Using quantum computers to solve combinatorial optimization problems

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Dirac/"Bra-ket" notation

- common notation for quantum states i.e. vectors in a complex Hilbert space V
- $|\rangle$ denotes a vector in a vector space V
- $\langle|$ denotes a linear functional on V, i.e. is an element of V^*
- we can identify a vector ("ket") with a linear functional ("bra") and vice versa
- $\langle|\rangle : V \times V \to \mathbb{C}$ denotes the inner product
- $|\rangle\langle| : V \times V \to V \otimes V$ denotes the outer product

A quantum bit

- A quantum bit (qubit) is a quantum mechanical system with a two-dimensional state space. A state $|\Phi\rangle$ is a unit vector in $\mathbb{C}^2$.
- Given an orthonormal basis $|\varphi_0\rangle, |\varphi_1\rangle$, (typically: $|\varphi_0\rangle = |0\rangle = (1,0)^T, |\varphi_1\rangle = |1\rangle = (0,1)^T$), a qubit can be written as

$$|\Phi\rangle = a_0 |\varphi_0\rangle + a_1 |\varphi_1\rangle \text{, with } a_0, a_1 \in \mathbb{C} \text{ and } |a_0|^2 + |a_1|^2 = 1. \tag{1}$$

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- In contrast to classical mechanics, a **superposition** of basis states is possible. An example is the state $|\Phi\rangle = -\frac{1}{\sqrt{2}}|0\rangle + i\frac{1}{\sqrt{2}}|1\rangle$.

Multiple qubits

The general state $|\Phi\rangle$ of n qubits is a unit vector in $(\mathbb{C}^2)^{\otimes n} = \underbrace{\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2}_{\text{n times}}$.

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Using the standard basis for $\mathbb{C}^2$, a basis for $(\mathbb{C}^2)^{\otimes n}$ is given by the following 2^n vectors

$$
\begin{aligned}
|0\rangle_n &:= |\underbrace{00\ldots00}_{\text{n digits}}\rangle = |0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle \otimes |0\rangle = \begin{pmatrix}1, 0 & \ldots & 0, 0\end{pmatrix}^\intercal \\
|1\rangle_n &:= |\underbrace{00\ldots01}_{\text{n digits}}\rangle = |0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle \otimes |1\rangle = \begin{pmatrix}0, 1 & \ldots & 0, 0\end{pmatrix}^\intercal \\
&\vdots \\
|2^n - 1\rangle_n &:= |\underbrace{11\ldots11}_{\text{n digits}}\rangle = |1\rangle \otimes |1\rangle \otimes \cdots \otimes |1\rangle \otimes |1\rangle = \begin{pmatrix}0, 0 & \ldots & 0, 1\end{pmatrix}^\intercal
\end{aligned} \tag{2}
$$

Multiple qubits

A general state can therefore be expressed as

$$|\Phi\rangle = \sum_{i=0}^{2^n-1} c_i |i\rangle = \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{2^n-2} \\ c_{2^n-1} \end{pmatrix}, \quad \sum_{i=0}^{2^n-1} |c_i|^2 = 1, \quad c_i \in \mathbb{C}. \tag{3}$$

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Remark.

- The space $(\mathbb{C}^2)^{\otimes n}$ is a 2^n-dimensional space. The dimension grows exponentially with the number of qubits.
- The state space of n classical bits, i.e., a binary string $\{0, 1\}^n$ is an n-dimensional space. The dimension grows linearly with the number of bits.

Product states and entanglement

A quantum state $|\Phi\rangle \in (\mathbb{C}^2)^{\otimes n}$ is a **product state** if it can be expressed as a tensor product of n single qubits $|\Phi_i\rangle$, i.e.,

$$|\Phi\rangle = \underbrace{|\Phi_1\rangle \otimes \cdots \otimes |\Phi_n\rangle}_{\text{n times}} \tag{4}$$

Otherwise, it is **entangled**.

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Examples.

- Product state: $\frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
- Entangled state: $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

Important states and conventions

- Two-qubit Bell states

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$
$$\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$
$$\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$
$$\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

  (They form a maximally entangled basis, known as the Bell basis, of the four-dimensional Hilbert space for two qubits.)

- Superposition states

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$
$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Operations on qubits

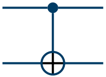
An operation applied by a quantum computer, which is also called a **gate**, to n qubits is a **unitary matrix** $U \in \mathbb{C}^{2^n \times 2^n}$.

- A matrix is U unitary, if $U^\dagger U = UU^\dagger = I$.
- Unitary matrices are norm-preserving, i.e., $\|U\left|\Phi\right\rangle\| = \|\left|\Phi\right\rangle\|$. This means that we get back a quantum state, which is a unit vector.
- Quantum operations are linear.
- Quantum operations are reversible.

Examples of 1 qubit gates

- Hadamard gate $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. We have that $H^2 = I, H\left|0\right\rangle = \left|+\right\rangle, H\left|1\right\rangle = \left|-\right\rangle, H\left|+\right\rangle = \left|0\right\rangle, H\left|-\right\rangle = \left|1\right\rangle$.
- Pauli gates $X = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. We have that $X^2 = I, X\left|0\right\rangle = \left|1\right\rangle, X\left|1\right\rangle = \left|0\right\rangle, X\left|+\right\rangle = \left|+\right\rangle, X\left|-\right\rangle = -\left|-\right\rangle$.
- Pauli gates $Y = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. We have that $Y^2 = I, Y\left|0\right\rangle = i\left|1\right\rangle, Y\left|1\right\rangle = -i\left|0\right\rangle$.
- Pauli gates $Z = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. We have that $Z^2 = I, Z\left|0\right\rangle = \left|0\right\rangle, Z\left|1\right\rangle = -\left|1\right\rangle$.
- Phase shift gates $R_\Phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\Phi} \end{pmatrix}$.
- Square root of NOT gate $\sqrt{X} = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+1 \end{pmatrix}$. We have that $\sqrt{X}\sqrt{X} = X$.
- . . .

