Date:23/09/25

TASK 10: Implement the QAOA algorithm

Aim: To implement the Quantum Approximate Optimization Algorithm (QAOA) using Qiskit and PyTorch to solve the Max-Cut problem, a classical NP-hard problem.

1 Mathematical Model of the QAOA Algorithm

1.1 Max-Cut Problem Formulation

Given a graph $G = (V, E)$ with weighted adjacency matrix w , the Max-Cut objective is

$$C(x) = \sum_{(,)} \quad w \,.\, x \square\, x$$

where $x \square \{0,1\}$ indicates the partition of node i.

The goal is $\square_{\{,\}} C(x)$

1.2 QAOA Ansatz

The QAOA prepares a quantum state parameterized by angles $\vec{\gamma}, \vec{\beta}$.

$$\square\, \vec{\gamma}, \vec{\beta}\, \rangle = \quad e \quad \Sigma \quad e \quad +\rangle\square$$

- $H \;= \sum_{(,)} w\, Z\, Z$ (cost Hamiltonian)
- $H \;= \sum X$ (mixer Hamiltonian)

1.3 Expectation Value

The objective is to maximize$F\, \vec{\gamma}, \vec{\beta} = \langle \square\, \vec{\gamma}, \vec{\beta}\ |\mathrm{H}|\ \square\, \vec{\gamma}, \vec{\beta}\, \rangle$, the optimization is performed using a classical optimizer (Adam with finite-difference gradients).

2 Algorithm - QAOA Algorithm

1. Graph Construction
   - Define adjacency matrix W.
   - Build a NetworkX graph for visualization.
2. Classical Baseline
   - Use brute-force enumeration to compute the optimal Max-Cut value (ground truth).

3. QAOA Circuit Construction

- Initialize qubits in $|+\rangle$.
- Apply alternating cost and mixer unitaries for depth p.
- Use controlled-Z rotation gates to implement $Z\ Z$ interactions.

4. Expectation Calculation

- Simulate circuit using Qiskit Aer statevector simulator.
- Compute expected cut value from measurement probabilities.

5. Hybrid Optimization

- Parameters $\vec{\gamma}$, $\vec{\beta}$ initialized randomly.
- Compute finite-difference gradients of expectation.
- Update parameters using PyTorch Adam optimizer.

6. Circuit Visualization

 Draw initial and optimized QAOA circuits using qiskit.visualization.

