

INTRODUCTION TO QUANTUM ANNEALING

Formulating and solve QUBO Problems

Daniele Ottaviani

The Quantum Annealing Algorithm

- In today's lesson we will study and learn how to program a particular type of quantum computer, the **Quantum Annealer**
- A Quantum Annealer is a **special purpose quantum computer**
- Its purpose, unlike the quantum computers seen in the previous lessons, called General Purpose Quantum Computers, **is not to be freely programmed** by the user.
- A Quantum Annealer is a quantum computer designed and built to host a **single quantum algorithm**, Quantum Annealing
- Quantum Annealing is a quantum algorithm capable of solving optimization problems



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The Quantum Annealing Algorithm

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PHYSICAL REVIEW E

VOLUME 58, NUMBER 5

NOVEMBER 1998

Quantum annealing in the transverse Ising model

Tadashi Kadowaki and Hidetoshi Nishimori

Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551, Japan

(Received 30 April 1998)

We introduce quantum fluctuations into the simulated annealing process of optimization problems, aiming at faster convergence to the optimal state. Quantum fluctuations cause transitions between states and thus play the same role as thermal fluctuations in the conventional approach. The idea is tested by the transverse Ising model, in which the transverse field is a function of time similar to the temperature in the conventional method. The goal is to find the ground state of the diagonal part of the Hamiltonian with high accuracy as quickly as possible. We have solved the time-dependent Schrödinger equation numerically for small size systems with various exchange interactions. Comparison with the results of the corresponding classical (thermal) method reveals that the quantum annealing leads to the ground state with much larger probability in almost all cases if we use the same annealing schedule. [S1063-651X(98)02910-9]

PACS number(s): 05.30.-d, 75.10.Nr, 89.70.+c

I. INTRODUCTION

The technique of simulated annealing (SA) was first proposed by Kirkpatrick *et al.* [1] as a general method to solve optimization problems. The idea is to use thermal fluctuations to allow the system to escape from local minima of the cost function so that the system reaches the global minimum under an appropriate annealing schedule (the rate of decrease of temperature). If the temperature is decreased too quickly, the system may become trapped in a local minimum. Too slow annealing, on the other hand, is practically useless although such a process would certainly bring the system to the global minimum. Geman and Geman proved a theorem on the annealing schedule for a generic problem of combinatorial optimization [2]. They showed that any system reaches the global minimum of the cost function asymptotically if the temperature is decreased as $T = c/\ln t$ or slower, where c is a constant determined by the system size and other structures of the cost function. This bound on the annealing schedule may be the optimal one under generic con-

specific model system, rather than to develop a general argument, to gain insight into the role of quantum fluctuations in the situation of optimization problem. Quantum effects have been found to play a very similar role to thermal fluctuations in the Hopfield model in a transverse field in thermal equilibrium [5]. This observation motivates us to investigate dynamical properties of the Ising model under quantum fluctuations in the form of a transverse field. We therefore discuss in this paper the transverse Ising model with a variety of exchange interactions. The transverse field controls the rate of transition between states and thus plays the same role as the temperature does in SA. We assume that the system has no thermal fluctuations in the QA context and the term "ground state" refers to the lowest-energy state of the Hamiltonian without the transverse field term.

Static properties of the transverse Ising model have been investigated quite extensively for many years [6]. There have, however, been very few studies on the dynamical behavior of the Ising model with a transverse field. We refer to the work by Sato *et al.* who carried out quantum Monte

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We introduce quantum annealing as a faster convergence to the same role as thermal fluctuations in the transverse Ising model, in which the system is driven by a transverse field. The goal is to find the ground state of the system as quickly as possible. We have simulated various exchange interactions and the results reveal that the quantum annealing method we use the same as the thermal method almost in all cases if

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I. INTRODUCTION

The technique of simulated annealing proposed by Kirkpatrick *et al.* [1] is widely used for solving optimization problems. The idea is to allow the system to escape from local minima by paying a cost function so that the system can reach the global minimum under an appropriate annealing schedule (i.e., a schedule of temperature). If the temperature is lowered slowly, the system may become trapped in a local minimum. However, if the system is cooled slowly enough, it will eventually reach the global minimum. Geman and Geman proposed a simulated annealing schedule for combinatorial optimization [2]. The system reaches the global minimum of the cost function if the temperature is decreased slowly enough, where c is a constant determined by the structure of the cost function. The annealing schedule may be the optimal one under generic con-



problems, aiming at the same role as thermal fluctuations in the transverse Ising model. The goal is to find the ground state of the system as quickly as possible. We have simulated various exchange interactions and the results reveal that the quantum annealing method we use the same as the thermal method almost in all cases if

than to develop a general argument on the role of quantum fluctuations in the transverse Ising problem. Quantum effects have a similar role to thermal fluctuations in the transverse Ising model. The transverse field in thermal equilibrium motivates us to investigate the transverse Ising model under quantum fluctuations. We therefore consider the transverse Ising model with a variable transverse field. The transverse field controls the dynamics of the system and thus plays the same role as thermal fluctuations. We assume that the system is in the lowest-energy state of the transverse Ising model.

The transverse Ising model have been studied for many years [6]. There have been many studies on the dynamical behavior of the system with a transverse field. We refer to the work by Sato *et al.* who carried out quantum Monte

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- The author of the paper, as well as the theorist of the algorithm, is **Professor Hidetoshi Nishimori**
- Professor Nishimori, now happily retired, used to work as a full professor at the University of Tokyo
- His studies in this field have opened a **real alternative path** for quantum computing
- From the moment of publication of this paper to the first realization of a machine prototype capable of implementing this algorithm **there is a gap of 14 years!**
- The first Quantum Annealer model from D-Wave, in fact, came out in **2012**
- In 2018 I had a beer with him!

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I. INTRODUCTION

The technique of simulated annealing proposed by Kirkpatrick *et al.* [1] is used for optimization problems. The idea is to allow the system to escape from local minima by increasing the cost function so that the system can find the global minimum under an appropriate annealing schedule (of temperature). If the temperature is too high, the system may become trapped in a local minimum. On the other hand, if the temperature is too low, the system may become trapped in a local minimum. However, such a process would not be efficient for finding the global minimum. Geman and Geman proposed an annealing schedule for combinatorial optimization [2]. The system reaches the global minimum of the cost function if the temperature is decreased slowly enough, where c is a constant determined by the structure of the cost function. The annealing schedule may be the optimal one under generic con-

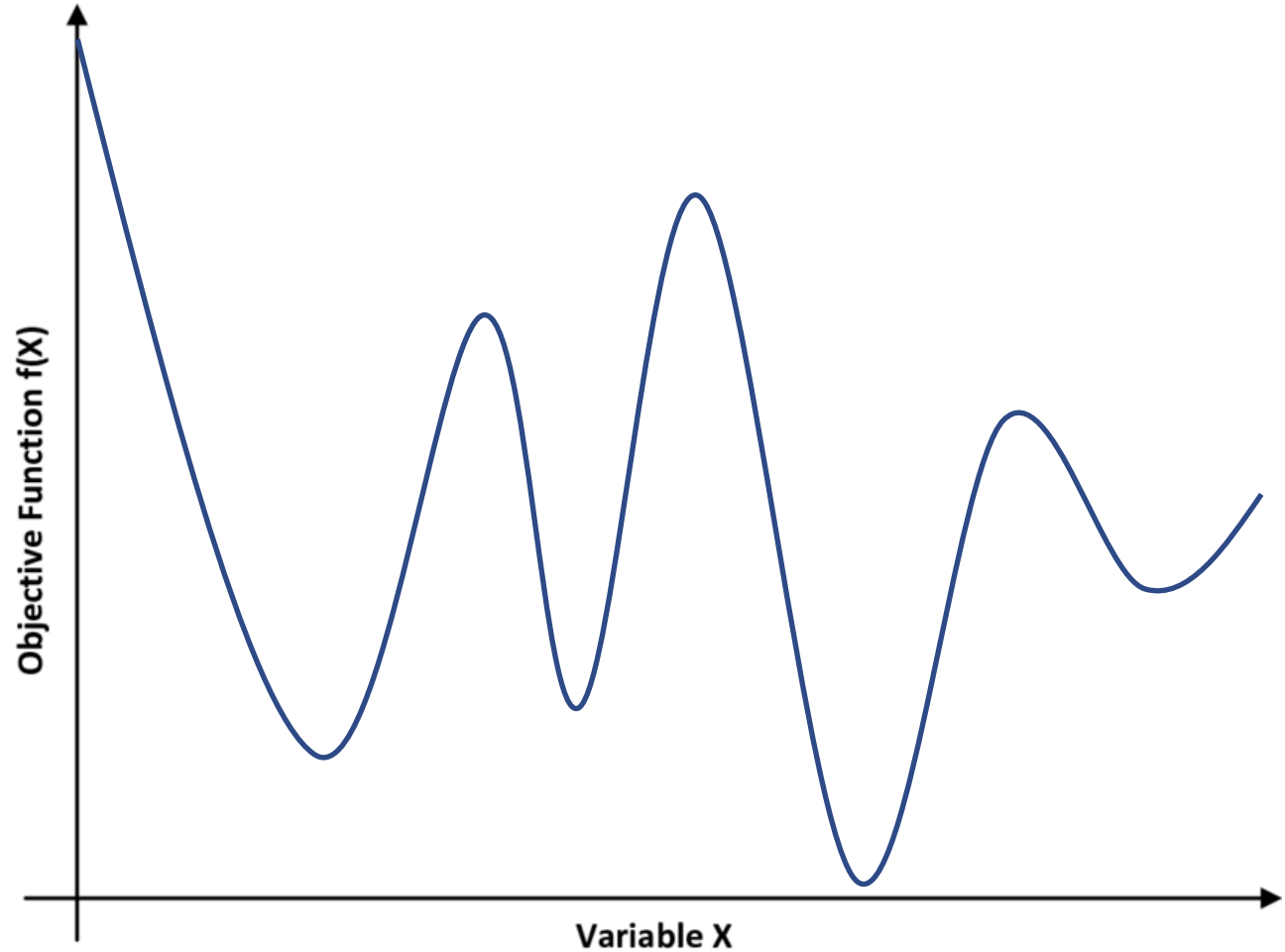


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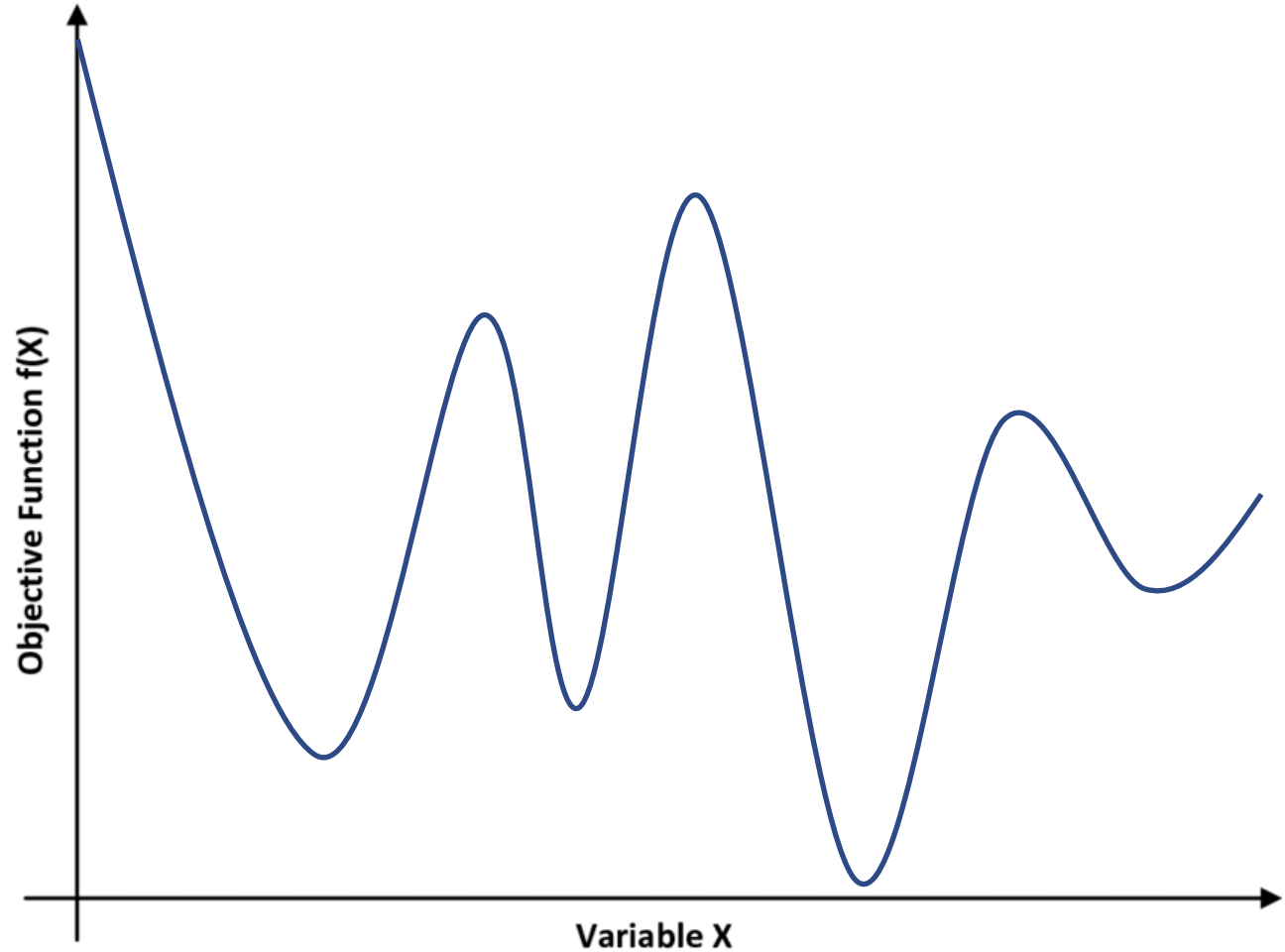
Annealing Algorithms

- Suppose we have an optimization problem, for example a minimization problem, whose objective function (i.e. the function to be minimized) is known and computable using a finite set of variables.
- The best way to solve a problem of this type is undoubtedly the so-called **brute force approach**: we calculate all the values of the objective function for all possible inputs and consider the smallest
- This approach, although undeniably functional, is **unfortunately not always practicable**. Sometimes the inputs with which to calculate the value of the objective function are not few ...
- Let's imagine for example the case of a function with N binary variables: the number of possible combinations is 2^N ...



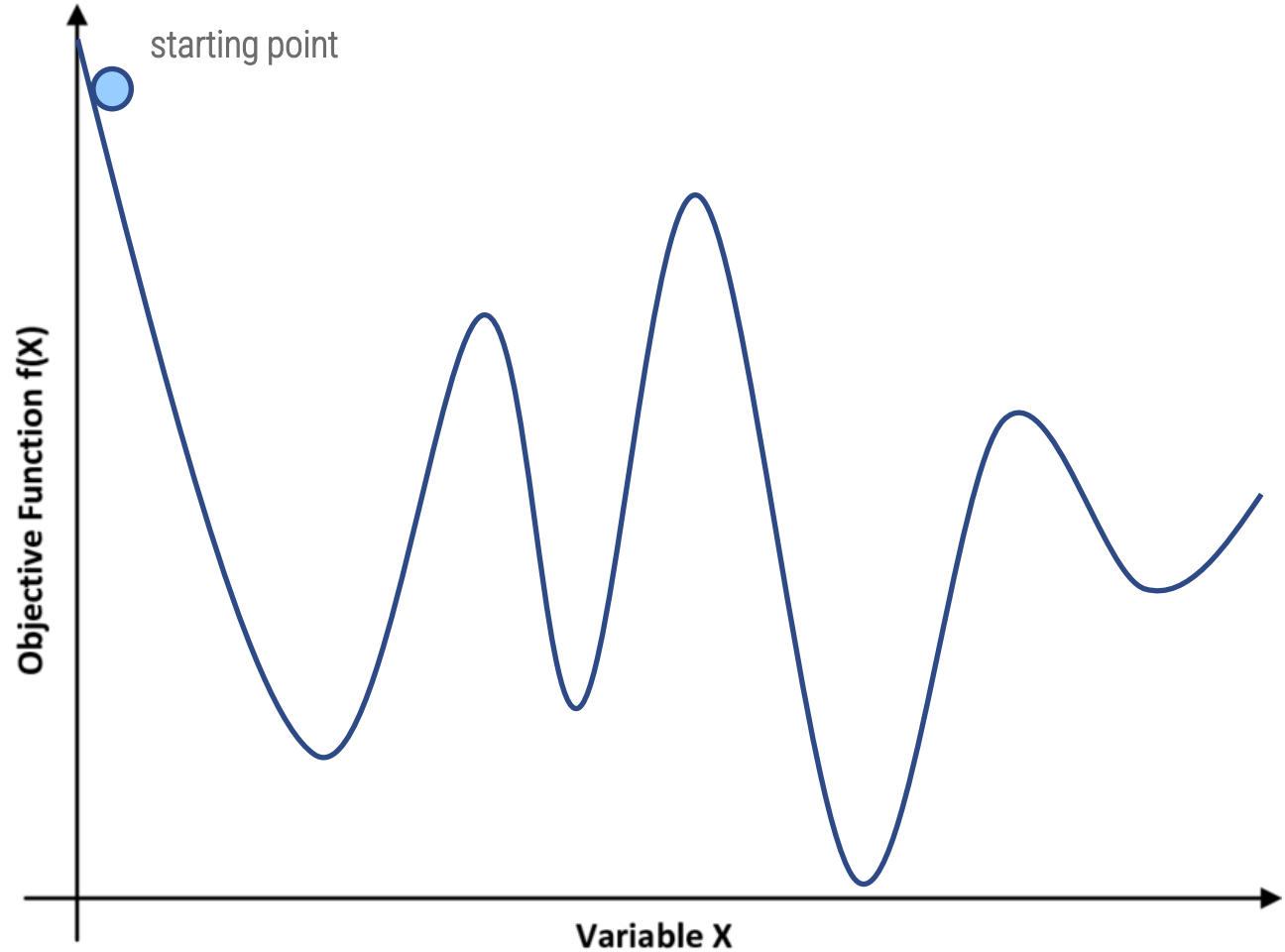
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- Fortunately, brute force is **not** the only algorithm for solving problems of this type.
- There are many algorithms capable of identifying the optimal point of an objective function without having to analyze each of its points
- One of these is known as **Simulated Annealing**
- Simulated annealing is a probabilistic strategy used to solve optimization problems