Examples of 2 qubit gates

- controlled not gate $CNOT = CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} =$ 

  It has the effect
  $CNOT \left|00\right\rangle = \left|00\right\rangle, CNOT \left|01\right\rangle = \left|01\right\rangle, CNOT \left|10\right\rangle = \left|11\right\rangle, CNOT \left|11\right\rangle = \left|10\right\rangle.$

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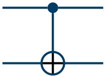
- controlled not gate $CNOT = CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} =$ 

  It has the effect
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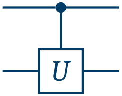
- controlled U gate $CU = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & u_{10} & u_{11} \end{pmatrix} =$ 

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- Physicist call eigenvalues of a Hamiltonian **energies**.
  - amounts of energy the system can have
  - typically order from smallest to largest, $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$.
- To each energy λ_j corresponds to an **energy eigenstate**.
  - **ground state**: energy eigenstate $|v_1\rangle$ corresponding to the lowest energy
  - **first excited state**, **second excited state**, ...: $|v_2\rangle$, $|v_3\rangle$, ...

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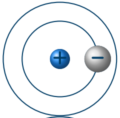
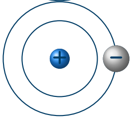
Electron sitting in the lowest shell is in the ground state



First excited state has the electron in the next shell up



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Expectation values

Given

- a state $|\phi\rangle$ and
- an observable H

Then the expectation value of H in the state $|\phi\rangle$ is given by

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Particularly: $\langle H \rangle_{|\psi_i\rangle} = \lambda_i$

SINTEF

The variational principle

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- Prepare parametrized state $|\psi(\theta)\rangle$
- Find θ^* s.t. $|\langle H \rangle_{|\phi(\theta^*)\rangle} - \lambda_{min}|$ minimal

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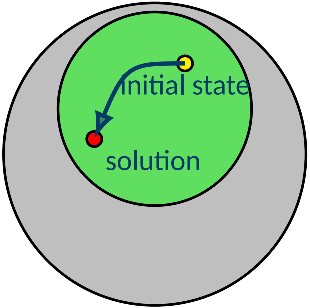
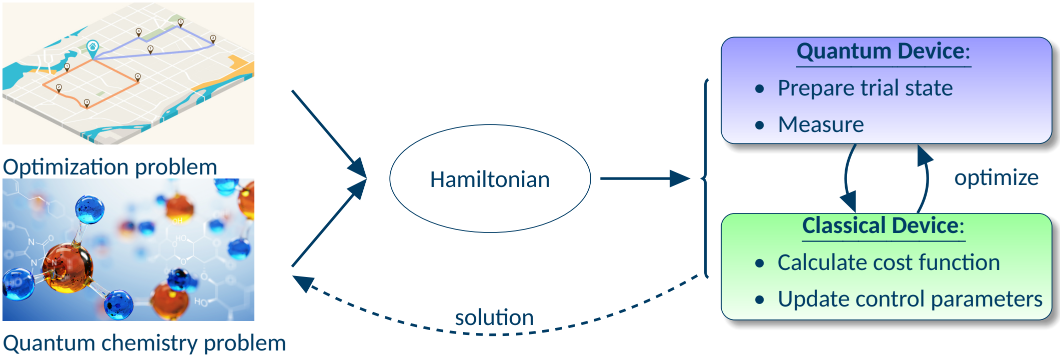
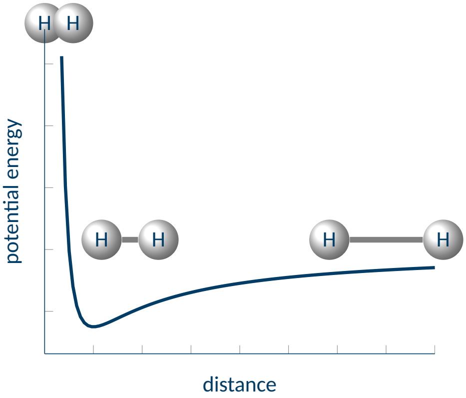


Overview Hybrid Quantum Classical Solvers



Quantum Chemistry



$$H(x) = \sum_{p,q} h_{p,q}(x) a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{p,q,r,s}(x) a_p^\dagger a_q^\dagger a_r a_s + h_{\text{nuc}} \tag{8}$$

Combinatorial optimization: MaxCut

- Given a graph $G = (V, E)$ consisting of vertices V and edges E with weights $w_{i,j} > 0$, for $(i,j) \in E$.

$$
\begin{aligned}
V =& \{0, 1, 2, 3, 4\} \\
E =& \{(0, 1, 1.0), (0, 2, 2.0), \\
& (0, 3, 1.0), (0, 4, 2.0), \\
& (1, 3, 1.0), (3, 2, 4.0), \\
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\end{aligned}
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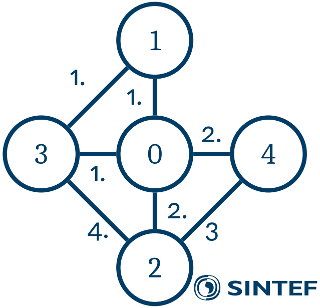

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- A cut is defined as a partition of the vertices V into two disjoint subsets $S, \overline{S}$.
- The cost function to be maximized is the sum of weights of edges with vertices in the two different subsets.

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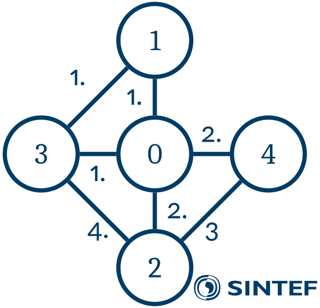

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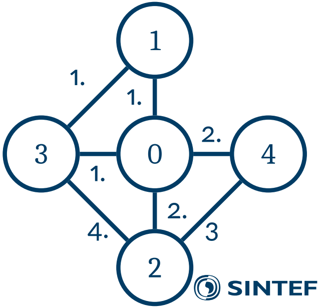
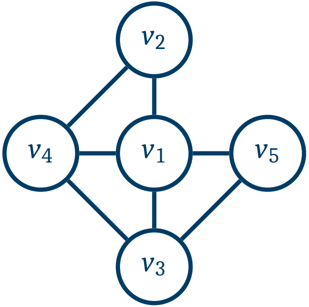