3 Program

```
#!pip install qiskit qiskit-optimization torch networkx numpy
#!pip install qiskit-aer #!pip install
pylatexenc
 import os import numpy as np
import networkx as nx import
torch
from qiskit import QuantumCircuit from qiskit_aer
import Aer
from qiskit.quantum_info import Statevector from qiskit_optimization.applications
import Maxcut from qiskit_optimization.problems import QuadraticProgram

# Visualization imports import matplotlib
# Use Agg backend in headless environments so saving works even without GUI
matplotlib.use(os.environ.get("MPLBACKEND", "Agg")) import matplotlib.pyplot
as plt

# ------------------------- # Problem
definition # ------------------------- def
make_graph():
    # Example: 4-node graph (same as Qiskit tutorial)
    w = np.array([
```

```
        [0.0, 1.0, 1.0, 0.0],
        [1.0, 0.0, 1.0, 1.0],
        [1.0, 1.0, 0.0, 1.0],
        [0.0, 1.0, 1.0, 0.0]
    ])
    G = nx.from_numpy_array(w)     return G, w

# computes classical objective (cut value) for bitstring x
(array of 0/1) def objective_value(x, w):     X =
np.outer(x, (1 - x))     w_01 = np.where(w != 0,
1, 0)     return np.sum(w_01 * X)

# brute-force best solution (for comparison) def
brute_force_maxcut(w):
    n = w.shape[0]     best = -1
best_x = None     for i in
range(2**n):
        x = np.array(list(map(int, np.binary_repr(i, width=n))))         val = objective_value(x, w)
if val > best:             best = val             best_x = x     return best_x, best

# -------------------------
# Build QAOA circuit (manual) # ------------------------- def
qaoa_circuit(n_qubits, edges, gammas, betas):
    """
    Build QAOA circuit:
      - start in |+>^n       - for each
layer l:
          cost unitary U_C(gamma_l) = exp(-i * gamma_l * C)           mixer U_B(beta_l) =
product Rx(2*beta_l)     edges: list of tuples (i, j, weight)     gammas, betas: lists or 1D
arrays (length p)
    """     p = len(gammas)
    qc = QuantumCircuit(n_qubits)
    # initial layer: Hadamards to create |+>^n     qc.h(range(n_qubits))

    for layer in range(p):
        gamma = float(gammas[layer])
        # cost layer: implement exp(-i * gamma * w_ij * Z_i Z_j)         for (i, j, w) in edges:
            if w == 0:                 continue
            # For ZZ interaction exp(-i * theta/2 * Z_i Z_j) -> use CNOT-RZ-CNOT with theta =
2*gamma*w             theta = 2.0 * gamma * w             qc.cx(i, j)             qc.rz(theta, j)
qc.cx(i, j)
        # mixer layer: RX(2*beta)         beta =
float(betas[layer])         for q in range(n_qubits):
qc.rx(2.0 * beta, q)

    return qc
```

```
# ------------------------
# Expectation value from statevector # ------------------------ def
expectation_from_statevector(statevector, w):     """Given a statevector and adjacency
matrix w, compute expected MaxCut objective."""     n = w.shape[0]
   probs = Statevector(statevector).probabilities_dict()     exp_val = 0.0     for bitstr, p
in probs.items():         # reverse so index 0 => qubit 0
       bits = np.array([int(b) for b in bitstr[::-1]])         exp_val +=
objective_value(bits, w) * p     return exp_val

# ------------------------
# QAOA + PyTorch classical loop # ---------------
----------
def run_qaoa_with_pytorch(w, p=1, init_std=0.5, maxiter=100, lr=0.1, finite_diff_eps=1e-3,
backend_name="aer_simulator_statevector"):
   n = w.shape[0]
   # edges list with weights (i>j to match earlier convention)     edges = [(i, j, w[i, j]) for i in
range(n) for j in range(i) if w[i, j] != 0]
   # initial params (gamma_1..gamma_p, beta_1..beta_p)     params = torch.randn(2 * p,
dtype=torch.double) * init_std     params.requires_grad = False  # we will supply grads
manually using finite differences
   optimizer = torch.optim.Adam([params], lr=lr)

   backend = Aer.get_backend(backend_name)

   best = {"val": -np.inf, "params": None, "bitstring": None}
    for it in range(maxiter):
      # unpack
      gammas = params.detach().numpy()[:p]         betas =
params.detach().numpy()[p:]

      # build circuit, get statevector         qc = qaoa_circuit(n, edges,
gammas, betas)         qc.save_statevector()         # using Aer simulator
res = backend.run(qc).result()         sv = res.get_statevector(qc)

      # compute expectation (we maximize expected cut)         exp_val =
expectation_from_statevector(sv, w)         loss = -float(exp_val)  # minimize negative
of expectation

      # keep best         if exp_val > best["val"]:
         # extract most likely bitstring             probs = Statevector(sv).probabilities_dict()
most = max(probs.items(), key=lambda kv: kv[1])[0]             bits = np.array([int(b) for b in
most[::-1]])             best.update({"val": exp_val, "params":
params.detach().clone(), "bitstring": bits})
```