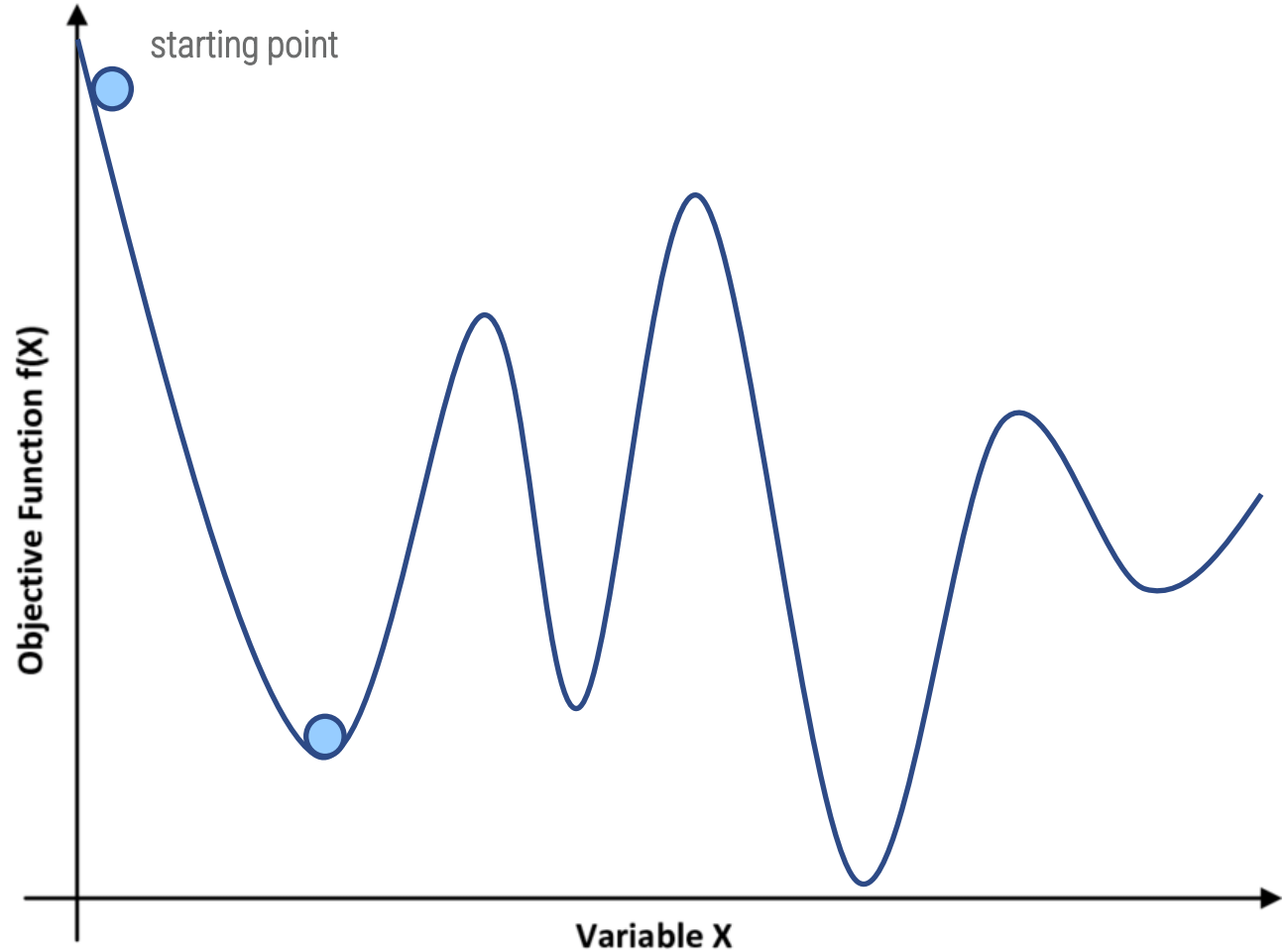
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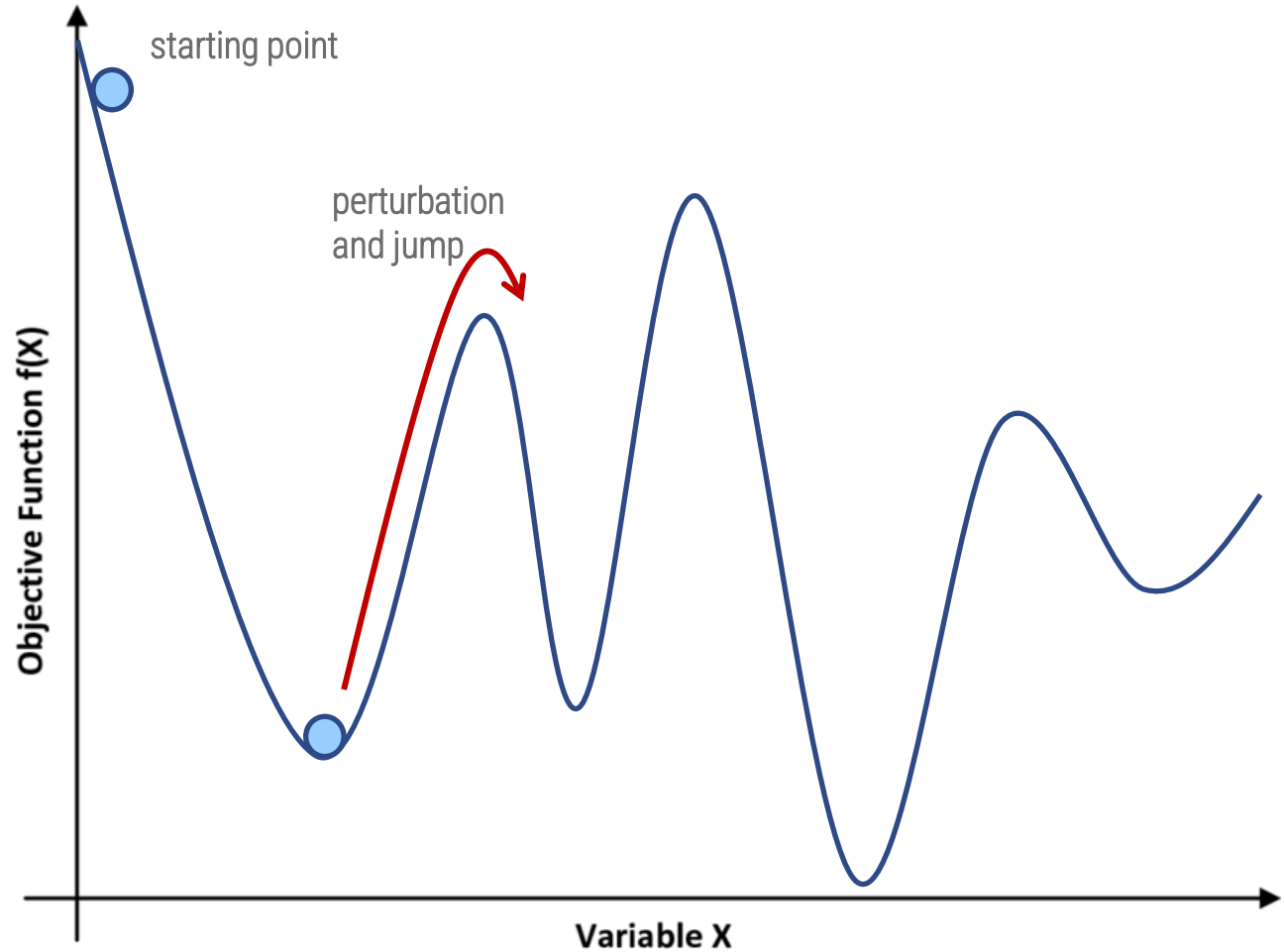
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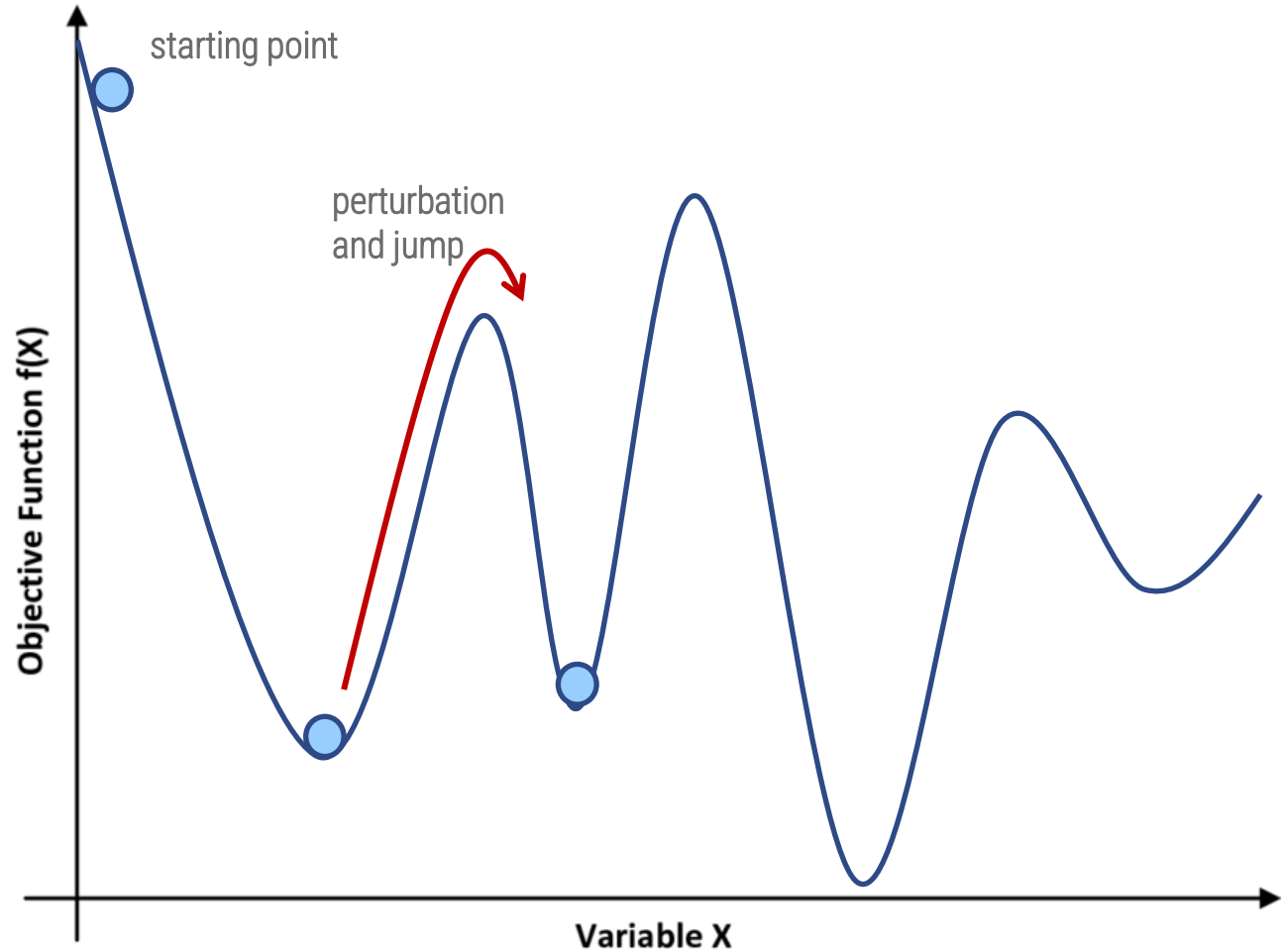
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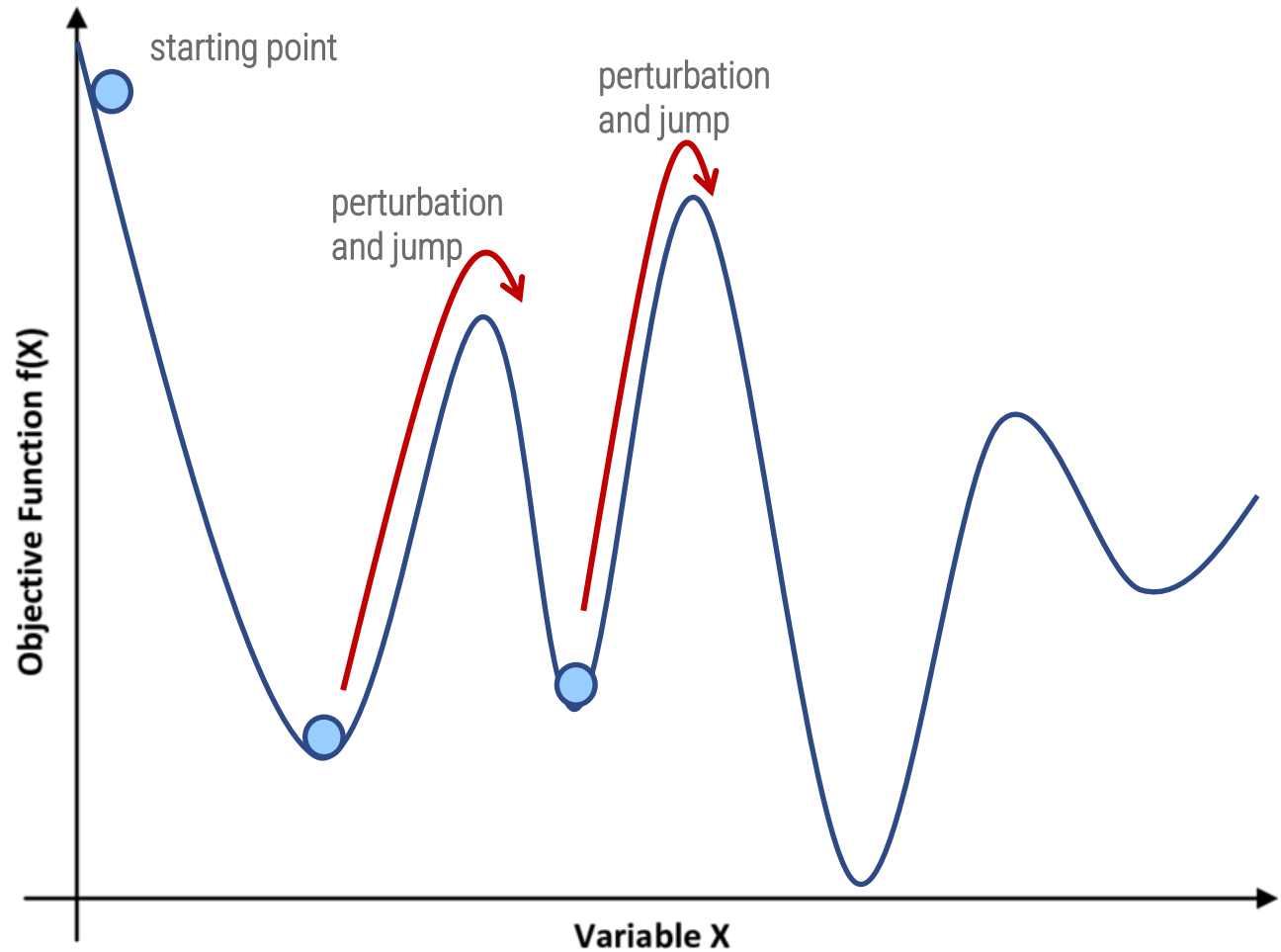
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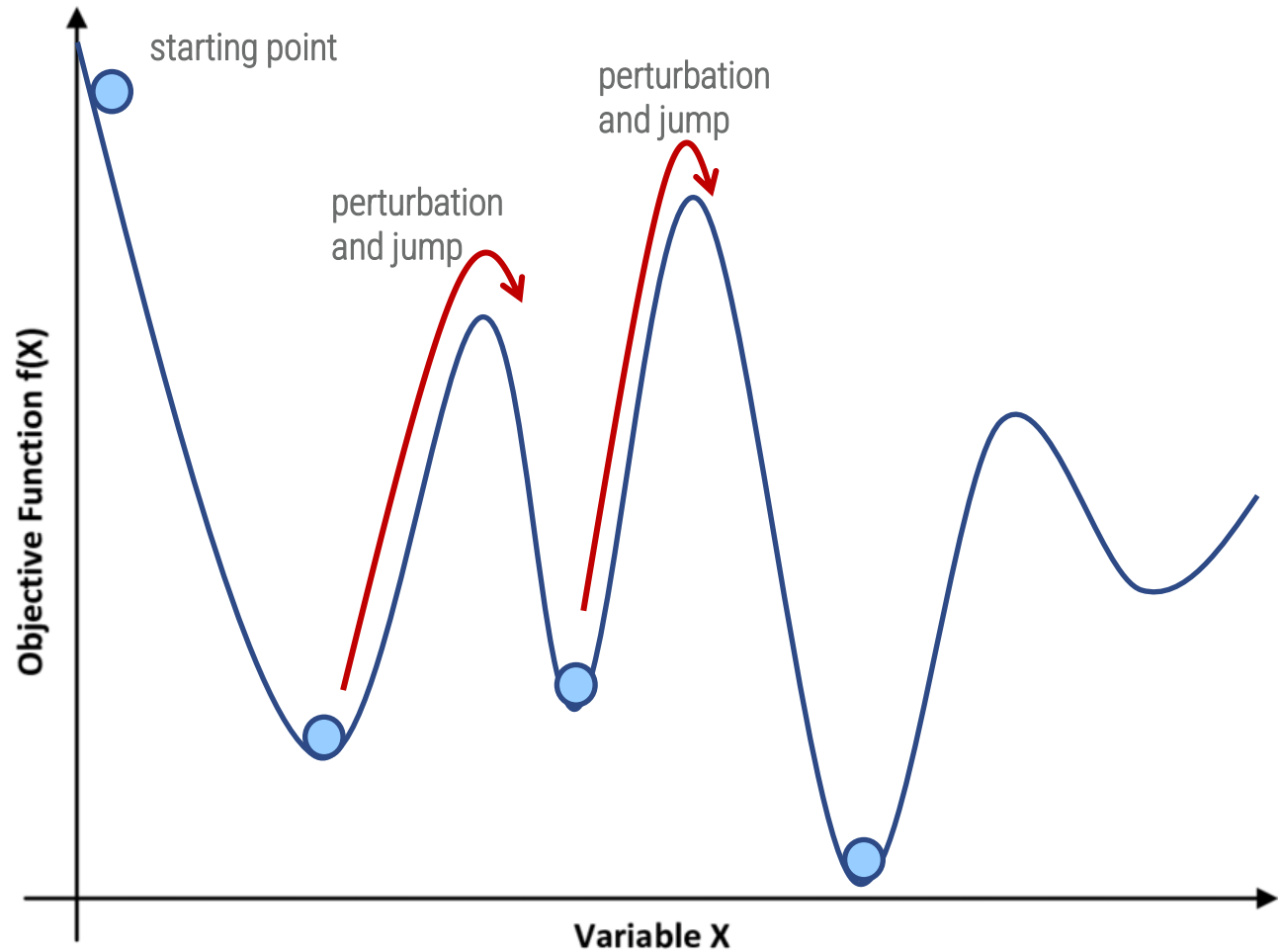
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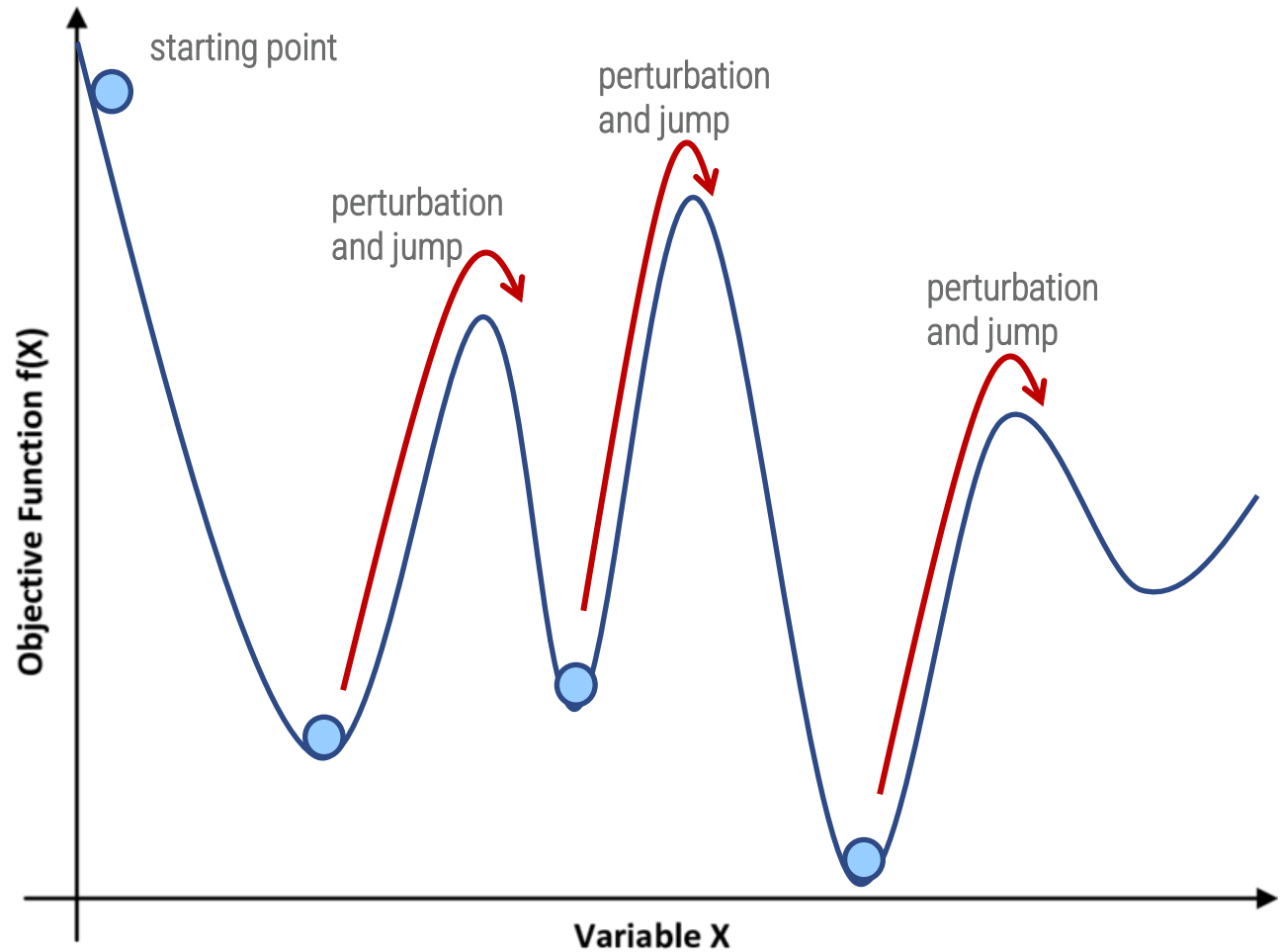
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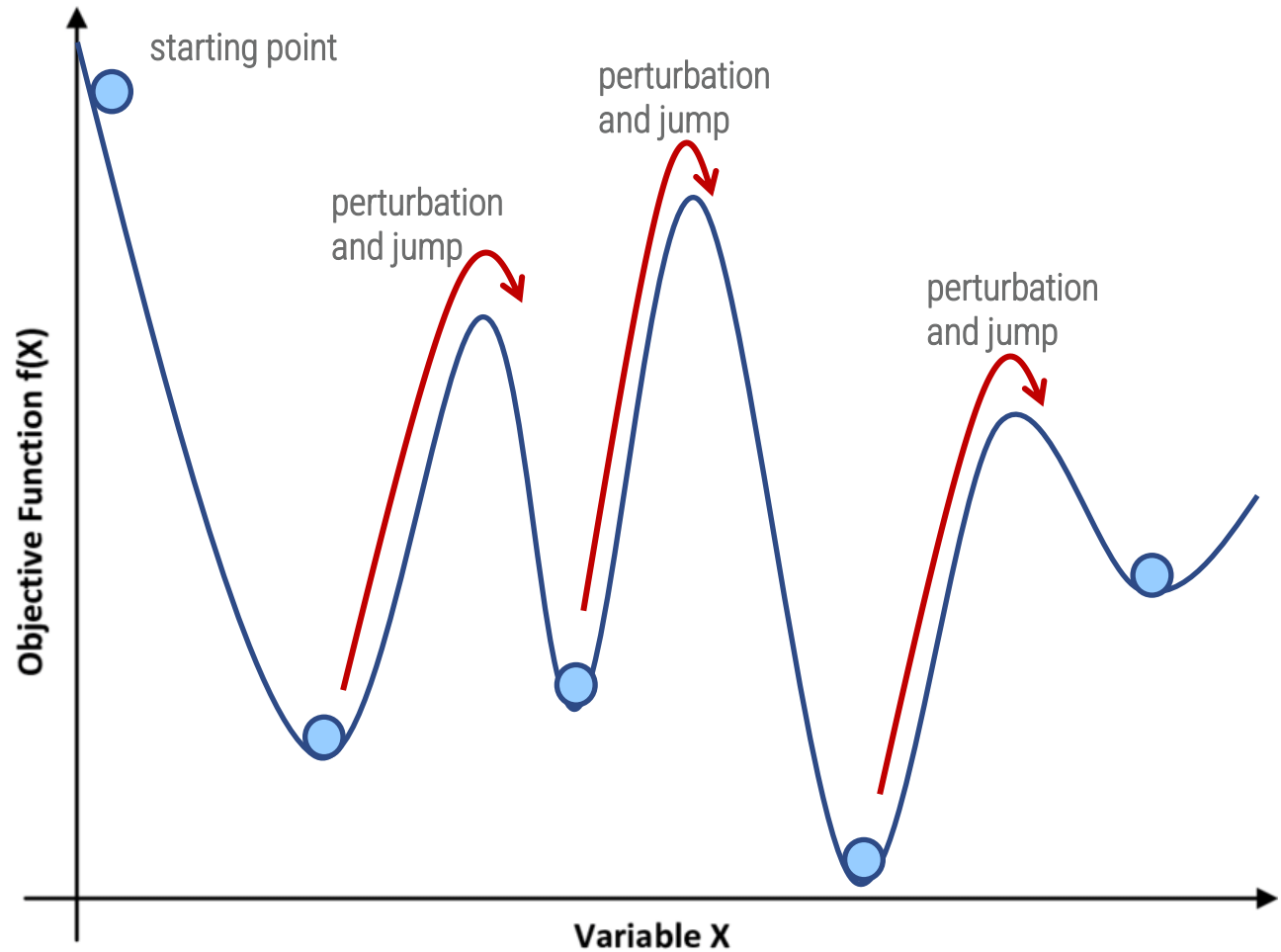
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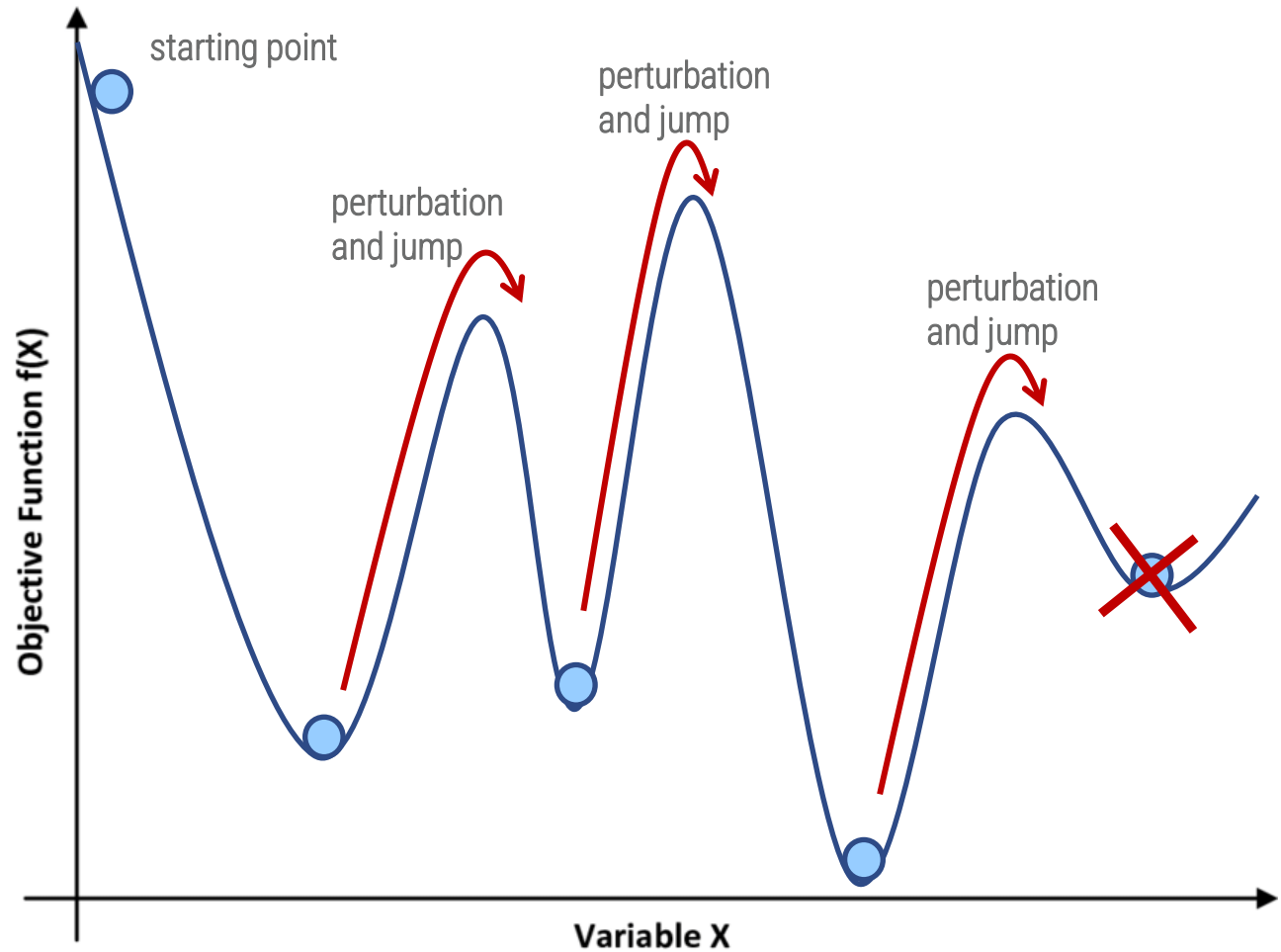
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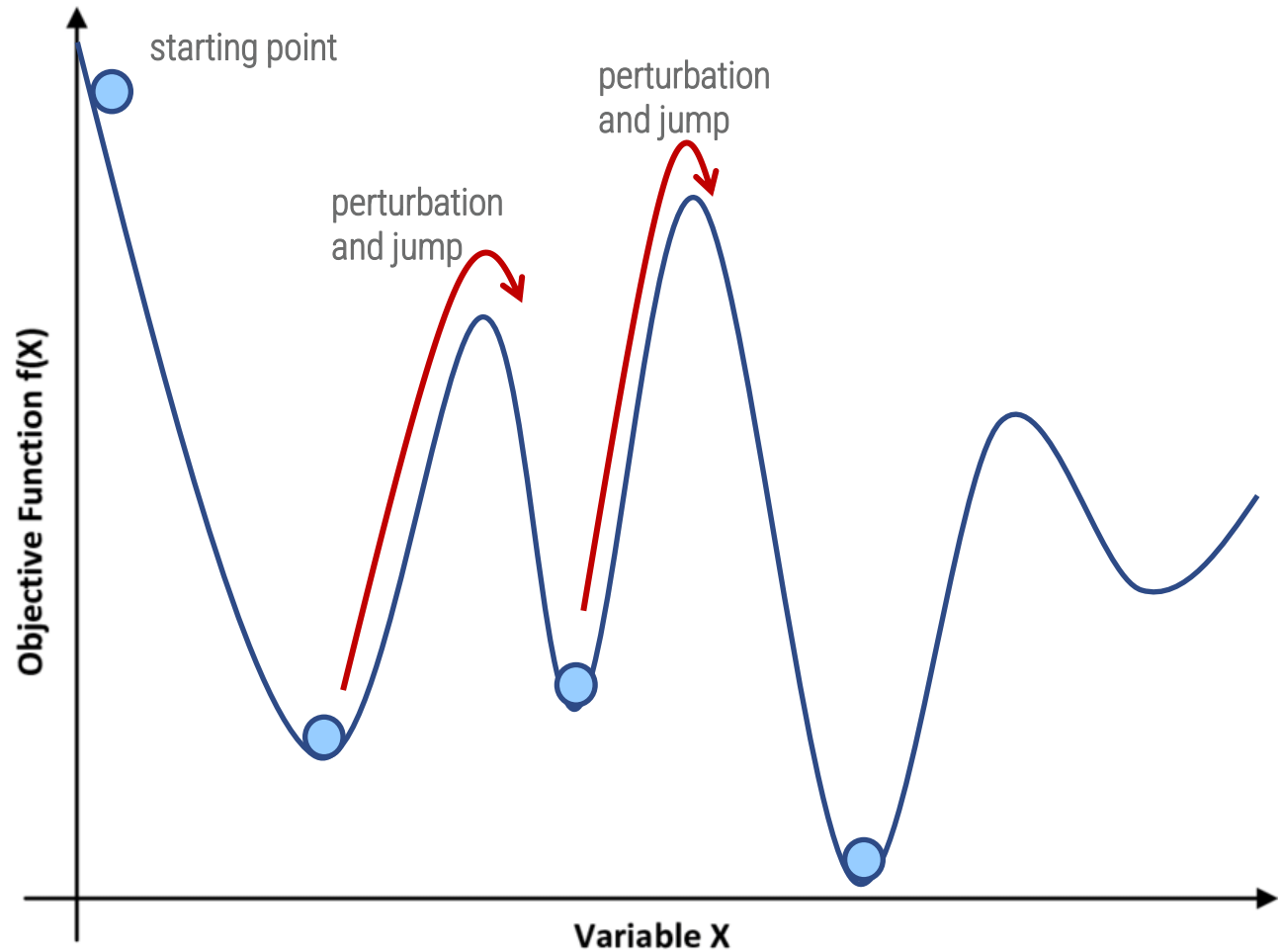
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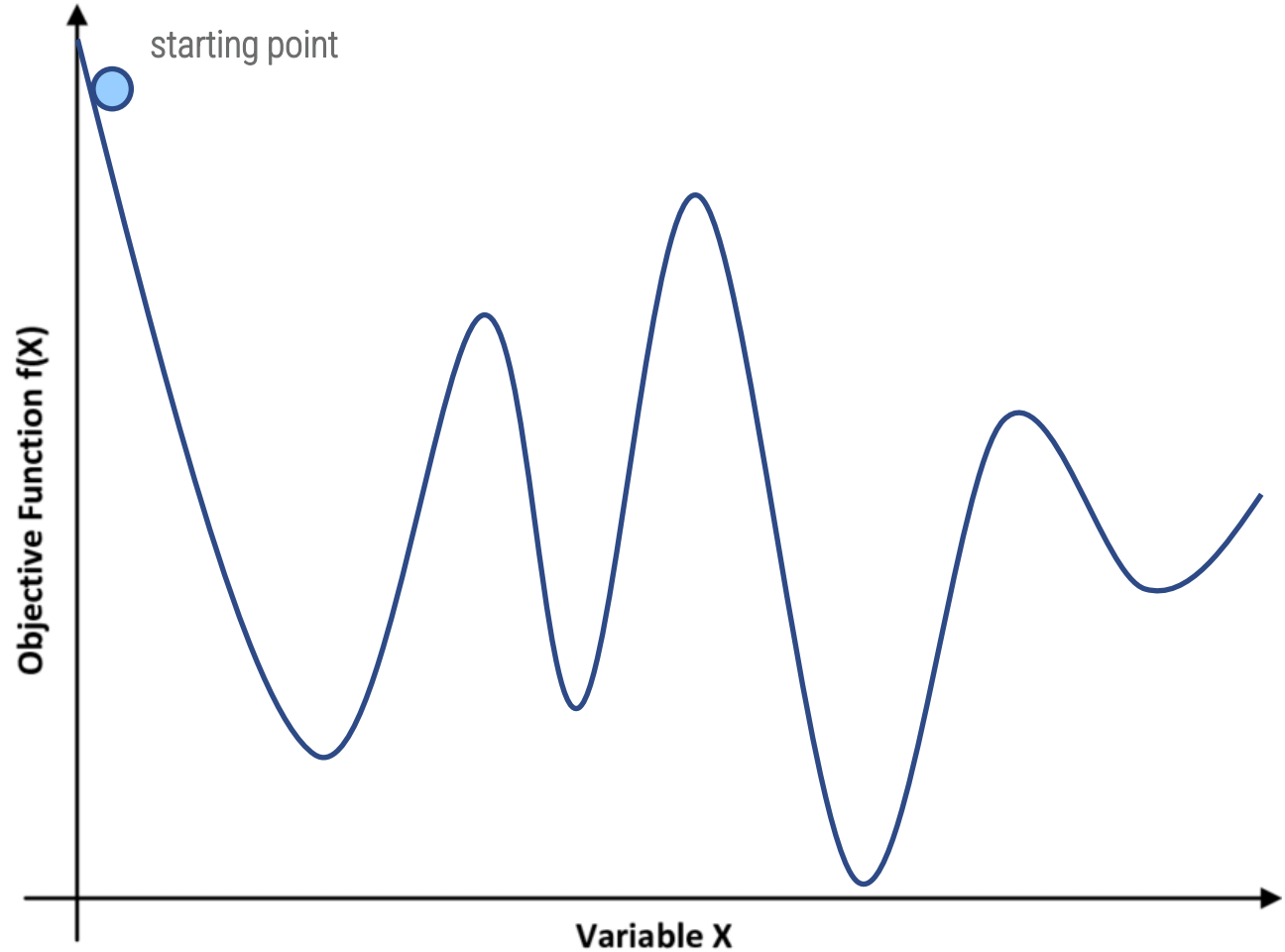
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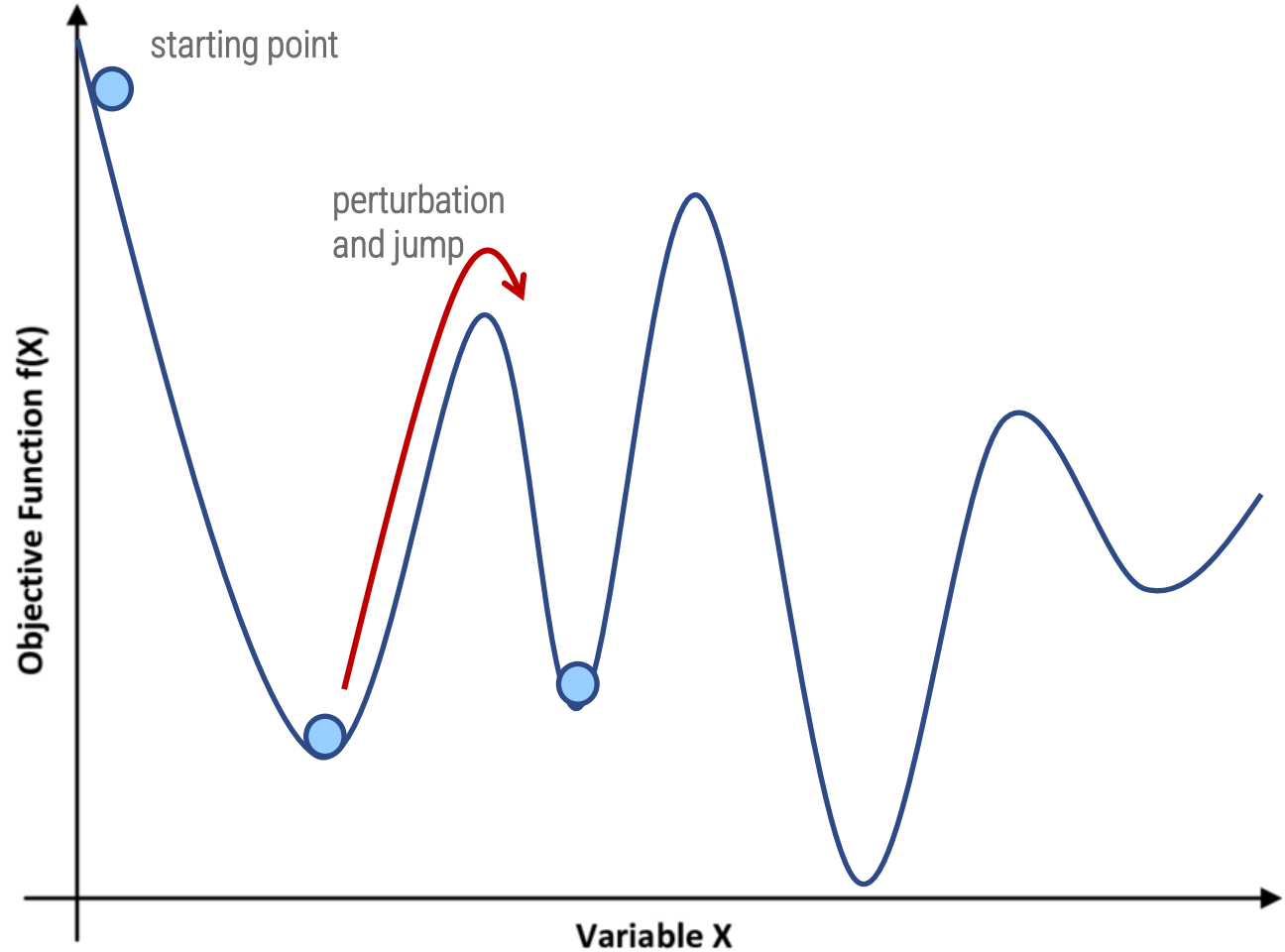
Quantum Annealing

- **Quantum Annealing** is the quantum version of simulated annealing
- The principle of quantum mechanics that is most exploited during the run of a quantum annealing is the **phenomenon of quantum tunneling**
- Visually, we can consider the quantum annealing process as a simulated annealing process where the ball, a macroscopic object, is replaced by a microscopic particle.



