

IonQ iQuHack2025 Challenge

Before proceeding, register once. Then, comment out the registration function call to avoid re-registering when running the notebook again.

```
In [7]: import requests
        def register():
            team_name = input("Enter your team name: ")
            in_person = input("Enter participation type - in-person or remote: ")
            data = []
            while email := input("Enter email separated by commas (enter to cancel): "):
                firstname = input("Enter your first name: ")
                lastname = input("Enter your last name: ")
                github = input("Enter your github handle: ")
                data.append((firstname, lastname, email, github))
            for firstname, lastname, email, github in data:
                url = f"https://ionquhack2025.azurewebsites.net/api/registration?TeamName={
                req = requests.post(url)
                print("\n\n\n"+req.text)
        # Comment this out after registration:
        # register()
```

Enter the key you've got on the previous step here:

```
In [27]: key = "61f7aaaf50e899e65f777e0e159408b5335faf68fd58ee21d8941de1907d3cfb"
```

Did you comment out the register() function call?

Please share your research process on GitHub: https://github.com/iQuHACK/2025-lonQ/discussions

Maximum Cut problem (max-cut) with variational Quantum Imaginary Time Evolution (varQITE) method

In this challenge, we demonstrate how to leverage IonQ Forte's industry-leading capabilities to solve instances of the NP-hard combinatorial optimization problem known as Maximum Cut (MaxCut) using a novel variational Quantum Imaginary Time Evolution (varQITE) algorithm developed by IonQ in conjunction with researchers at Oak Ridge National Labs (ORNL).

What's the problem?

MaxCut 101

The Maximum Cut Problem (MaxCut) is a classic combinatorial optimization problem commonly used as an algorithm benchmark by scientific computing researchers. It has numerous applications in a variety of fields: for example, it is used in circuit desing as part of Very Large Scale Integration (VLSI) to find the optimal layout of circuit components; it is used in the study of social networks to identify communities; it is used in computer vision for image segmentation, etc.

MaxCut is a graph problem: given a graph G=(V,E) with vertex set V and edge set E, it asks for a partition of V into sets S and T maximizing the number of edges crossing between S and T.

Think of it like this: you're trying to cut the graph into two pieces, and you want to make the cut so that it slices through as many edges as possible.

Prepare the code environment

First, we'll set up the coding environment and install necessary dependencies.

```
In [1]: pip install qiskit qiskit-aer networkx numpy pandas -q
```

Note: you may need to restart the kernel to use updated packages.

To ensure your code runs correctly everywhere, please only use the imported dependencies. Using external libraries may cause your submission to fail due to missing dependencies on our servers.

```
# Hackathon at iQuHack2025 hosted by MIT and only during the Feb 1-2, 2025
# duration of such event.

import matplotlib.pyplot as plt
from IPython import display

import networkx as nx
import numpy as np
import pandas as pd
import time

from typing import List
from qiskit import QuantumCircuit, transpile
from qiskit.circuit import ParameterVector
from qiskit.quantum_info import SparsePauliOp
from qiskit_aer import AerSimulator
```

Graph definition

A simple graph, defined using the Python NetworkX library, will serve to illustrate the problem and you can explore further complexities.

```
In [3]: # other graphs candidates to check
        import networkx as nx
        import matplotlib.pyplot as plt
        import random
        #-> Cycle Graph C8
        def cycle_graph_c8():
            G = nx.cycle_graph(8)
            plt.figure(figsize=(6, 6))
            pos = nx.circular_layout(G)
            nx.draw(G, pos, with labels=True, node color='lightblue', edge color='gray', no
            plt.title("Cycle Graph C8")
            plt.show()
            return G
        # Path Graph P16
        def path_graph_p16():
            G = nx.path graph(16)
            plt.figure(figsize=(12, 2))
            pos = nx.spring_layout(G, seed=42)
            nx.draw(G, pos, with_labels=True, node_color='lightgreen', edge_color='gray', n
            plt.title("Path Graph P16")
            plt.show()
            return G
        #-> Complete Bipartite Graph K8,8
        def complete_bipartite_graph_k88():
            G = nx.complete_bipartite_graph(8, 8)
            plt.figure(figsize=(8, 6))
            pos = nx.bipartite_layout(G, nodes=range(8))
```

```
nx.draw(G, pos, with_labels=True, node_color=['lightcoral'] * 8 + ['lightblue']
            edge_color='gray', node_size=300)
   plt.title("Complete Bipartite Graph K8,8")
   plt.show()
   return G
#-> Complete Bipartite Graph K8,8
def complete_bipartite_graph_k_nn(n):
   G = nx.complete bipartite graph(n, n)
   plt.figure(figsize=(8, 6))
   pos = nx.bipartite_layout(G, nodes=range(n))
   nx.draw(G, pos, with_labels=True, node_color=['lightcoral'] * n + ['lightblue']
            edge_color='gray', node_size=300)
   plt.title("Complete Bipartite Graph K{},{}".format(n,n))
   plt.show()
   return G
# Star Graph S16
def star_graph_s16():
   G = nx.star_graph(16)
   plt.figure(figsize=(8, 8))
   pos = nx.spring_layout(G, seed=42)
   nx.draw(G, pos, with_labels=True, node_color='gold', edge_color='gray', node_si
   plt.title("Star Graph S16")
   plt.show()
   return G
# Grid Graph 8x4
def grid_graph_8x4():
   G = nx.grid_graph(dim=[8, 4])
   plt.figure(figsize=(12, 6))
   pos = {node: node for node in G.nodes()}
   nx.draw(G, pos, with_labels=True, node_color='lightblue', edge_color='gray', no
   plt.title("Grid Graph 8x4")
   plt.show()
   return G
# Grid Graph 8x4
def grid_graph_nxm(n,m):
   G = nx.grid_graph(dim=[n, m])
   plt.figure(figsize=(12, 6))
   pos = {node: node for node in G.nodes()}
   nx.draw(G, pos, with_labels=True, node_color='lightblue', edge_color='gray', no
   plt.title("Grid Graph {}x{}".format(n,m))
   plt.show()
   return G
#-> 4-Regular Graph with 8 Vertices
def regular graph 4 8():
   G = nx.random_regular_graph(d=4, n=8, seed=42)
   plt.figure(figsize=(6, 6))
   pos = nx.circular_layout(G)
   nx.draw(G, pos, with_labels=True, node_color='lightgreen', edge_color='gray', n
   plt.title("4-Regular Graph with 8 Vertices")
   plt.show()
```

```
return G
#-> Cubic (3-Regular) Graph with 16 Vertices
def cubic_graph_3_16():
   G = nx.random_regular_graph(d=3, n=16, seed=42)
   plt.figure(figsize=(8, 6))
   pos = nx.spring_layout(G, seed=42)
   nx.draw(G, pos, with_labels=True, node_color='lightcoral', edge_color='gray', n
   plt.title("Cubic (3-Regular) Graph with 16 Vertices")
   plt.show()
   return G
# Disjoint Union of Four C4 Cycles
def disjoint_union_c4():
   cycles = [nx.cycle_graph(4) for _ in range(4)]
   G = nx.disjoint_union_all(cycles)
   plt.figure(figsize=(12, 6))
   pos = \{\}
   shift x = 0
   for component in nx.connected components(G):
        subgraph = G.subgraph(component)
        pos_sub = nx.circular_layout(subgraph, scale=1, center=(shift_x, 0))
        pos.update(pos_sub)
        shift_x += 3
   nx.draw(G, pos, with_labels=True, node_color='lightblue', edge_color='gray', no
   plt.title("Disjoint Union of Four C4 Cycles")
   plt.show()
   return G
# Complete Bipartite Graph K16,16
def complete bipartite graph k1616():
   G = nx.complete bipartite graph(16, 16)
   plt.figure(figsize=(12, 6))
   pos = nx.bipartite layout(G, nodes=range(16))
   nx.draw(G, pos, with_labels=False, node_color=['lightcoral'] * 16 + ['lightblue']
            edge_color='gray', node_size=100)
   plt.title("Complete Bipartite Graph K16,16")
   plt.show()
   return G
# 5-Dimensional Hypercube Graph Q5
def hypercube_graph_q5():
   G = nx.hypercube_graph(5)
   plt.figure(figsize=(10, 8))
   pos = nx.spring_layout(G, seed=42)
   nx.draw(G, pos, with_labels=False, node_color='lightgreen', edge_color='gray',
   plt.title("5-Dimensional Hypercube Graph Q5")
   plt.show()
   return G
# Tree Graph with 8 Vertices
def tree_graph_8():
   G = nx.balanced_tree(r=2, h=2)
   G.add edge(6, 7)
   plt.figure(figsize=(8, 6))
   pos = nx.spring layout(G, seed=42)
```

```
nx.draw(G, pos, with_labels=True, node_color='lightblue', edge_color='gray', no
    plt.title("Tree Graph with 8 Vertices")
    plt.show()
    return G
# Wheel Graph W16
def wheel graph w16():
    G = nx.wheel_graph(16)
    plt.figure(figsize=(8, 8))
    pos = nx.circular_layout(G)
    nx.draw(G, pos, with_labels=True, node_color='lightcoral', edge_color='gray', n
    plt.title("Wheel Graph W16")
    plt.show()
    return G
#-> Random Connected Graph with 16 Vertices
def random_connected_graph_16(p=0.15):
    \#n, p = 16, 0.25
    n=16
    while True:
        G = nx.erdos_renyi_graph(n, p, seed=random.randint(1, 10000))
        if nx.is_connected(G):
            break
    plt.figure(figsize=(10, 8))
    pos = nx.spring_layout(G, seed=42)
    nx.draw(G, pos, with_labels=False, node_color='lightgreen', edge_color='gray',
    plt.title("Random Connected Graph with 16 Vertices")
    plt.show()
    return G
# Expander Graph with 32 Vertices
def expander graph 32():
    G = nx.random_regular_graph(4, 32, seed=42)
    plt.figure(figsize=(10, 8))
    pos = nx.spring_layout(G, seed=42)
    nx.draw(G, pos, with_labels=False, node_color='lightblue', edge_color='gray', n
    plt.title("Expander Graph with 32 Vertices")
    plt.show()
    return G
#-> Expander Graph with n Vertices
def expander_graph_n(n):
    G = nx.random_regular_graph(4, n, seed=42)
    plt.figure(figsize=(10, 8))
    pos = nx.spring_layout(G, seed=42)
    nx.draw(G, pos, with_labels=False, node_color='lightblue', edge_color='gray', n
    plt.title("Expander Graph with {} Vertices".format(n))
    plt.show()
    return G
# Planar Connected Graph with 16 Vertices
def planar_connected_graph_16():
    G = nx.grid_graph(dim=[8, 2])
    G = nx.convert_node_labels_to_integers(G)
    additional_edges = [(0, 9), (1, 10), (2, 11), (3, 12), (4, 13), (5, 14), (6, 15
                        (7, 15), (8, 7)]#, (6, 15), (14, 1), (1, 13), (10, 9), (0, 15)
```

```
G.add_edges_from([e for e in additional_edges if e[0] < 16 and e[1] < 16])
assert nx.check_planarity(G)[0], "Graph is not planar."
pos = {node: (node // 2, node % 2) for node in G.nodes()}
plt.figure(figsize=(16, 8))
nx.draw(G, pos, with_labels=False, node_color='lightcoral', edge_color='gray',
plt.title("Planar Connected Graph with 16 Vertices")
plt.axis('equal')
plt.show()
return G</pre>
```

