA



(a) *2D*.

IQT



(a) *2D*. (b) *3D*.

QA: Golyanik and Theobalt. A Quantum Computational Approach to Correspondence Problems on Point Sets. CVPR, 2020.
IQT: Kuete Meli, Mannel, and Lellmann. An iterative quantum approach for transformation estimation from point sets. CVPR, 2022.

Application (Notebook)

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Given N pairs of points $(x_i, y_i) \in \mathbb{R}^d$, solve $\min_{R \in SO(d)} \sum_{i=1}^{N} \|x_i - Ry_i\|^2$.

IQT strategy: Write R as

$$R = \exp(M(v)),$$

where

in 2D for $v \in \mathbb{R}$	in 3D for $v := (v_1, v_2, v_3)^\top \in \mathbb{R}^3$
$M(v) = v \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$M(v) = \|v\|_2 \begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix}.$

- Binarize using K-bit representation: $v_i = \sum_k 2^k q_{i_k}$
- Linearize using first order Taylor's expansion

Optimizing over $q \Rightarrow$ QUBO!!!

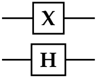
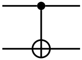
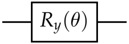
QA: Golyanik and Theobalt. A Quantum Computational Approach to Correspondence Problems on Point Sets. CVPR, 2020.
IQT: Kuete Meli, Mannel, and Lellmann. An iterative quantum approach for transformation estimation from point sets. CVPR, 2022.

Section 3

Universal Quantum Computing

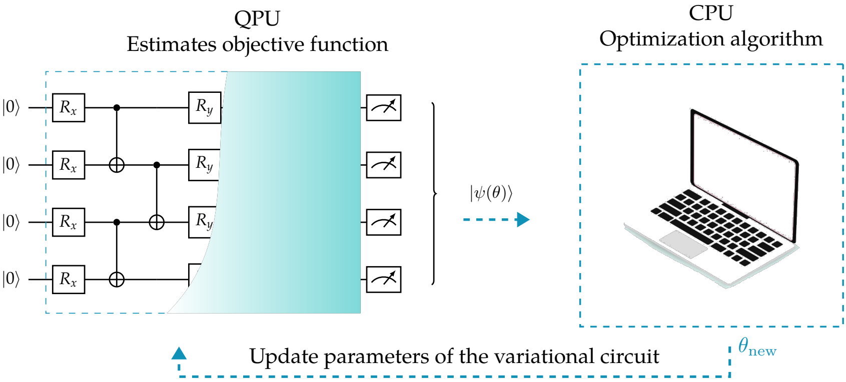
$$|\psi(t)\rangle = \mathbf{U}(t)\,|\psi(0)\rangle$$

Quantum gates

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	$R_y(2\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$		$R_y(2\theta)\lvert 0\rangle = \cos(\theta)\lvert 0\rangle - \sin(\theta)\lvert 1\rangle$

Universal QC: *Nielsen 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: A Concrete Case

Recall: we want to solve

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

for

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

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

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

VQC for QUBO: Farhi et al. A quantum approximate optimization algorithm. arXiv, 2014.

VQC for QUBO: A Concrete Case

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

for

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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

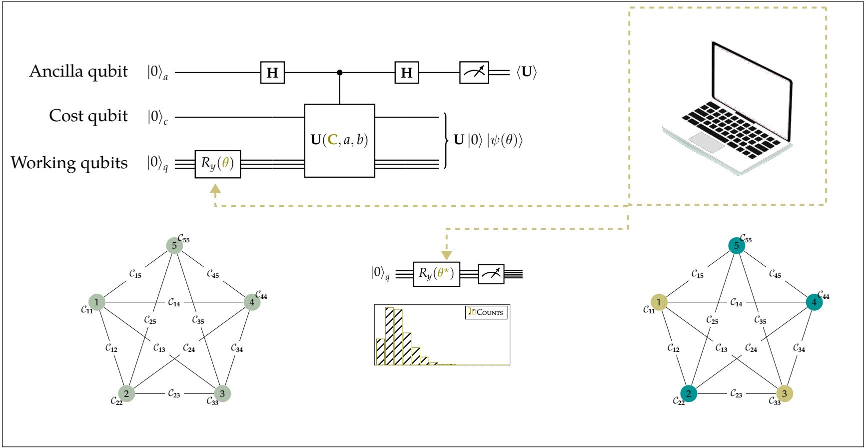
$$\arg \min_{\theta \in \Theta} \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \langle \psi(\theta) | \mathbf{C} | \psi(\theta) \rangle \,.$$