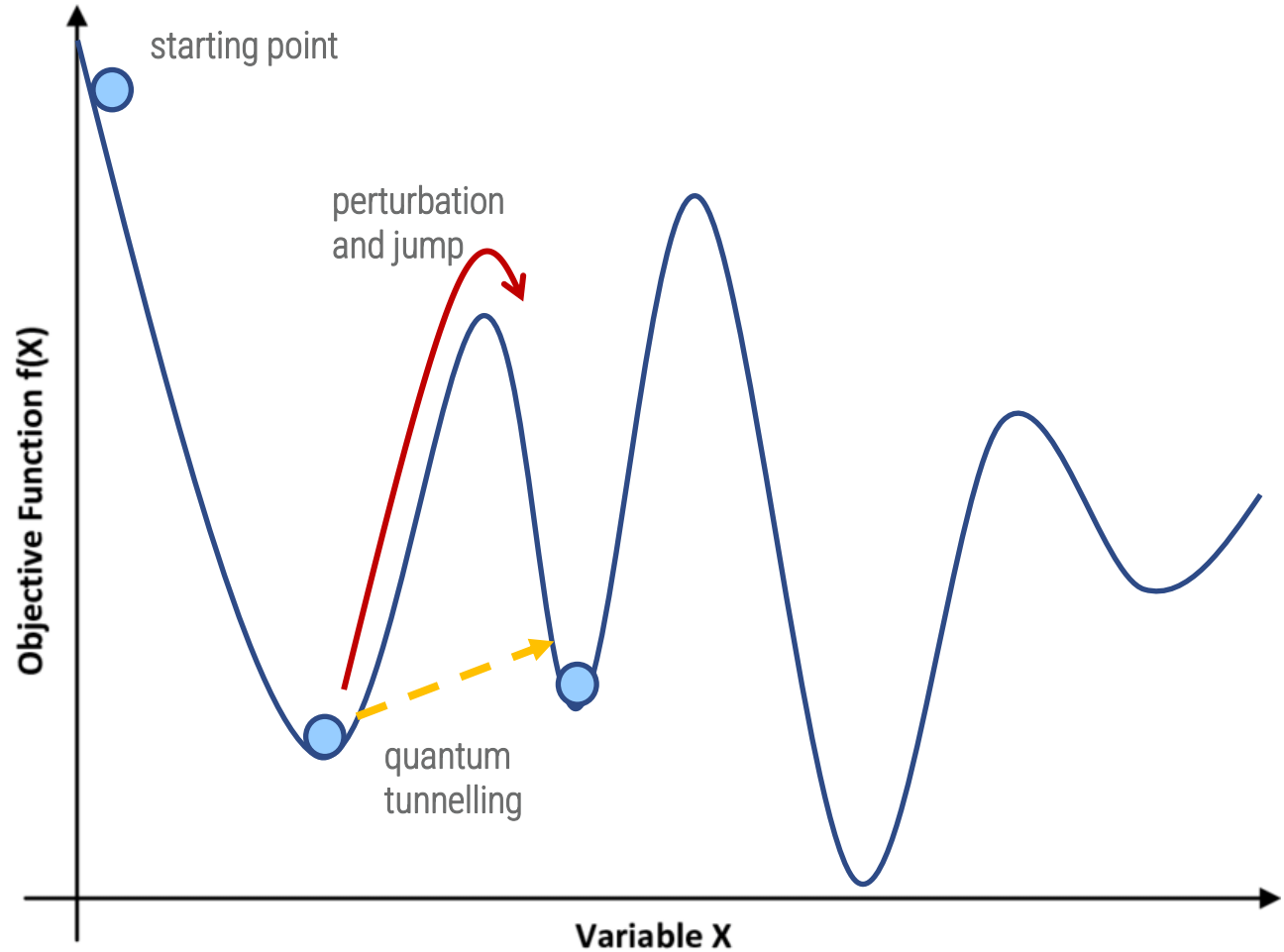
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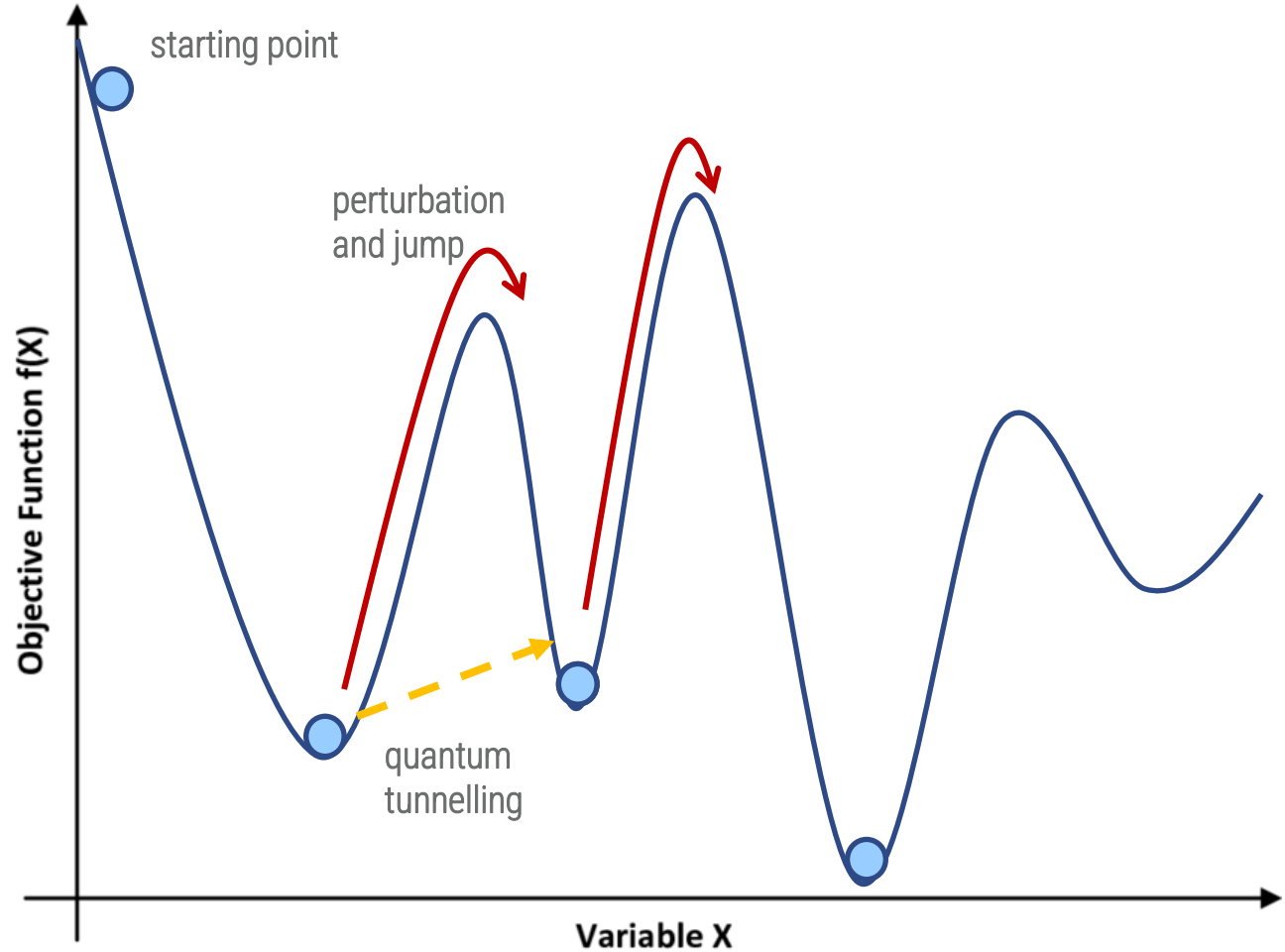
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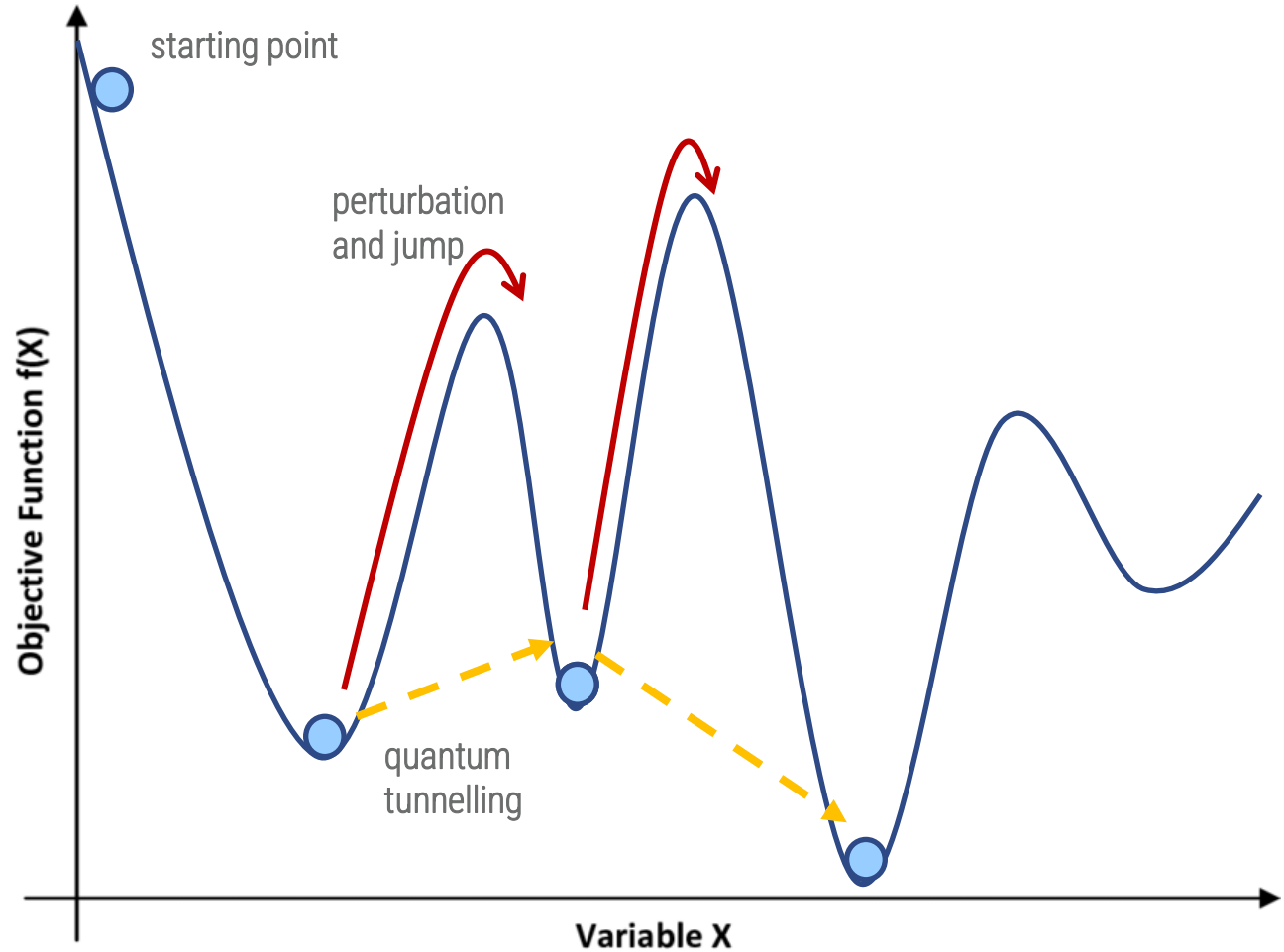
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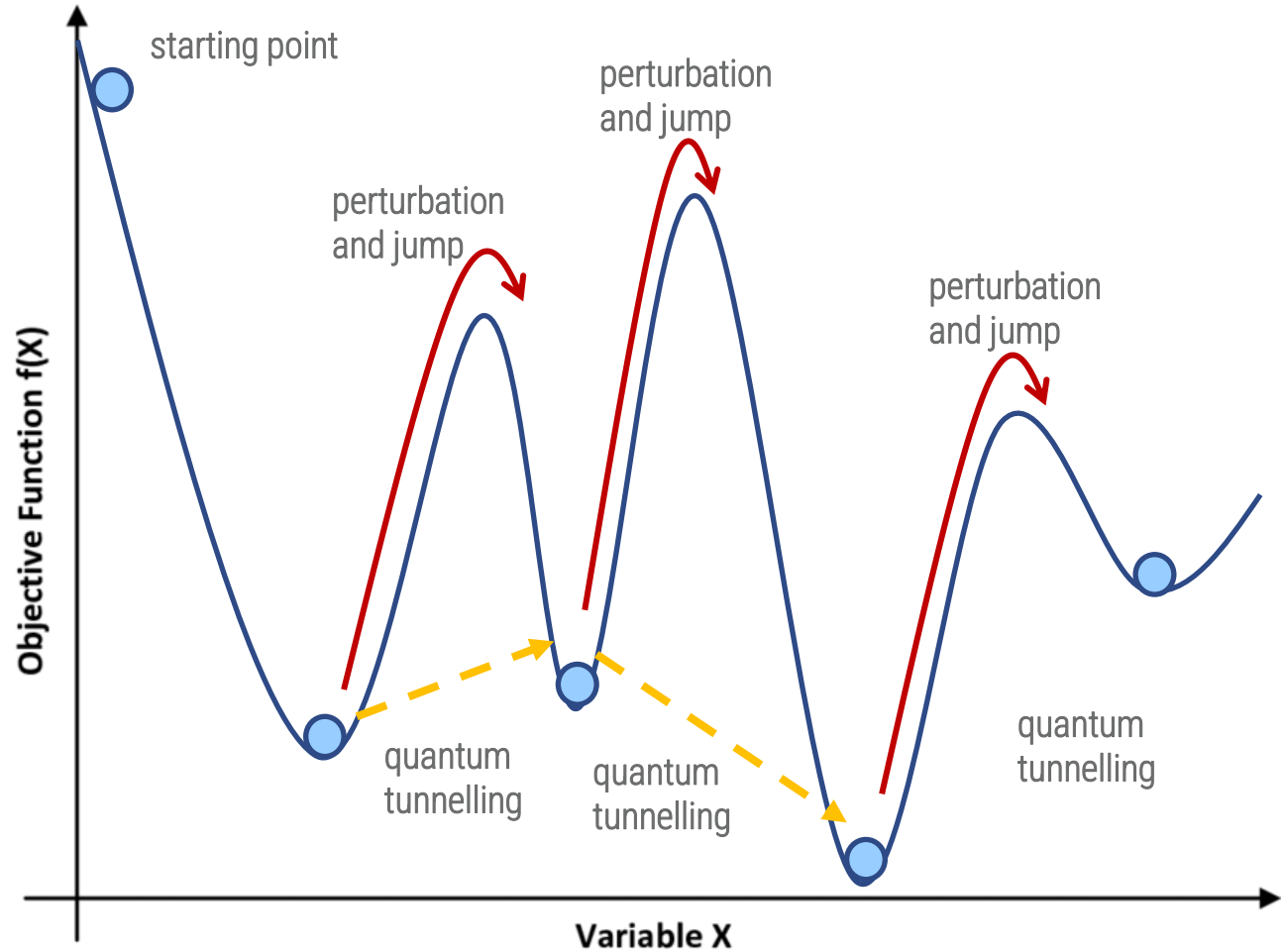
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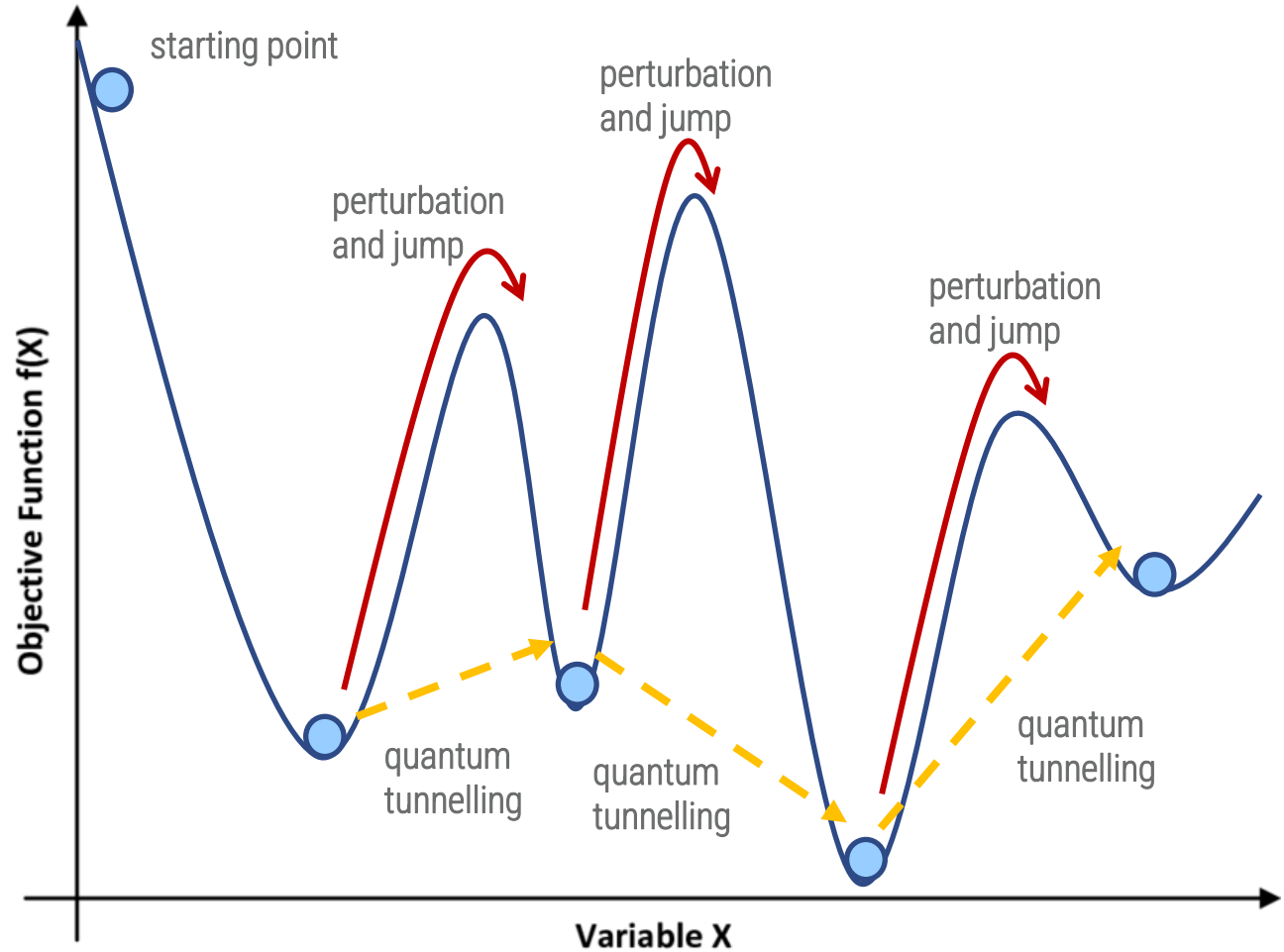
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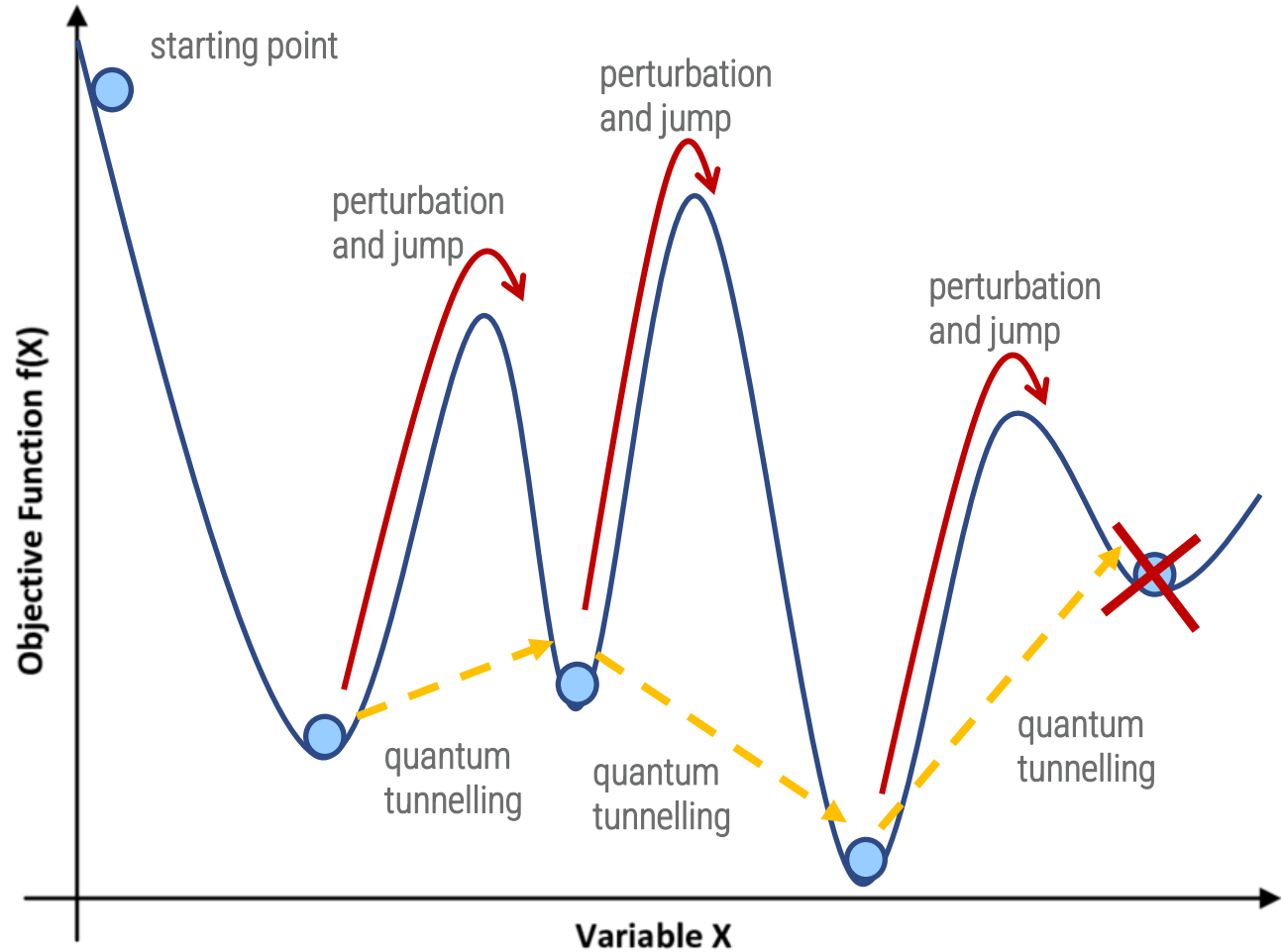
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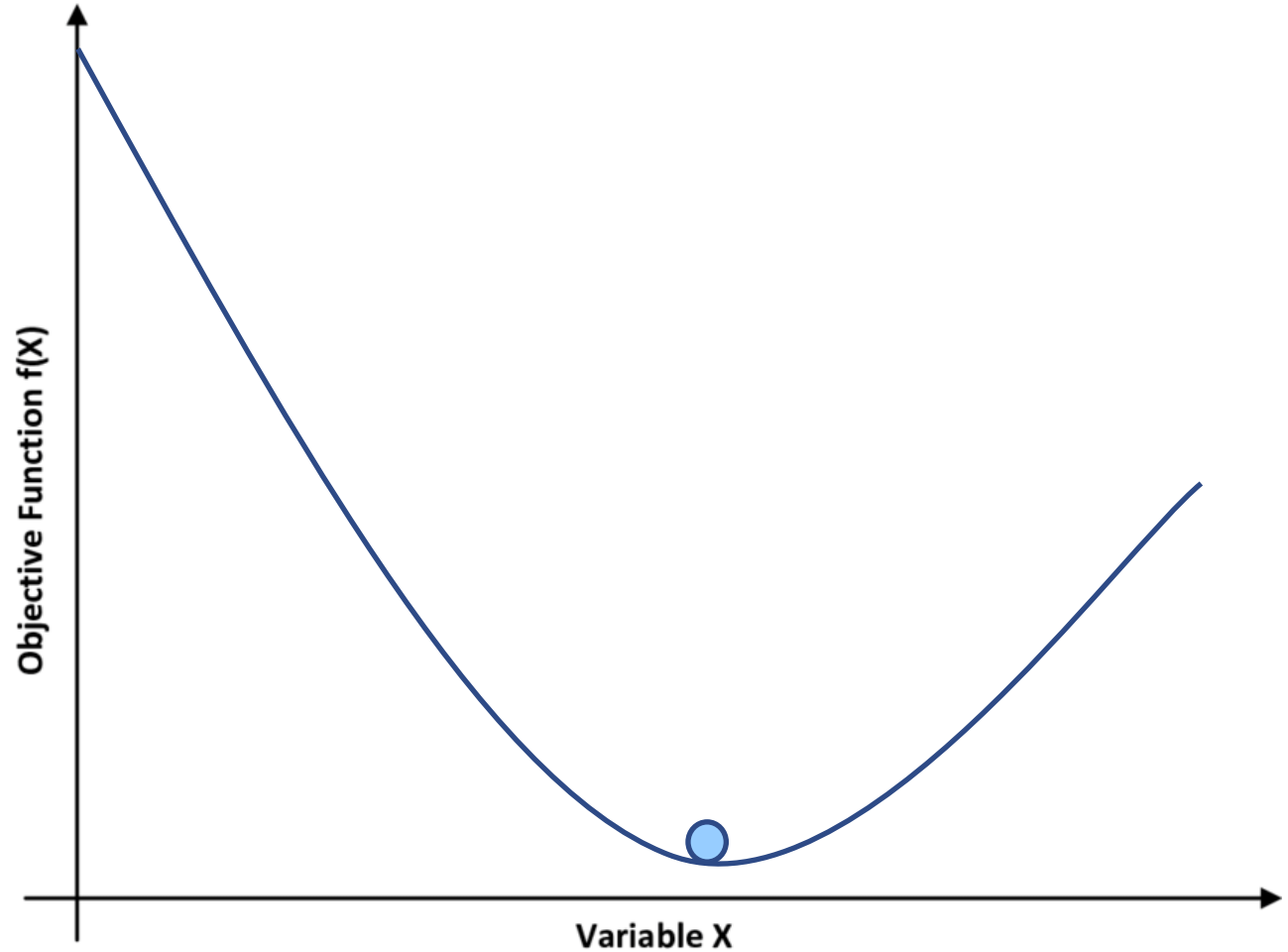
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- How does the Quantum Annealing process work? The core of the algorithm is in the **Adiabatic Theorem**:
A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum



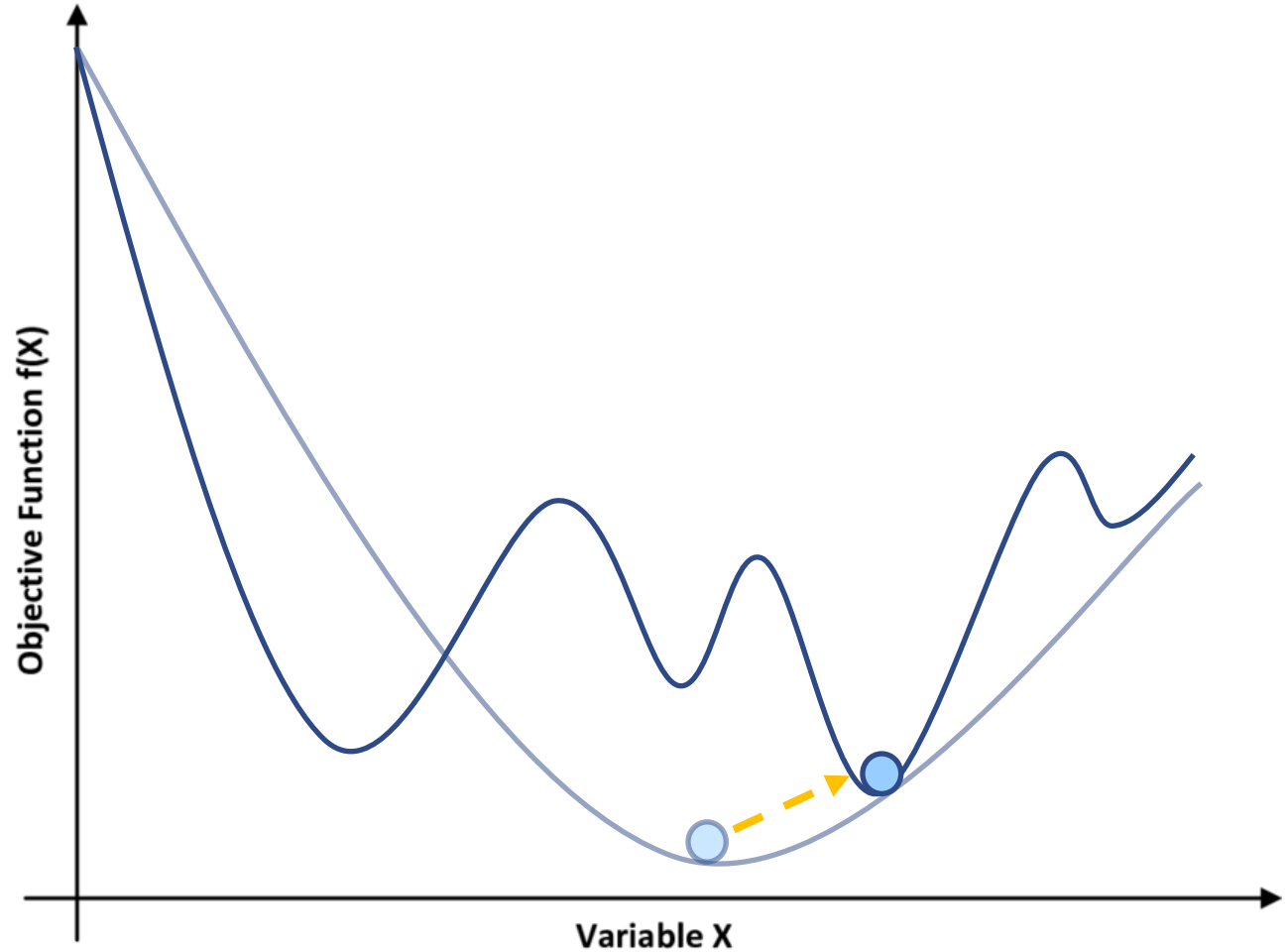
Quantum Annealing

- Optimization through quantum annealing begins with choosing an objective function **different** than the one you want to optimize.
- The choice always falls on a **simple function**, of which the **global minimum is known** (for example).



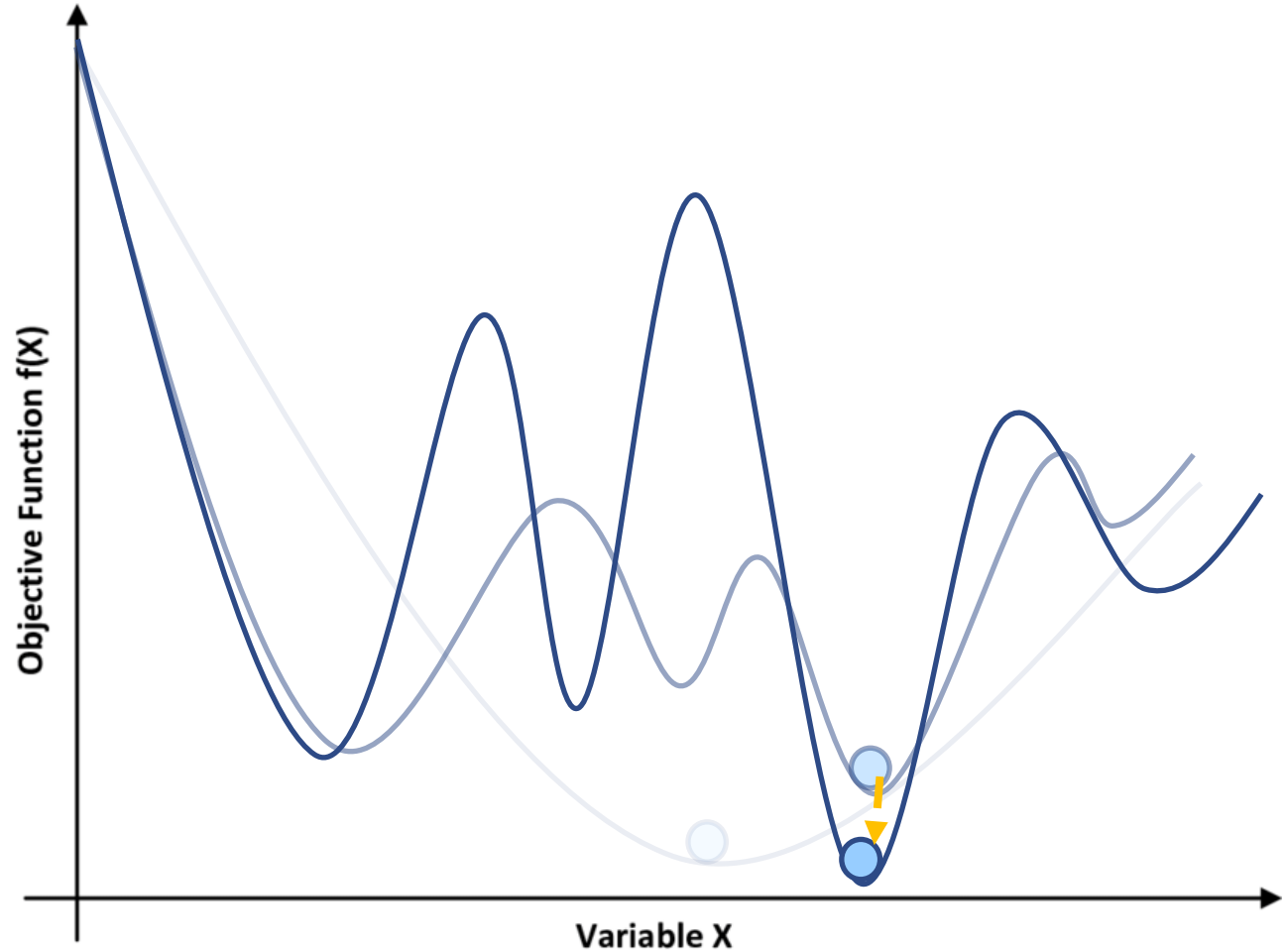
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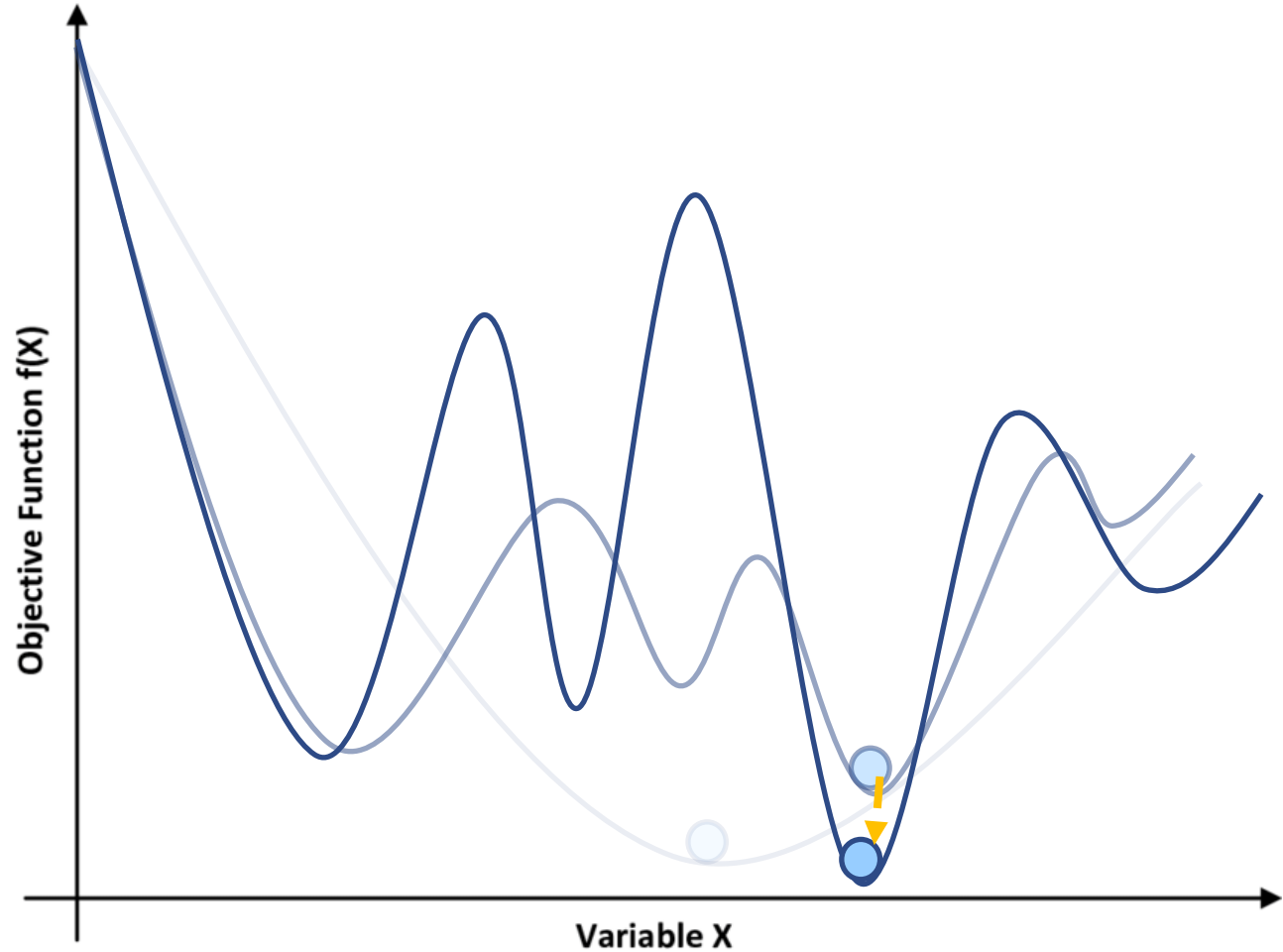
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- The process lasts until the initial objective function **becomes equivalent** to the objective function whose you really want to optimize



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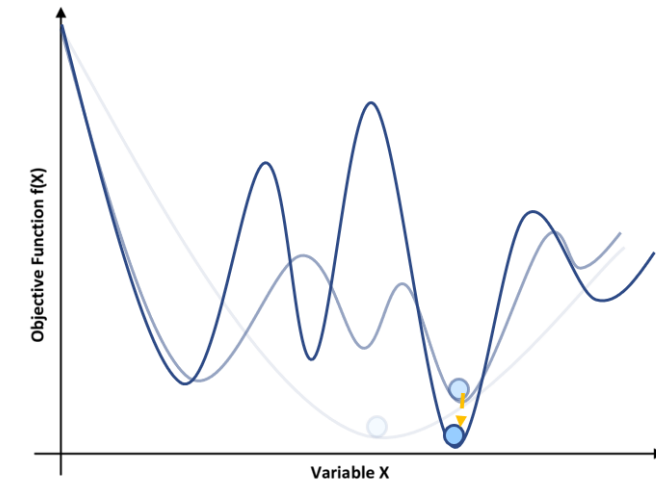
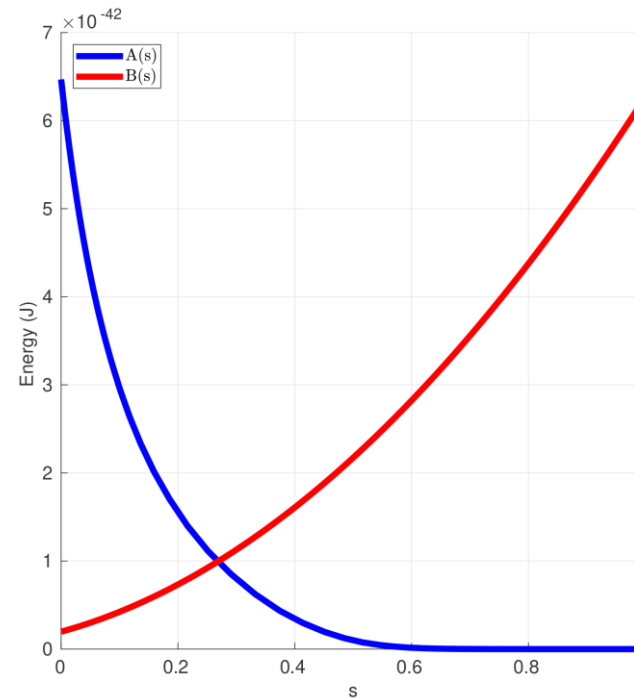
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$$\underbrace{-\frac{A(s)}{2} \left(\sum_i \hat{\sigma}_x^{(i)} \right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2} \left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \right)}_{\text{Final Hamiltonian}}$$



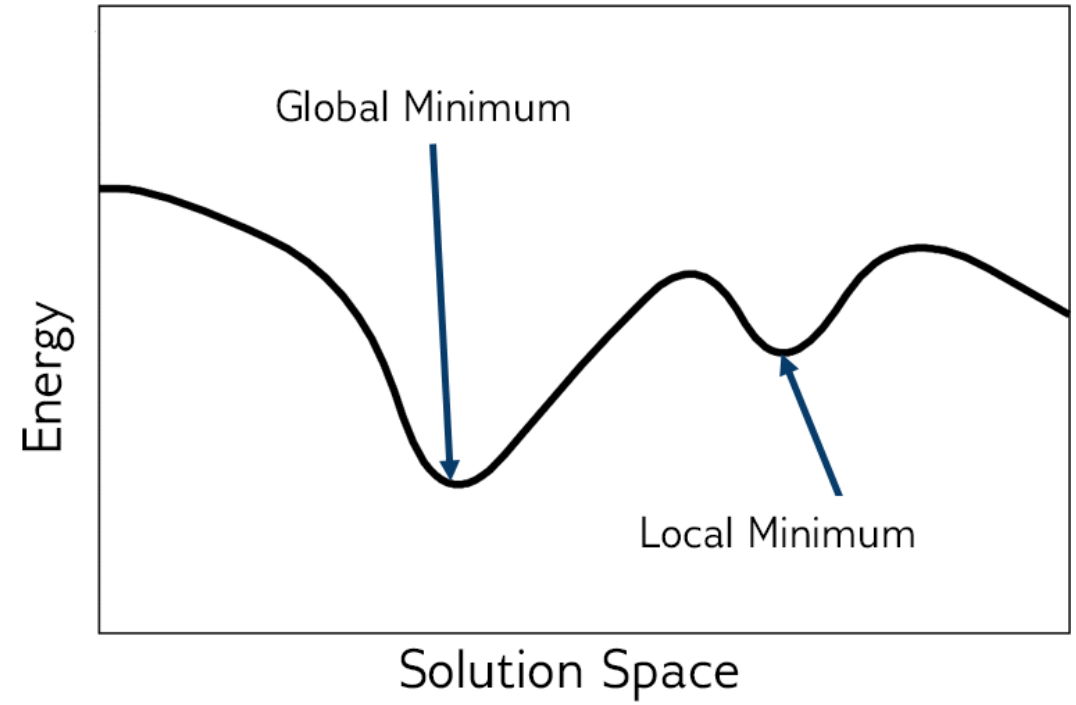
The Quantum Annealer

- Currently, we can talk about **The** quantum annealer and not about **a** generic quantum annealer **since today there is only one manufacturer** for this type of device.
- The company in question is called **D-Wave**
- At the moment the latest quantum annealer model has more than 5000 qubits and about 30,000 connectors
- We will see in the course of the lesson the importance of these numbers
- To understand how to interact with a quantum annealer, we need the following concepts:
 - Objective functions
 - Ising model (Ising Hamiltonian)
 - Quadratic Unconstrained Binary Optimization problems (QUBO problems)
 - Graphs and embedding



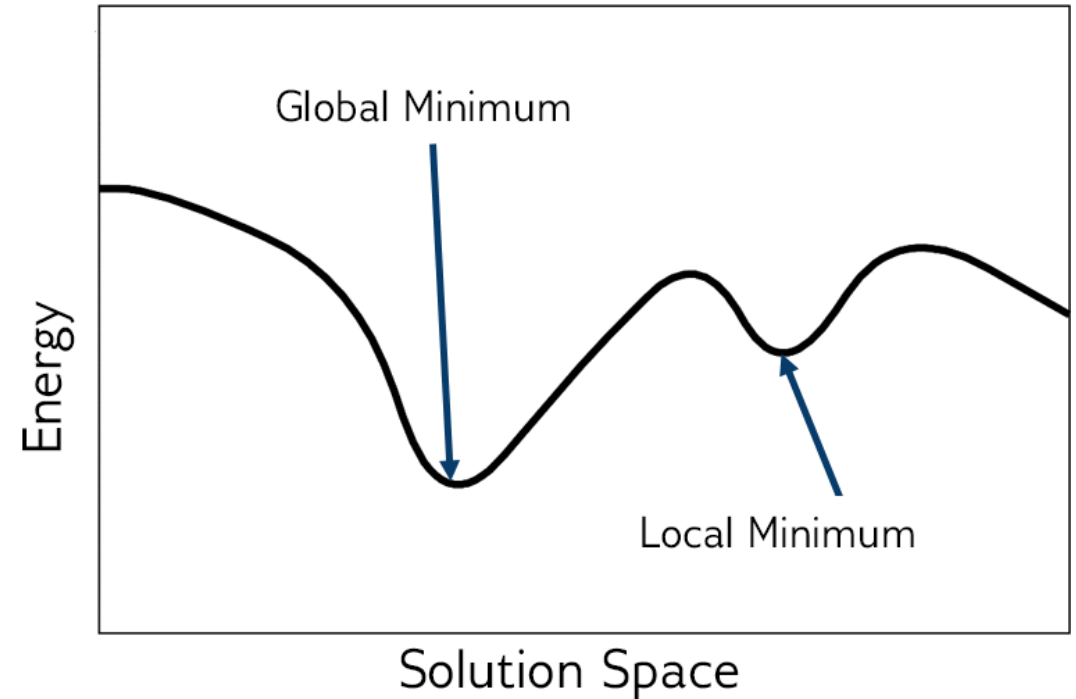
Objective Function

- To express a problem in a form that allows its resolution through quantum annealing, we need first of all an objective function,
- An objective function is a mathematical expression of the energy of a system. Put simply, it represents the function whose minimum you want to find
- When the solver is a QPU, energy is a function of the binary variables that represent its qubits; for classical quantum hybrid solvers, energy might be a more abstract function.
- For most problems, the lower the energy of the objective function, the better the solution. Sometimes any state of local minimum for energy is an acceptable solution to the original problem; for other problems only optimal solutions are acceptable.



Objective Function

- Expressing a problem through a minimizable objective function means **thinking of every problem as a minimization problem**
- Mathematically speaking, this is always a possible operation
- Although, in some cases it becomes very difficult.
- The objective functions accepted by the quantum annealer of D-Wave are of two types (equivalent to each other): **Ising Hamiltonians and QUBO formulations**



$$x + 1 = 2$$

$$\min_x [2 - (x + 1)]^2$$

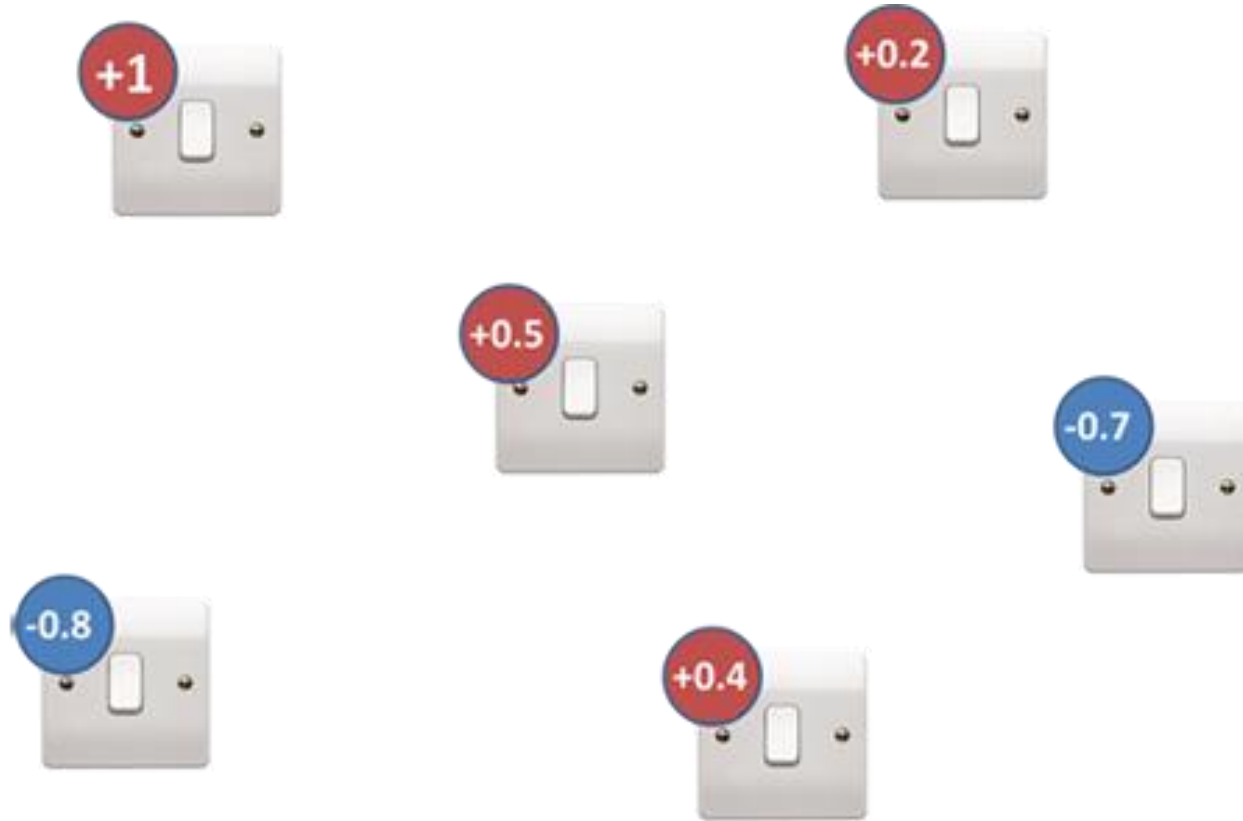
Ising Model

- The Ising Model is a well-known model in statistical mechanics.
- Quadratic and binary model, an Ising Hamiltonian has as variables +1 and -1 (commonly called **spin variables**: spin up for the value +1, spin down for the value -1).
- The relationships between the spins, represented by the coupling values of the Hamiltonian, represent the **correlations or anti-correlations**.
- Mathematically, it is expressed in this form

$$E_{\text{ising}}(s) = \sum_{i=1}^N h_i s_i + \sum_{i=1}^N \sum_{j=i+1}^N J_{i,j} s_i s_j$$

- Where the coefficients h represent the bias values associated with the qubits and the coefficients J represent the strength of the coupling bonds

Game of Switches

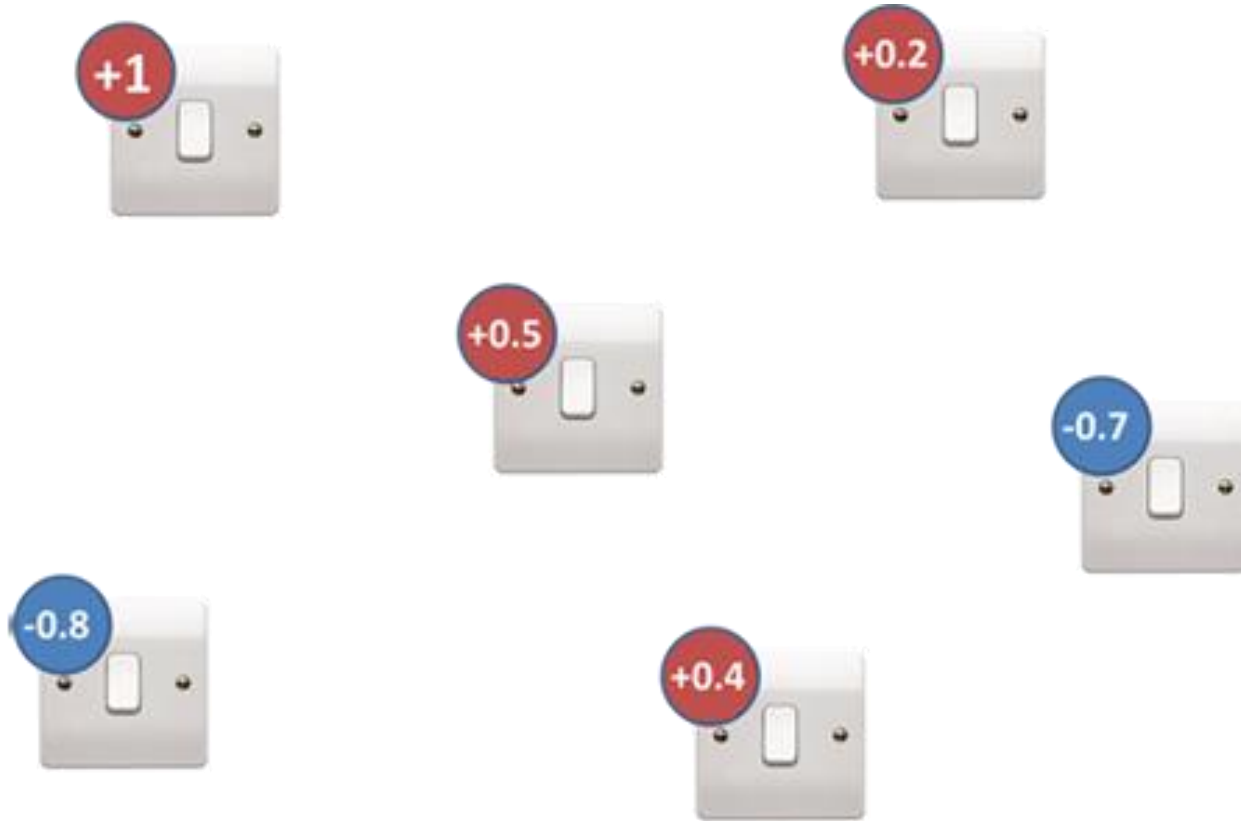


- The switch game is a very simple game that can help you understand the nature of an optimization problem that can be solved by a quantum annealer.
- Suppose we have a certain number of switches, each settable on two possible states represented by the values 1 and -1
- Furthermore, each switch has a univocally associated weight

