Optimization in quantum domain

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Optimization Problems

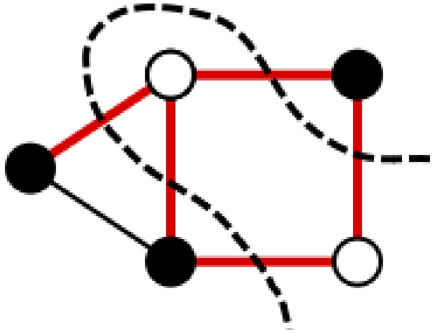
- Many problems in quantitative fields such as finance and engineering are optimization problems.
- Optimization problems lay at the core of complex decision-making and definition of strategies.
- Optimization (or combinatorial optimization) means searching for an optimal solution in a finite or countably infinite set of potential solutions.
- Optimality is defined with respect to some criterion function, which is to be minimized or maximized. This is typically called cost function, loss function, or objective function.

Typical optimization problems

- **Minimization**: cost, distance, length of a traversal, weight, processing time, material, energy consumption, number of objects
- **Maximization**: profit, value, output, return, yield, utility, efficiency, capacity, number of objects
- We consider here max-cut problem of practical interest in many fields, and show how they can mapped on quantum computers.
- Traveling salesman problem, **investment portfolio problem**, ….

Max-cut problem

- **Max-Cut is an NP-complete problem**, with applications in clustering, network science, and statistical physics.



- Consider an n-node undirected graph $G = (V, E)$ where $|V| = n$ with edge weights $w_{ij} > 0$, $w_{ij} = w_{ji}$, for $(i,j) \in E$.
- A cut is defined as a partition of the original set V into two subsets.
- One wants a subset S of the vertex set such that **the number of edges between *S* and the complementary subset is as large as possible**.
- The cost function to be optimized is in this case **the sum of weights of edges connecting points in the two different subsets, *crossing* the cut.**
- By assigning x_i=0 or x_i=1 to each node i, one tries to maximize the global profit function (here and in the following summations run over indices 0,1,...n-1)

$$\tilde{C}(\mathbf{x}) = \sum_{i,j} w_{ij} x_i (1 - x_j).$$

Marketing Problem

- To grasp how practical applications are mapped into given Max-Cut instances, consider a system of many people that can interact and influence each other.
- Individuals can be represented by vertices of a graph, and their interactions seen as pairwise connections between vertices of the graph, or edges.
- Suppose that it is assumed that individuals will influence each other's buying decisions, and knowledge is given about how strong they will influence each other.
- The influence can be modeled by weights assigned on each edge of the graph.
- It is possible then to predict the outcome of a marketing strategy in which products are offered for free to some individuals, and then ask which is the optimal subset of individuals that should get the free products, in order to maximize revenues.

Formulation of weighted max-cut problem

- In our simple marketing model, w_{ij} represents the probability that the person j will buy a product after i gets a free one.
- Note that the weights w_{ij} can in principle be greater than 1, corresponding to the case where the individual j will buy more than one product.
- **Maximizing the total buying probability corresponds to maximizing the total future revenues**.
- In the case where the profit probability will be greater than the cost of the initial free samples, the strategy is a convenient one.
- An extension to this model has the nodes themselves carry weights, which can be regarded, in our marketing model, as the likelihood that a person granted with a free sample of the product will buy it again in the future.
- With this additional information in our model, the objective function to maximize becomes

$$C(\mathbf{x}) = \sum_{i,j} w_{ij} x_i (1 - x_j) + \sum_i w_i x_i .$$

Mapping to Ising Hamiltonian model

- **Encoding**: $x_i \rightarrow n_i=(1-Z_i)/2$ where Z_i is the Pauli Z operator that has eigenvalues ± 1. The objective function to maximize becomes:

$$C(\mathbf{Z}) = \sum_{i,j} \frac{w_{ij}}{4}(1 - Z_i)(1 + Z_j) + \sum_i \frac{w_i}{2}(1 - Z_i) = -\frac{1}{2}\left(\sum_{i<j} w_{ij} Z_i Z_j + \sum_i w_i Z_i\right) + \text{const},$$

where const = $\sum_{i<j} w_{ij}/2 + \sum_i w_i/2$.