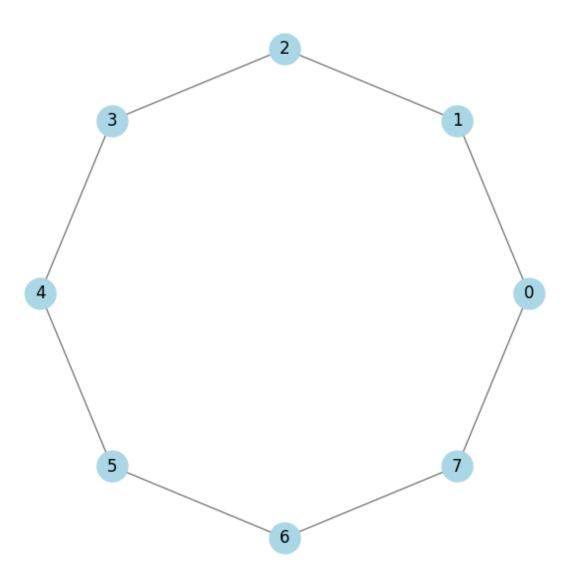
We've suggested a few graph ideas above.

The list below highlights those achievable with minimal computational resources, whether on a local laptop or a cloud instance. Some are simply too large.

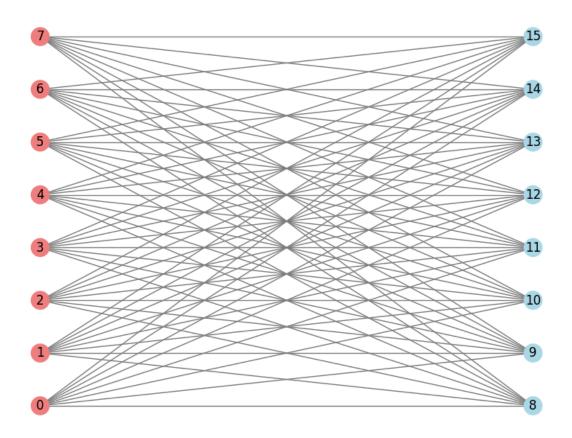
```
In [4]: # Choose your favorite graph and build your winning ansatz!

graph1 = cycle_graph_c8()
graph2 = complete_bipartite_graph_k88()
graph3 = complete_bipartite_graph_k_nn(5)
graph4 = regular_graph_4_8()
graph5 = cubic_graph_3_16()
graph6 = random_connected_graph_16(p=0.18)
graph7 = expander_graph_n(16)
#graph8 = -> make your own cool graph
```