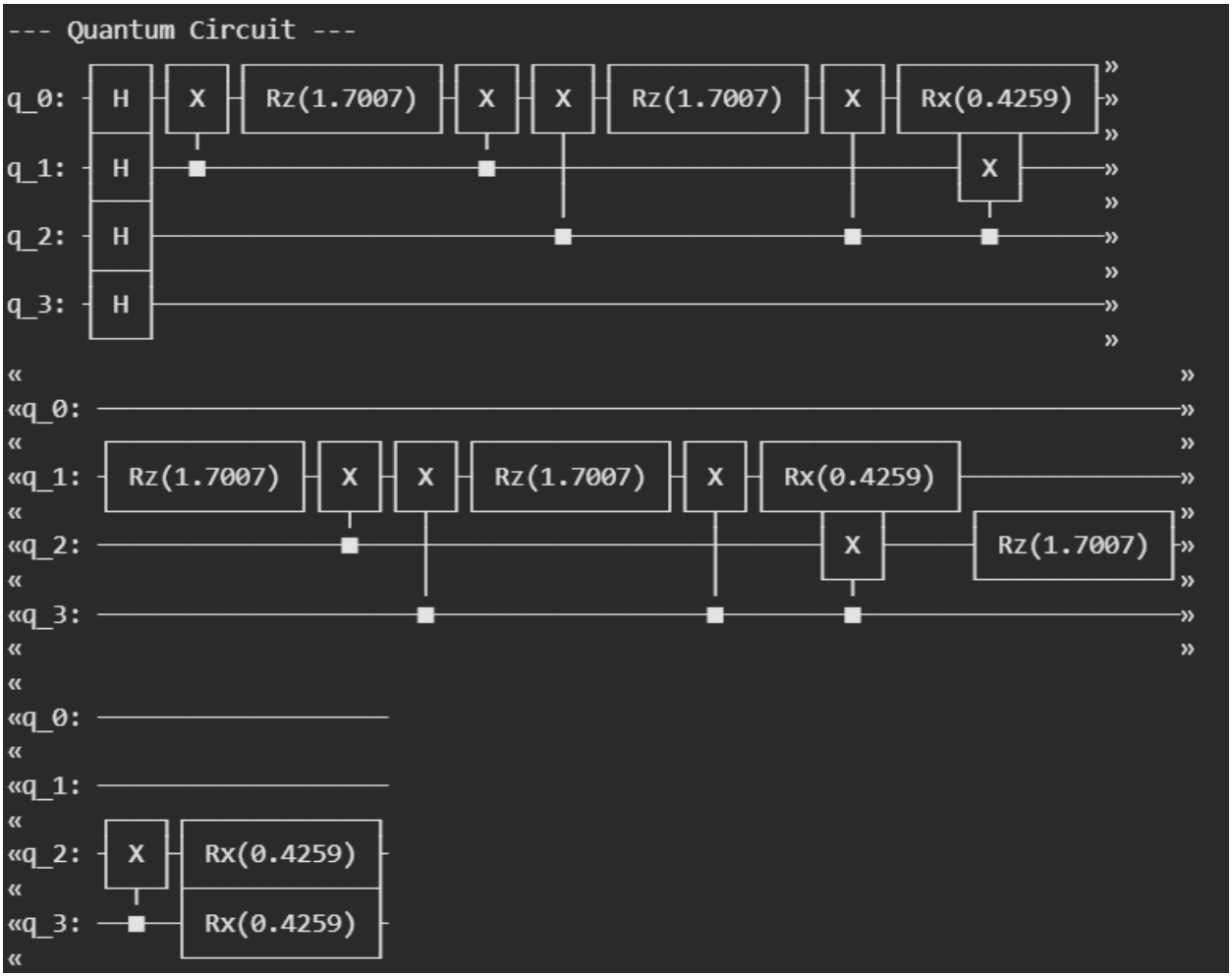
```
        # finite-difference gradient (central difference)         grads =
np.zeros_like(params.detach().numpy())         base = params.detach().numpy()
eps = finite_diff_eps         for k in range(len(base)):             plus = base.copy()
minus = base.copy()             plus[k] += eps             minus[k] -= eps

            g_plus = _qaoa_expectation_with_params(plus, n, edges, backend, w, p)
            g_minus = _qaoa_expectation_with_params(minus, n, edges, backend, w, p)
            grad_k = (-(g_plus - g_minus) / (2 * eps))  # derivative of loss = -expectation
grads[k] = grad_k

        # set grads into params manually and step optimizer         params_grad =
torch.from_numpy(grads).to(dtype=torch.double)         params.grad = params_grad

        optimizer.step()         optimizer.zero_grad()
         if it % 10 == 0 or it == maxiter - 1:
            print(f"Iter {it:03d}: expected cut = {exp_val:.6f}, loss = {loss:.6f}")

    return best
 def _qaoa_expectation_with_params(flat_params, n, edges, backend, w, p):
    """Helper to evaluate expected cut quickly for given params
(no PyTorch)"""      gammas =
flat_params[:p]     betas = flat_params[p:]
    qc = qaoa_circuit(n, edges, gammas, betas)
qc.save_statevector()     res = backend.run(qc).result()     sv =
res.get_statevector(qc)
    exp_val = expectation_from_statevector(sv, w)     return exp_val

# -------------------------
# Circuit display helpers # ----------------
---------
def show_circuit(qc: QuantumCircuit, filename: str = None, style: str = "mpl"):

    print("\n--- Quantum Circuit ---")     try:
        print(qc.draw(output="text"))     except Exception as e:
        print("Failed to draw Quantum Circuit:", e)
     if style == "mpl":         try:
            fig = qc.draw(output="mpl", interactive=False)             fig.tight_layout()
if filename:
                fig.savefig(filename, dpi=200, bbox_inches="tight")
                print(f"[Saved circuit figure to {filename}]")             else:
                # if no filename provided, still save to a temporary PNG and show inline if
possible                 tempname = "qaoa_circuit.png"                 fig.savefig(tempname,