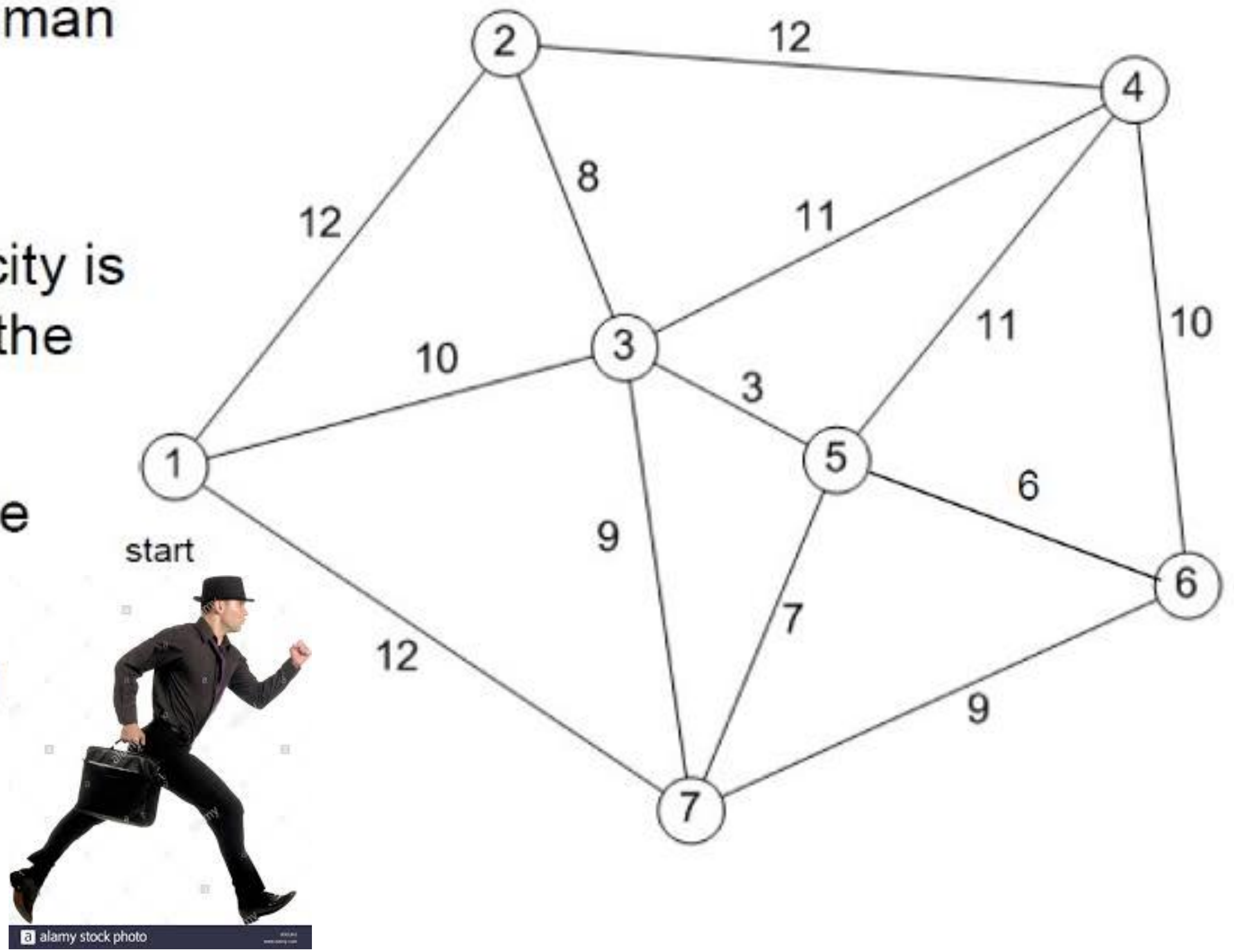
- The weighted Max-Cut problem is equivalent to minimizing the Ising Hamiltonian:

$$H = \sum_i w_i Z_i + \sum_{i<j} w_{ij} Z_i Z_j.$$

Aqua can generate the Ising Hamiltonian for the profit functions C̃ and C.