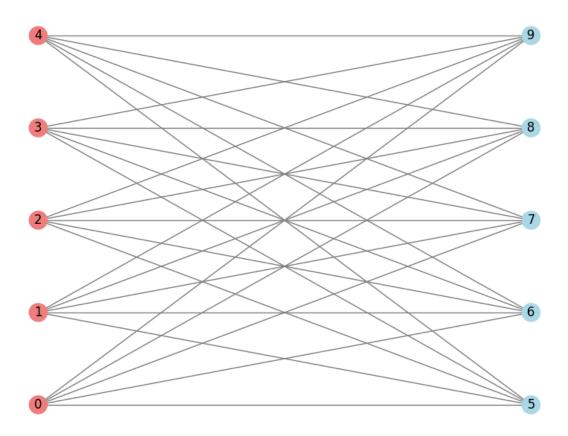
Cycle Graph C8



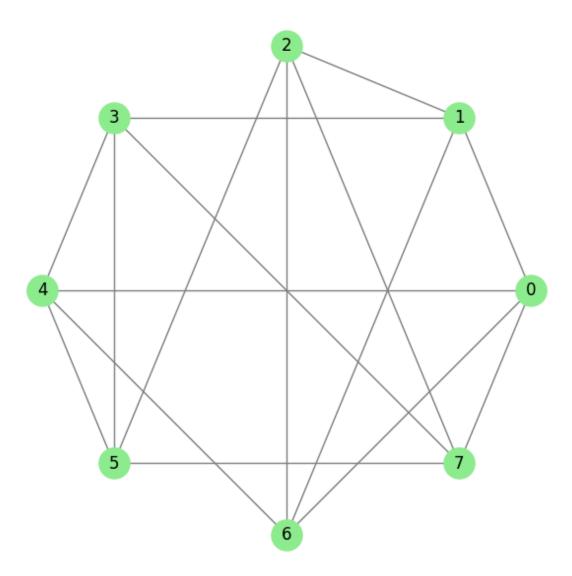
Complete Bipartite Graph K8,8



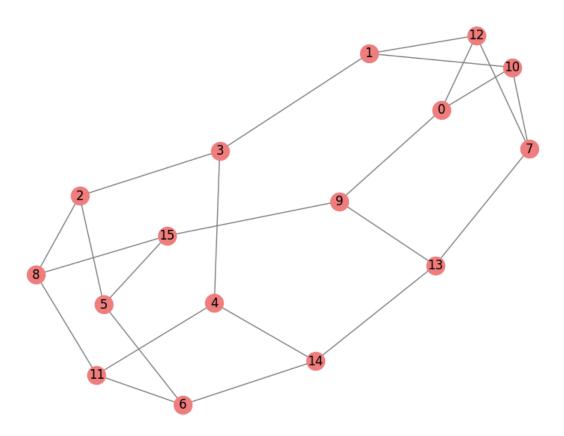
Complete Bipartite Graph K5,5



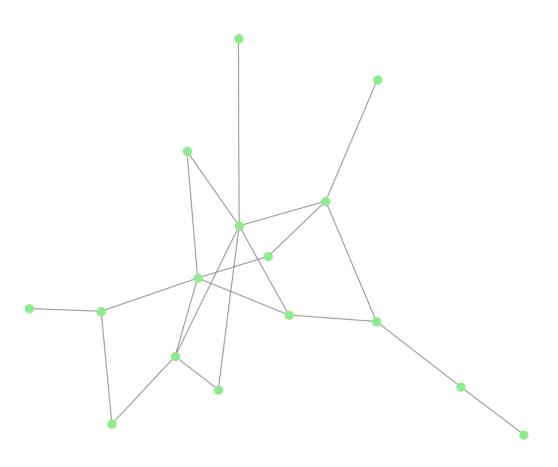
4-Regular Graph with 8 Vertices



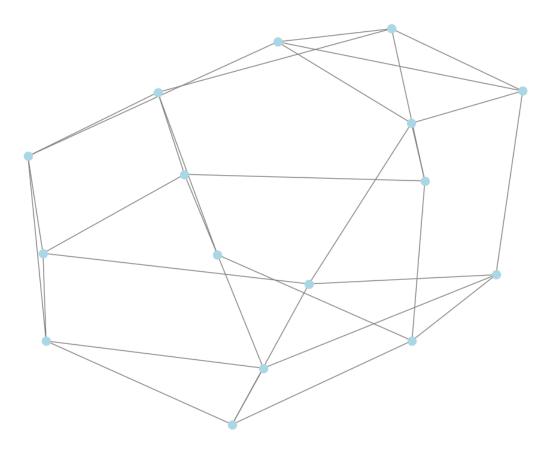
Cubic (3-Regular) Graph with 16 Vertices



Random Connected Graph with 16 Vertices



Expander Graph with 16 Vertices



Input graph

In [290... graph = graph5 graph

Out[290... <networkx.classes.graph.Graph at 0x2085132c390>

Play around with all of them

Quantum Circuit Generator

We start by generating parameterized circuit based on a given graph.

Note: Future experiments will focus on optimizing this circuit generator (this function below). Maximizing your score requires minimizing the number of gates in the generated parameterized circuit.

Set of Rules:

Rules: Do not rename the function, import external libraries (except Qiskit), or use classical solvers. Implement any needed algorithms (e.g., sorting) within the function. Minimize gate count. Run locally for all the graphs before submitting the results.

Let's iterate again.

This challenge requires you to work within the provided function's name and scope. You may only use Qiskit libraries. Do not import additional libraries or call external functions. If your solution requires operations like sorting, implement them directly within the function. Critically, do *not* use a classical algorithm to solve the problem and simply input the result. Optimize your code to minimize the number of quantum gates, while aiming for the correct solutions distribution. Thoroughly get your solution results to report at the end.

Important note: To confirm your results, please save this notebook including all cell outputs and upload it in the form here: https://forms.gle/tAjnUd7b5t3oX3b2A . To avoid exceeding the notebook's 10MB file size limit, please be mindful of the number of print statements you use. Feel free to modify the notebook as needed. However, please ensure your code is readable. Please thoroughly comment your code; we will evaluate your problem-solving approach based on the educational clarity of your explanations.

Good luck, and have fun!

```
In [291... # Visualization will be performed in the cells below;

def build_ansatz(graph: nx.Graph) -> QuantumCircuit:
    ansatz = QuantumCircuit(graph.number_of_nodes())
    ansatz.h(range(graph.number_of_nodes()))

theta = ParameterVector(r"$\theta$", graph.number_of_edges())
    for t, (u, v) in zip(theta, graph.edges):
        ansatz.cx(u, v)
        ansatz.ry(t, v)
        ansatz.cx(u, v)

return ansatz
```

```
# alternate method to make the ansatz

# function to generate a maximum spanning tree of the graph
def generate_max_spanning_tree(G):
    # for u, v in G.edges:
    # G[u][v]['weight'] *= -1
    return nx.minimum_spanning_tree(G, algorithm='kruskal')

# function to return the graph with the spanning tree edges removed
def remove_spanning_tree_edges(G, T):
    H = G.copy()
    for edge in T.edges:
```

```
H.remove_edge(*edge)
return H
```

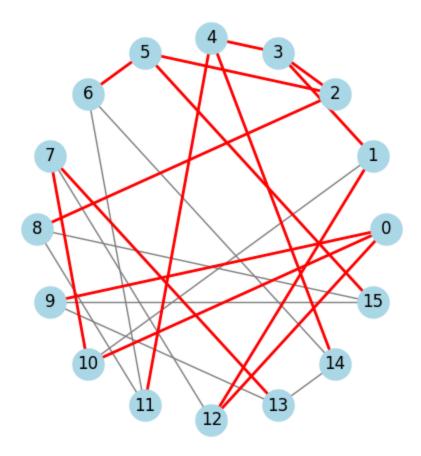
```
# get the maximum spanning tree of the graph by negating all the edge weights and c
T = generate_max_spanning_tree(graph)

# remove the edges of the spanning tree from the graph
H = remove_spanning_tree_edges(graph, T)

# visualize the tree and the graph with the tree edges removed
plt.figure(figsize=(12, 6))
plt.subplot(121)
pos = nx.circular_layout(graph)
nx.draw(graph, pos, with_labels=True, node_color='lightblue', edge_color='gray', no
nx.draw_networkx_edges(T, pos, edge_color='red', width=2)
plt.title("Graph with Maximum Spanning Tree")
```

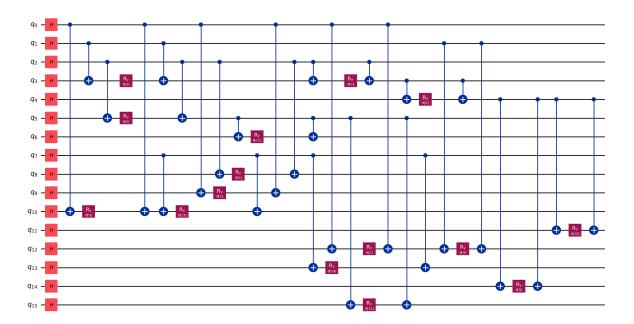
Out[293... Text(0.5, 1.0, 'Graph with Maximum Spanning Tree')

Graph with Maximum Spanning Tree



```
In [294... # build the ansatz circuit for both T and H
ansatz_T = build_ansatz(T)
ansatz_H = build_ansatz(H)
In [295... # visualize the ansatz circuit for the tree
ansatz_T.draw("mpl", fold=-1)
```

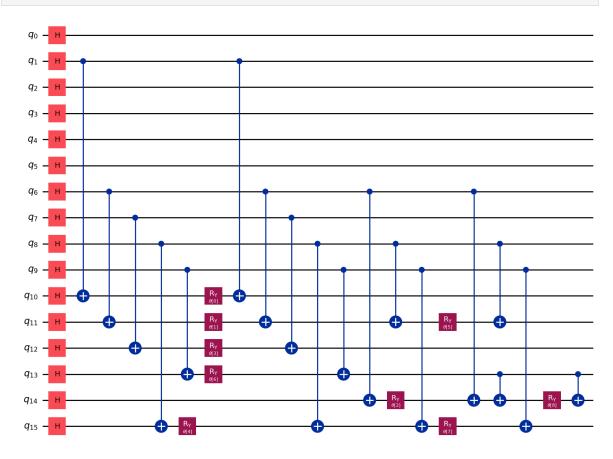
Out[295...