Game of Switches

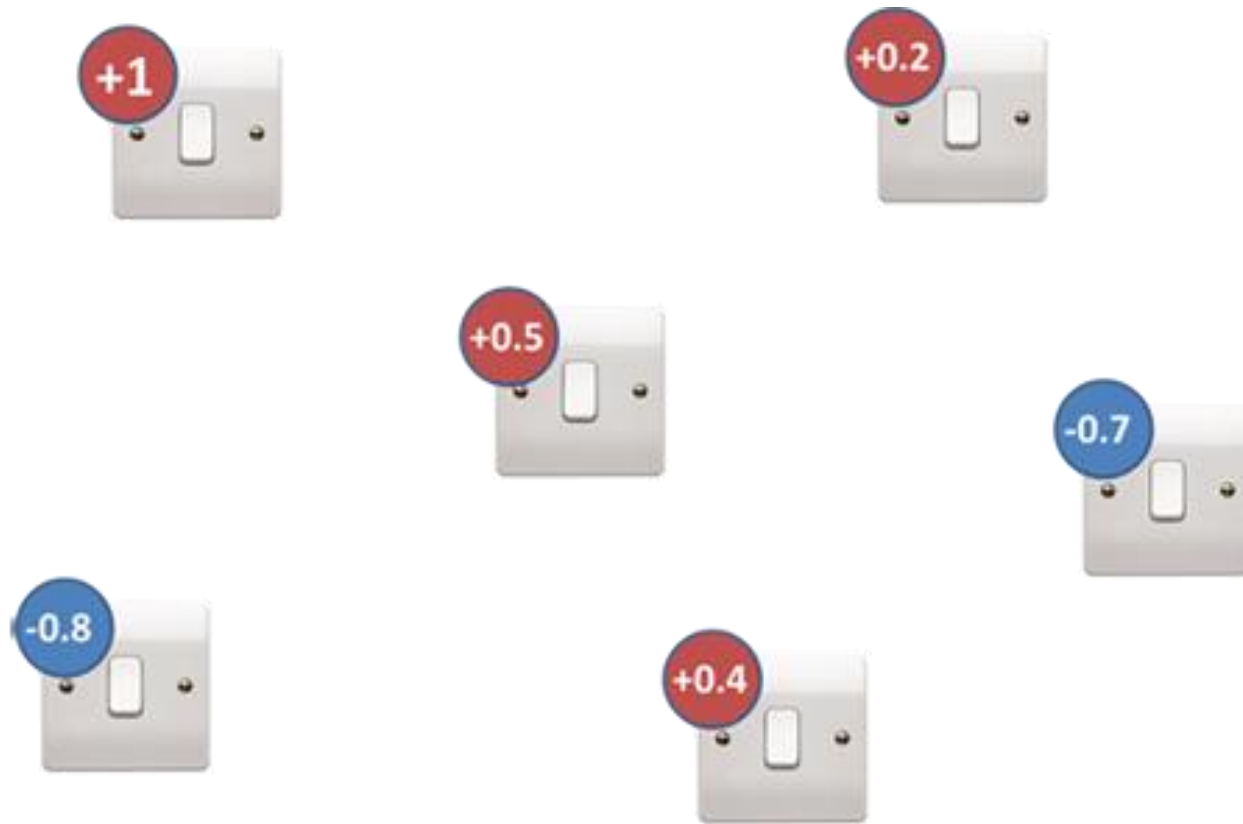


Game of Switches



- The switch game is a very simple game that can help you understand the nature of an optimization problem that can be solved by a quantum annealer.
- Suppose we have a certain number of switches, each settable on two possible states represented by the values 1 and -1
- Furthermore, each switch has a univocally associated weight
- The value of a switch is calculated by multiplying its weight by its state
- The game consists in finding the combination of states for the switches such that the sum of their values is as low as possible

Game of Switches



$$E(\mathbf{s}) = \sum_i h_i s_i$$

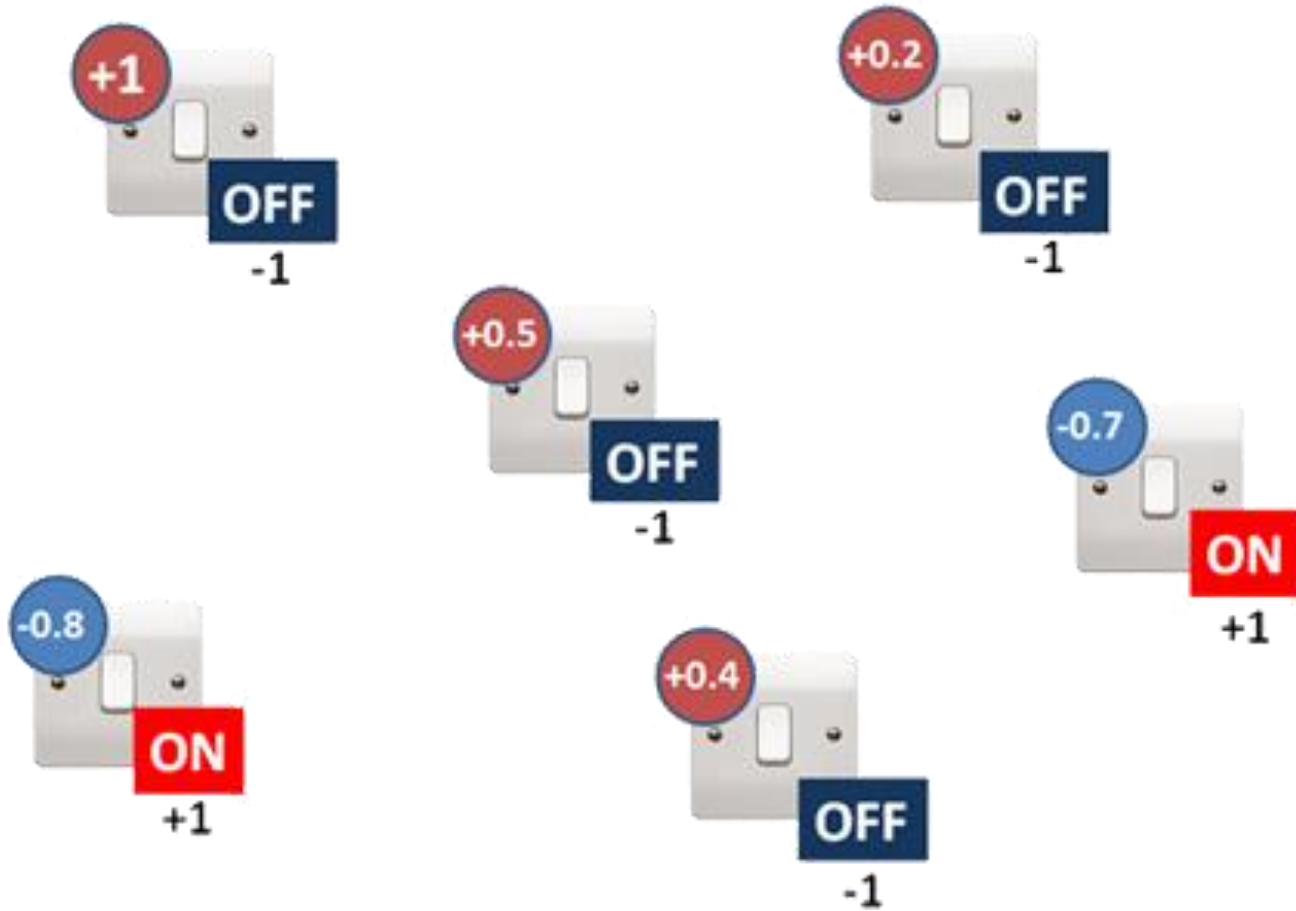


h = 'bias' value associated with each switch



s = the ON/OFF setting of each switch, +1 or -1

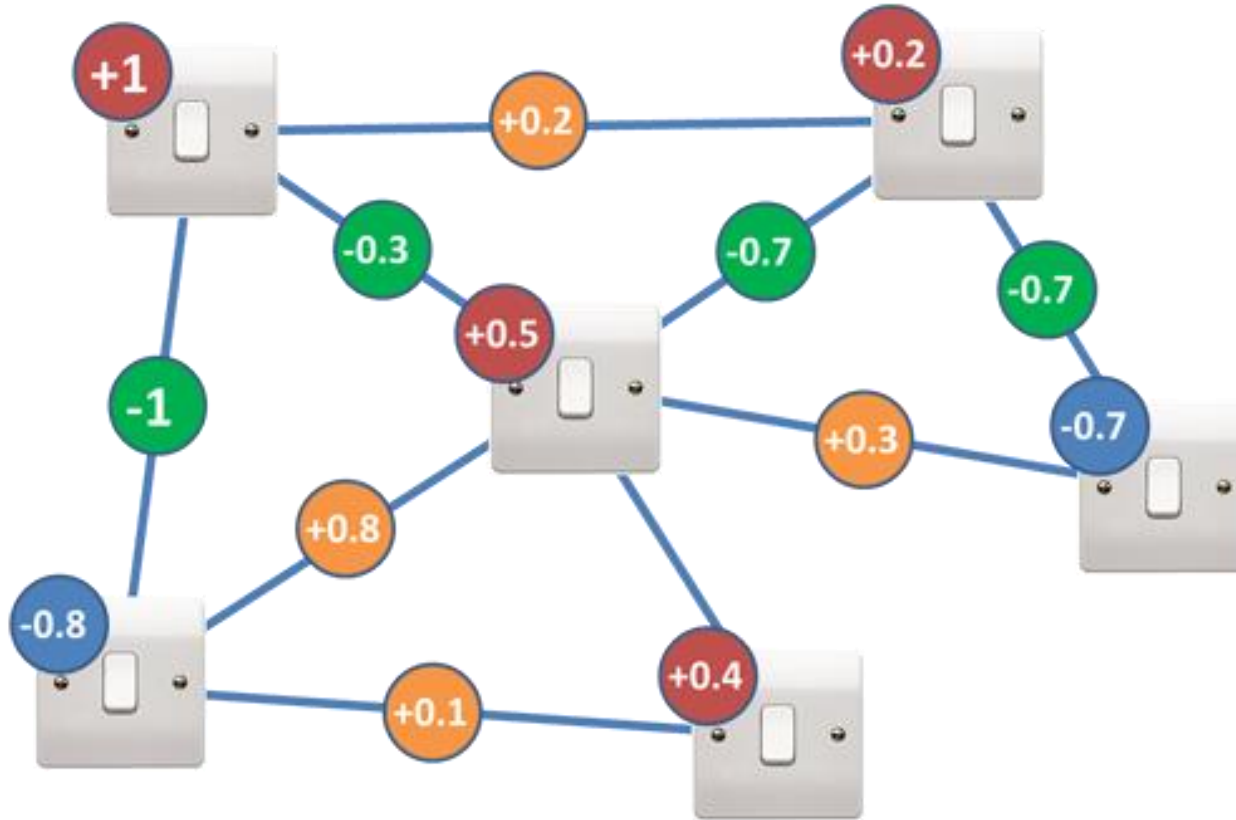
Game of Switches



$$\begin{array}{rclcl} +1 & \times & -1 & = & -1 \\ +0.2 & \times & -1 & = & -0.2 \\ +0.5 & \times & -1 & = & -0.5 \\ -0.8 & \times & +1 & = & -0.8 \\ +0.4 & \times & -1 & = & -0.4 \\ -0.7 & \times & +1 & = & -0.7 \end{array}$$

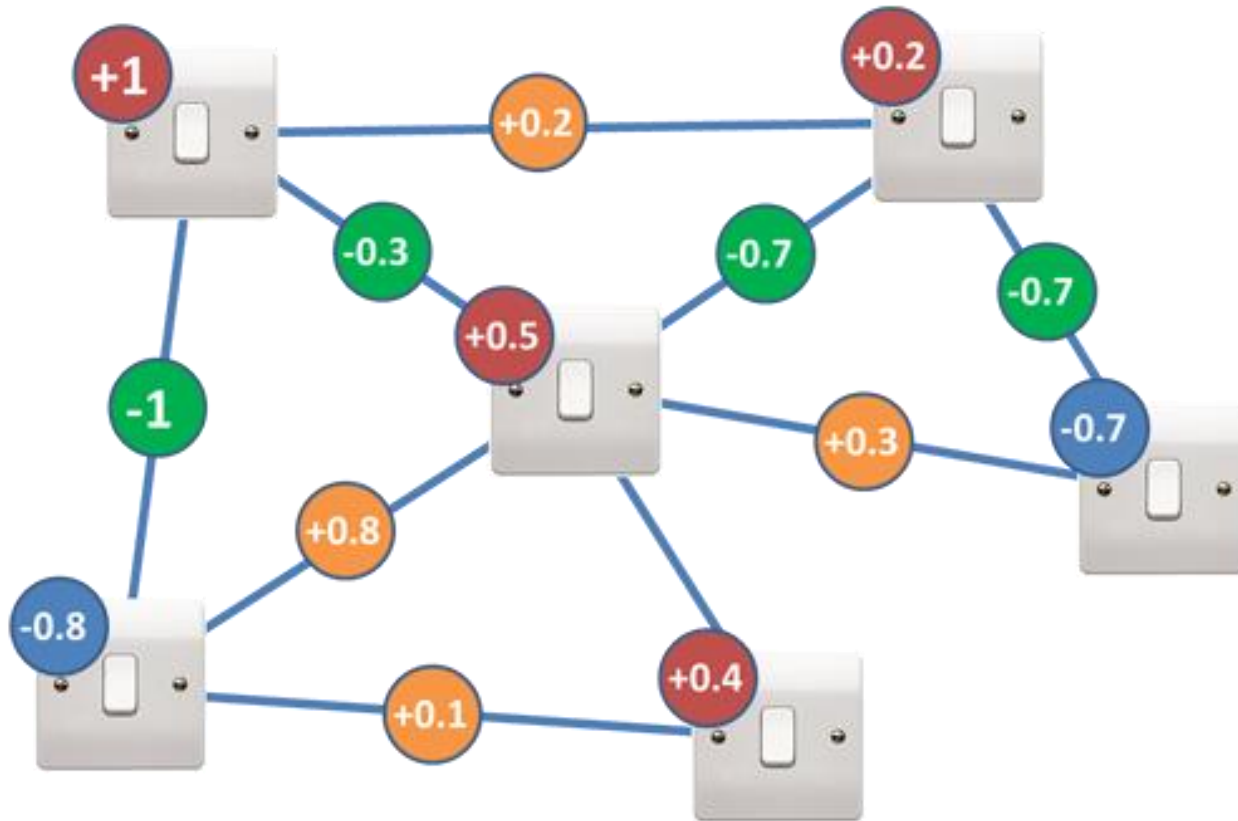
Total: -3.6

Game of Switches



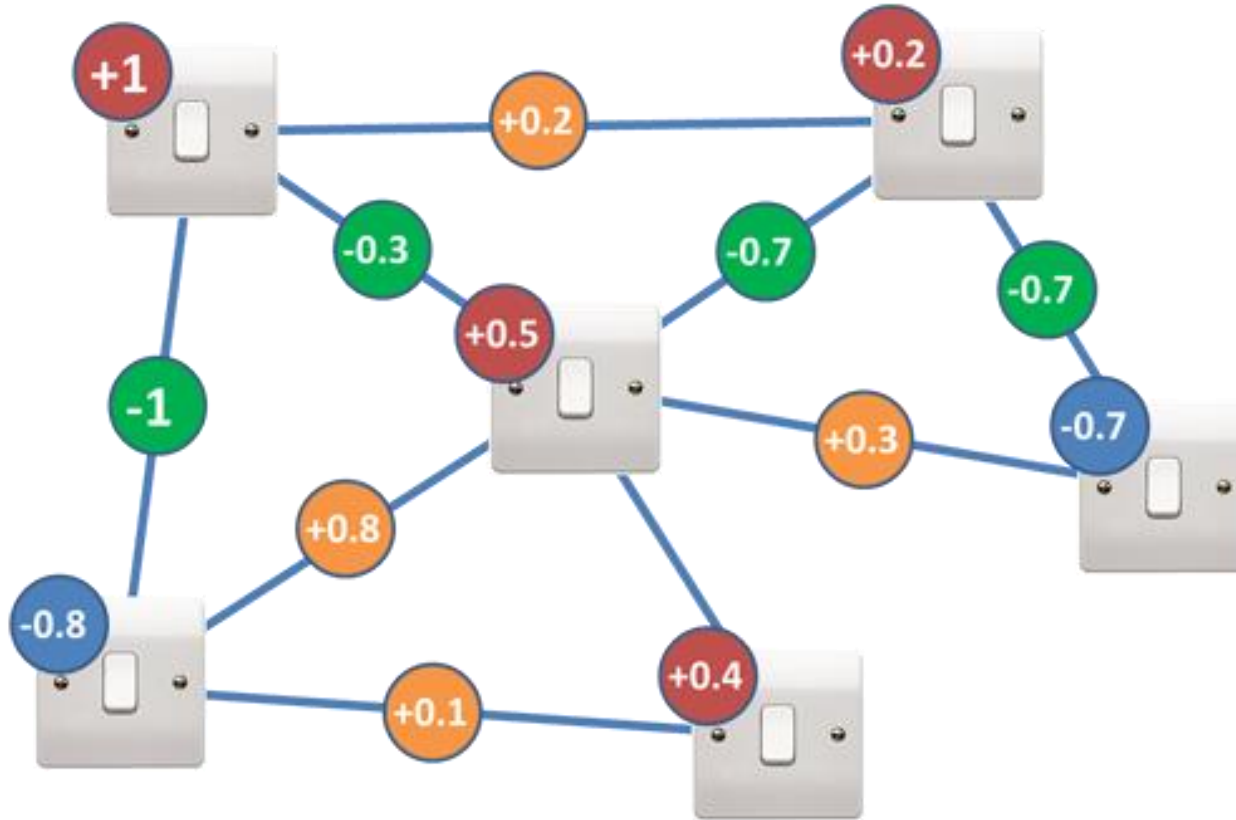
- Let us now consider another factor, namely the presence of couplers between the switches
- Couplers, just like switches, are endowed with a certain numerical weight
- The value of the couplers is given by their own weight multiplied by the state of the switches to which the coupler is associated

Game of Switches



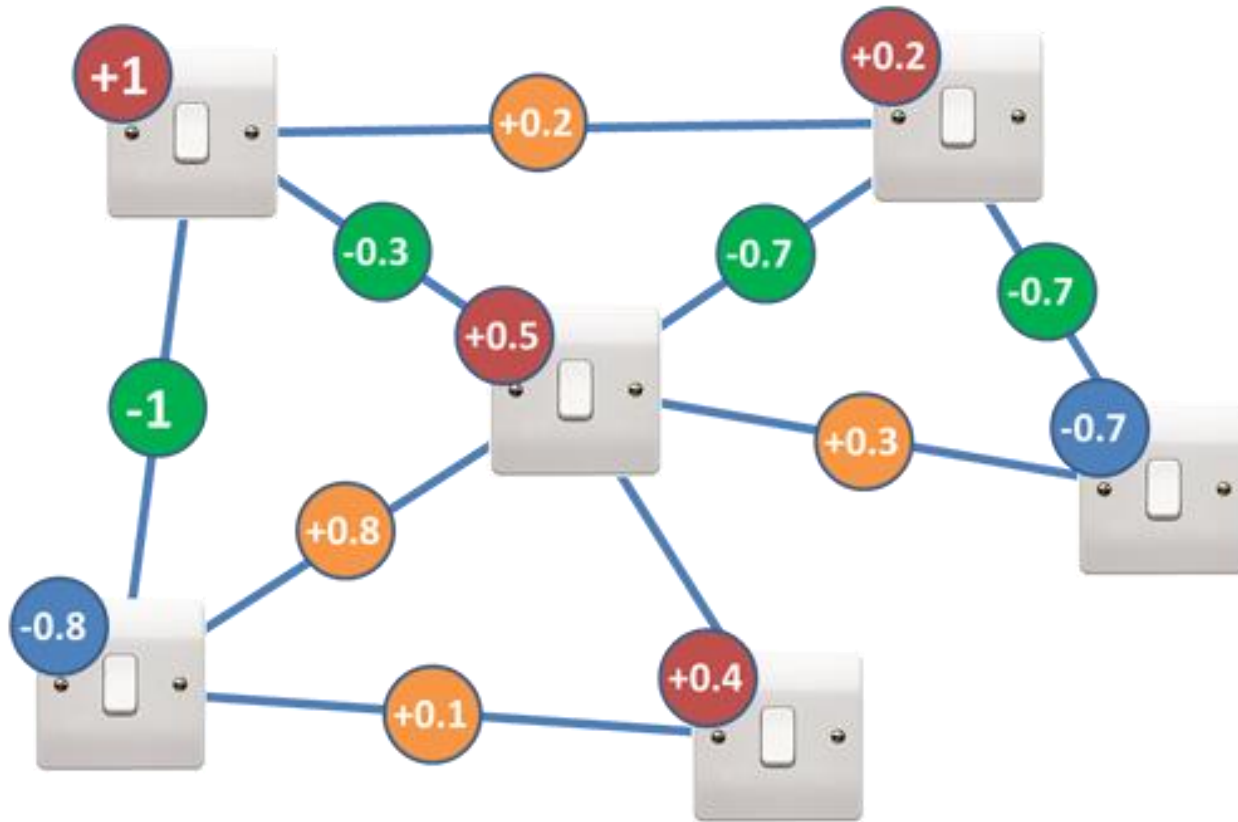
Adding another weight, J , which multiplies the product of the two switch settings.

Game of Switches



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- Couplers, just like switches, are endowed with a certain numerical weight
- The value of the couplers is given by their own weight multiplied by the state of the switches to which the coupler is associated
- In our case, the coupler will therefore have a state -1 if the two switches it connects are discordant, +1 otherwise
- We therefore add to the quantity to be minimized the contribution introduced by the couplers

Game of Switches



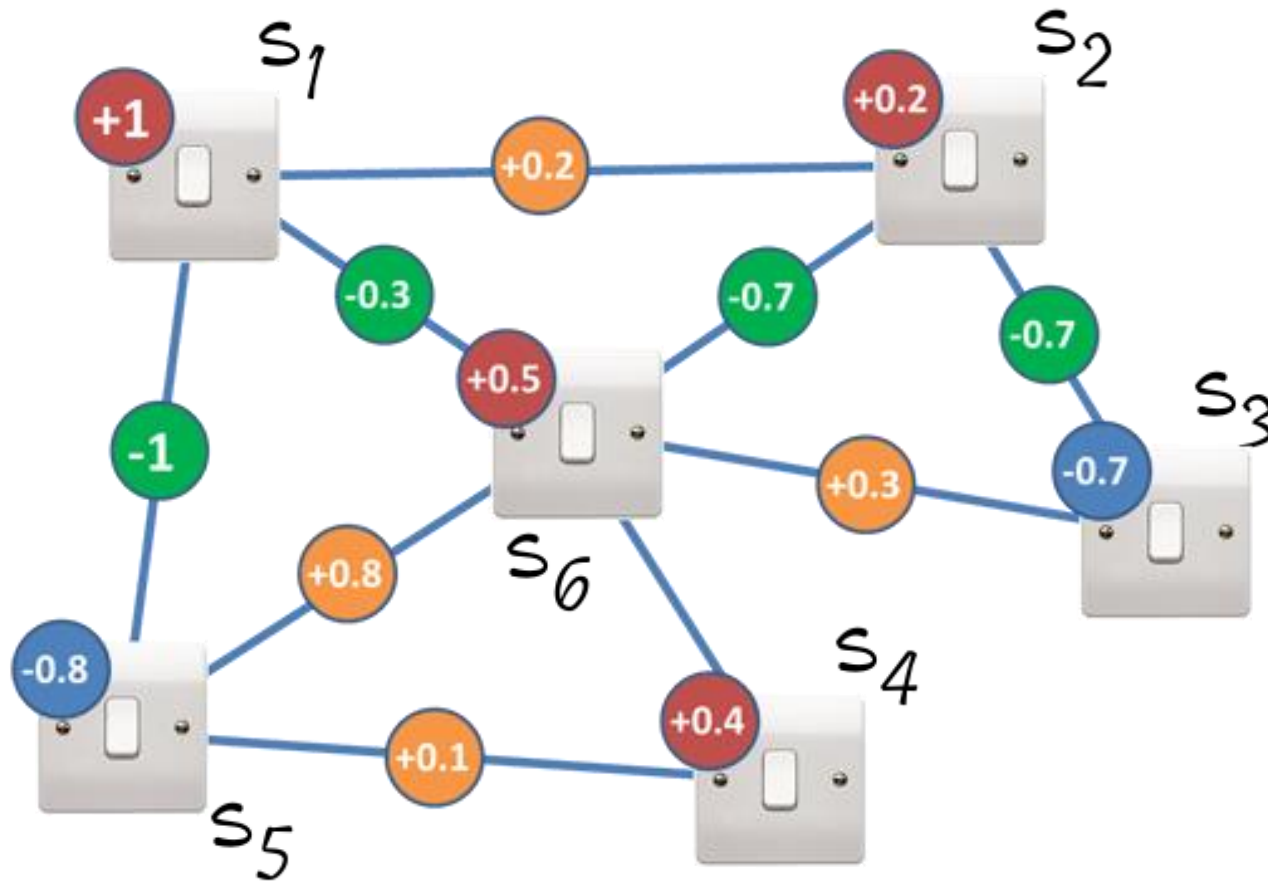
A small network diagram showing 3 switches (represented by light gray rectangular icons) connected by weighted edges (represented by blue lines). Each switch has a circular label with a numerical value. The connections and weights are as follows:

- Switch 1 (top, red +1) is connected to Switch 2 (middle, green -1) with weight -1.
- Switch 2 is connected to Switch 3 (bottom, blue -0.8) with weight -0.8.

$$E(\mathbf{s}) = \sum_i h_i s_i + \sum_{i,j} J_{i,j} s_i s_j$$

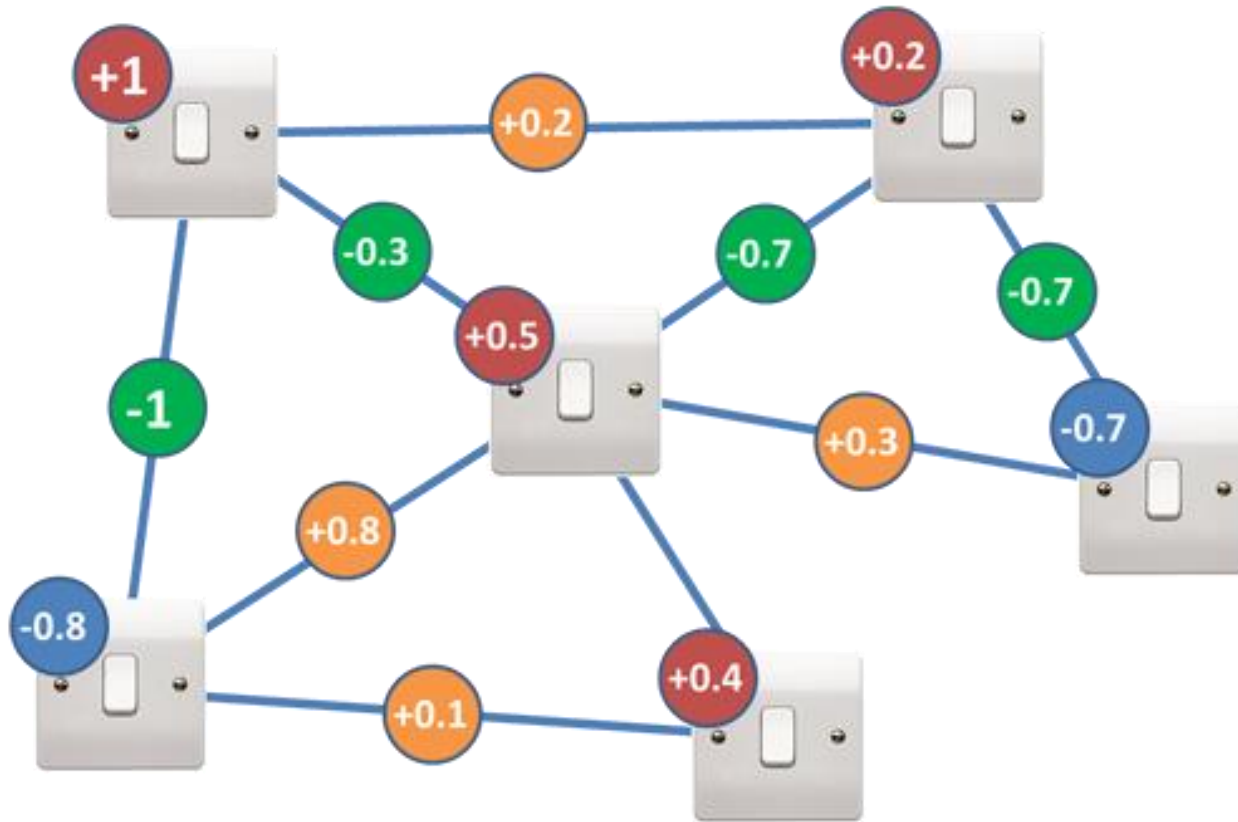
Adding another weight, J , which multiplies the product of the two switch settings.