The Traveling Salesman Problem

- Starting from city 1, the salesman must travel to all cities once before returning home
- The distance between each city is given, and is assumed to be the same in both directions
- Only the links shown are to be used
- Objective - Minimize the total distance to be travelled



Formulation of traveling salesman problem

- **The TSP on the nodes of a graph asks for the shortest Hamiltonian cycle that can be taken through each of the nodes.** A Hamilton cycle is a closed path that uses every vertex of a graph once
- Find the shortest Hamiltonian cycle in a graph $G=(V,E)$ with $n=|V|$ nodes and distances, w_{ij} (distance from vertex i to vertex j). A Hamiltonian cycle is described by n^2 variables $x_{i,p}$, where i represents the node and p represents its order in a prospective cycle.
- The decision variable takes the value 1 if the solution occurs at node i at time order p.
- We require that every node can only appear once in the cycle, and for each time a node has to occur.

$$\sum_i x_{i,p} = 1 \quad \forall p \qquad\qquad \sum_p x_{i,p} = 1 \quad \forall i.$$

Mapping to Ising Hamiltonian model

- The distance that needs to be minimized is

$$C(\mathbf{x}) = \sum_{i,j} w_{ij} \sum_{p} x_{i,p} x_{j,p+1}$$

- Putting this all together in a single objective function to be minimized, we get the following:

$$C(\mathbf{x}) = \sum_{i,j} w_{ij} \sum_{p} x_{i,p} x_{j,p+1} + A \sum_{p} \left(1 - \sum_{i} x_{i,p}\right)^2 + A \sum_{i} \left(1 - \sum_{p} x_{i,p}\right)^2$$

- where A is a free parameter. One needs to ensure that A is large enough so that these constraints are respected. One way to do this is to choose A such that $A > \max(w_{ij})$.
- **Encoding**: $x_{i,p} \rightarrow n_{i,p} = (1 - Z_{i,p})/2$ where $Z_{i,p}$ is the Pauli Z operator that has eigenvalues ± 1.
- The TSP is equivalent to minimizing the Ising Hamiltonian:

Quantum approximate optimization algorithm (VQE)

The Algorithm works as follows:

1. Choose the w_i and w_{ij} in the target Ising problem. In principle, even higher powers of Z are allowed.
2. Choose the depth of the quantum circuit m. Note that the depth can be modified adaptively.
3. Choose a set of controls θ and make a trial function $|\psi(\boldsymbol{\theta})\rangle$, built using a quantum circuit made of C-Phase gates and single-qubit Y rotations, parameterized by the components of $\boldsymbol{\theta}$.
4. Evaluate $C(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})\,|H|\,\psi(\boldsymbol{\theta})\rangle = \sum_i w_i \langle\psi(\boldsymbol{\theta})\,|Z_i|\,\psi(\boldsymbol{\theta})\rangle + \sum_{i<j} w_{ij} \langle\psi(\boldsymbol{\theta})\,|Z_i Z_j|\,\psi(\boldsymbol{\theta})\rangle$ by sampling the outcome of the circuit in the Z-basis and adding the expectation values of the individual Ising terms together. In general, different control points around $\boldsymbol{\theta}$ have to be estimated, depending on the classical optimizer chosen.
5. Use a classical optimizer to choose a new set of controls.
6. Continue until $C(\boldsymbol{\theta})$ reaches a minimum, close enough to the solution $\boldsymbol{\theta}^*$.
7. Use the last $\boldsymbol{\theta}$ to generate a final set of samples from the distribution $|\langle z_i\,|\psi(\boldsymbol{\theta})\rangle|^2 \;\forall i$ to obtain the answer.