In [296...

visualize the ansatz circuit for the graph with the tree edges removed
ansatz_H.draw("mpl", fold=-1)

Out[296...



On Parametrized Quantum Circuits

Parametrized quantum circuits (PQC) recently have gained significant attention as a prominent way to reach quantum advantage in many different fields. They are characterized

by their use of varying parameters within quantum gates and can be optimized to solve specific problems, such as machine learning, quantum optimization, or quantum chemistry.

PQCs usually consist of three main parts:

- 1. Initialization: The qubits are set to a known starting state (usually $|0\rangle$) and then set into superposition with Hadamard gates.
- 2. Parameterized gates, such as rotation gates (Rx, Ry, Rz), and entanglement gates are adjustable. Their parameters can be optimized to reflect the relationships between the encoded problem data.
- 3. Measurement: After applying the parameterized gates, the qubits are measured to get results.

These circuits are important elements in Variational Quantum Algorithms (VQA), hybrid quantum-classical systems where classical optimization helps to improve quantum operations. Two most notable examples of VQAs are Variational Quantum Eigensolver (VQE), an algorithm that finds a ground state energy of a given Hamiltonian, and Quantum Approximate Optimization Algorithm (QAOA), which is designed for solving combinatorial optimization problems. Near-term quantum computers are noisy and limited in size, and PQCs provide a practical way for us to use them more effectively.

More on that topic: https://arxiv.org/abs/2207.06850

Back to the problem in hand

This function produces parametrized quantum circuits (PQCs), a visualization of which is provided below.

In [297... ansatz = build_ansatz(graph)
ansatz.draw("mpl", fold=-1)
Out[297...

Building the MaxCut Hamiltonian

Formally, we write MaxCut as a Quadratic Program (QP) with binary decision variables as follows. For each node $v \in V$, we let x_v denote a binary variable indicating whether v

belongs to S or T. The objective is to maximize the number of cut edges:

$$ext{maximize}_x \quad \sum_{(v,w) \in E} (x_v + x_w - 2x_v x_w)$$

Let's break this down. Notice that for each edge e=(v,w) in the graph, the quantity $(x_v+x_w-2x_vx_w)$ indicates whether e is cut by the partition represented by x; that is, the quantity $(x_v+x_w-2x_vx_w)$ is zero or one, and it equals one only if v and w lie on different sides of the partition specified by x.

The code cell below obtains a symbolic representation of the maximization objective corresponding to the graph above.

```
def build maxcut_hamiltonian(graph: nx.Graph) -> SparsePauliOp:
In [298...
               Build the MaxCut Hamiltonian for the given graph H = (|E|/2)*I - (1/2)*\Sigma_{\{(i,j)\}}
               num_qubits = len(graph.nodes)
               edges = list(graph.edges())
               num_edges = len(edges)
               pauli_terms = ["I"*num_qubits] # start with identity
               coeffs = [-num edges / 2]
               for (u, v) in edges: # for each edge, add -(1/2)*Z_i Z_j
                   z_term = ["I"] * num_qubits
                   z_{term[u]} = "Z"
                   z_{term[v]} = "Z"
                   pauli_terms.append("".join(z_term))
                   coeffs.append(0.5)
               return SparsePauliOp.from_list(list(zip(pauli_terms, coeffs)))
          # get the maxcut hamiltonian for the tree
In [299...
          H_maxcut_T = build_maxcut_hamiltonian(T)
           # get the maxcut hamiltonian for the graph with the tree edges removed
          H_maxcut_H = build_maxcut_hamiltonian(H)
In [300...
          print(H_maxcut_T)
          print(H maxcut H)
```

Let's keep this function contained within its own cell, as you might need to adapt it for various max-cut problem types later.

```
ham = build maxcut hamiltonian(graph)
In [301...
     SparsePauliOp(['IIIIIIIIIIIII', 'ZIIIIIIIIIII', 'ZIIIIIIII', 'ZIIIIIIII', 'ZIIIIII
Out[301...
      IIIIIIZIII', 'IZIZIIIIIIIIIIII', 'IZIIIIIIIIIZIII', 'IZIIIIIIIIZIIII', 'IZIIIIIIII', 'IIZIIZII
      Z', 'IIIIIIIIIIIIZZI'],
              coeffs=[-12. +0.j, 0.5+0.j, 0.5+0.j, 0.5+0.j, 0.5+0.j,
                                                  0.5
      +0.j,
       0.5+0.j, 0.5+0.j, 0.5+0.j, 0.5+0.j, 0.5+0.j,
       0.5+0.j, 0.5+0.j, 0.5+0.j, 0.5+0.j, 0.5+0.j,
       0.5+0.i, 0.5+0.i, 0.5+0.i, 0.5+0.i, 0.5+0.i, 0.5+0.i,
       0.5+0.j
```

As a Hamiltonian energy minimization problem

Quantum MaxCut

Quantum computers are good at finding the ground state of particle systems evolving under the action of a given Hamiltonian. In this section, we'll construct a Hamiltonian whose energies are exactly the values of the MaxCut objective function. This correspondence will effectively translate our classical combinatorial optimization problem into a quantum problem, which we'll approach using our novel heuristic.

Given an objective function C(x), with domain $x \in \{0,1\}^n$, we'll produce a Hamiltonian H_C on n gubits such that

$$H_C \setminus \mathbf{ket} x = C(x) \setminus \mathbf{ket} x$$
.

In the last equation, $\backslash ket x$ denotes the n-qubit computational basis state indexed by the bit-string $x \in \{0,1\}$. Thus the last equation says each of the 2^n computational basis states

is an eigenvector of H_C , and the eigenvalue corresponding to $\backslash \ker x$ is C(x); that is, H_C is diagonal with respect to the computational basis, and its energies are the values of the objective function C.

We'll obtain the Hamiltonian H_C by replacing each x_j in the expression of C(x) by the operator

$$\hat{X}_j \setminus \operatorname{coloneqq} \frac{1}{2} (I - Z_j),$$

where I denotes the identity operator on n qubits and Z_j denotes the Pauli-Z operator acting on the jth qubit. Notice that \hat{X}_j is diagonal with respect to the computational basis, and its eigenvalues are zero and one; in particular,

$$\hat{X}_i \backslash \text{ket} x = x_i \backslash \text{ket} x.$$

MaxCut Hamiltonian

When we apply the Ising map construction to the MaxCut objective

$$M(x) = \sum_{(v,w) \in E} (x_v + x_w - 2x_v x_w)$$

we obtain the Hamiltonian

$$H_M = \sum_{(v,w) \in E} (X_v + X_w - 2X_v X_w) = rac{1}{2} \sum_{(v,w) \in E} ig(2I - Z_v - Z_w - (I - Z_v)(I - Z_w) ig) = rac{1}{2} ert$$

In the last equation, |E| denotes the number of edges in the graph.

Energy minimization via QITE

Enter varQITE

With the MaxCut Hamiltonian in hand, we can turn to minimizing its energy using our novel quantum-classical varQITE heuristic. Much like any Variataional Quantum Algorithm (VQA), our novel varQITE method provides a recipe for iteratively updating the parameters in a variational quantum circuit to minimize the expectation value of the MaxCut Hamiltonian, measured with respect to the parametrized state.