dpi=200, bbox_inches="tight")
                print(f"[Saved circuit figure to {tempname}]")             plt.close(fig)         except
Exception as e:
```

```
        print("Matplotlib drawing failed:", str(e))          print("Fallback: Quantum Circuit diagram above.")
 def demo_display_initial_circuit(w, p=1, filename="qaoa_initial_circuit.png"):
    n = w.shape[0]
    # random params for demo     gammas = np.random.randn(p) * 0.8     betas = np.random.randn(p) * 0.8
    edges = [(i, j, w[i, j]) for i in range(n) for j in range(i) if w[i, j] != 0]
    qc = qaoa_circuit(n, edges, gammas, betas)     show_circuit(qc, filename=filename, style="mpl")
 def demo_display_best_circuit(w, best_params, p=1, filename="qaoa_best_circuit.png"):
    n = w.shape[0]     if isinstance(best_params, torch.Tensor):         flat = best_params.detach().cpu().numpy()     else:
        flat = np.array(best_params)     gammas = flat[:p]     betas = flat[p:]
    edges = [(i, j, w[i, j]) for i in range(n) for j in range(i) if w[i, j] != 0]
    qc = qaoa_circuit(n, edges, gammas, betas)     show_circuit(qc, filename=filename, style="mpl")

# ------------------------- # Run example
# ------------------------- if __name__ == "__main__":
    G, w = make_graph()
    print("Graph edges:", list(G.edges()))     bf_x, bf_val = brute_force_maxcut(w)
    print("Brute-force best:", bf_x, "value:", bf_val)

    # show an initial example circuit (random parameters)     demo_display_initial_circuit(w, p=1, filename="qaoa_initial_circuit.png")

    # run QAOA p=1 (toy)
    best = run_qaoa_with_pytorch(w, p=1, init_std=0.8, maxiter=80, lr=0.2, finite_diff_eps=1e-3)     print("QAOA best expected value:", best["val"])     print("Most-likely bitstring found:", best["bitstring"])
    # evaluate most-likely bitstring exactly     exact_val = objective_value(best["bitstring"], w)     print("Exact value of that bitstring:", exact_val)

    # Display the optimized circuit using the best parameters (and save)     if best["params"] is not None:         demo_display_best_circuit(w, best["params"], p=1, filename="qaoa_best_circuit.png")     else:
        print("No best params found to display.")
```