Assign $x_i = \begin{cases} -1, & \text{if edge } i \text{ is in set } S \\ +1, & \text{otherwise} \end{cases}$, then the cost function is given by

$$C(x) = \sum_{(i,j)\in E} w_{i,j} \frac{1}{2}(1 - x_i x_j) \qquad (9)$$

SINTEF

Example



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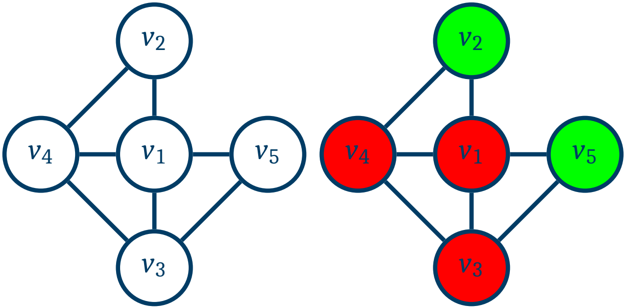

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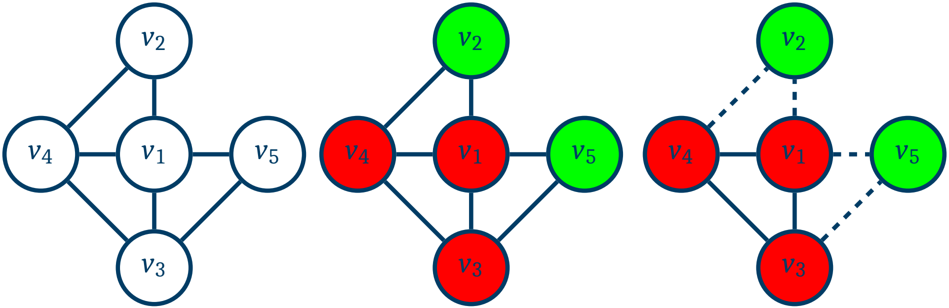
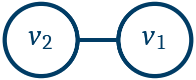


Smallest case



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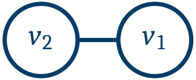

- For each vertex we define $|x_i\rangle = \begin{cases} |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & \text{if vertex } i \in S \\ |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, & \text{if vertex } i \in \overline{S} \end{cases}$

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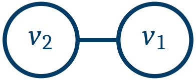

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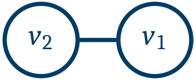

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- Hamiltonian

$$H = ZZ \tag{10}$$

has ground states $|01\rangle, |10\rangle$

SINTEF

MaxCut for general graph

Remember that the cost function is given by

$$C(x) = \sum_{(i,j)\in E} w_{i,j} \frac{1}{2}(1 - x_i x_j) \tag{11}$$

- The Hamiltonian encoding our problem is therefore

$$H_C = \sum_{(i,j)\in E} w_{i,j} \frac{1}{2}(I - \sigma_z^i \otimes \sigma_z^j), \tag{12}$$

where I^m denotes the identity matrix in $(\mathbb{C}^2)^{\otimes m}$

QUBO

In general any QUBO

$$x^T A x + b^T x + c \to \min \tag{13}$$

can be formulated as an Ising-Hamiltonian by the transformation

$$x_i \to \frac{1}{2}\left(I - \sigma_z^i\right) \tag{14}$$

SINTEF

The adiabatic theorem

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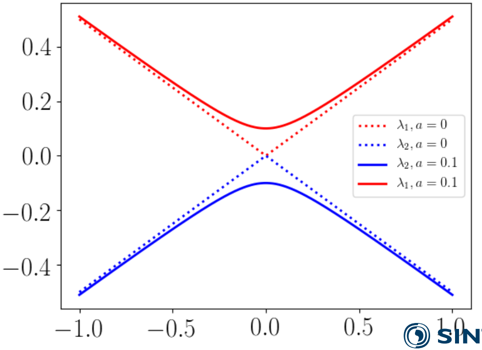
Consider a time dependent Hamiltonian

$$H(t) = \begin{pmatrix} \alpha t & a \\ a & -\alpha t \end{pmatrix} \tag{15}$$

$$\lambda_{1,2} = \pm\sqrt{a^2 + (\alpha t)^2} \tag{16}$$

The probability of a diabatic transition is given by (Landau-Zener)

$$P_D = e^{2\pi a^2/|\alpha|} \tag{17}$$



SINTEF

Quantum annealing

$$H_{QA}(s) = (1 - t)H_B + tH_C, \tag{18}$$

- Choose H_B s.t. ground state easy to prepare
- Choose H_C s.t. ground state encodes solution

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Quantum annealing

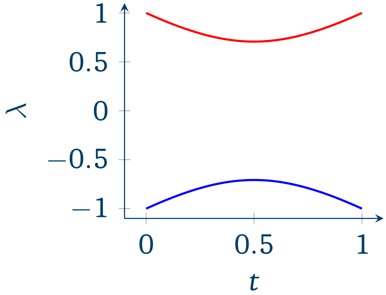
$$H_{QA}(s) = (1 - t)H_B + tH_C, \tag{18}$$

- Choose H_B s.t. ground state easy to prepare
- Choose H_C s.t. ground state encodes solution
- run time of the algorithm typically scales as $\mathcal{O}(1/\Delta^2_{\text{min}})$, where $\Delta_{\text{min}} = \min_{s\in[0,1]}(\lambda_2(t) - \lambda_1(t))$ is the minimum spectral gap.
- It turns out that for hard instances, Δ_{min} is exponentially small with respect to the problem size.