A key novelty is that our varQITE algorithm does *not* rely on a classical optimizer to update the circuit parameters; instead, it specifies an explicit update rule based on the solution of a system linear Ordinary Differential Equations (ODEs). The ODEs relate the gradient of the variational circuit parameters to the expected value of certain operators related to the MaxCut Hamiltonian, and they are derived from an Ehrenfest Theorem that applies to imaginary time evolution. For details, see Equation (5) in our varQITE paper.

In any case, setting up the ODE system at each step of the algorithm requires executing a batch of quantum circuits and running some post-processing to evaluate the results.

The code cell below illustrates how to set up the variational ansatz $\backslash \ker \Psi(\theta)$ introduced by our varQITE paper in Equation (2). We'll set up the required circuits and the ODEs further down.

Below is simplified version of Quantum Imaginary Time Evolution (QITE). It uses a finite differences approach to estimate gradients, then performs gradient descent updates.

In [302... class OITEvolver: A class to evolve a parametrized quantum state under the action of an Ising Hamiltonian according to the variational Quantum Imaginary Time Evolution (QITE) principle described in IonQ's latest joint paper with ORNL. def init (self, hamiltonian: SparsePauliOp, ansatz: QuantumCircuit): self.hamiltonian = hamiltonian self.ansatz = ansatz # Define some constants self.backend = AerSimulator() self.num shots = 10000self.energies, self.param_vals, self.runtime = list(), list(), list() def evolve(self, num steps: int, lr: float = 0.4, verbose: bool = True): Evolve the variational quantum state encoded by ``self.ansatz`` under the action of ``self.hamiltonian`` according to varQITE. curr_params = np.zeros(self.ansatz.num_parameters) for k in range(num_steps): # Get circuits and measure on backend iter_qc = self.get_iteration_circuits(curr_params) job = self.backend.run(iter_qc, shots=self.num_shots) q0 = time.time() measurements = job.result().get_counts() quantum_exec_time = time.time() - q0 # Update parameters-- set up defining ODE and step forward Gmat, dvec, curr_energy = self.get_defining_ode(measurements) dcurr params = np.linalg.lstsq(Gmat, dvec, rcond=1e-2)[0] curr_params += lr * dcurr_params # Progress checkpoint! if verbose: self.print_status(measurements) self.energies.append(curr energy) self.param_vals.append(curr_params.copy()) self.runtime.append(quantum_exec_time)

def get_defining_ode(self, measurements: List[dict[str, int]]):

```
Construct the dynamics matrix and load vector defining the varQITE
    # Load sampled bitstrings and corresponding frequencies into NumPy arrays
    dtype = np.dtype([("states", int, (self.ansatz.num_qubits,)), ("counts", "f
    measurements = [np.fromiter(map(lambda kv: (list(kv[0]), kv[1]), res.items(
    # Set up the dynamics matrix by computing the gradient of each Pauli word
    # with respect to each parameter in the ansatz using the parameter-shift ru
    pauli_terms = [SparsePauliOp(op) for op, _ in self.hamiltonian.label_iter()
    Gmat = np.zeros((len(pauli_terms), self.ansatz.num_parameters))
    for i, pauli_word in enumerate(pauli_terms):
        for j, jth_pair in enumerate(zip(measurements[1::2], measurements[2::2]
            for pm, pm_shift in enumerate(jth_pair):
                Gmat[i, j] += (-1)**pm * expected_energy(pauli_word, pm_shift)
    # Set up the load vector
    curr_energy = expected_energy(self.hamiltonian, measurements[0])
    dvec = np.zeros(len(pauli terms))
    for i, pauli word in enumerate(pauli terms):
        rhs_op_energies = get_ising_energies(pauli_word, measurements[0]["state
        rhs_op_energies *= get_ising_energies(self.hamiltonian, measurements[0]
        dvec[i] = -np.dot(rhs_op_energies, measurements[0]["counts"]) / self.nu
    return Gmat, dvec, curr_energy
def get_iteration_circuits(self, curr_params: np.array):
    Get the bound circuits that need to be evaluated to step forward
    according to QITE.
    # Use this circuit to estimate your Hamiltonian's expected value
    circuits = [self.ansatz.assign parameters(curr params)]
    # Use these circuits to compute gradients
    for k in np.arange(curr_params.shape[0]):
        for j in range(2):
            pm_shift = curr_params.copy()
            pm \ shift[k] += (-1)**j * np.pi/2
            circuits += [self.ansatz.assign_parameters(pm_shift)]
    # Add measurement gates and return
    [qc.measure_all() for qc in circuits]
    return circuits
def plot_convergence(self):
    Plot the convergence of the expected value of ``self.hamiltonian`` with
    respect to the (imaginary) time steps.
    plt.plot(self.energies)
    plt.xlabel("(Imaginary) Time step")
    plt.ylabel("Hamiltonian energy")
    plt.title("Convergence of the expected energy")
def print_status(self, measurements):
```

```
Print summary statistics describing a QITE run.
"""

stats = pd.DataFrame({
    "curr_energy": self.energies,
    "num_circuits": [len(measurements)] * len(self.energies),
    "quantum_exec_time": self.runtime
})

stats.index.name = "step"
display.clear_output(wait=True)
display.display(stats)
```

A few utility functions:

```
def interpret_solution(graph, bitstring):
In [306...
              Visualize the given ``bitstring`` as a partition of the given ``graph``.
              pos = nx.spring_layout(graph, seed=42)
              set_0 = [i for i, b in enumerate(bitstring) if b == '0']
              set_1 = [i for i, b in enumerate(bitstring) if b == '1']
              plt.figure(figsize=(4, 4))
              nx.draw_networkx_nodes(graph, pos=pos, nodelist=set_0, node_color='blue', node_
              nx.draw_networkx_nodes(graph, pos=pos, nodelist=set_1, node_color='red', node_s
              cut_edges = []
              non_cut_edges = []
              for (u, v) in graph.edges:
                  if bitstring[u] != bitstring[v]:
                      cut_edges.append((u, v))
                  else:
                      non_cut_edges.append((u, v))
              nx.draw_networkx_edges(graph, pos=pos, edgelist=non_cut_edges, edge_color='gray
              nx.draw_networkx_edges(graph, pos=pos, edgelist=cut_edges, edge_color='green',
              nx.draw_networkx_labels(graph, pos=pos, font_color='white', font_weight='bold')
              plt.axis('off')
              plt.show()
```

curr_energy num_circuits quantum_exec_time

step			
0	-11.9851	49	2.926789
1	-11.9698	49	2.581497
2	-12.0819	49	2.381946
3	-12.7734	49	2.433768
4	-11.9958	49	2.204524
5	-11.3017	49	2.401866
6	-11.3164	49	2.465045
7	-11.8922	49	2.201644
8	-12.0624	49	2.432921
9	-12.1391	49	2.302248
10	-12.4059	49	2.482618
11	-12.1881	49	2.464386
12	-12.3540	49	2.361092
13	-12.6030	49	2.435034
14	-12.6092	49	2.271876
15	-12.8726	49	2.972570
16	-12.8067	49	2.202216
17	-12.7812	49	2.169699
18	-12.2843	49	2.214199
19	-12.3846	49	2.285783
20	-12.4820	49	2.368450
21	-12.4200	49	2.289847
22	-12.4804	49	2.435036
23	-12.5000	49	2.404916
24	-12.5778	49	2.402697
25	-12.6824	49	2.489310
26	-12.6948	49	2.389317
27	-12.8738	49	2.459233
28	-12.7837	49	2.433296