Trial wavefunction

- Consider a simple trial function of the form

$$|\psi(\theta)\rangle = [U_{\text{single}}(\boldsymbol{\theta})U_{\text{entangler}}]^m|+\rangle$$

where $U_{entangler}$ is a collection of C-Phase gates (fully entangling gates), and

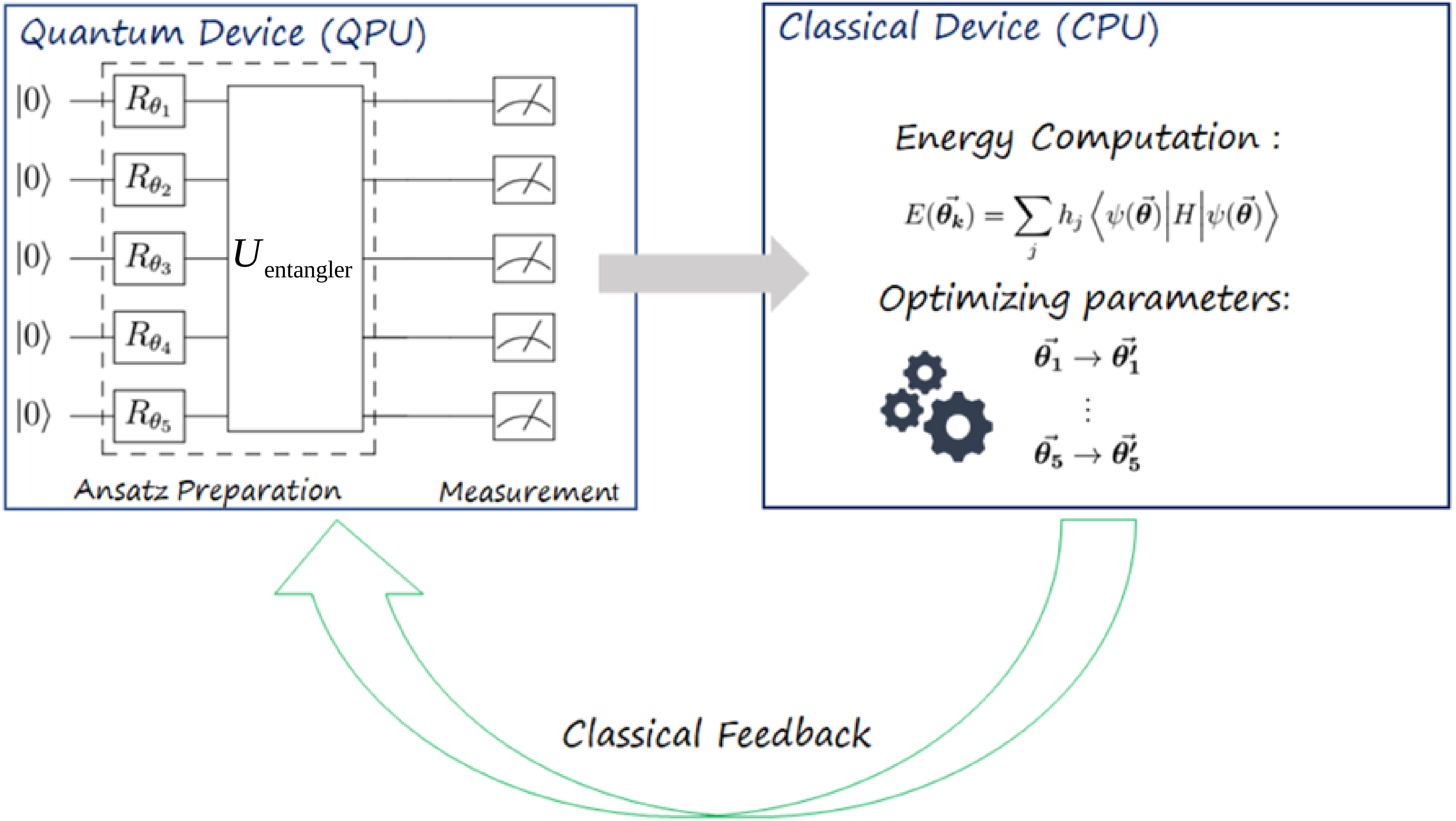
$$U_{\text{single}}(\theta) = \prod_{i=1}^{n} Y(\theta_i),$$

where *n* is the number of qubits and *m* is the depth of the quantum circuit.

- The motivation for this choice is that for these classical problems **this choice allows us to search over the space of quantum states that have only real coefficients, still exploiting the entanglement to potentially converge faster to the solution.**
- One advantage of using this sampling method compared to adiabatic approaches is that the target Ising Hamiltonian does not have to be implemented directly on hardware, allowing this algorithm not to be limited to the connectivity of the device.
- Furthermore, higher-order terms in the cost function, such as $Z_i Z_j Z_k$ can also be sampled efficiently, whereas in adiabatic or annealing approaches they are generally impractical to deal with.

Variational Quantum Eigensolver (VQE)

- Use the VQE method to minimize cost function $C(Z)$.



Investment portfolio problem

- Portfolio:
  - "A **portfolio** is a collection of investments held by an investment company, hedge fund, financial institution or individual." — wikipedia

- Optimization

  Don't put all your eggs in one basket.

Background

- For N assets, an N-dim vector $x=(x_1, x_2, \ldots, x_{N-1}) \in \{0,1\}^N$ represents an investment portfolio.
  ($x_i=1$ indicates picking the i-th asset, and vice versa.)

- $\mu \in \boldsymbol{R}^N$ denotes the expected returns for the assets.
- $\Sigma \in \boldsymbol{R}^{N \times N}$ denotes covariance between and variance of assets.
  (Variance/Covariance are indicators of risk.)

Mathematical Formulation

- Expected profit function (*P*):

$$P = \mu^T x - q\, x^T \Sigma\, x$$

  where *q*>0 is the "risk appetite" of the decision maker.

- Constraint (limited budget *B*)

  Assume that

  - all assets have same price (normalized to 1),
  - full budget has to be used.

$$(1, 1, ..., 1)x = B$$

Cost Function

- The cost function to minimized composes of –*P* and penalty term for constraint with scaling factor *p*.

$$C = qx^T \Sigma x - \mu^T x + p|(1, 1, ..., 1)x - B|^2$$

- Goal: Find *x** that minimizes *C*:

$$x^* = \min_{x \in \{0,1\}^N} C(x)$$

Encoding to Pauli Matrices and Ising Hamiltonian

1. x_i is either 0 or 1; while Pauli-Z has eigenvalues +1 and -1.

   Encoding: $x_i \rightarrow n_i=(1-Z_i)/2$

   $0 \rightarrow n_i = 0 \rightarrow Z_i = 1$

   $1 \rightarrow n_i = 1 \rightarrow Z_i = -1$

2. Substitute it into $C(x)$:

$$C(Z) = \sum_{i \neq j} c_{ij} Z_i Z_j + \sum_i c_i Z_i + \text{const.}$$

3. The portfolio problem is equivalent to minimizing the Ising Hamiltonian

Ising Hamiltonians and QUBO problems

- Ising Hamiltonians can also be converted to what are called quadratic unconstrained binary optimization problems, or QUBOs.
- Quantum annealing (QA) is a metaheuristic for finding the global minimum of a given objective function over a given set of candidate solutions (candidate states), by a process using quantum fluctuations
- Quantum annealing is used mainly for problems where the search space is discrete (combinatorial optimization problems) with many local minima; such as finding the ground state of a spin glass[1] or the traveling salesman problem
- Digital Annealer developed by Fujitsu is a quantum-inspired digital technology architecture, capable of performing parallel, real-time optimization calculations at speed, with precision and on a scale classical computing cannot.