$H(t) = (1-t)(-X) + tZ$

Eigenvalues:

$$\lambda_{1/2} = \pm\sqrt{2t^2 - 2t + 1}$$



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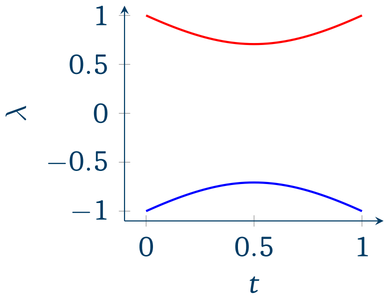

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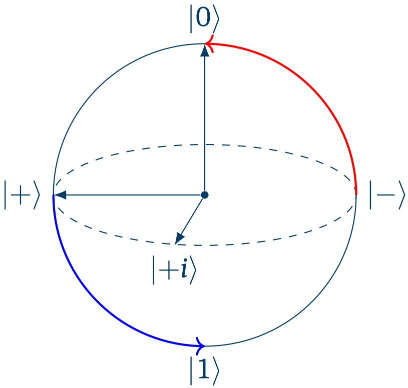

weighted MaxCut

$$H_C = \sum_{(j,k)\in E} \frac{1}{2} w_{i,j} \left(I - \sigma_z^i \sigma_z^j \right) \tag{19}$$

- H_C is sum of $|E|$ local terms
- H_C is a diagonal matrix

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- H_C is sum of $|E|$ local terms
- H_C is a diagonal matrix

$$H_B = \sum_{i \in nodes} \sigma_x^i \tag{20}$$

- H_B has only off-diagonal non-zero entries
- H_B induces a swap operation between neighboring qubits, and thus can move the excitation around for the purpose of state transfer

How to find quantum gates for QA?

We need to find gates for

$$e^{-iH_{QA}(s)}, \tag{21}$$

where

$$H_{QA}(s) = -(sH_C + (1-s)H_B), \quad s = t/T \tag{22}$$

Matrix exponentials

If H_1, H_2 are matrices (Hamiltonians), then

$$e^{H_1+H_2} \neq e^{H_1} e^{H_2}, \tag{23}$$

except when H_1 and H_2 commute, i.e., $H_1 H_2 = H_2 H_1$.

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Trotterization, (Lie-Trotter-Suzuki product formula[Trotter(1959), Suzuki(1976)])

$$e^{-i(H_1+H_2)t} = \left(e^{-iH_1\frac{t}{n}} e^{-iH_2\frac{t}{n}}\right)^n + \mathcal{O}\left(\frac{t^2}{n}\right) \tag{24}$$

First and second order versions

$$\begin{aligned} e^{-i(H_1+H_2)t} &= e^{-iH_1 t} e^{-iH_2 t} + \mathcal{O}\left(t^2\right) \\ e^{-i(H_1+H_2)t} &= e^{-iH_1 t/2} e^{-iH_2 t} e^{-iH_1 t/2} + \mathcal{O}\left(t^3\right) \end{aligned} \tag{25}$$

Overall QAOA

1. Using $2p$ parameters $\gamma = \gamma_1, \ldots, \gamma_p$, $\beta = \beta_1, \ldots, \beta_p$, prepare state

$$|\Psi(\gamma, \beta)\rangle = U_{B_p} U_{C_p} \ldots U_{B_1} U_{C_1} |+\rangle^{\otimes n}, \quad (26)$$

   where the operators have the explicit form

$$U_{B_l} = e^{-i\beta_l H_B} = \prod_{j=1}^{n} e^{-i\beta_l \sigma_x^j},$$
$$U_{C_l} = e^{-i\beta_l H_C} = \prod_{(j,k)\in E} e^{-i\gamma_l w_{j,k}/2(I-\sigma_z^j \sigma_z^k)}, \quad (27)$$

2. Obtain $\langle\Psi(\gamma, \beta)|H_C|\Psi(\gamma, \beta)\rangle$.
3. Run an outer, classical, optimization loop to find γ, β that minimizes the expectation value $\langle\Psi(\gamma, \beta)|H_C|\Psi(\gamma, \beta)\rangle$.

SINTEF

How to obtain the expectation value

H_C is a diagonal Hamiltonian, and we have that

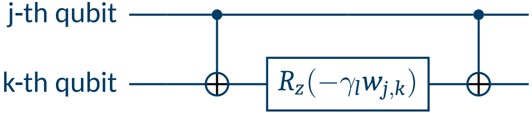
$$H_C = \sum_{x \in \{0,1\}^n} C(x) |x\rangle \langle x| \tag{28}$$

Therefore,

$$\begin{aligned} \langle \Psi_p(\vec{\gamma}, \vec{\beta}) | H | \Psi_p(\vec{\alpha}, \vec{\beta}) \rangle &= \langle \Psi_p(\vec{\gamma}, \vec{\beta}) | \sum_{x \in \{0,1\}^n} C(x) |x\rangle \langle x| | \Psi_p(\vec{\alpha}, \vec{\beta}) \rangle \\ &= \sum_{x \in \{0,1\}^n} C(x) \langle \Psi_p(\vec{\gamma}, \vec{\beta}) | x \rangle \langle x | \Psi_p(\vec{\alpha}, \vec{\beta}) \rangle = \sum_{x \in \{0,1\}^n} C(x) p(x) \end{aligned} \tag{29}$$

How to implement with gates efficiently?

$e^{-i\gamma_l w_{j,k}/2(I-\sigma_z^j\sigma_z^k)}$ can be implemented as



- Observe that $e^{-i\gamma_l w_{j,k}/2I}$ is a global phase and can be ignored
-

$$(CX)(I\otimes Rz(\theta))(CX) = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}1&0\\0&1\end{pmatrix}\otimes\begin{pmatrix}e^{-i\theta/2}&0\\0&e^{i\theta/2}\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$$

$$= \begin{pmatrix}e^{-i\theta/2}&0&0&0\\0&e^{i\theta/2}&0&0\\0&0&e^{i\theta/2}&0\\0&0&0&e^{-i\theta/2}\end{pmatrix} = e^{-i\theta/2\sigma_z\sigma_z}$$

How to implement with gates efficiently?

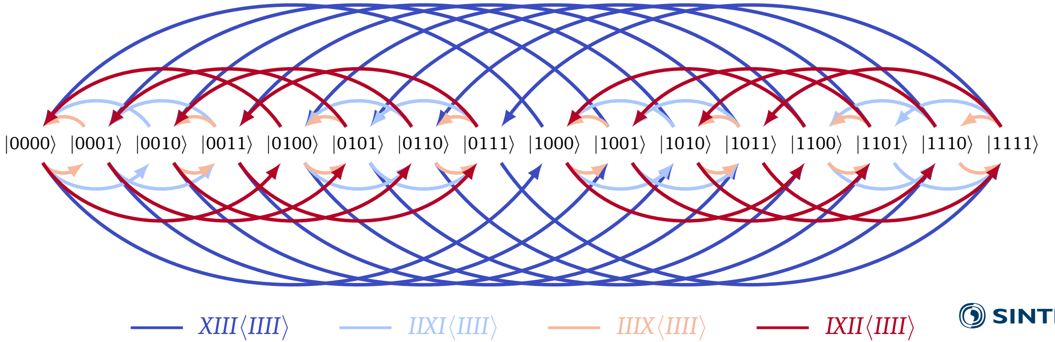
$e^{-i\beta_l X}$ can be implemented as

$$Rx(\theta) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \tag{31}$$

How to implement with gates efficiently?

$e^{-i\beta_l X}$ can be implemented as j-th qubit ——$\boxed{R_x(2\beta_l)}$——

$$Rx(\theta) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \tag{31}$$



Types of approaches

Solving NP hard optimization problems.

- Calculating the cost of all partitions takes exponential time.

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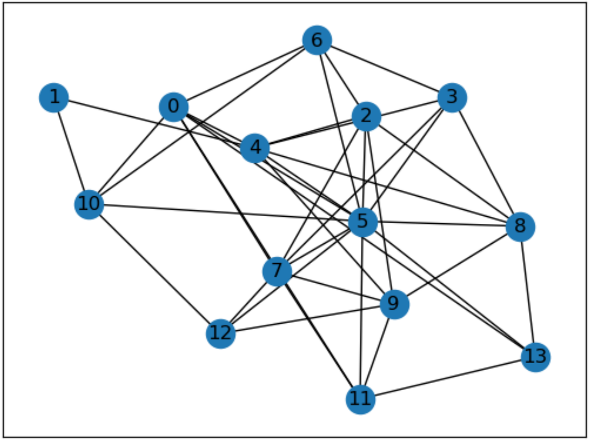
Solving NP hard optimization problems.

- Calculating the cost of all partitions takes exponential time.
- **Heuristic algorithms**. No polynomial run time guarantee; appear to perform well on some instances.
- **Approximate algorithms**. Efficient and provide provable guarantees.
  With high probability we get a solution x^* such that

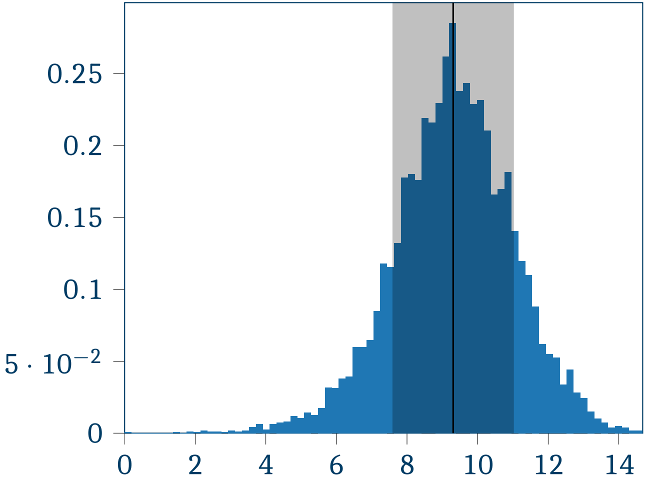
$$\frac{C(x^*) - \min_x C(x)}{\max_x C(x) - \min_x C(x)} \geq \alpha, \tag{32}$$

  where $0 < \alpha \leq 1$ is the approximation ratio.

Example graph



Random sampling



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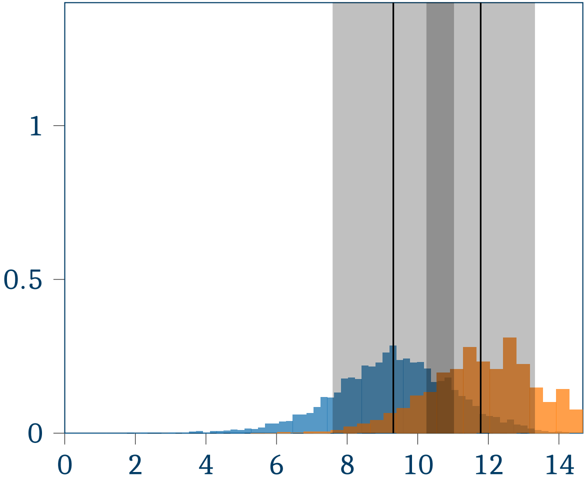
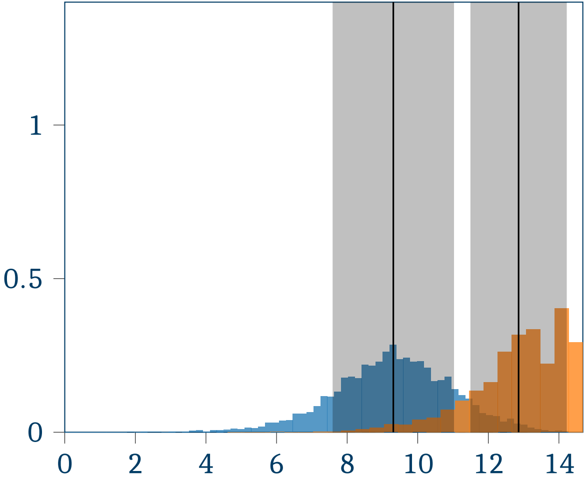
QAOA depth = 1