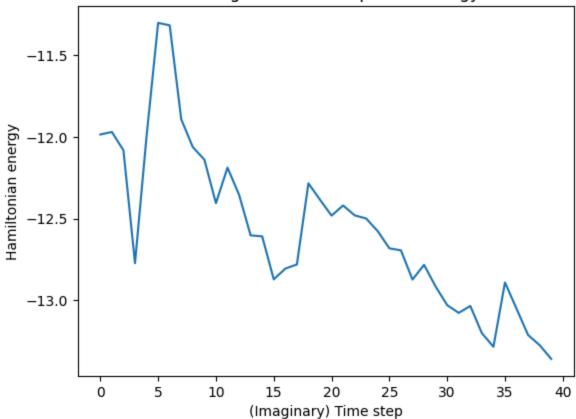
curr_energy num_circuits quantum_exec_time

step			
29	-12.9162	49	2.434023
30	-13.0303	49	2.196268
31	-13.0779	49	2.270947
32	-13.0356	49	2.403818
33	-13.2019	49	2.385900
34	-13.2855	49	2.427895
35	-12.8916	49	2.349488
36	-13.0525	49	2.201709
37	-13.2135	49	2.256346
38	-13.2758	49	2.351604

CPU times: total: 16min 27s

Wall time: 2min 6s

Convergence of the expected energy



```
qit_evolver_T.evolve(num_steps=40, lr=0.1, verbose=True)
# Visualize your results!
qit_evolver_T.plot_convergence()
```

curr_energy num_circuits quantum_exec_time

step			
0	-7.5027	31	1.863185
1	-7.5505	31	1.653444
2	-7.6127	31	1.414492
3	-7.7688	31	1.600814
4	-7.7711	31	1.665730
5	-7.8288	31	1.536808
6	-7.9712	31	1.461215
7	-8.0513	31	1.435824
8	-8.1033	31	1.402839
9	-8.1649	31	1.451447
10	-8.2454	31	1.400297
11	-8.3400	31	1.441431
12	-8.4890	31	1.335682
13	-8.4652	31	1.365992
14	-8.5871	31	1.431898
15	-8.6236	31	1.447386
16	-8.8158	31	1.364285
17	-8.7170	31	1.491132
18	-8.8512	31	1.404974
19	-8.9750	31	1.468778
20	-9.0490	31	1.382346
21	-9.2094	31	1.363024
22	-9.2806	31	1.415356
23	-9.4053	31	1.267308
24	-9.5321	31	1.369168
25	-9.5800	31	1.425491
26	-9.6566	31	1.401311
27	-9.7179	31	1.384993
28	-9.8157	31	1.319627

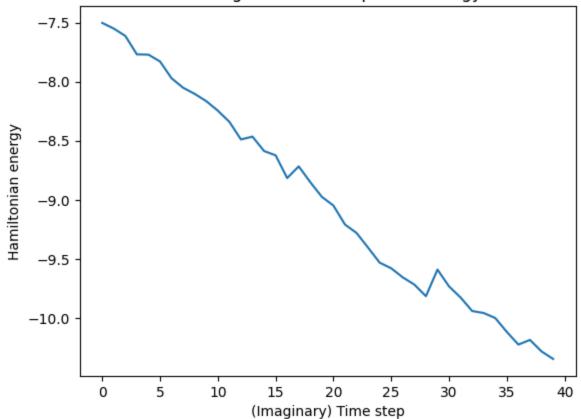
curr_energy num_circuits quantum_exec_time

step			
29	-9.5907	31	1.360190
30	-9.7332	31	1.433958
31	-9.8273	31	1.389221
32	-9.9413	31	1.358191
33	-9.9585	31	1.439763
34	-10.0010	31	1.354221
35	-10.1189	31	1.287035
36	-10.2255	31	1.400928
37	-10.1861	31	1.367295
38	-10.2836	31	1.232846

CPU times: total: 10min 16s

Wall time: 1min 10s

Convergence of the expected energy



In [309...

%%time

Set up your QITEvolver for the graph with the tree edges removed
qit_evolver_H = QITEvolver(H_maxcut_H, ansatz_H)

```
qit_evolver_H.evolve(num_steps=40, lr=0.1, verbose=True)
# Visualize your results!
qit_evolver_H.plot_convergence()
```

curr_energy num_circuits quantum_exec_time

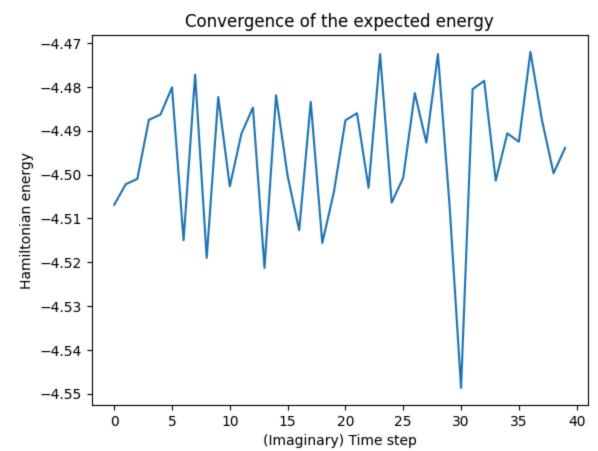
step			
0	-4.5069	19	1.179153
1	-4.5022	19	0.899106
2	-4.5010	19	0.983723
3	-4.4875	19	1.094769
4	-4.4863	19	1.053946
5	-4.4801	19	0.958224
6	-4.5150	19	1.002547
7	-4.4772	19	1.011643
8	-4.5190	19	1.051871
9	-4.4823	19	1.058879
10	-4.5027	19	1.044394
11	-4.4907	19	0.980603
12	-4.4847	19	1.016350
13	-4.5213	19	1.192840
14	-4.4819	19	0.902930
15	-4.5003	19	1.092071
16	-4.5127	19	1.024948
17	-4.4834	19	1.097475
18	-4.5156	19	0.988022
19	-4.5040	19	0.965503
20	-4.4876	19	0.952781
21	-4.4860	19	1.114725
22	-4.5030	19	0.977443
23	-4.4725	19	0.970870
24	-4.5064	19	1.053168
25	-4.5007	19	1.018006
26	-4.4814	19	1.003280
27	-4.4927	19	1.137343
28	-4.4725	19	1.013669

curr_energy num_circuits quantum_exec_time

step			
29	-4.5068	19	1.105107
30	-4.5487	19	0.933466
31	-4.4805	19	0.863265
32	-4.4786	19	0.864900
33	-4.5014	19	0.917141
34	-4.4906	19	0.904462
35	-4.4925	19	1.055041
36	-4.4720	19	0.997501
37	-4.4876	19	0.783672
38	-4.4997	19	0.829785

CPU times: total: 6min 26s

Wall time: 54.6 s



Check out your best / most frequent cut!

Following the variational quantum imaginary time evolution (vQITE) loop, we sample the quantum circuit to obtain classical bitstrings. The most frequent bitstring represents our solution, the final score though will take into account all of the right solutions...

print(counts_T)

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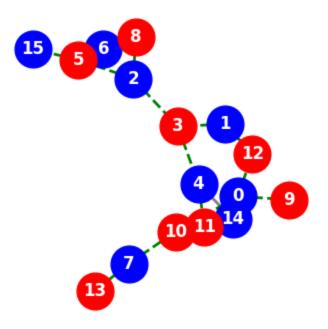
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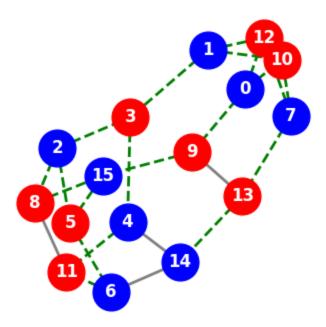
```
interpret_solution(T, best_bs_T)
print("Cut value: "+str(compute_cut_size(T, best_bs_T)))
print(T, best_bs_T)
```



Cut value: 14

Graph with 16 nodes and 15 edges 00010100111111100

```
# interpret the same solution, but with the whole graph instead of the tree
interpret_solution(graph, best_bs_T)
print("Cut value: "+str(compute_cut_size(graph, best_bs_T)))
print(graph, best_bs_T)
```