Output:

Graph edges: [(0, 1), (0, 2), (1, 2), (1, 3), (2, 3)]

Brute-force best: [0 1 1 0] value: 4



Matplotlib drawing failed: "The 'pylatexenc' library is required to use 'MatplotlibDrawer'. You can install it with 'pip install pylatexenc'."

Fallback: Quantum Circuit diagram above.

Iter 000: expected cut = 2.023362, loss = -2.023362

Iter 010: expected cut = 2.791205, loss = -2.791205

Iter 020: expected cut = 2.948465, loss = -2.948465

Iter 030: expected cut = 3.032813, loss = -3.032813

Iter 040: expected cut = 3.069579, loss = -3.069579

Iter 050: expected cut = 3.084200, loss = -3.084200

Iter 060: expected cut = 3.084985, loss = -3.084985

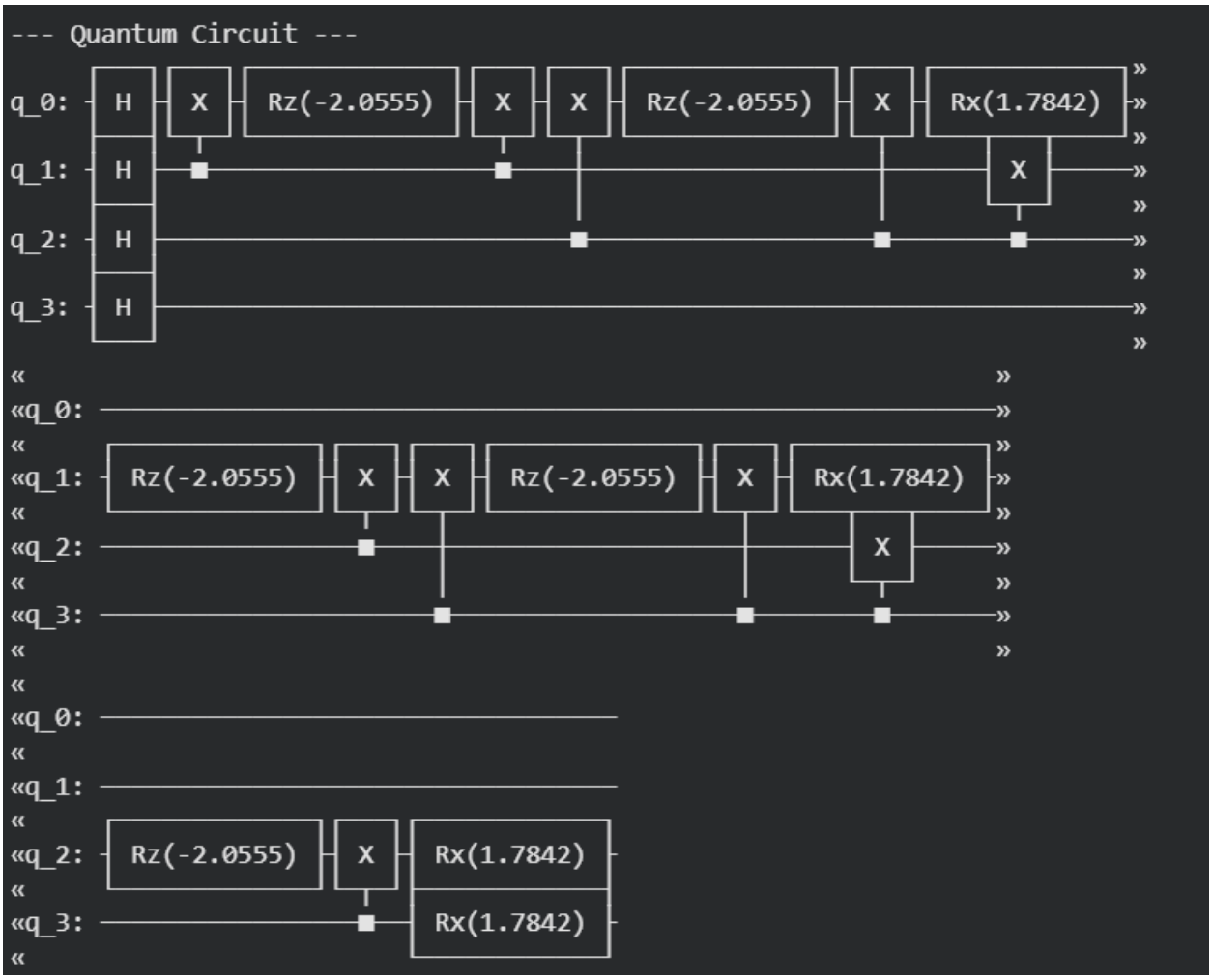
Iter 070: expected cut = 3.085243, loss = -3.085243

Iter 079: expected cut = 3.085654, loss = -3.085654

QAOA best expected value: 3.085886870240427

Most-likely bitstring found: [0 1 1 0]

Exact value of that bitstring: 4



Matplotlib drawing failed: "The 'pylatexenc' library is required to use 'MatplotlibDrawer'. You can install it with 'pip install pylatexenc'."

Fallback: Quantum Circuit diagram above.

4 Result

The QAOA implementation successfully demonstrates a hybrid quantum-classical optimization approach to solving the Max-Cut problem.