QAOA depth = 2



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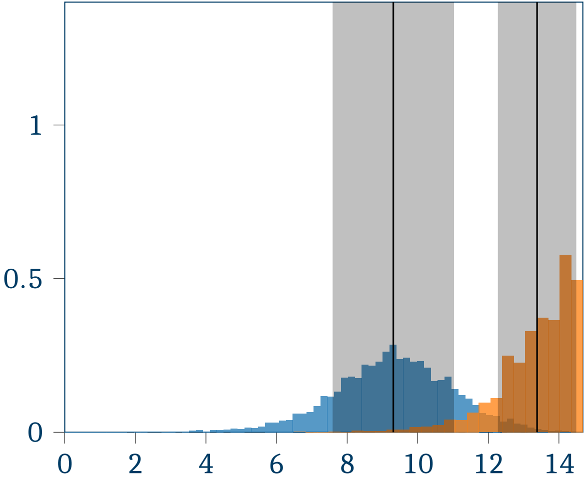
QAOA depth = 3



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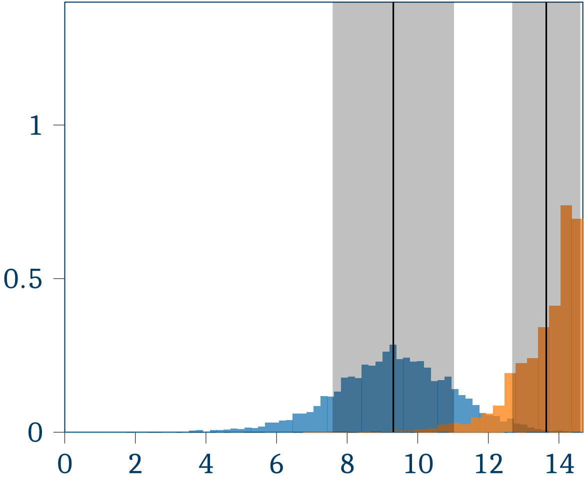
QAOA depth = 4



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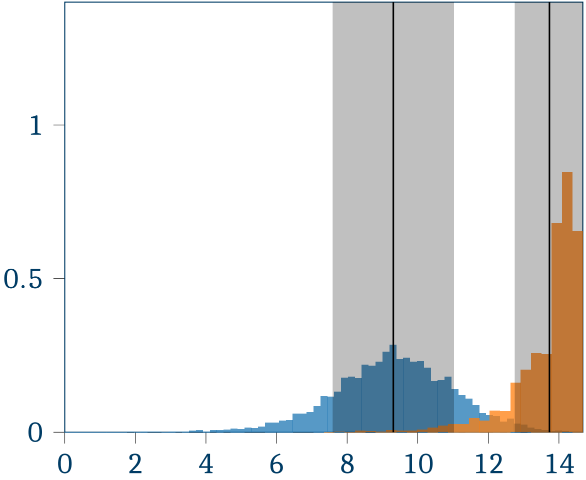
QAOA depth = 5



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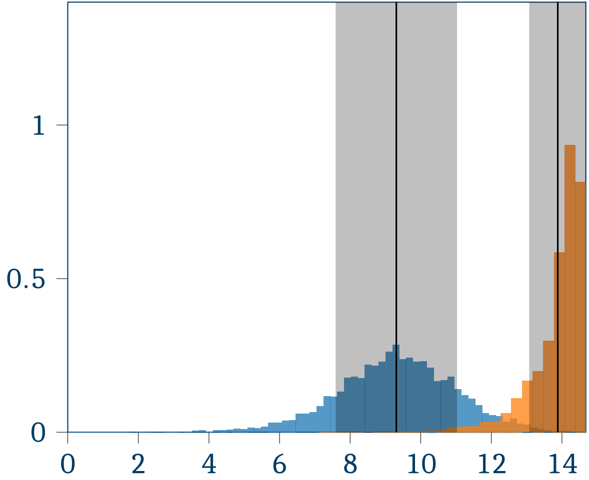
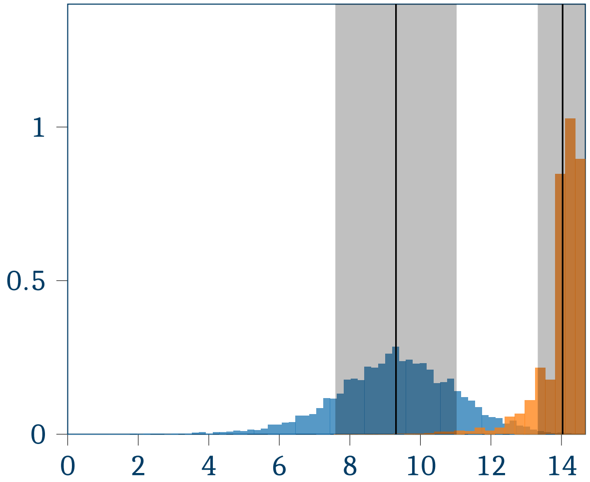
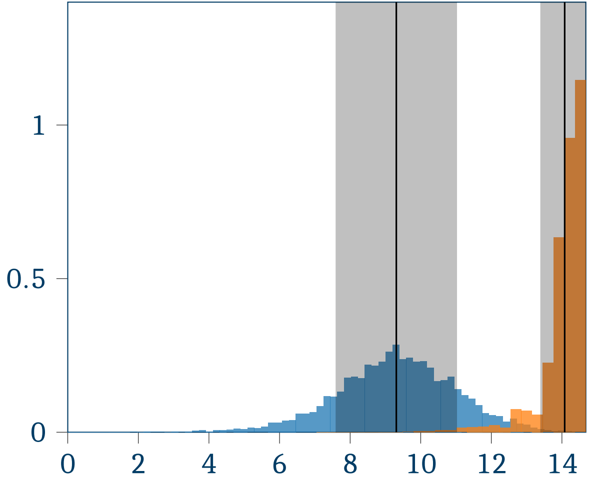
QAOA depth = 6



QAOA depth = 7



QAOA depth = 8



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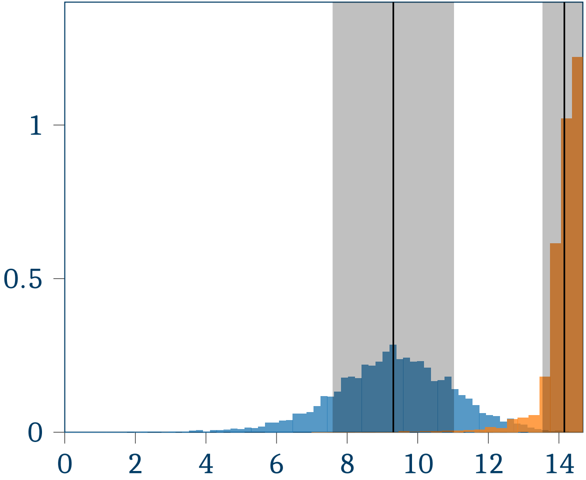
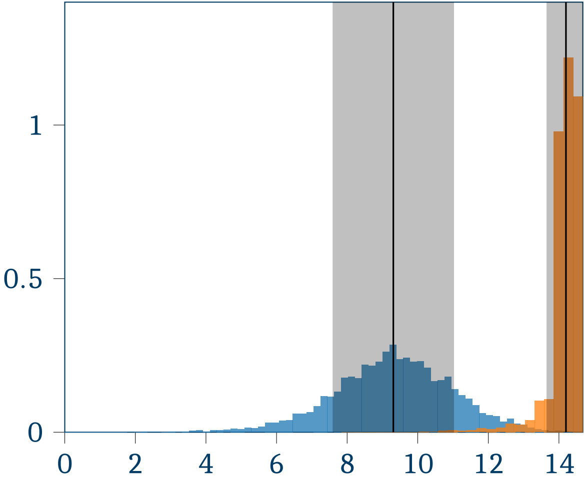
QAOA depth = 9



QAOA depth = 10



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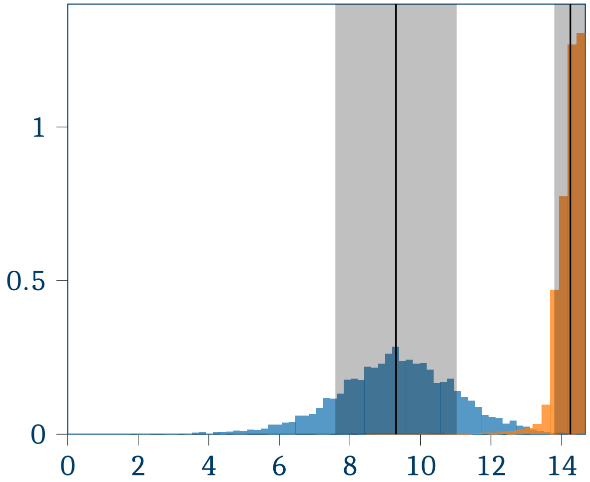
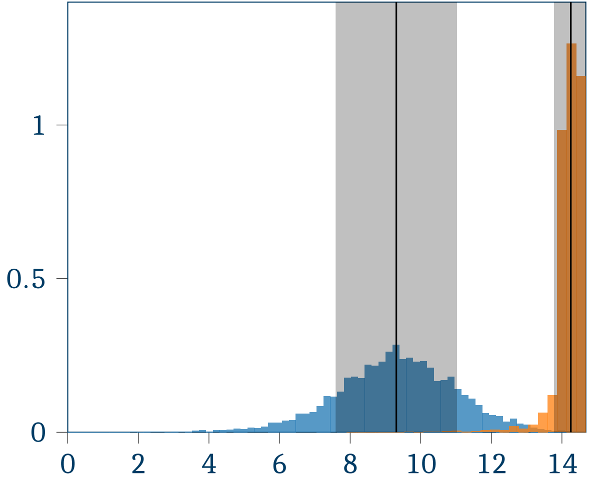
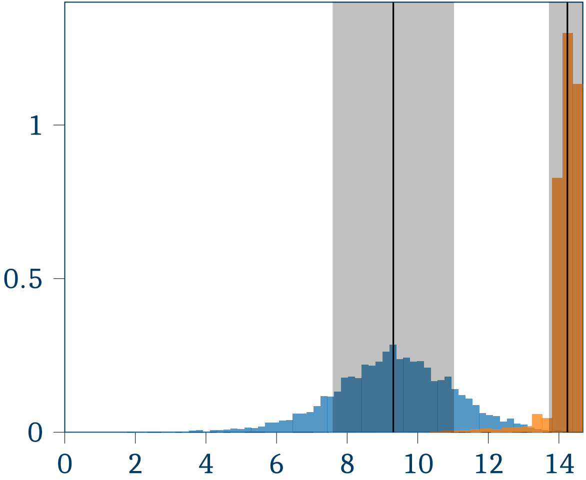
QAOA depth = 11



QAOA depth = 12



QAOA depth = 13



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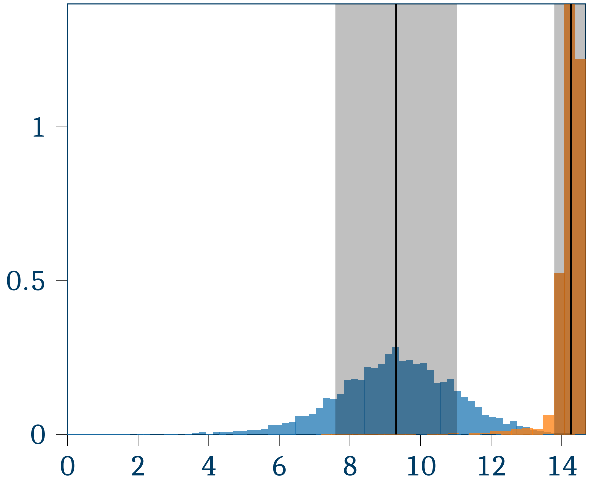
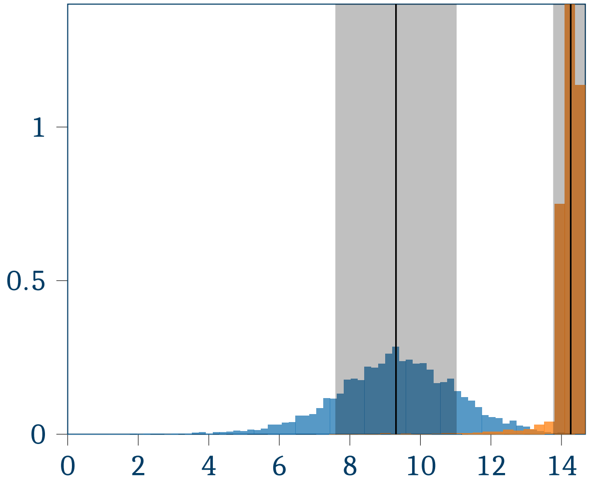
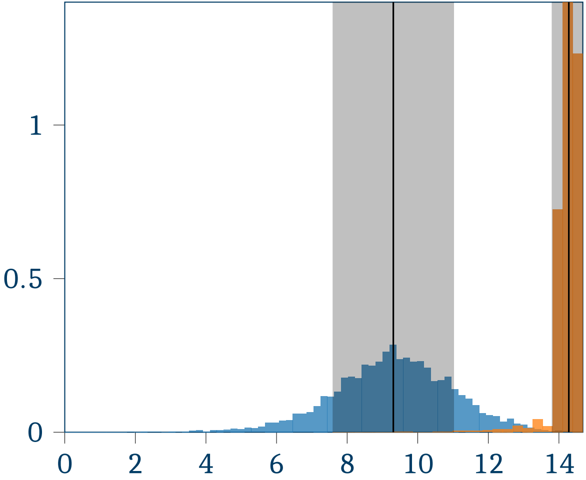
QAOA depth = 14



QAOA depth = 15



QAOA depth = 16



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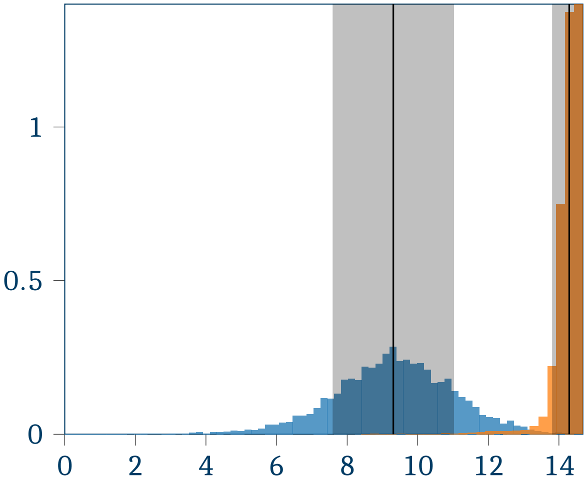
QAOA depth = 17



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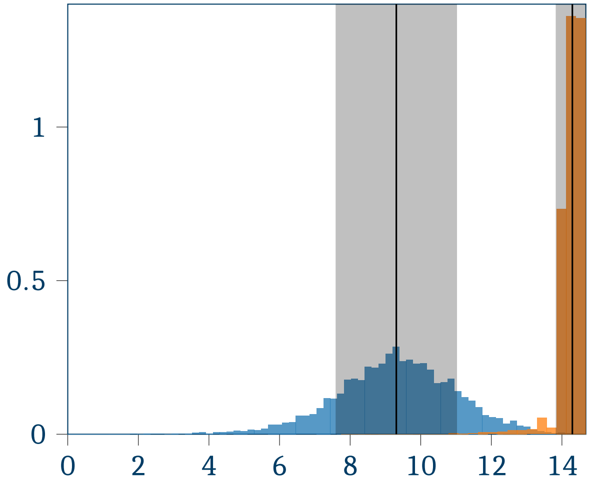
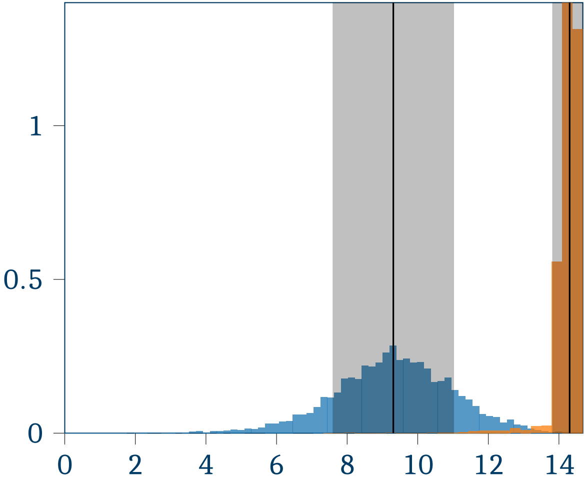
QAOA depth = 18



QAOA depth = 19



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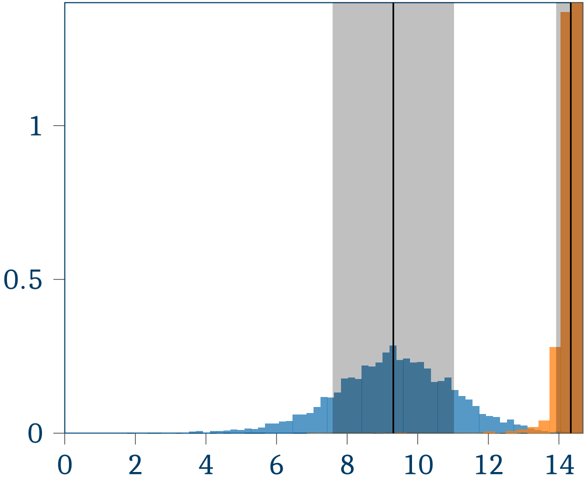
QAOA depth = 20



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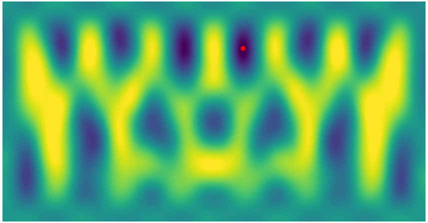
Global continuous optimization problem

original problem $\overset{Hamiltonian}{\longrightarrow}$ minimize $\mathrm{cost}(\theta) = \langle \phi(\theta) | \boldsymbol{A} | \phi(\theta) \rangle$



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Communications in Mathematical Physics, 51(2):183–190, 1976.

Hale F Trotter.
On the product of semi-groups of operators.
Proceedings of the American Mathematical Society, 10(4):545–551, 1959.