Cut value: 20 Graph with 16 nodes and 24 edges 00010100111111100

```
In [346... # Sample your optimized quantum state using Aer for the tree

optimized_state_H = ansatz_H.assign_parameters(qit_evolver_H.param_vals[-1])
    optimized_state_H.measure_all()
    counts_H = backend.run(optimized_state_H, shots=shots).result().get_counts()

# Find the sampled bitstring with the largest cut value
    cut_vals_H = sorted(((bs, compute_cut_size(H, bs))) for bs in counts_H), key=lambda
    best_bs_H = cut_vals_H[-1][0]

# Now find the most likely MaxCut solution as sampled from your optimized state
# We'll leave this part up to you!!!
    most_likely_soln = ""

print(counts_H)
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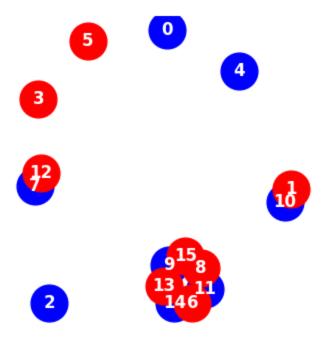
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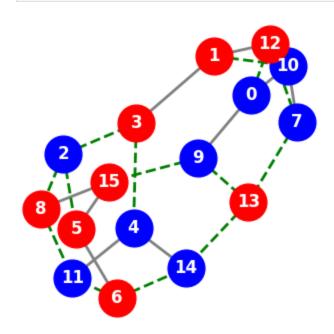
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```
interpret_solution(H, best_bs_H)
print("Cut value: "+str(compute_cut_size(H, best_bs_H)))
print(H, best_bs_H)
```



Cut value: 8
Graph with 16 nodes and 9 edges 0101011010001101

```
interpret_solution(graph, best_bs_H)
print("Cut value: "+str(compute_cut_size(graph, best_bs_H)))
print(graph, best_bs_H)
```

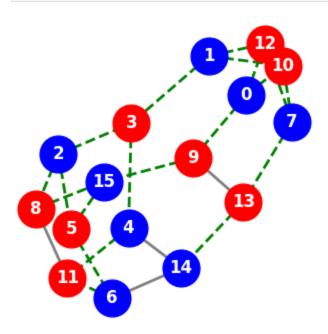


Cut value: 14 Graph with 16 nodes and 24 edges 0101011010001101

```
In [349... # choose the better result from best_bs_T and best_bs_H
best_bs_final = best_bs_H if compute_cut_size(graph, best_bs_H) > compute_cut_size(
final_cut_value = compute_cut_size(graph, best_bs_final)

# choose the better result ansatz from ansatz_T and ansatz_H
ansatz_final = ansatz_H if compute_cut_size(graph, best_bs_H) > compute_cut_size(graph)
```

```
interpret_solution(graph, best_bs_final)
print("Cut value: "+str(final_cut_value))
print(graph, best_bs_final)
```



Cut value: 20
Graph with 16 nodes and 24 edges 00010100111111100

```
In [350... # from qiskit_aer import AerSimulator

# shots = 100_000

# Sample your optimized quantum state using Aer
# backend = AerSimulator()
optimized_state = ansatz.assign_parameters(qit_evolver.param_vals[-1])
optimized_state.measure_all()
counts = backend.run(optimized_state, shots=shots).result().get_counts()

# Find the sampled bitstring with the largest cut value
cut_vals = sorted(((bs, compute_cut_size(graph, bs)) for bs in counts), key=lambda
best_bs = cut_vals[-1][0]

# Now find the most likely MaxCut solution as sampled from your optimized state
# We'll leave this part up to you!!!
most_likely_soln = ""
print(counts)
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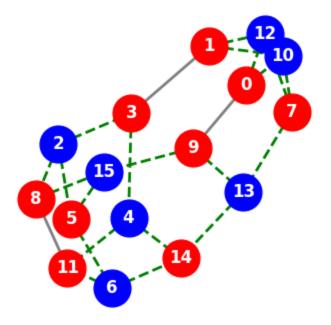
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```
interpret_solution(graph, best_bs)
print("Cut value: "+str(compute_cut_size(graph, best_bs)))
print(graph, best_bs)
```



Cut value: 21 Graph with 16 nodes and 24 edges 1101010111010010

Drumroll please... the scores!

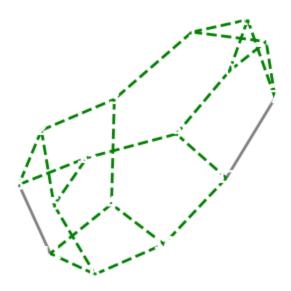
```
In [352...
          %%time
          # Brute-force approach with conditional checks
          verbose = False
          G = graph
          n = len(G.nodes())
          w = np.zeros([n, n])
          for i in range(n):
              for j in range(n):
                  temp = G.get_edge_data(i, j, default=0)
                   if temp != 0:
                      w[i, j] = 1.0
          if verbose:
              print(w)
          best_cost_brute = 0
          best_cost_balanced = 0
          best_cost_connected = 0
          for b in range(2**n):
              x = [int(t) for t in reversed(list(bin(b)[2:].zfill(n)))]
              # Create subgraphs based on the partition
              subgraph0 = G.subgraph([i for i, val in enumerate(x) if val == 0])
              subgraph1 = G.subgraph([i for i, val in enumerate(x) if val == 1])
              bs = "".join(str(i) for i in x)
```

```
# Check if subgraphs are not empty
     if len(subgraph0.nodes) > 0 and len(subgraph1.nodes) > 0:
         cost = 0
         for i in range(n):
             for j in range(n):
                  cost = cost + w[i, j] * x[i] * (1 - x[j])
         if best_cost_brute < cost:</pre>
             best_cost_brute = cost
             xbest brute = x
             XS_brut = []
         if best_cost_brute == cost:
             XS_brut.append(bs)
         outstr = "case = " + str(x) + " cost = " + str(cost)
         if (len(subgraph1.nodes)-len(subgraph0.nodes))**2 <= 1:</pre>
             outstr += " balanced"
             if best_cost_balanced < cost:</pre>
                  best_cost_balanced = cost
                  xbest balanced = x
                 XS_balanced = []
             if best_cost_balanced == cost:
                 XS_balanced.append(bs)
         if nx.is connected(subgraph0) and nx.is connected(subgraph1):
             outstr += " connected"
             if best_cost_connected < cost:</pre>
                  best_cost_connected = cost
                  xbest\_connected = x
                 XS_connected = []
             if best cost connected == cost:
                  XS connected.append(bs)
         if verbose:
             print(outstr)
CPU times: total: 4.47 s
Wall time: 9.21 s
# This is classical brute force solver results:
```

```
In [353... # This is classical brute force solver results:
    interpret_solution(graph, xbest_brute)
    print(graph, xbest_brute)
    print("\nBest solution = " + str(xbest_brute) + " cost = " + str(best_cost_brute))
    print(XS_brut)

interpret_solution(graph, xbest_balanced)
    print(graph, xbest_balanced)
    print("\nBest balanced = " + str(xbest_balanced) + " cost = " + str(best_cost_balan print(XS_balanced))

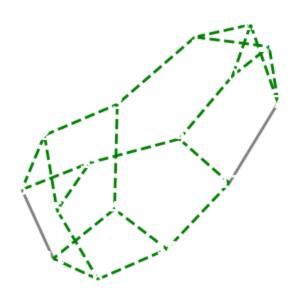
interpret_solution(graph, xbest_connected)
    print(graph, xbest_connected)
    print("\nBest connected = " + str(xbest_connected) + " cost = " + str(best_cost_con print(XS_connected))
    print(XS_connected)
    plt.show()
```



Graph with 16 nodes and 24 edges [0, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1, 1, 1, 0, 1, 0]

Best solution = [0, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1, 1, 1, 0, 1, 0] cost = 22.0

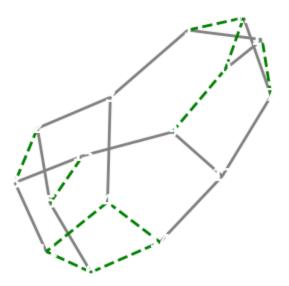
['0001010011111010', '1110101100000101']