Strategy: Embed the Hamiltonian **C** into a unitary operator **U** and solve relaxation

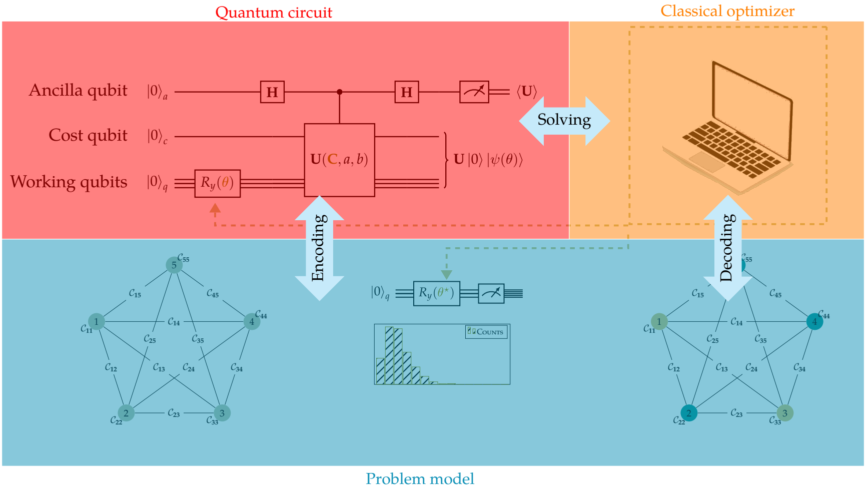
$$\arg \min_{\theta \in \Theta} \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \langle 0, \psi(\theta) | \mathbf{U} | 0, \psi(\theta) \rangle \,.$$

VQC for QUBO: *Farhi et al. A quantum approximate optimization algorithm. arXiv, 2014.*
Block Encoding: *Kuete Meli et al. A universal quantum algorithm for weighted maximum cut and Ising problems. Springer, 2023.*

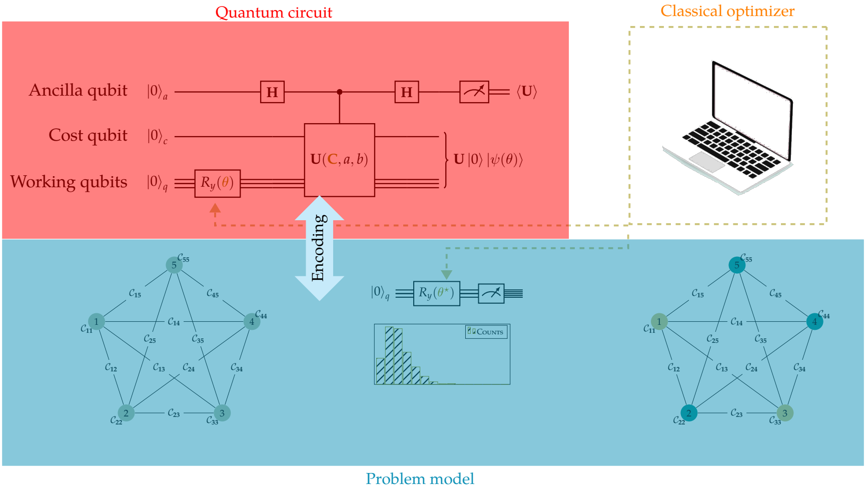
VQC for QUBO: Overview



VQC for QUBO: Overview



VQC for QUBO: Overview



VQC for QUBO: Block Encoding

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

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

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

- On a basis states it holds

$$\langle 0, q \,|\, \mathbf{U} \,|\, 0, q\rangle = \langle 0|\mathbf{U}_{2\times 2}(q)|0\rangle \otimes \langle q|q\rangle = \cos(\langle q|\hat{\mathbf{C}}|q\rangle).$$

- On an arbitrary state il holds

$$\langle 0, \psi(\theta) \,|\, \mathbf{U} \,|\, 0, \psi(\theta)\rangle = \sum_q \left|\alpha_q(\theta)\right|^2 \cos(\langle q|\hat{\mathbf{C}}|q\rangle).$$

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

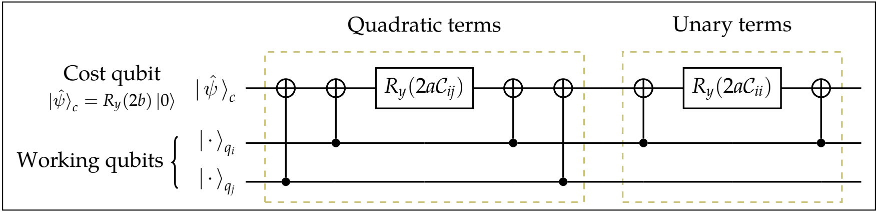
VQC for QUBO: Circuit Implementation

Using that

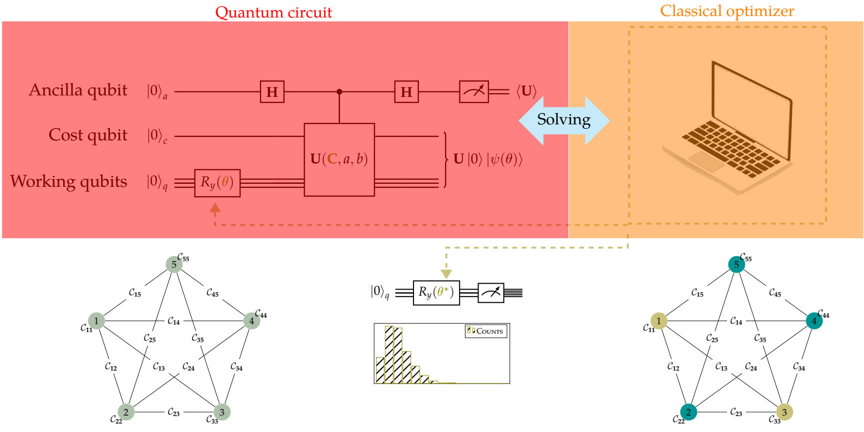
$$\langle q|\hat{\mathbf{C}}|q\rangle = a\,\langle q|\mathbf{C}|q\rangle + b, \quad \langle q|\mathbf{C}|q\rangle = \sum_{i=1}^{n}(-1)^{q_i}\mathcal{C}_{ii} + \sum_{1\le i<j\le n}(-1)^{q_i+q_j}\mathcal{C}_{ij},$$

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

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



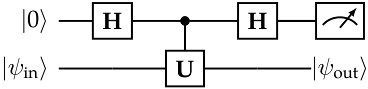
VQC for QUBO: Overview



Problem model

VQC for QUBO: 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 $\text{Re}\left(\langle \psi_{\text{in}} \,|\, \mathbf{U} \,|\, \psi_{\text{in}} \rangle\right) = p(0) - p(1)$.

In our application

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

VQC for QUBO: Optimization

In an iterative process, we solve

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

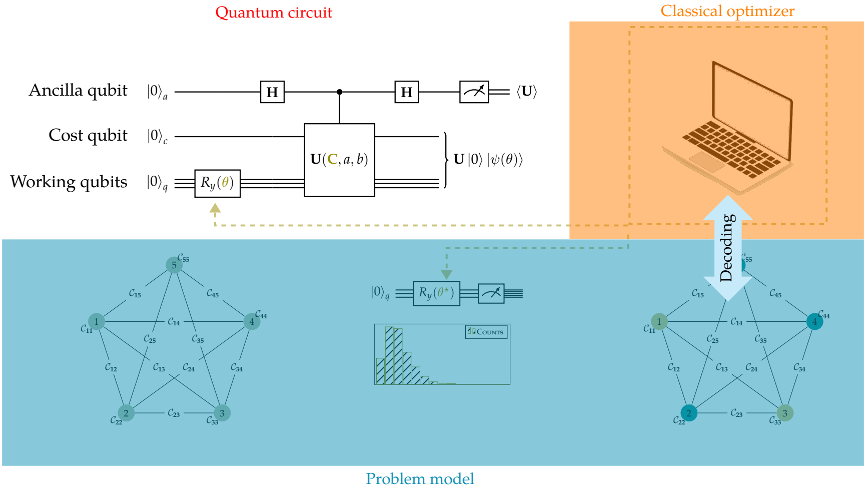
where we evaluate $\mathcal{L}(\theta)$ with Hadamard test.
Optimization with normalized gradient descent and decreasing step size:

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

Parameter shift rule [Mitara et al. '2018]

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

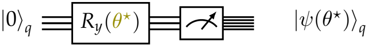
VQC for QUBO: Overview



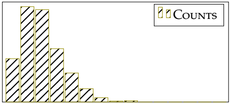
Decoding

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

- Prepare and measure ansatz



- Measure and get count histogram



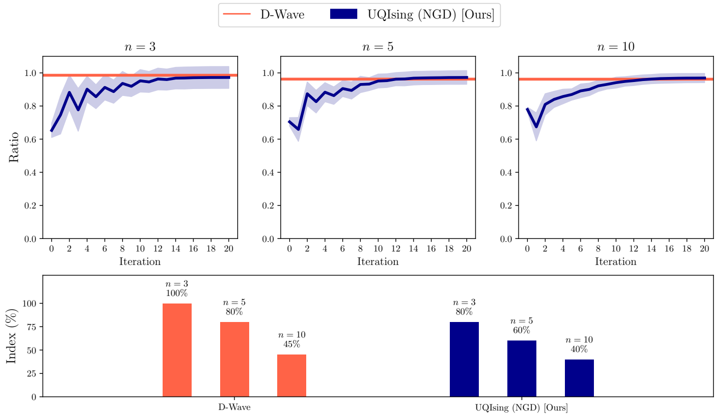
- Select solution (without loss of generality)

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

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

Demo (Notebook)

Comparison against D-Wave:



Metrics: $\text{Ratio} = 1 - \frac{\langle \psi^\star | \mathbf{C} | \psi^\star \rangle - \mathcal{C}_{\min}}{\mathcal{C}_{\max} - \mathcal{C}_{\min}}, \quad \text{Index} = \# \{\psi^\star = q^\star\}.$

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

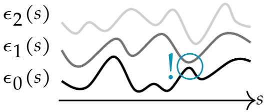
Section 4

Take-Home

Take-Home

1. Adiabatic quantum computing solves QUBOs:

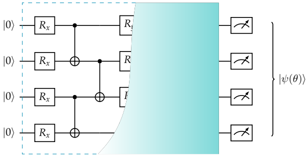
$$\arg\min_{s\in\{-1,1\}^n} \mathcal{J}(s), \qquad \mathcal{J}(s) := \sum_{i=1}^{n} C_{ii} s_i + \sum_{1\leq i<j\leq n} C_{ij} s_i s_j .$$



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

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

   - Gradient computable via parameter shift rule.



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Thank You!