Game of Switches



$$\begin{aligned} & s_1 + 0.2s_2 - 0.7s_3 + \\ & 0.4s_4 - 0.8s_5 + 0.5s_6 + \\ & 0.2s_1s_2 - 0.7s_2s_3 + \\ & 0.3s_3s_6 - 0.7s_2s_6 + \\ & - 0.3s_1s_6 - s_1s_5 + \\ & 0.1s_5s_4 + s_6s_4 \end{aligned}$$

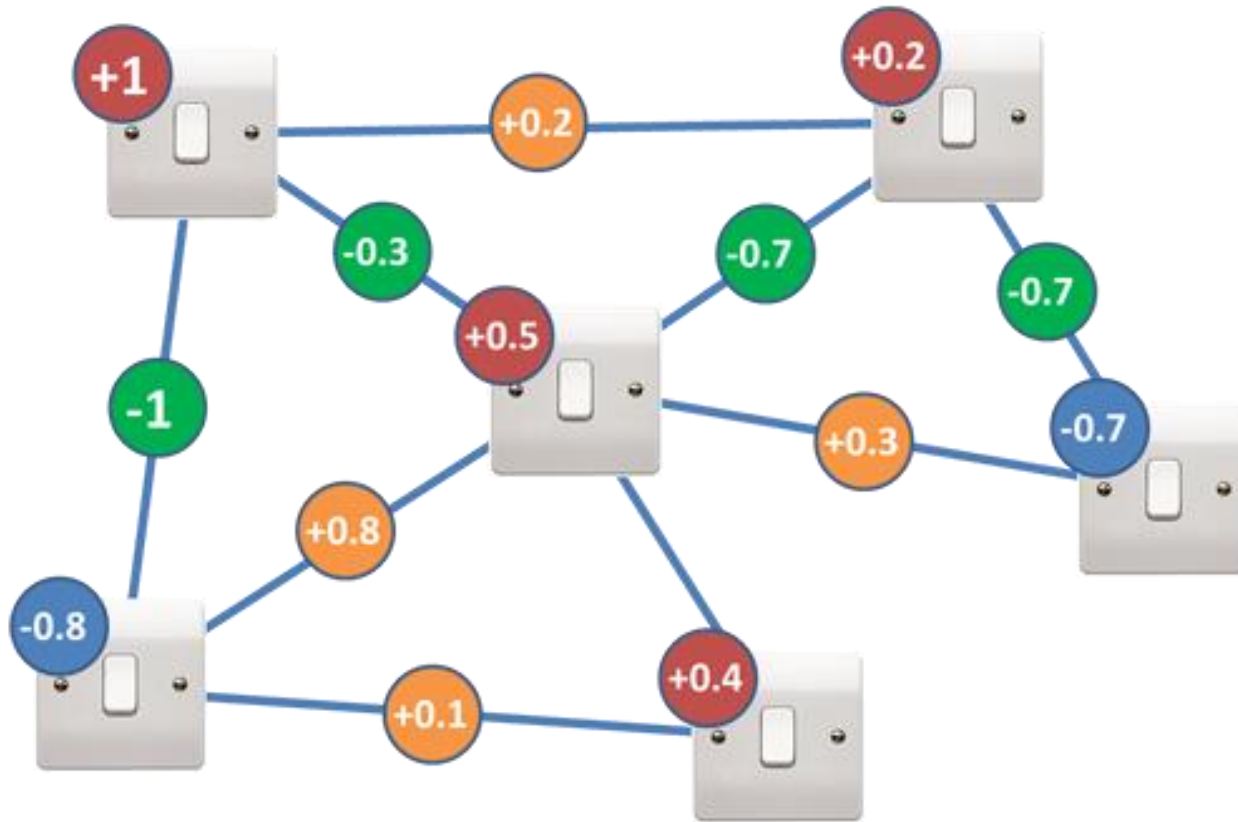
Game of Switches



2 switches = $2^2 =$
4 possible answers



Game of Switches

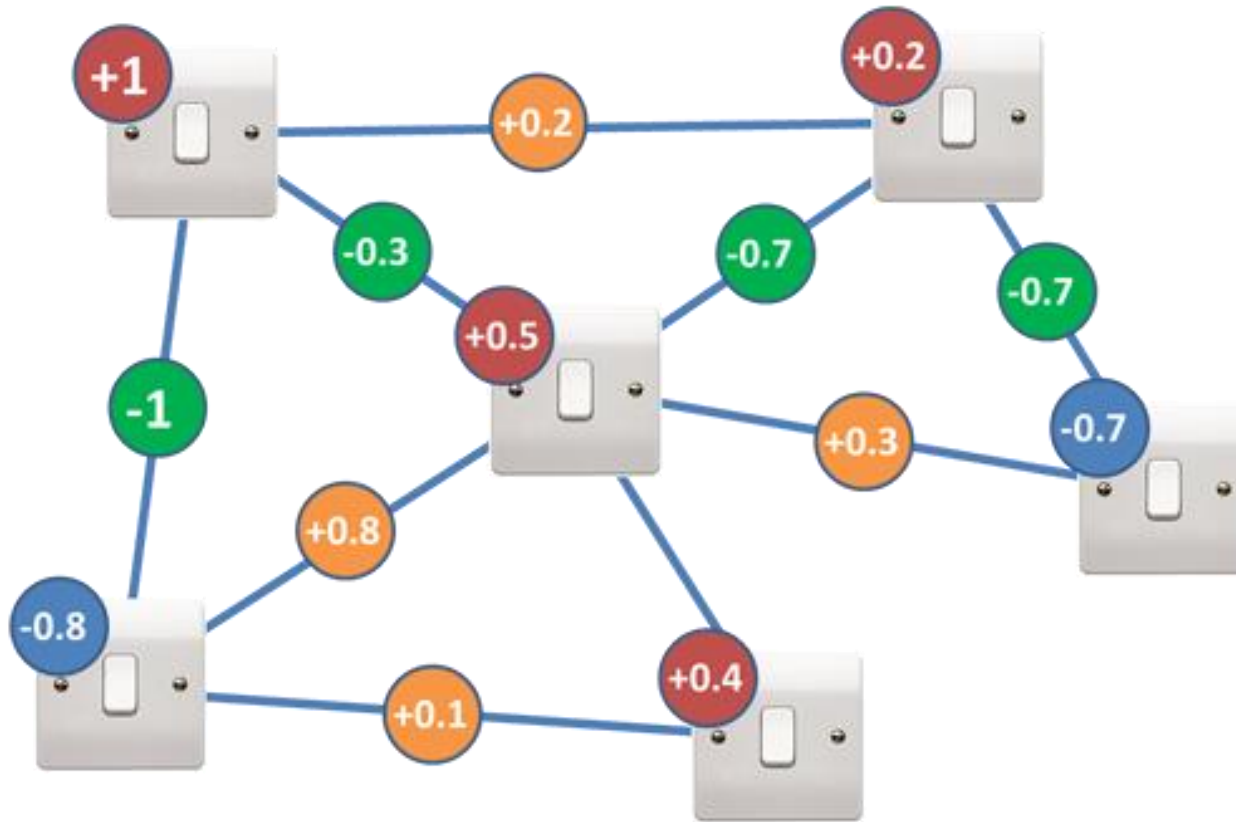


2 switches = $2^2 =$
4 possible answers

10 switches = $2^{10} =$
1024 possible answers



Game of Switches



2 switches = $2^2 =$
4 possible answers

10 switches = $2^{10} =$
1024 possible answers

100 switches = $2^{100} =$
1,267,650,600,228,229,401,496,703,205,376
possible answers



QUBO Problems

- QUBO (Quadratic Unconstrained Binary Optimization) problems are well known problems in the field of combinatorial optimization.
- A QUBO problem is defined by a **matrix** Q (upper triangular) and a **vector of binary variables** x .
- Its mathematical form is

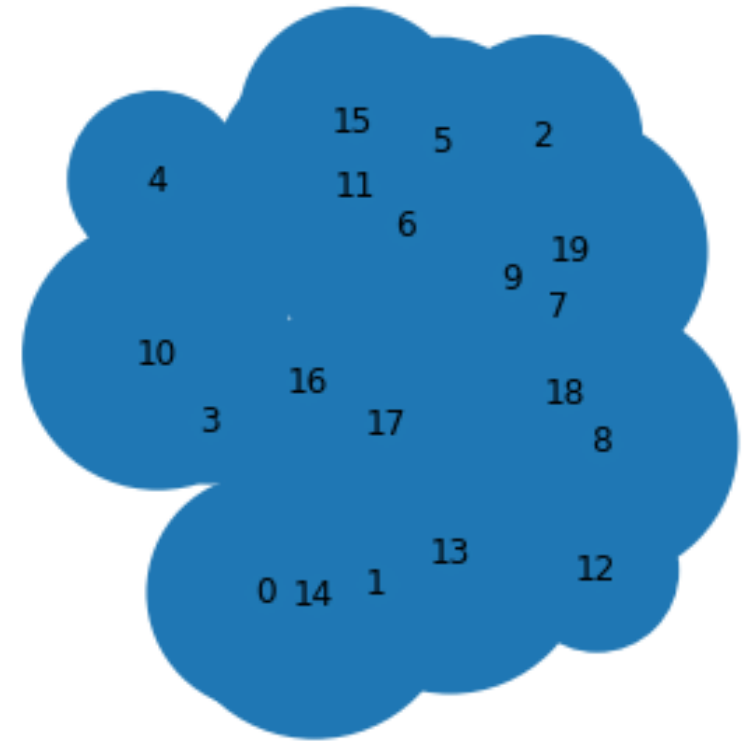
$$f(x) = \sum_i Q_{i,i} x_i + \sum_{i < j} Q_{i,j} x_i x_j$$

- Where the diagonal terms of the matrix Q play the role of linear coefficients while the other non-zero elements are the quadratic coefficients. In matrix form

$$\min_{x \in \{0,1\}^n} x^T Q x.$$

QUBO Problems

- To familiarize yourself with the QUBO formulation, let's make an example of a realistic problem whose structure can be mapped in this form
- Suppose we have a certain number of antennas and a certain number of possible sites to place these antennas.
- Each antenna with its signal can cover a certain area. When multiple signals overlap, however, unpleasant interference is generated
- Our task is to position the antennas in order to maximize the surface covered by the signal and at the same time minimize interference between the antennas.



QUBO Problems

We define:

- The area covered by a single antenna such as the area of the circle whose radius is the parameter that describes the range of action of each individual antenna (problem data)

$$A_i = r_i^2 \cdot \pi$$

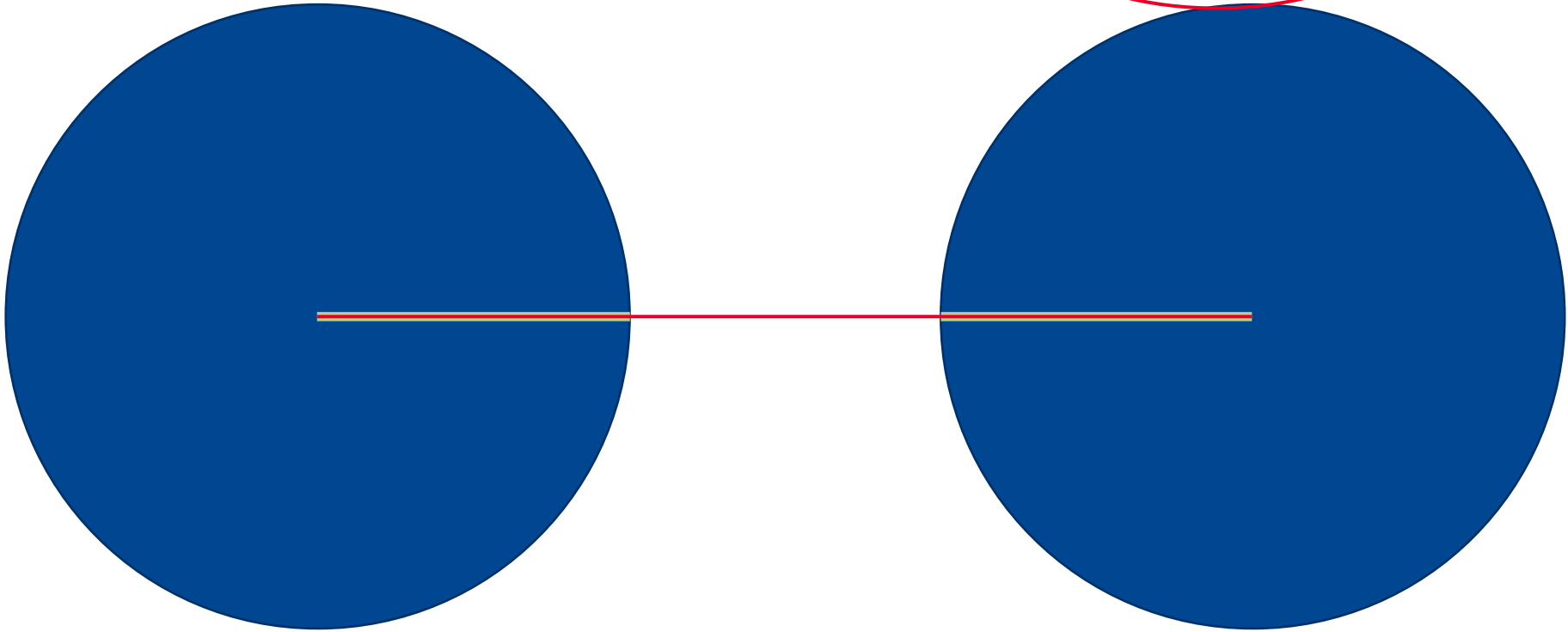
- The interference surface between two antennas as the area of the circle whose radius is given by the following formula

$$\rho_{ij} = \max \left\{ 0, r_i + r_j - \text{dist} \left(c_i, c_j \right) \right\}$$

- where r_i and r_j are the parameters relating to the range of action of the antennas i and j and $\text{dist}(c_i, c_j)$ is the distance between the points where the antennas are positioned

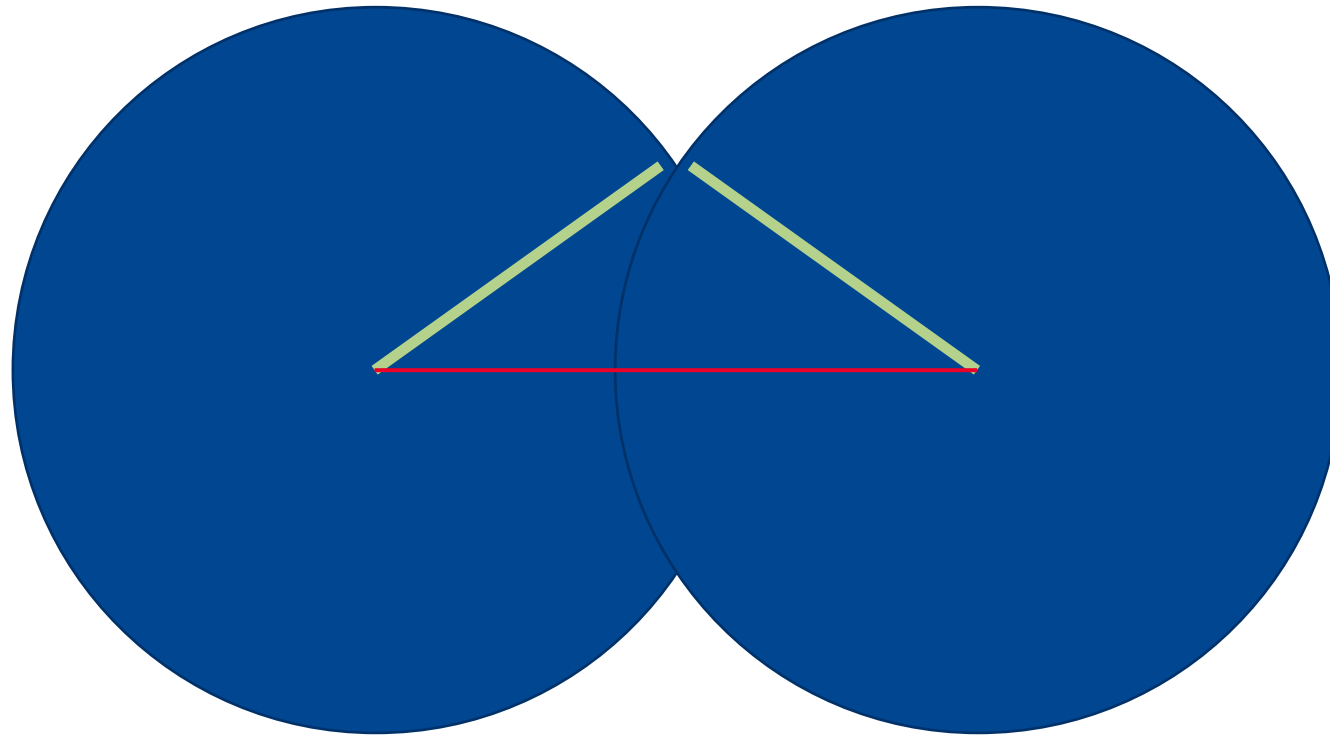
QUBO Problems

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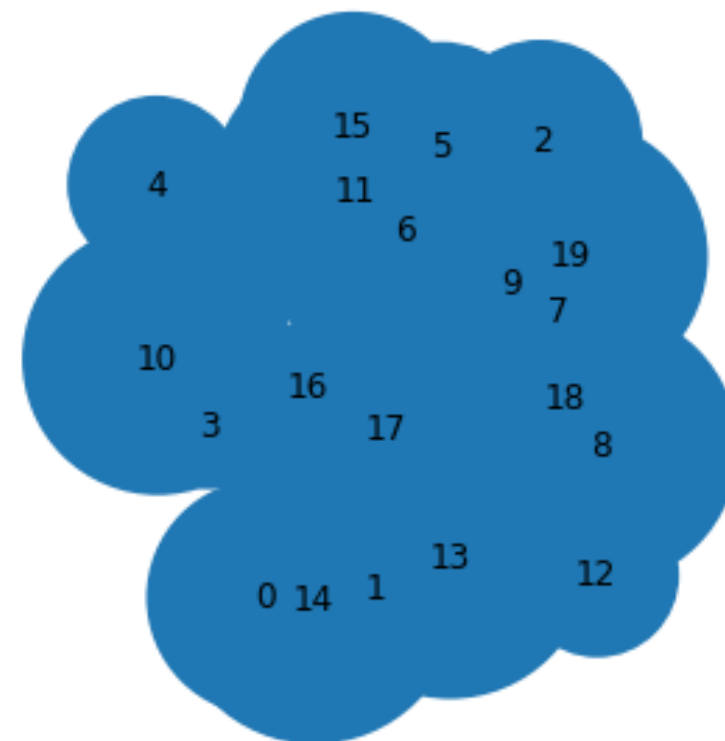
QUBO Problems

- With the definition of the rho radius, we can define the interference area between the overlap of two antennas i and j as

$$B_{ij} = \rho_{ij}^2 \cdot \pi$$

- Now we just have to model the antennas with the help of a vector of binary variables. We simply associate a binary variable q_i with each possible site. The variable will take the value 1 if it is a place where it is recommended to install an antenna, 0 otherwise

$$[q_0, \dots, q_{19}]$$

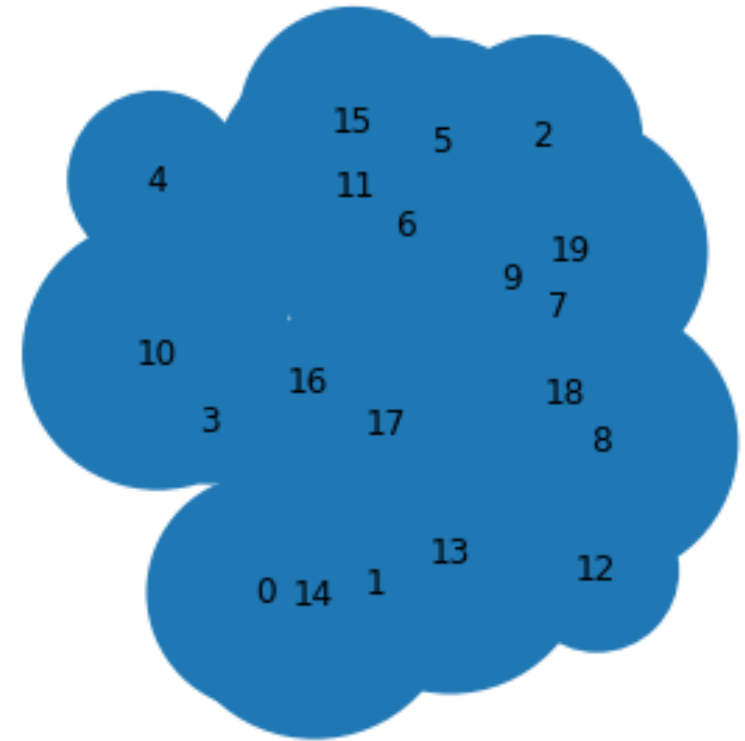


QUBO Problems

- Let's formulate our problem. At this stage, we must always think about a minimization problem. To maximize, simply reverse the sign. Keeping in mind that

$$A_i = r_i^2 \cdot \pi$$

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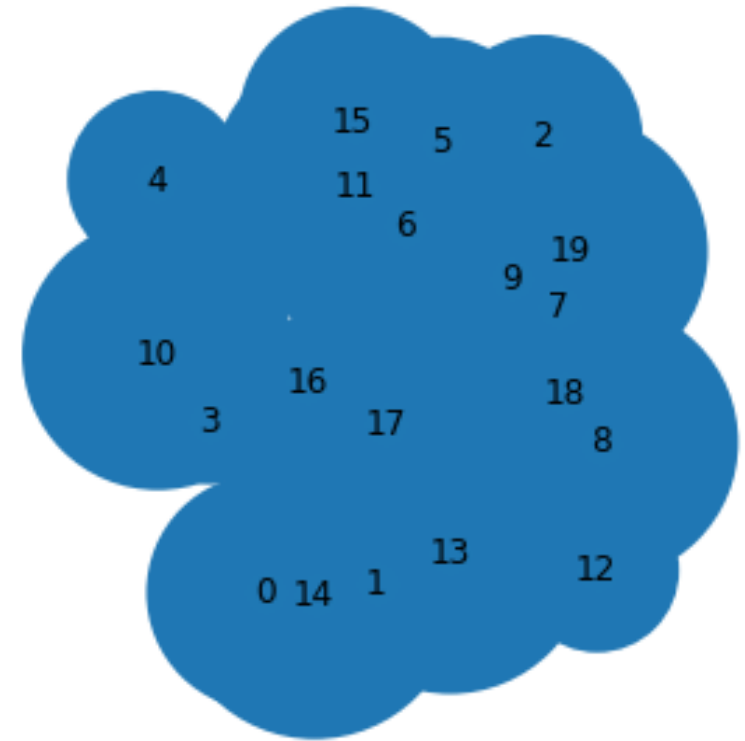
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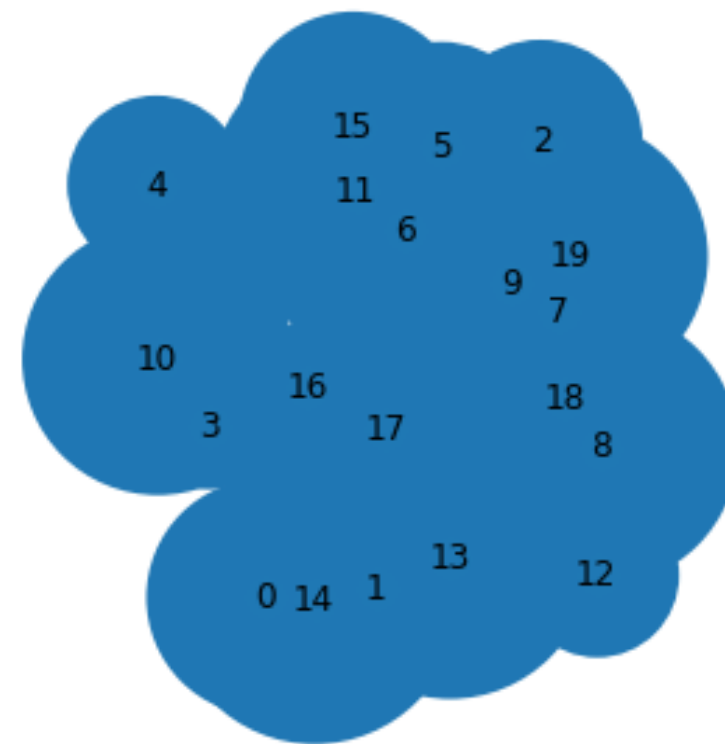
$$A_i = r_i^2 \cdot \pi$$

$$B_{ij} = \rho_{ij}^2 \cdot \pi$$

- Minimize interference

$$\text{QUBO} =$$

$$\sum_{i < j} B_{ij} q_i q_j$$



QUBO Problems

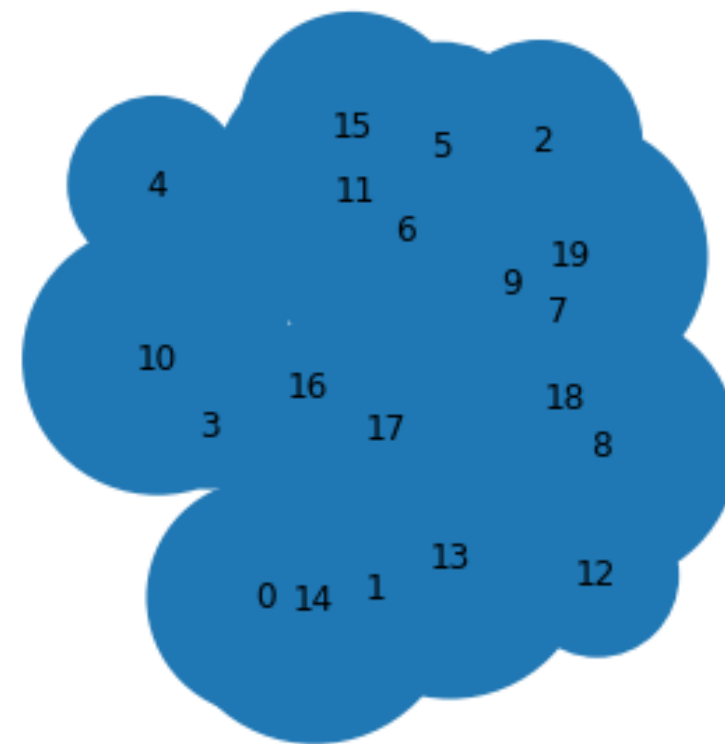
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- Maximize covering area

$$\text{QUBO} = \sum_{i=0}^N A_i q_i + \sum_{i < j} B_{ij} q_i q_j$$



QUBO Problems

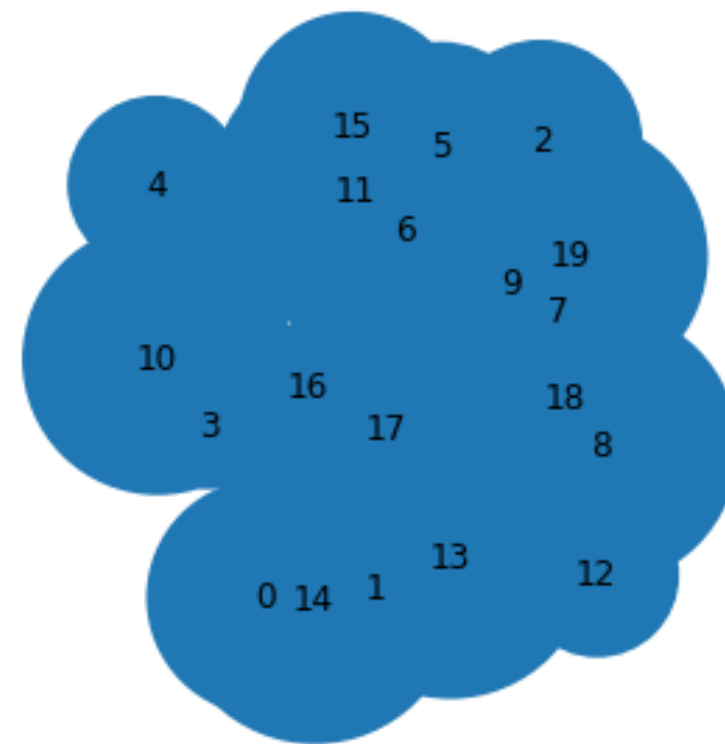
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- Maximize covering area

$$\text{QUBO} = - \sum_{i=0}^N A_i q_i + \sum_{i < j} B_{ij} q_i q_j$$



QUBO Problems

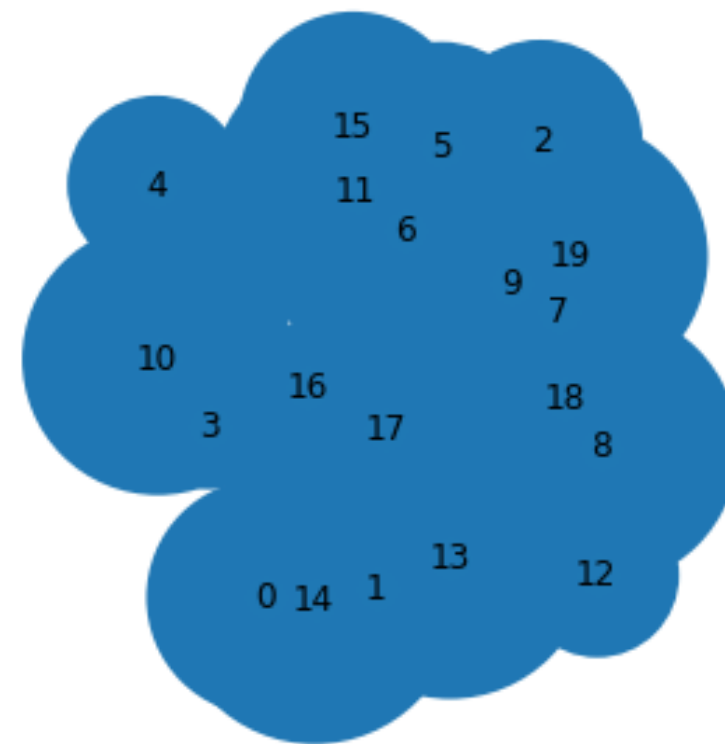
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$$B_{ij} = \rho_{ij}^2 \cdot \pi$$

- Maximize covering area

$$\text{QUBO} = -\sum_{i=0}^N A_i q_i + \alpha \sum_{i < j} B_{ij} q_i q_j$$



Programming a Quantum Annealer

- PyQUBO is a python library, with a C ++ backend, written by DWAVE to use its quantum annealer.

Programming a Quantum Annealer

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- PyQUBO is included in the D-Wave Ocean Suite. Installation is quite easy:

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python -m venv ocean  
. ocean/bin/activate
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pip install dwave-ocean-sdk
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- PyQUBO is a very handy utility for writing problems in QUBO or ISING form. Let's see how to use it
- Variables: Type Binary (0/1)

```
>>> from pyqubo import Binary  
>>> x1, x2 = Binary('x1'), Binary('x2')  
>>> H = 2*x1*x2 + 3*x1  
>>> pprint(H.compile().to_qubo()) # doctest: +SKIP  
{('x1', 'x1'): 3.0, ('x1', 'x2'): 2.0, ('x2', 'x2'): 0.0}, 0.0)
```

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```

- PyQUBO is a very handy utility for writing problems in QUBO or ISING form. Let's see how to use it
- Variables: Type Spin (+1/-1)

```
>>> from pyqubo import Spin  
>>> s1, s2 = Spin('s1'), Spin('s2')  
>>> H = 2*s1*s2 + 3*s1  
>>> pprint(H.compile().to_qubo()) # doctest: +SKIP  
{('s1', 's1'): 2.0, ('s1', 's2'): 8.0, ('s2', 's2'): -4.0}, -1.0)
```

Programming a Quantum Annealer

- Arrays of Binary type variables (same for Spin type variables)

```
>>> from pyqubo import Array
>>> x = Array.create('x', shape=(2, 3), vartype='BINARY')
>>> x[0, 1] + x[1, 2]
(Binary(x[0][1])+Binary(x[1][2]))
```

Programming a Quantum Annealer

- Arrays of Binary type variables (same for Spin type variables)

```
>>> from pyqubo import Array
>>> numbers = [4, 2, 7, 1]
>>> s = Array.create('s', shape=4, vartype='SPIN')
>>> H = sum(n * s for s, n in zip(s, numbers))**2
>>> model = H.compile()
>>> qubo, offset = model.to_qubo()
>>> pprint(qubo) # doctest: +SKIP
{('s[0]', 's[0]'): -160.0,
 ('s[0]', 's[1]'): 64.0,
 ('s[0]', 's[2]'): 224.0,
 ('s[0]', 's[3]'): 32.0,
 ('s[1]', 's[1]'): -96.0,
 ('s[1]', 's[2]'): 112.0,
 ('s[1]', 's[3]'): 16.0,
 ('s[2]', 's[2]'): -196.0,
 ('s[2]', 's[3]'): 56.0,
 ('s[3]', 's[3]'): -52.0}
```

Programming a Quantum Annealer

- Construct a QUBO problem with PyQUBO

```
>>> from pyqubo import Binary
>>> a, b = Binary('a'), Binary('b')
>>> M = 5.0
>>> H = 2*a + b + M*(a+b-1)**2
>>> model = H.compile()
>>> qubo, offset = model.to_qubo() # QUBO with M=5.0
>>> M = 6.0
>>> H = 2*a + b + M*(a+b-1)**2
>>> model = H.compile()
>>> qubo, offset = model.to_qubo() # QUBO with M=6.0
```

Programming a Quantum Annealer

- Construct a QUBO problem with PyQUBO (with Placeholders)

```
>>> from pyqubo import Binary
>>> a, b = Binary('a'), Binary('b')
>>> M = 5.0
>>> H = 2*a + b + M*(a+b-1)**2
>>> model = H.compile()
>>> qubo, offset = model.to_qubo() # QUBO with M=5.0
>>> M = 6.0
>>> H = 2*a + b + M*(a+b-1)**2
>>> model = H.compile()
>>> qubo, offset = model.to_qubo() # QUBO with M=6.0
```

```
>>> from pyqubo import Placeholder
>>> a, b = Binary('a'), Binary('b')
>>> M = Placeholder('M')
>>> H = 2*a + b + M*(a+b-1)**2
>>> model = H.compile()
>>> qubo, offset = model.to_qubo(feed_dict={'M': 5.0})
```

Programming a Quantum Annealer

- Solve a problem set via pyQUBO
- After setting the Hamiltonian of the problem, it must be compiled and transformed into a bqm object

```
>>> from pyqubo import Binary
>>> x1, x2 = Binary('x1'), Binary('x2')
>>> H = (x1 + x2 - 1)**2
>>> model = H.compile()
>>> bqm = model.to_bqm()
```

Programming a Quantum Annealer

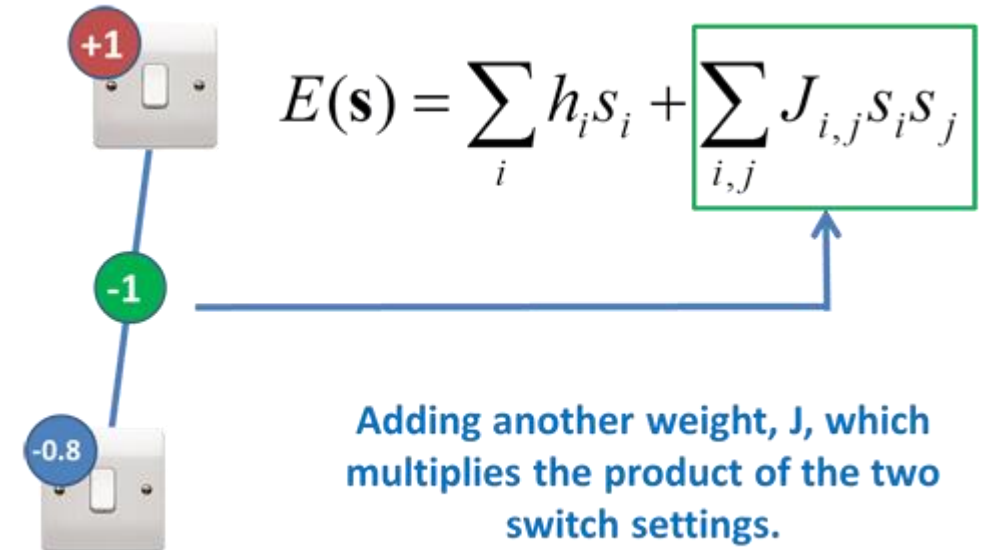
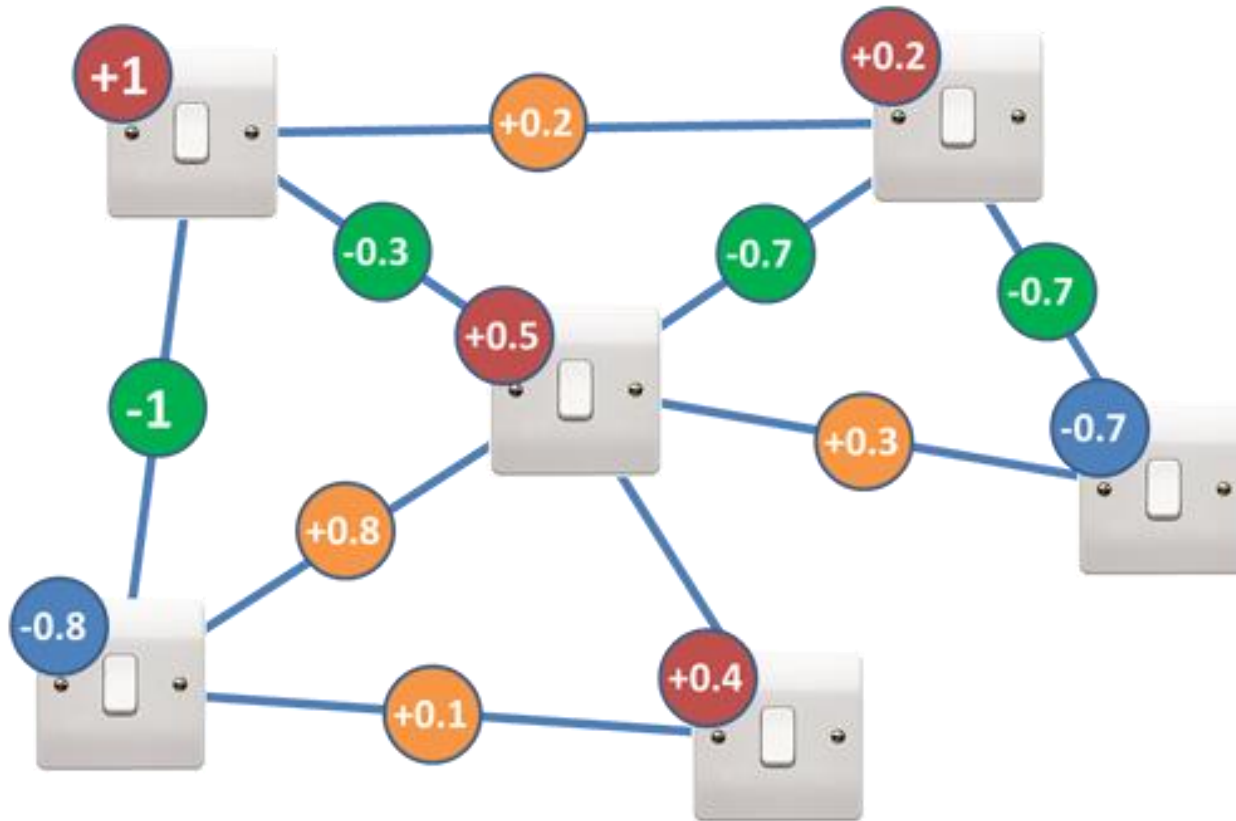
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>>> x1, x2 = Binary('x1'), Binary('x2')
>>> H = (x1 + x2 - 1)**2
>>> model = H.compile()
>>> bqm = model.to_bqm()
```

```
>>> import neal
>>> sa = neal.SimulatedAnnealingSampler()
>>> sampleset = sa.sample(bqm, num_reads=10)
>>> decoded_samples = model.decode_sampleset(sampleset)
>>> best_sample = min(decoded_samples, key=lambda x: x.energy)
>>> pprint(best_sample.sample)
{'x1': 0, 'x2': 1}
```


Exercise 1: Game of Switches

- Try to implement the Game of Switches



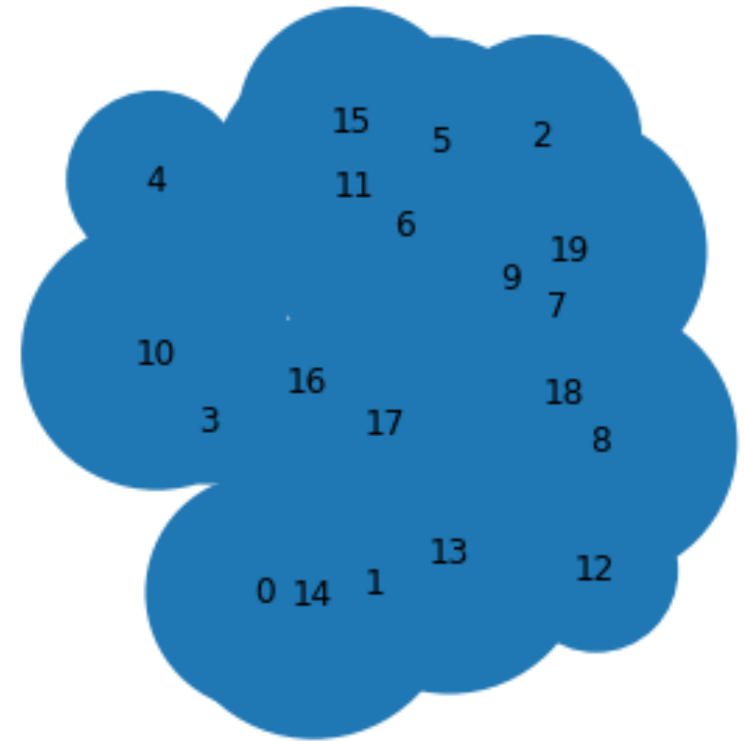
Exercise 2: Antenna Placement

- Try to implement the Antenna Placement Problem

$$A_i = r_i^2 \cdot \pi$$

$$B_{ij} = \rho_{ij}^2 \cdot \pi$$

$$\text{QUBO} = -\sum_{i=0}^N A_i q_i + \alpha \sum_{i < j} B_{ij} q_i q_j$$



Add a Constraint to a QUBO Problem

- By definition, a QUBO problem admits no constraints

Quadratic Unconstrained Binary Optimization

- Still, there is a way.

Add a Constraint to a QUBO Problem

- Let's see how to implement a linear constraint in a QUBO problem.
- Everything relies around the concept of **penalty function**
- A penalty function is in fact an **additional quantity** to the original minimization problem, **which must be optimized** in order for the entire problem to be optimized
- Suppose we want to add the following constraint to our antenna optimization problem
- *Let F be the exact number of antennas to be placed*
- Remembering the mathematical formulation of our problem, requested constraint can be seen as

$$\sum_{i=0}^N q_i = F$$

Add a Constraint to a QUBO Problem

- Let's do some math

$$\sum_{i=0}^N q_i = F$$

Add a Constraint to a QUBO Problem

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$$\sum_{i=0}^N q_i = F \quad \Rightarrow \quad \min \left(\sum_{i=0}^N q_i - F \right)^2$$

Add a Constraint to a QUBO Problem

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$$\sum_{i=0}^N q_i = F \Rightarrow \min \left(\sum_{i=0}^N q_i - F \right)^2$$
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Add a Constraint to a QUBO Problem

- Let's do some math

$$\sum_{i=0}^N q_i = F \Rightarrow \min \left(\sum_{i=0}^N q_i - F \right)^2$$
$$\left(\sum_{i=0}^N q_i - F \right)^2 = \left(\sum_{i=0}^N q_i \right)^2 + F^2 - 2F \sum_{i=0}^N q_i$$

Add a Constraint to a QUBO Problem

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$$\sum_{i=0}^N q_i = F \Rightarrow \min \left(\sum_{i=0}^N q_i - F \right)^2$$
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Add a Constraint to a QUBO Problem

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$$\begin{aligned}\sum_{i=0}^N q_i = F &\Rightarrow \min \left(\sum_{i=0}^N q_i - F \right)^2 \\ \left(\sum_{i=0}^N q_i - F \right)^2 &= \left(\sum_{i=0}^N q_i \right)^2 + \cancel{F^2} - 2F \sum_{i=0}^N q_i = \left(\sum_{i=0}^N q_i \right)^2 - 2F \sum_{i=0}^N q_i = \\ &= \sum_{i=0}^N q_i^2 + 2 \sum_{i < j} q_i q_j - 2F \sum_{i=0}^N q_i\end{aligned}$$

Add a Constraint to a QUBO Problem

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Add a Constraint to a QUBO Problem

- Let's do some math

$$\begin{aligned}\sum_{i=0}^N q_i = F &\Rightarrow \min \left(\sum_{i=0}^N q_i - F \right)^2 \\ \left(\sum_{i=0}^N q_i - F \right)^2 &= \left(\sum_{i=0}^N q_i \right)^2 + \cancel{F^2} - 2F \sum_{i=0}^N q_i = \left(\sum_{i=0}^N q_i \right)^2 - 2F \sum_{i=0}^N q_i = \\ &= \sum_{i=0}^N q_i^2 + 2 \sum_{i < j} q_i q_j - 2F \sum_{i=0}^N q_i = \sum_{i=0}^N q_i + 2 \sum_{i < j} q_i q_j - 2F \sum_{i=0}^N q_i = \\ &= \sum_{i=0}^N (1 - 2F) q_i + \sum_{i < j} 2q_i q_j\end{aligned}$$

Add a Constraint to a QUBO Problem

$$\sum_{i=0}^N q_i = F \quad \Rightarrow \quad \min \left(\sum_{i=0}^N q_i - F \right)^2$$

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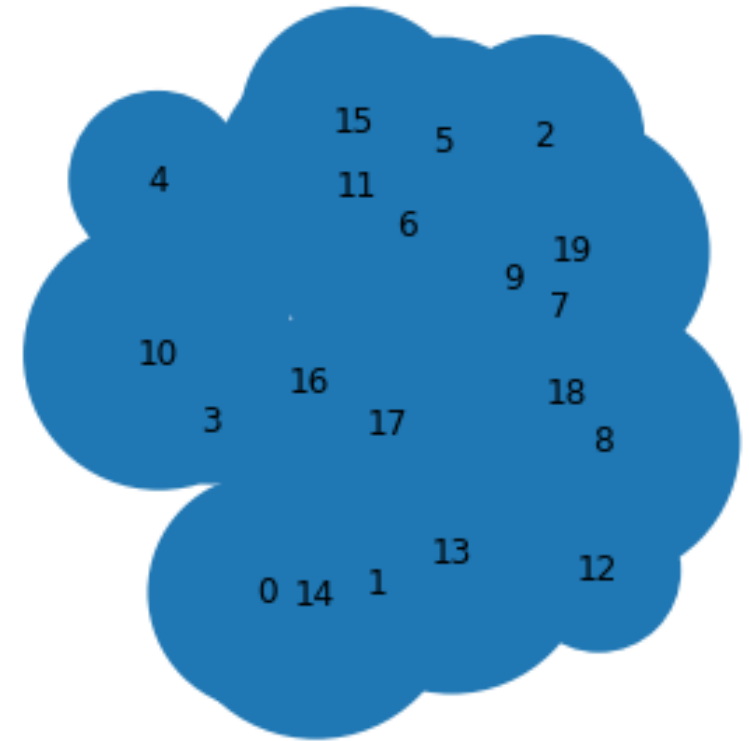
Exercise 2: Antenna Placement

- Implement constraint into the Antenna Placement Problem

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$$\min \left(\left(\sum_{i=0}^N \beta (1 - 2F) q_i + \sum_{i < j} 2\beta q_i q_j \right) \right)$$



Add a Constraint to a QUBO Problem

- Now suppose we want to add another constraint.
- For some reason, we have received orders from above telling us that certain antennas must be placed, regardless of any other conditions.
- How can we implement this type of request?
- First of all we consider a vector L , of length equal to the number of antennas available. We mark with 0 the free antennas and with 1 the antennas that must necessarily be activated.
- Consequently, penalty function can be seen as

$$\sum_{i=1}^N L_i (q_i - 1)^2$$

Add a Constraint to a QUBO Problem

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Add a Constraint to a QUBO Problem

$$\sum_{i=1}^N L_i (q_i - 1)^2 = \sum_{i=1}^N L_i q_i + \sum_{i=1}^N L_i - \sum_{i=1}^N 2L_i q_i =$$

Add a Constraint to a QUBO Problem

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Exercise 2: Antenna Placement

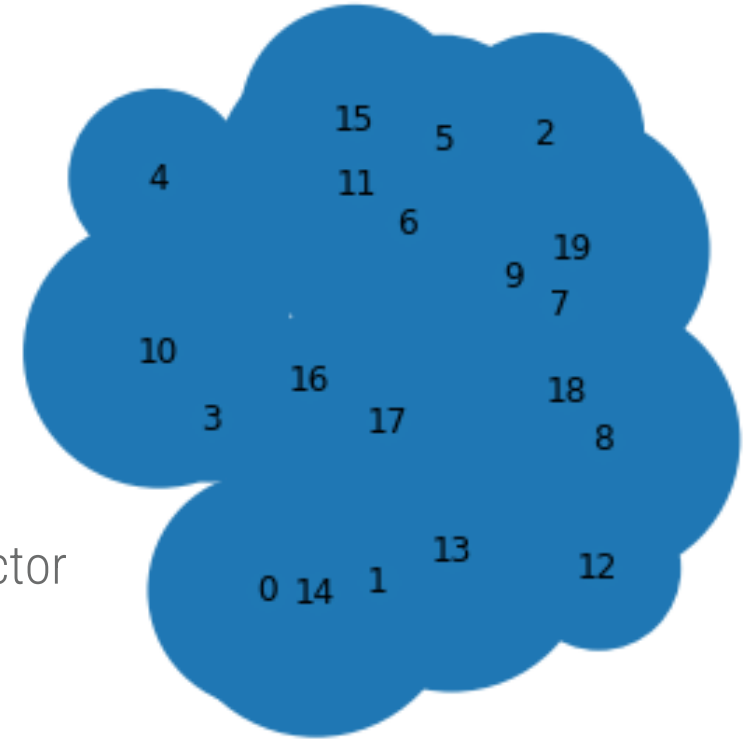
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$$\min \left(\left(\sum_{i=0}^N \beta (1 - 2F) q_i + \sum_{i < j} 2\beta q_i q_j \right) \right)$$



$$-\sum_{i=1}^N \gamma L_i q_i$$

- Implement and configure L vector
- Add values to QUBO problem formulation

Add a Constraint to a QUBO Problem

- Now suppose we want to add an **inequality** constraint to our problem.
- An example could be
- *Let F be the maximum number of antennas that can be placed*
- Mathematically, the constraint appears in the form

$$\sum_{i=0}^N q_i \leq F$$

Add a Constraint to a QUBO Problem

- So far we have seen how to transform constraints involving equalities into penalty functions
- How to deal with an inequality?
- One way can be to **reduce inequality to equality**
- To do that, we need additional binary variables. For this interpretation, we need F more variables

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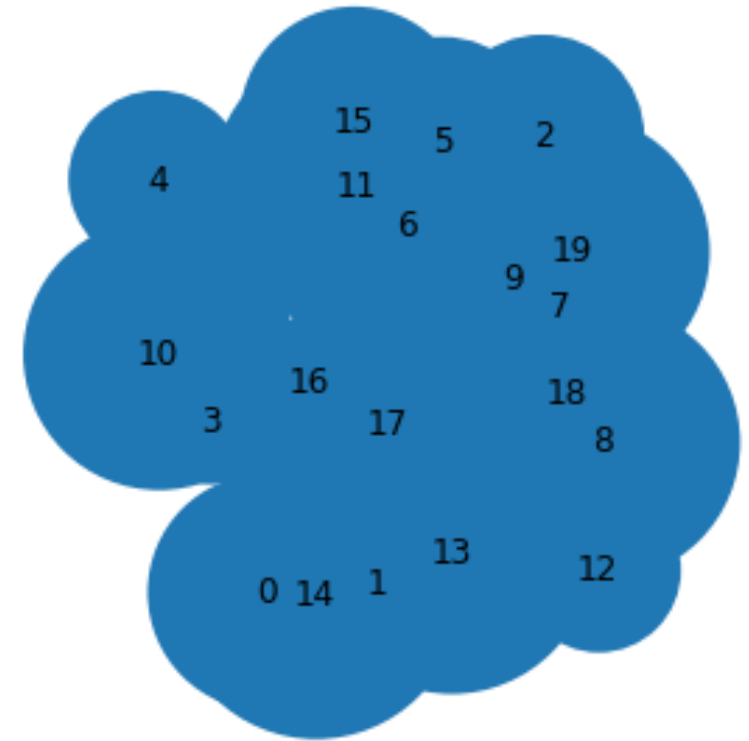
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- Add F more qubits to the formulation
- These qubits are a sort of ghost qubits: they MUST don't interact with the other part of the problem formulation



Add a Constraint to a QUBO Problem

- Now suppose we want to add another inequality constraint to our problem
- For example:

Let A_m be a measure of area. Turn on the antennas so that the minimum covered area is greater than or equal to A_m

$$\sum_{i=1}^N A_i q_i \geq A_m$$

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$$\sum_{i=1}^N A_i q_i - \sum_{k=1}^N A_k q_k = A_m \Rightarrow \sum_{i=1}^{2N} C_i A_i q_i = A_m$$

Add a Constraint to a QUBO Problem

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Add a Constraint to a QUBO Problem

$$\sum_{i=1}^{2N} C_i A_i q_i = A_m \Rightarrow \left(\sum_{i=1}^{2N} C_i A_i q_i - A_m \right)^2$$

Add a Constraint to a QUBO Problem

$$\sum_{i=1}^{2N} C_i A_i q_i = A_m \Rightarrow \left(\sum_{i=1}^{2N} C_i A_i q_i - A_m \right)^2 = \left(\sum_{i=1}^{2N} C_i A_i q_i \right)^2 - 2 \sum_{i=1}^{2N} A_m C_i A_i q_i$$

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$$\sum_{i=1}^{2N} A_i^2 q_i + 2 \sum_{i < j} C_i C_j A_i A_j q_i - 2 \sum_{i=1}^{2N} A_m C_i A_i q_i = \sum_{i=1}^{2N} (A_i^2 - 2 A_m C_i A_i) q_i + \sum_{i < j} 2 C_i C_j A_i A_j q_i$$

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$$QUBO = -\sum_{i=0}^N A_i q_i + \alpha \sum_{i < j} B_{ij} q_i q_j \quad \min \left(\left(\sum_{i=0}^N \beta (1 - 2F) q_i + \sum_{i < j} 2\beta q_i q_j \right) \right) - \sum_{i=1}^N \gamma L_i q_i \quad \sum_{i=1}^{N+F} q_i = F$$

$$\sum_{i=1}^{2N} C_i A_i q_i = A_m$$

- Add N more qubits to the formulation
- These qubits are a sort of ghost qubits: they don't interact with the other part of the problem formulation
- Do the math!



Add High Order terms to our problem

- Sometimes it is necessary to add some terms of order 3 or higher to our problem.
- How can we relate to a QUBO problem?

$$xyz = \max_w \{w(x + y + z - 2)\}$$

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- How can we relate to a QUBO problem?

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x, y, z	xyz	$x + y + z - 2$	$\max_w \{w(x + y + z - 2)\}$
0, 0, 0	0	-2	$0 _{w=0}$
0, 0, 1	0	-1	$0 _{w=0}$
0, 1, 0	0	-1	$0 _{w=0}$
0, 1, 1	0	0	$0 _{w=0,1}$
1, 0, 0	0	-1	$0 _{w=0}$
1, 0, 1	0	0	$0 _{w=0,1}$
1, 1, 0	0	0	$0 _{w=0,1}$
1, 1, 1	1	1	$1 _{w=1}$

Exercise 2: Antenna Placement

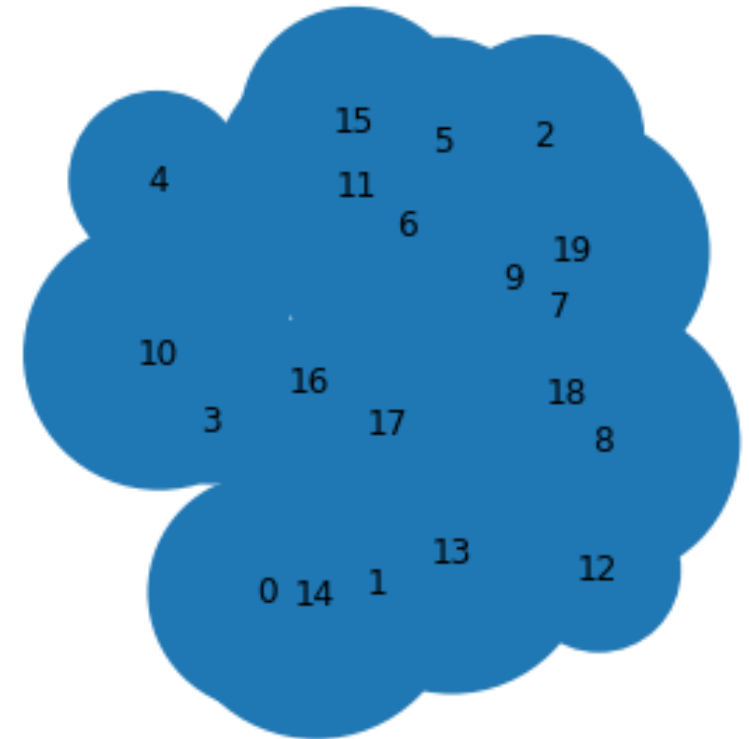
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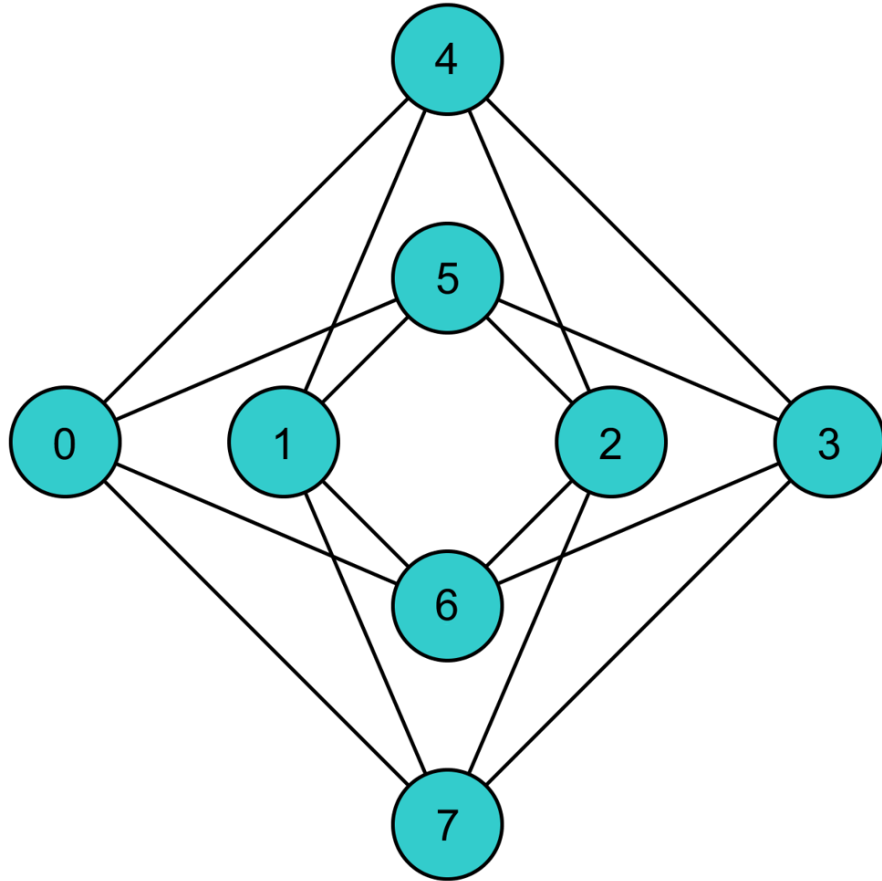
$$\text{QUBO} = -\sum_{i=0}^N A_i q_i + \alpha \sum_{i < j} B_{ij} q_i q_j \quad \min \left(\left(\sum_{i=0}^N \beta (1 - 2F) q_i + \sum_{i < j} 2\beta q_i q_j \right) \right) \quad -\sum_{i=1}^N \gamma L_i q_i \quad \sum_{i=1}^{N+F} q_i = F$$

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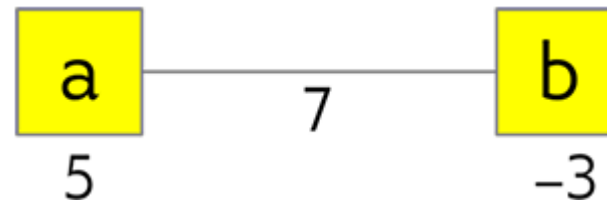
- Add High Order Terms to QUBO problem with pyqubo

Graphs

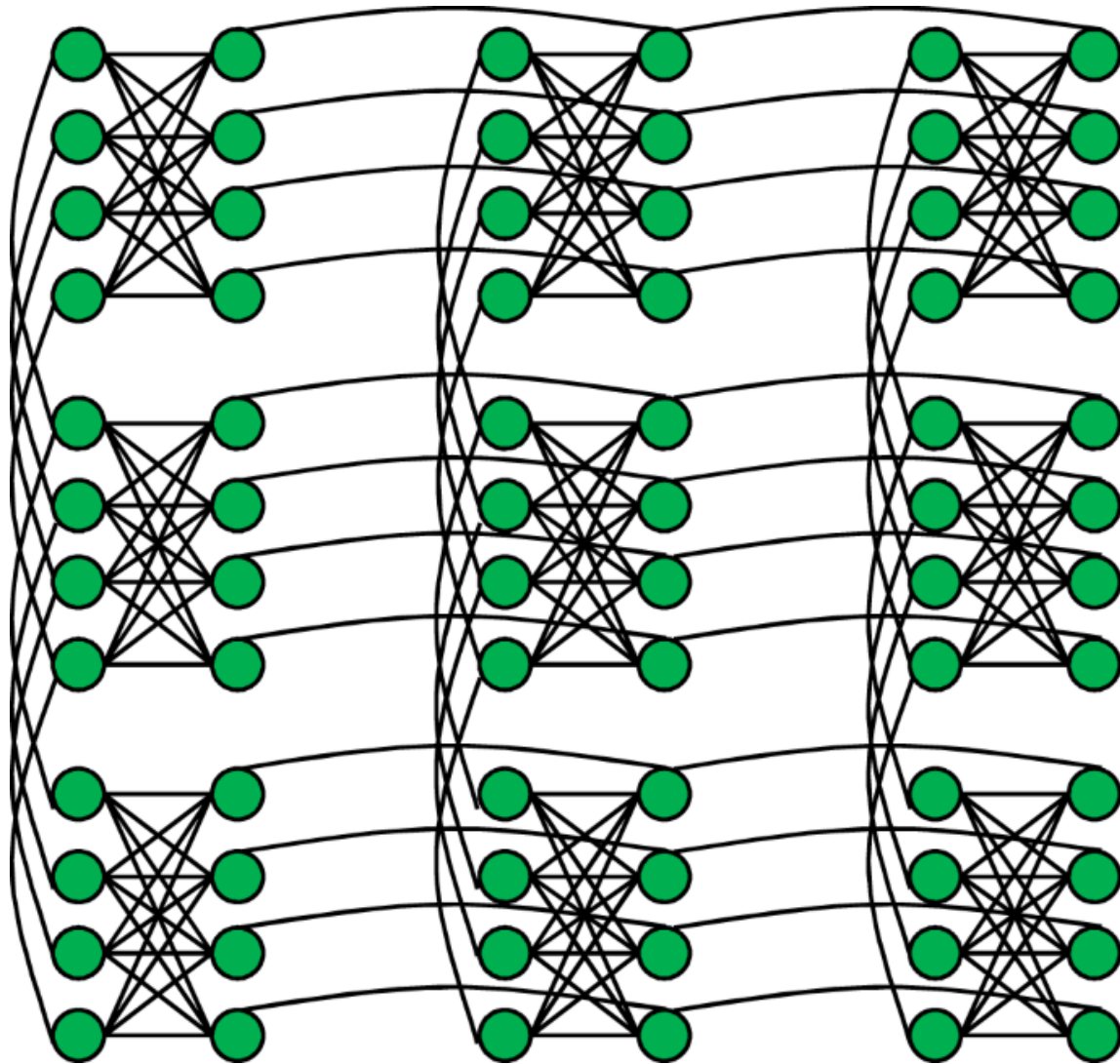


- Mathematically speaking, an undirected graph is defined as a set of vertices $V = \{v_1, \dots, v_N\}$
- and a set of edges $E \subseteq V \times V$
- Each node and each edge can be weighted with an arbitrary value (in this case we are talking about a weighted graph)
- In this way it is possible to establish a one-to-one correspondence between a weighted graph and a QUBO function

$$H(a, b) = 5a + 7ab - 3b$$



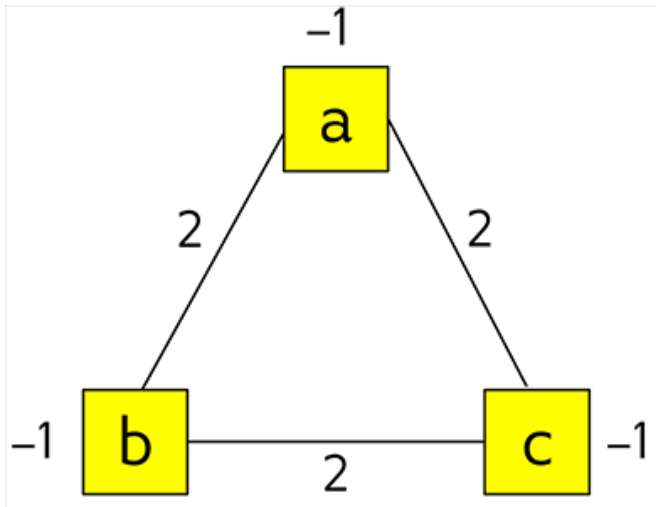
Embedding a problem on a graph



- But what if the graph with which we want to represent the QUBO function does not have enough vertices or edges to do so?
- In the case of the vertices, there is nothing to do: we have to change the problem and / or graph!
- In the case of the edges, however, something is possible to do
- The core of a quantum annealer is represented by a graph: in the figure, we can observe the Chimera graph, that is the topology of one of the D-Wave models (the penultimate model)
- This means that to solve a QUBO problem it is necessary to map your problem on the graph of the selected quantum annealer
- This procedure is called embedding

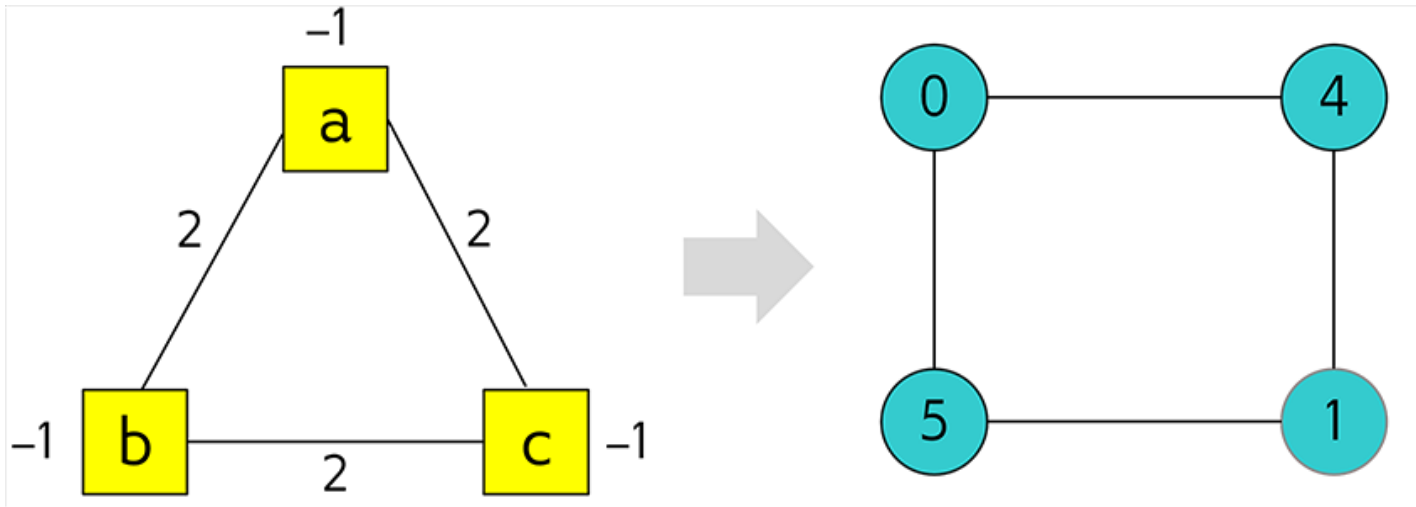
Embedding a problem on a graph

- Suppose we have a QUBO problem that can be translated with the following graph



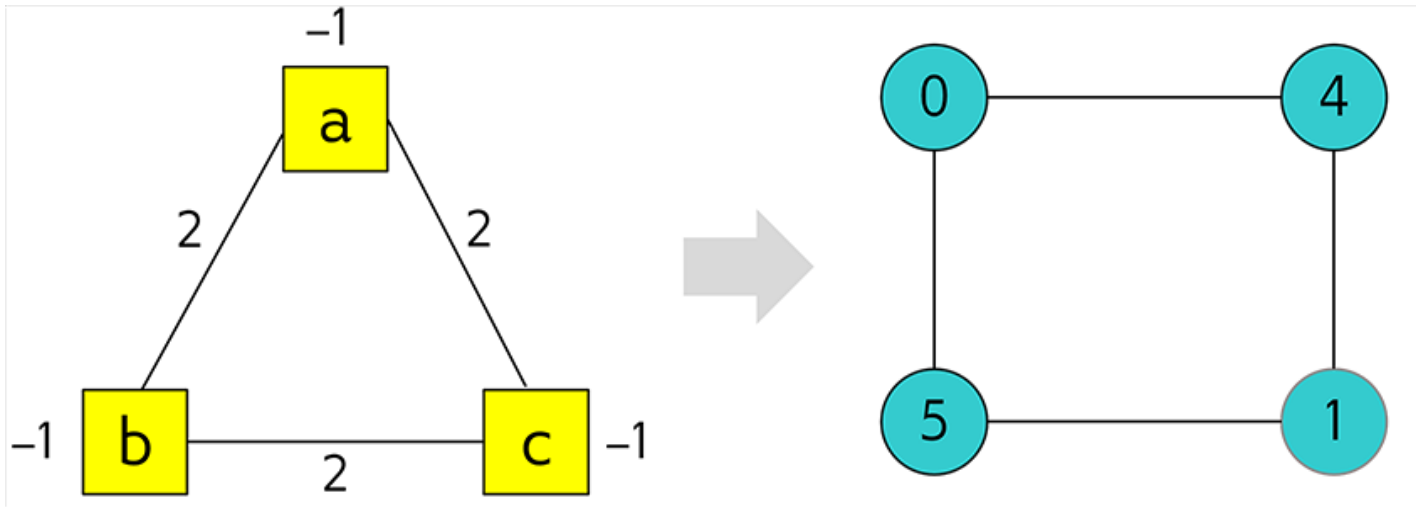
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- Suppose we have a QUBO problem that can be translated with the following graph
- Suppose we also have a quantum annealer with a graph of this shape



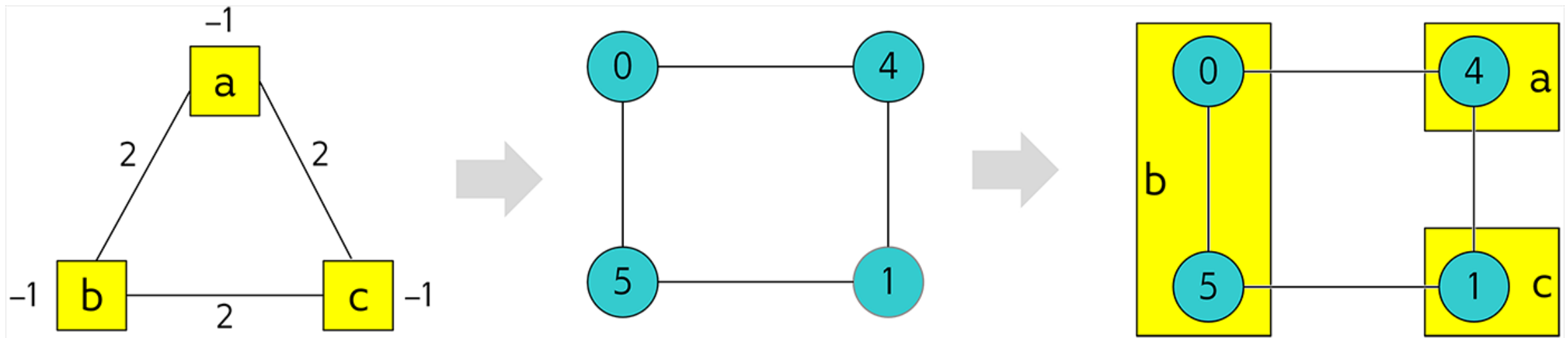
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- Suppose we have a QUBO problem that can be translated with the following graph
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- By looking at them, it seems impossible to map our problem to the target graph



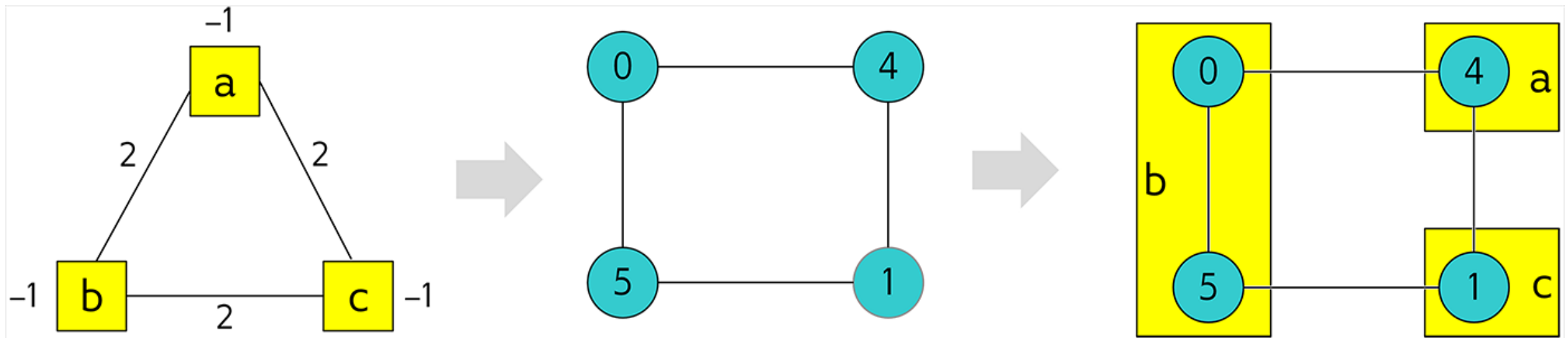
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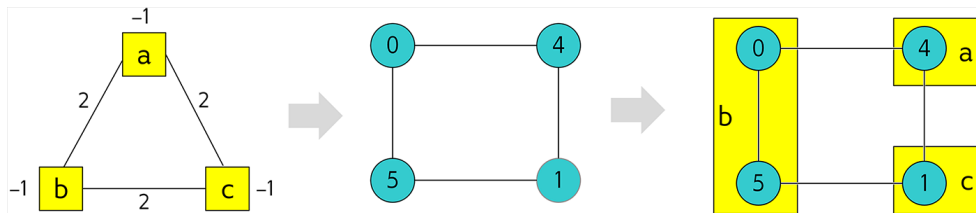
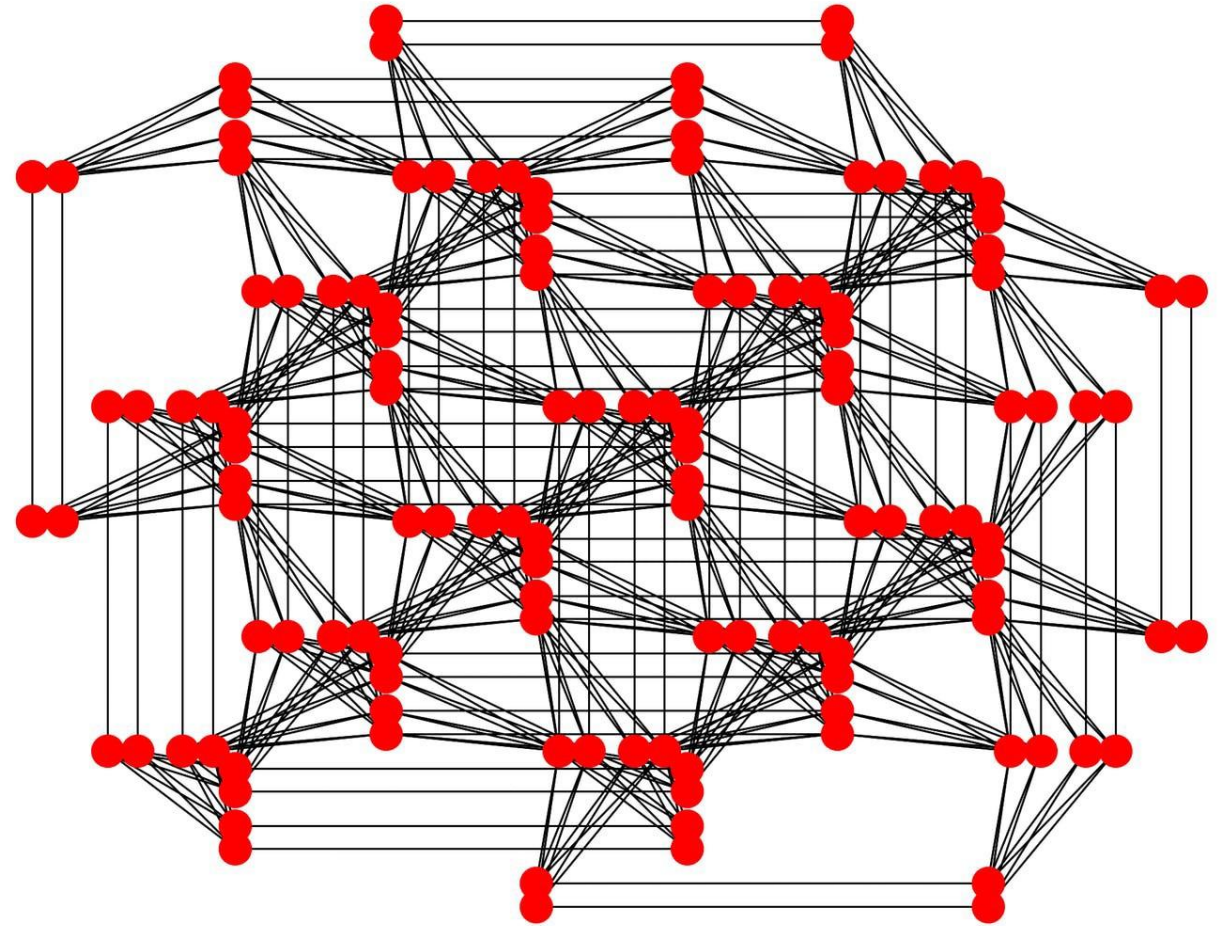
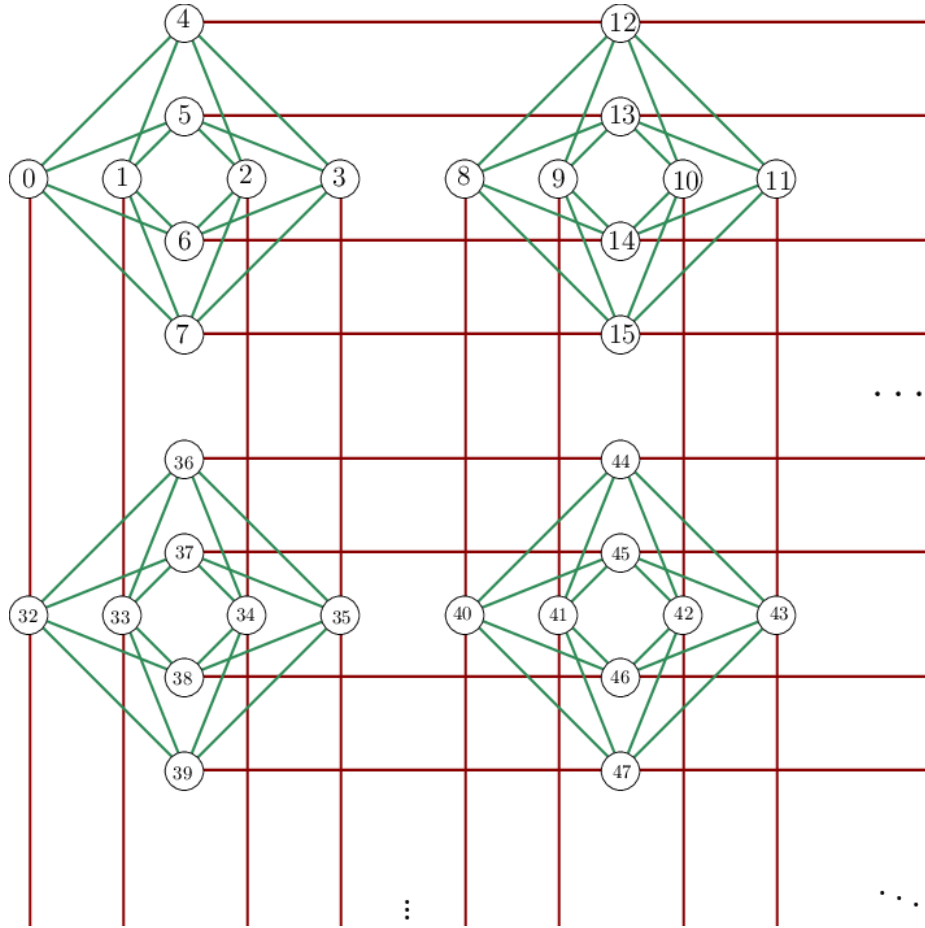


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- Suppose we have a QUBO problem that can be translated with the following graph
- Suppose we also have a quantum annealer with a graph of this shape
- By looking at them, it seems impossible to map our problem to the target graph
- The embedding procedure allows for this mapping by forcing multiple qubits to behave as one
- In a certain sense, we can say that the qubits engaged in embedding are placed in entanglement relationship: they are forced to collapse in the same classical state



Embedding on Chimera and Pegasus



Exercise 2: Antenna Placement

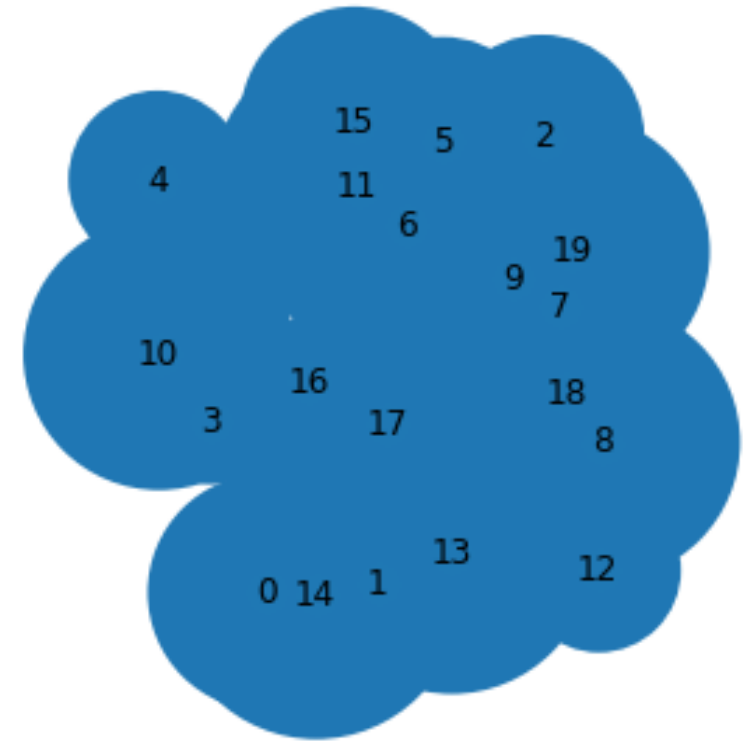
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- Try the embedding on Pegasus and Chimera