Graph with 16 nodes and 24 edges [0, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1, 1, 1, 0, 1, 0]

Best balanced = [0, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1, 1, 1, 0, 1, 0] cost = 22.0

['0001010011111010', '1110101100000101']



Graph with 16 nodes and 24 edges [1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0]

Best connected = [1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0] cost = 10.0 ['1111111000100000', '01111111100100000', '11111110010100000', '111101101010100000', '01 110000', '0111110100110000', '0111101100110000', '0111011100110000', '010111111001100 '0111001110110000', '0101101110110000', '1111100001110000', '1111000011110000', '110 1100011110000', '11111111000001000', '01111111100001000', '11111110010001000', '11111111 010001000', '0111110110001000', '0111011110001000', '11111110001001000', '11110110010 01000', '1111100011001000', '01111111000101000', '01111110010101000', '0111011011010100 0', '1111110000011000', '1111101000011000', '1111011000011000', '1101111000011000', 1010010011000', '1111001010011000', '1101101010011000', '0111010110011000', '0111001 110011000', '0101101110011000', '1111100001011000', '1111000011011000', '11011000110 11000', '0111110000111000', '0111101000111000', '01111011000111000', '010111100011100 0', '0111010010111000', '0111001010111000', '0101101010111000', '0111110100100100', '0111011100100100', '0111100110100100', '0111100100110100', '0111000110110100', '010 100011100', '0111000110011100', '0101100110011100', '11111110000100010', '11111010001 00010', '1111011000100010', '1101111000100010', '0111110100100010', '0111110110010001 0', '0111011100100010', '0101111100100010', '11111100010100010', '01111100110100010', '1111100000110010', '0111100100110010', '1101100010110010', '0101100110110010', '111 1110000001010', '1111101000001010', '1111011000001010', '11011111000001010', '0111110 100001010', '0111101100001010', '0111011100001010', '0101111100001010', '11111000100 01010', '0111100110001010', '0111110000101010', '0111101000101010', '0111101100010101 0', '0101111000101010', '0111100010101010', '11111100000011010', '0111100100011010', '1101100010011010', '0101100110011010', '01111100000111010', '0101100010111010', '011 1110100000110', '0111101100000110', '0111011100000110', '0101111100000110', '01111100 110000110', '1010011101000110', '1000111101000110', '0111110000100110', '01111010001 00110', '0111011000100110', '0101111000100110', '01111010100100110', '001111010010011 '0101011100100110', '0011011100100110', '1000111100100110', '0100111100100110', '001 0111100100110', '0001111100100110', '0111100010100110', '0111000110100110', '0011100 110100110', '0010011110100110', '1010011001100110', '1000111001100', '00100111011 00110', '0000111101100110', '0111100100010110', '0101100110010110', '100001110101011 0', '1000100111010110', '1000001111010110', '01111100000110110', '0011100100110110', 0100110110110', '0100100110110110', '0010100110110110', '0001100110110110', '1000001 110110110', '0100001110110110', '0010001110110110', '0000011110110110', '10000110011 10110', '0000011101110110', '1000100011110110', '1000001011110110', '000010011111011 0', '0000001111110110', '0111110000001110', '0111101000001110', '0111011000001110', '0101111000001110', '0111010100001110', '0011110100001110', '0111001100001110', '001 1101100001110', '1010011100001110', '0110011100001110', '01010111100001110', '0011011 100001110', '1000111100001110', '0100111100001110', '0010111100001110', '00011111000 0', '1010011001001110', '1000111001001110', '0010011101001110', '0000111101001110', '0010011100101110', '0000111100101110', '0111100000011110', '0011100100011110', '100 0011100011110', '0100011100011110', '0010011100011110', '0101100010011110', '1000100 110011110', '0100100110011110', '0010100110011110', '0001100110011110', '10000011100 0', '0000011101011110', '1000100011011110', '1000001011011110', '0000100111011110', '0000001111011110', '0000011100111110', '0000100110111110', '0000001110111110', '111 000100001', '0111110100100001', '0111011100100001', '11111100010100001', '01111001101

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```
In [354... # And this is how we calculate the shots counted toward scores for each class of th
sum_counts = 0
for bs in counts:
    if bs in XS_brut:
        sum_counts += counts[bs]
```

```
print(f"Pure max-cut: {sum_counts} out of {shots}")

sum_balanced_counts = 0
for bs in counts:
    if bs in XS_balanced:
        sum_balanced_counts += counts[bs]

print(f"Balanced max-cut: {sum_balanced_counts} out of {shots}")

sum_connected_counts = 0
for bs in counts:
    if bs in XS_connected:
        sum_connected_counts += counts[bs]

print(f"Connected max-cut: {sum_connected_counts} out of {shots}")
```

Pure max-cut: 0 out of 100000

Balanced max-cut: 0 out of 100000

Connected max-cut: 172 out of 100000

```
def final_score(graph, XS_brut,counts,shots,ansatz,challenge):
In [355...
              if(challenge=='base'):
                  sum counts = 0
                  for bs in counts:
                      if bs in XS_brut:
                           sum_counts += counts[bs]
              elif(challenge=='balanced'):
                  sum_balanced_counts = 0
                  for bs in counts:
                      if bs in XS balanced:
                           sum_balanced_counts += counts[bs]
                  sum_counts = sum_balanced_counts
              elif(challenge=='connected'):
                  sum_connected_counts = 0
                  for bs in counts:
                      if bs in XS connected:
                           sum_connected_counts += counts[bs]
                  sum_counts = sum_connected_counts
              transpiled_ansatz = transpile(ansatz, basis_gates = ['cx','rz','sx','x'])
              cx count = transpiled ansatz.count ops()['cx']
              score = (4*2*graph.number_of_edges())/(4*2*graph.number_of_edges() + cx_count)
              return np.round(score,5)
```

In [356...
print("Base score: " + str(final_score(graph,XS_brut,counts,shots,ansatz,'base')))
print("Balanced score: " + str(final_score(graph,XS_brut,counts,shots,ansatz,'balan
print("Connected score: " + str(final_score(graph,XS_brut,counts,shots,ansatz,'conn

Base score: 0.0
Balanced score: 0.0
Connected score: 0.00138

```
# calculate our version of the score for the final solution
print("Base score: " + str(final_score(graph,XS_brut,counts,shots,ansatz_H,'base'))
print("Balanced score: " + str(final_score(graph,XS_brut,counts,shots,ansatz_H,'bal
print("Connected score: " + str(final_score(graph,XS_brut,counts,shots,ansatz_H,'co
```

Base score: 0.0
Balanced score: 0.0
Connected score: 0.00157

```
In [358...
```

```
# calculate our version of the score for the final solution
print("Base score: " + str(final_score(graph,XS_brut,counts,shots,ansatz_T,'base'))
print("Balanced score: " + str(final_score(graph,XS_brut,counts,shots,ansatz_T,'bal
print("Connected score: " + str(final_score(graph,XS_brut,counts,shots,ansatz_T,'co
```

Base score: 0.0
Balanced score: 0.0
Connected score: 0.00149

This is the main challenge: design optimal ansatz generators and Hamiltonians for the maxcut problem, subject to three specific conditions. Solutions for each condition can be submitted independently; however, a unified approach applicable to all three conditions will receive additional credit.

Submit your results

I guess this is the most important part. You probably want to report your results.

Please, follow the link: https://forms.gle/gkpSCe7HGr7QHZXQ6

Let's revisit the problem statement. **This is important!!!** We have three scoring methods to report:

- 1. Counts shots achieving the optimal max-cut value. Sorry, no approximation value this time.
- 2. Adds a balance constraint—subgraphs must have equal cardinality.
- 3. Requires connected subgraphs—all vertices within a subgraph must be mutually reachable.

For **in-person participants**: Prepare a presentation that explains your research and demonstrates the value of your proposed solution.

Can you solve this? Good luck!

Feedback

If you have any suggestions or recommendations abou the hackathon challange, please, don't hesitatate to leave your comment here: https://iter.ly/u42um



In []: