



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



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- A Quantum Annealer is a **special purpose quantum computer**



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- 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.



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- A Quantum Annealer is a quantum computer designed and built **to host a single quantum algorithm, Quantum Annealing**



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- A Quantum Annealer is a **special purpose quantum computer**
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- 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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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 conventional method.

PACS number(s): 05.50.+a

I. INTRODUCTION

The technique of simulated annealing proposed by Kirkpatrick *et al.* [1] is widely used for optimization problems. The idea is to allow the system to escape from local minima by increasing the temperature to allow the system to escape from local minima and then slowly decreasing the temperature to allow the system to settle into the global minimum. Geman and Geman [2] applied this technique to image restoration. The technique of simulated annealing is based on the idea of the Metropolis algorithm [3]. The technique of simulated annealing is based on the idea of the Metropolis algorithm [3]. The technique of simulated annealing is based on the idea of the Metropolis algorithm [3].



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We introduce quadratic exchange to achieve faster convergence to the global minimum. It plays the same role as thermal exchange in the Metropolis model, in which the system is allowed to exchange energy with a heat bath. The goal is to find the minimum energy configuration if possible. We have studied various exchange interactions and found that quadratic exchange reveals that the quadratic approximation is a good approximation. We use the same approximation for the quadratic approximation.

PACS number(s): 0

I. INTRO

The technique of simulated annealing proposed by Kirkpatrick *et al.* [1] is used for solving optimization problems. The idea is to allow the system to escape from local minima of the 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 decreases too fast, the system may become trapped in a local minimum. In slow annealing, on the other hand, the system can reach the global minimum, though such a process would require a very long time. Geman and Geman [2] proposed an annealing schedule for simulated annealing [2]. The system reaches the global minimum of the cost function locally if the temperature is decreased according to the schedule where c is a constant determined by the structure of the cost function. The annealing schedule may be the optimal one for a given problem.



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- In 2018 I had a beer with him!

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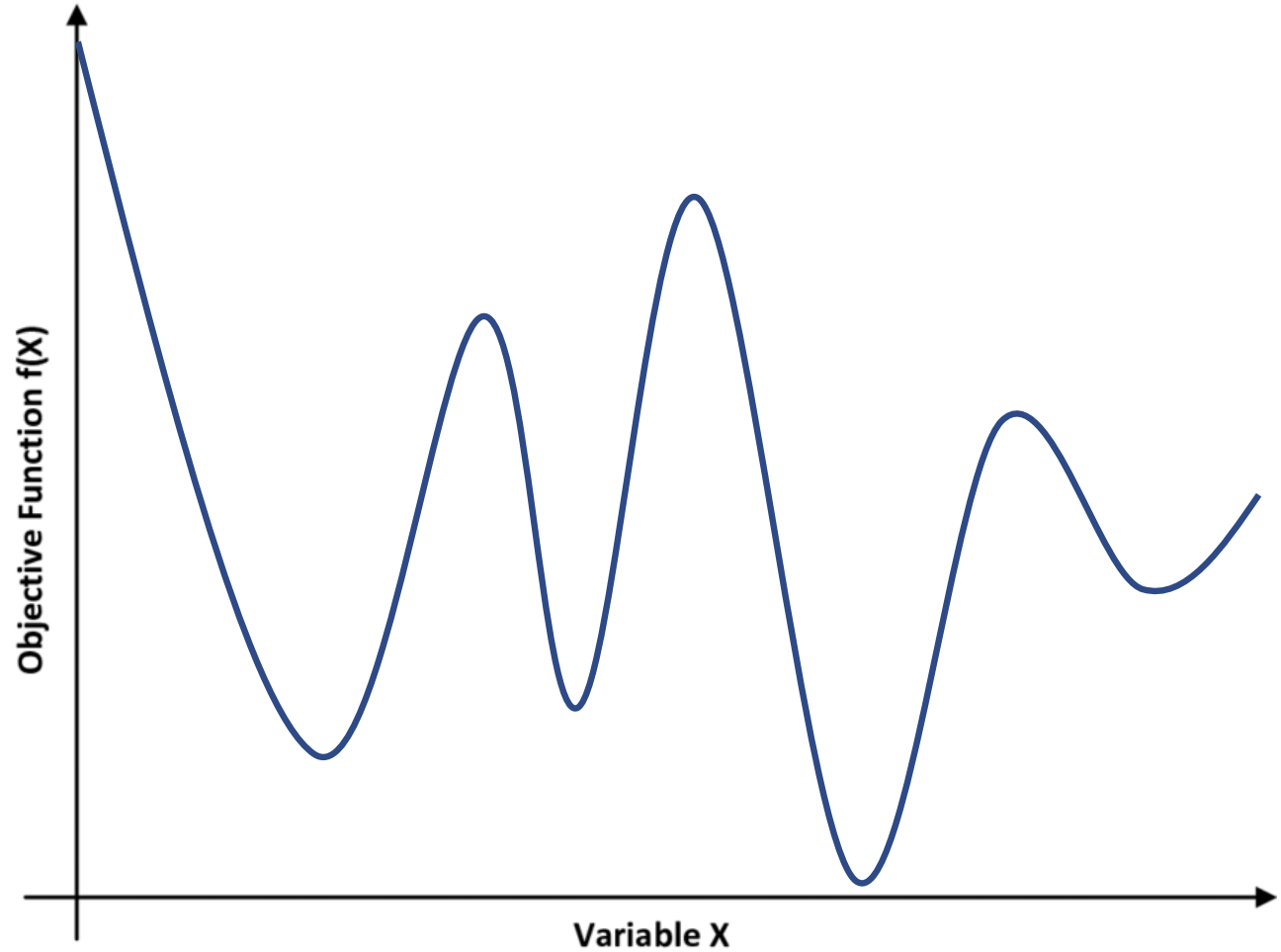
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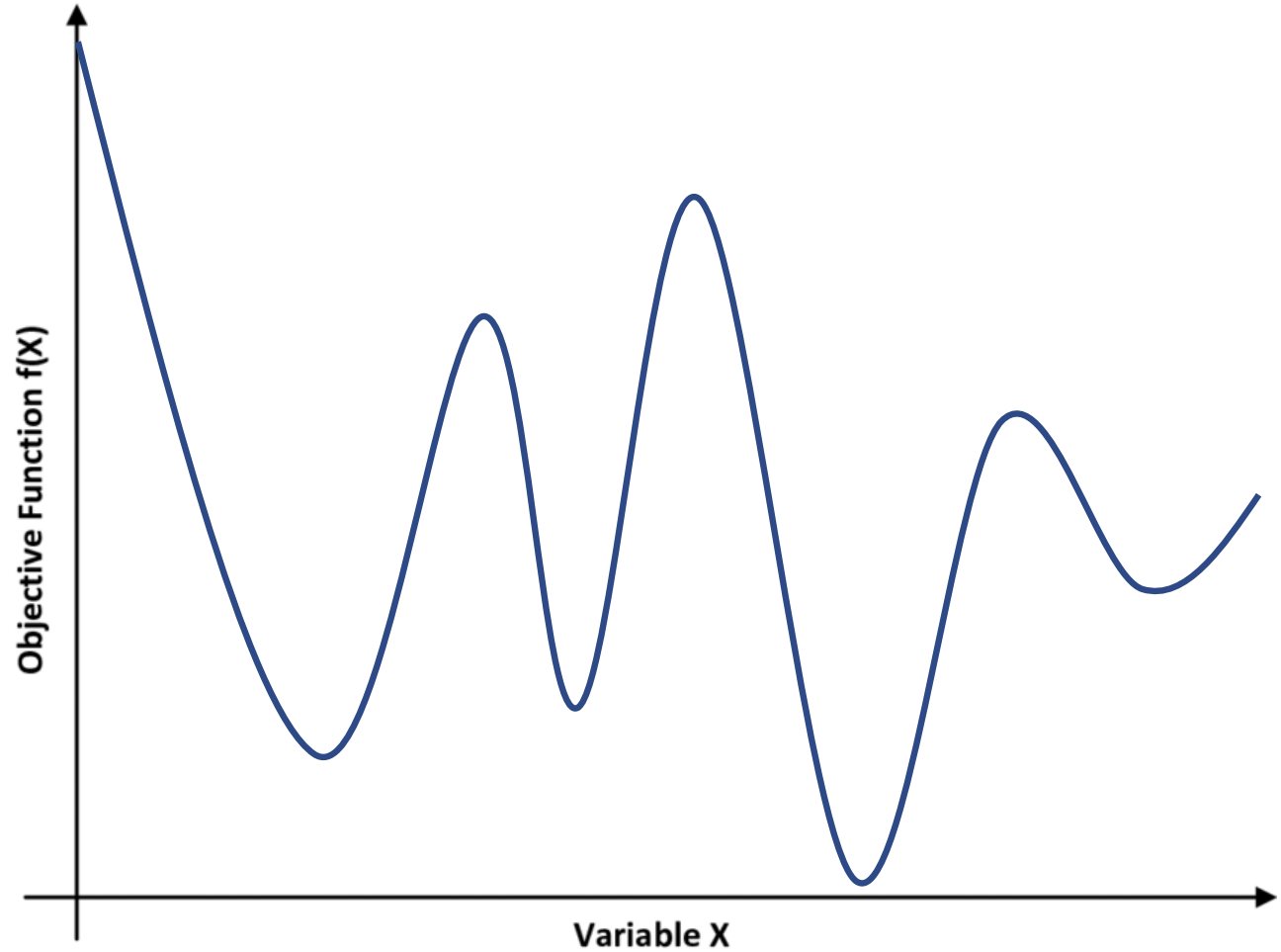
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- Suppose we have an optimization problem, for example a minimization problem, whose objective function (i.e. the function to be minimized) is known and computable using a finite set of variables.



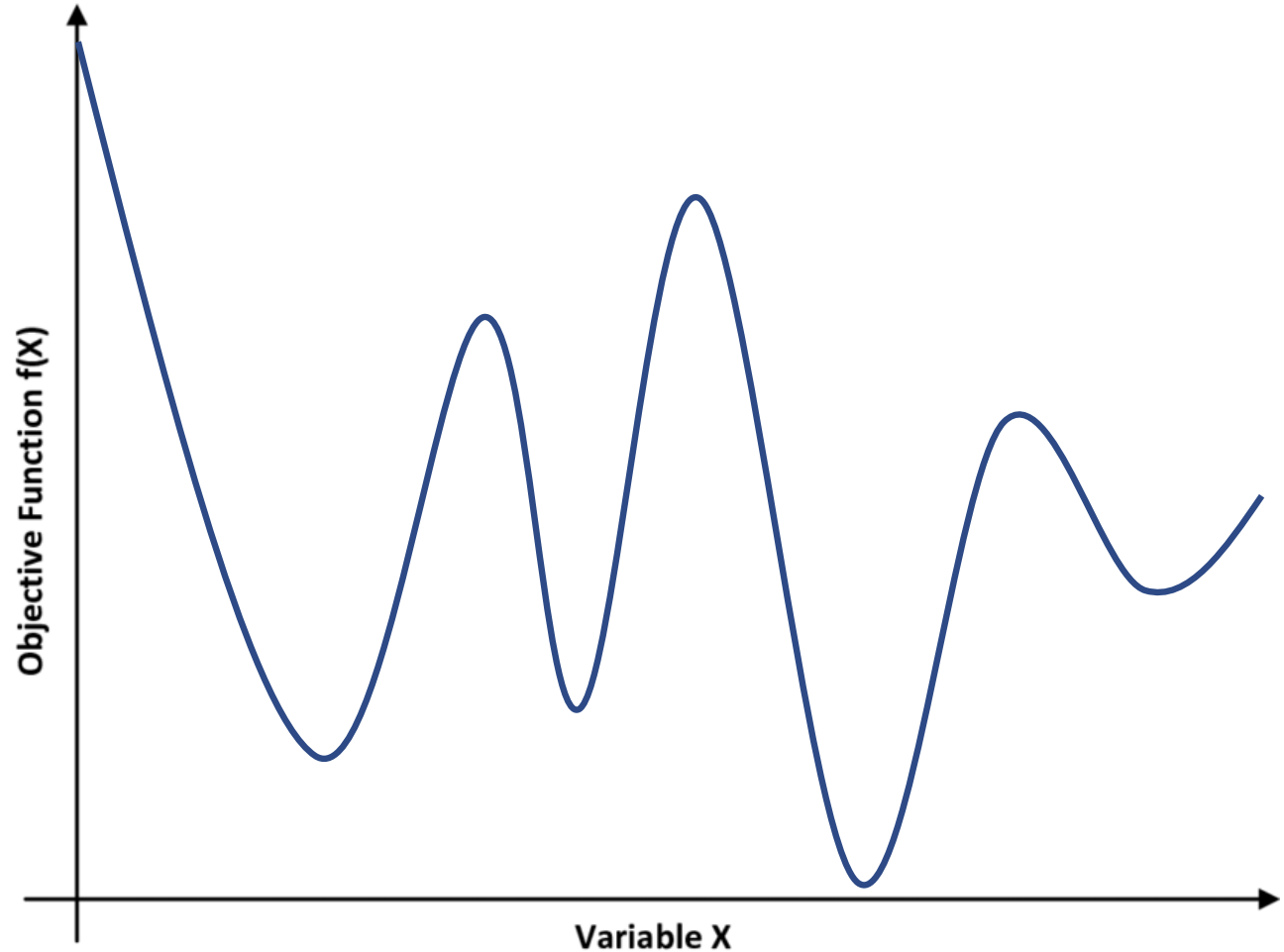
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- Suppose we have an optimization problem, for example a minimization problem, whose objective function (i.e. the function to be minimized) is known and computable using a finite set of variables.
- The best way to solve a problem of this type is undoubtedly the so-called **brute force approach**: we calculate all the values of the objective function for all possible inputs and consider the smallest



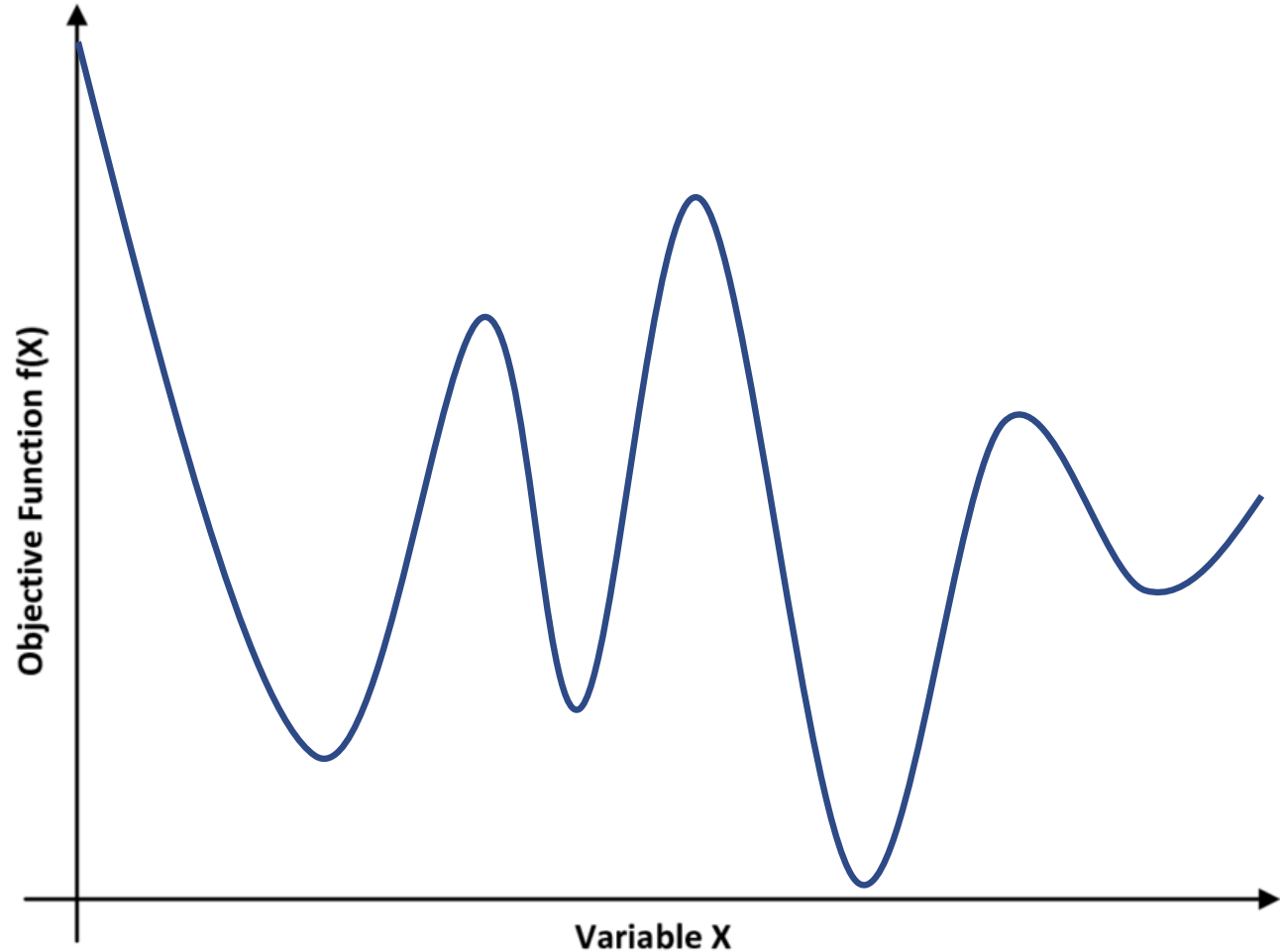
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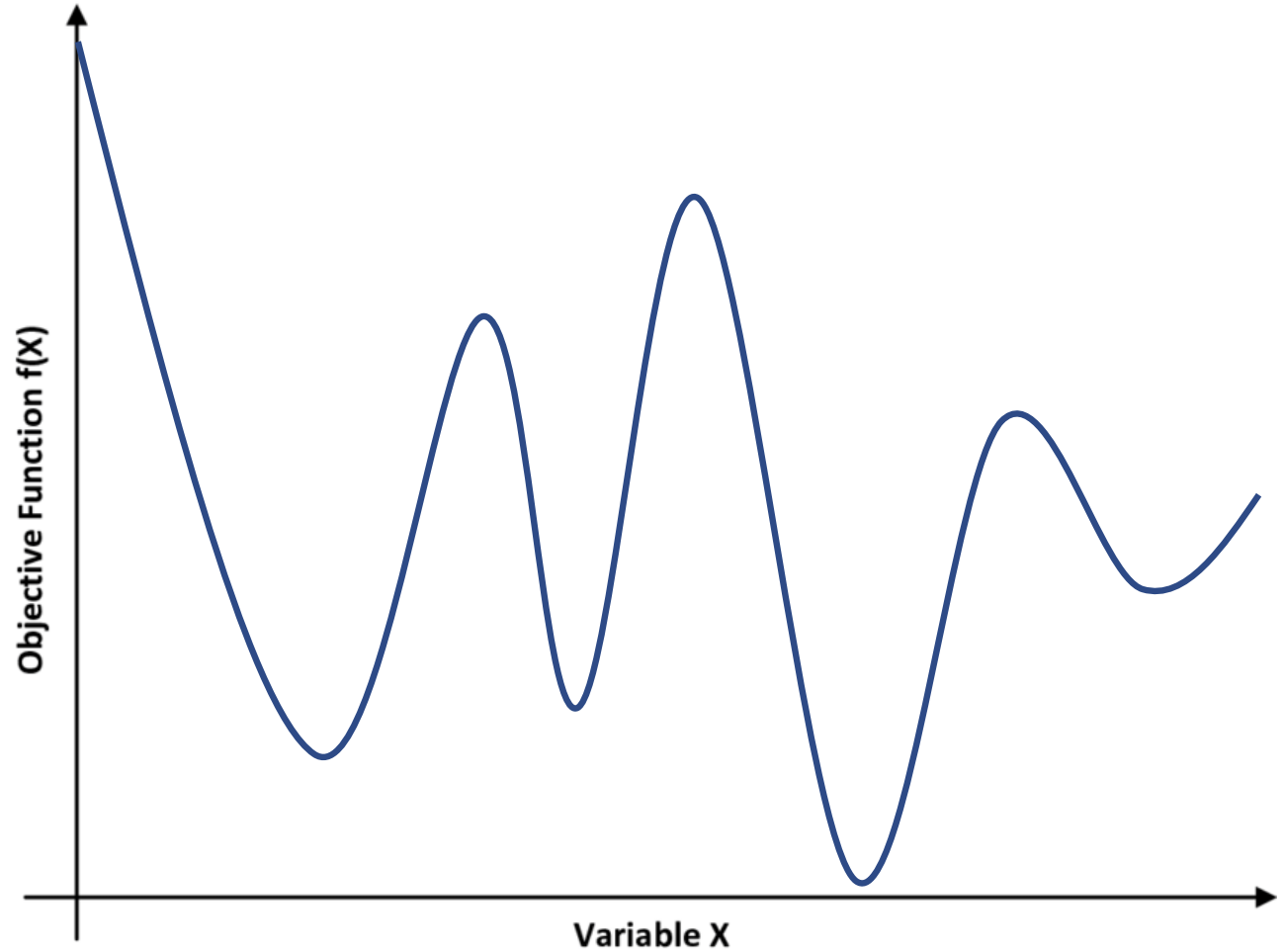
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- Let's imagine for example the case of a function with **N** binary variables: the number of possible combinations is 2^N ...



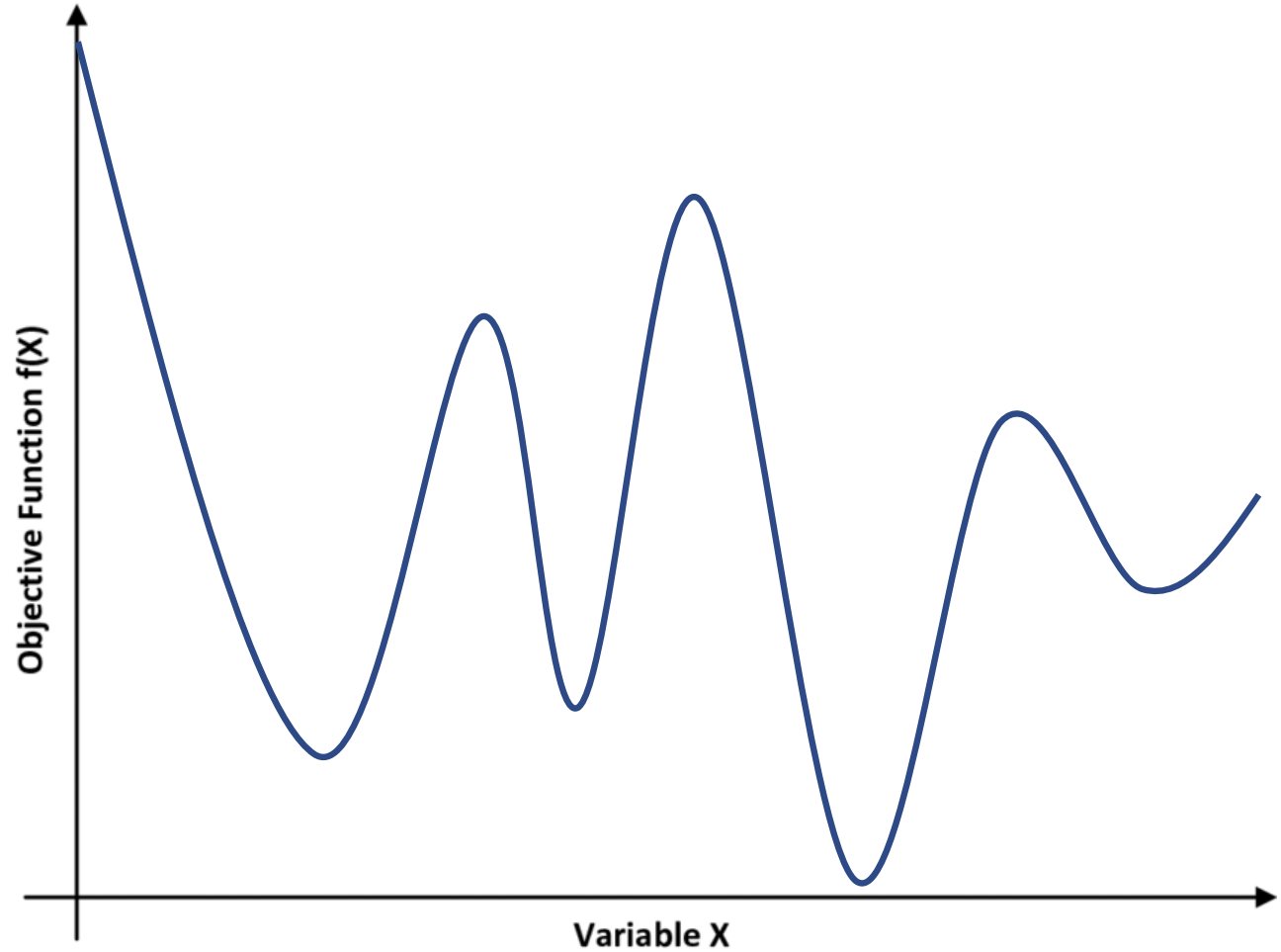
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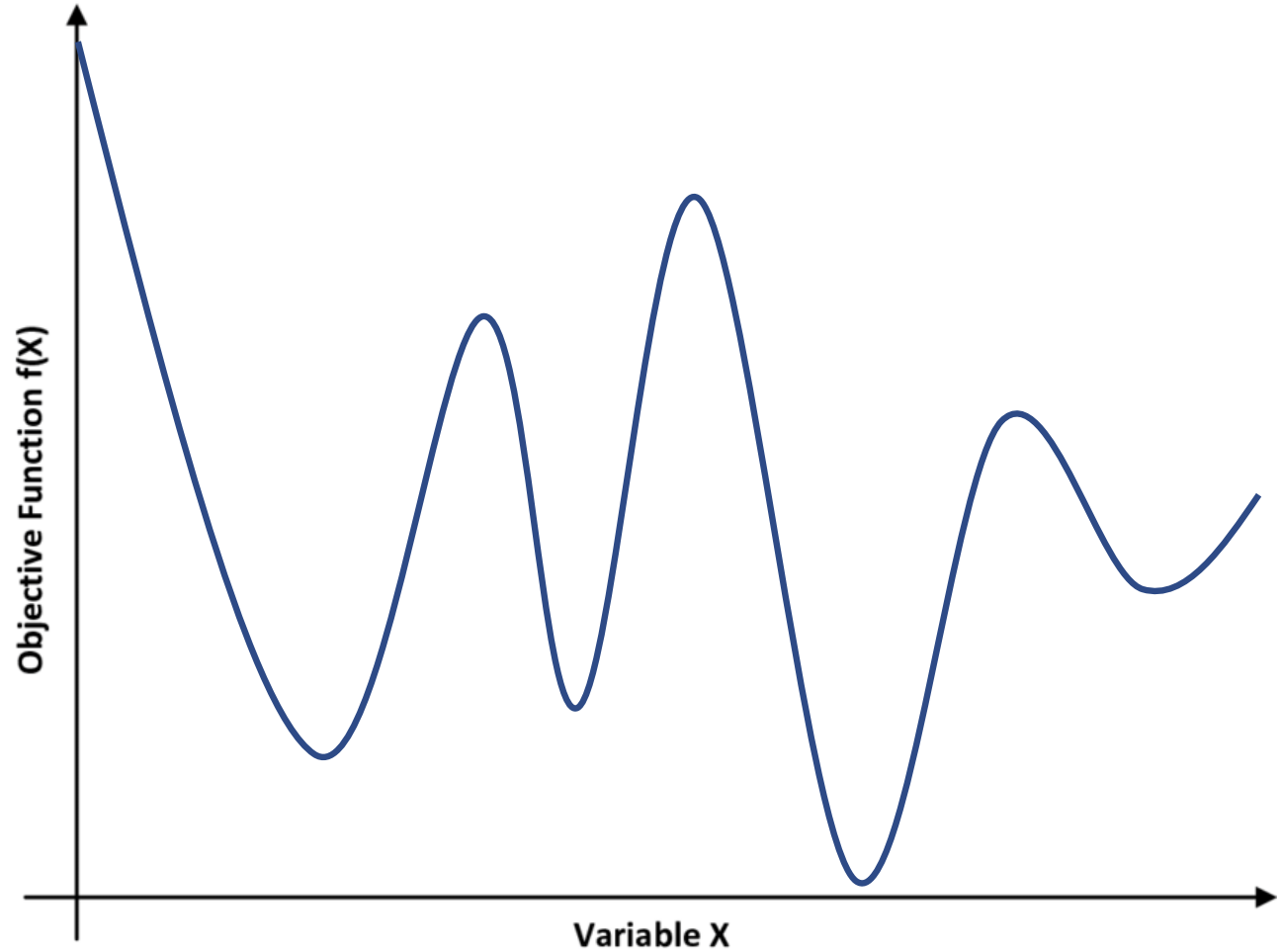
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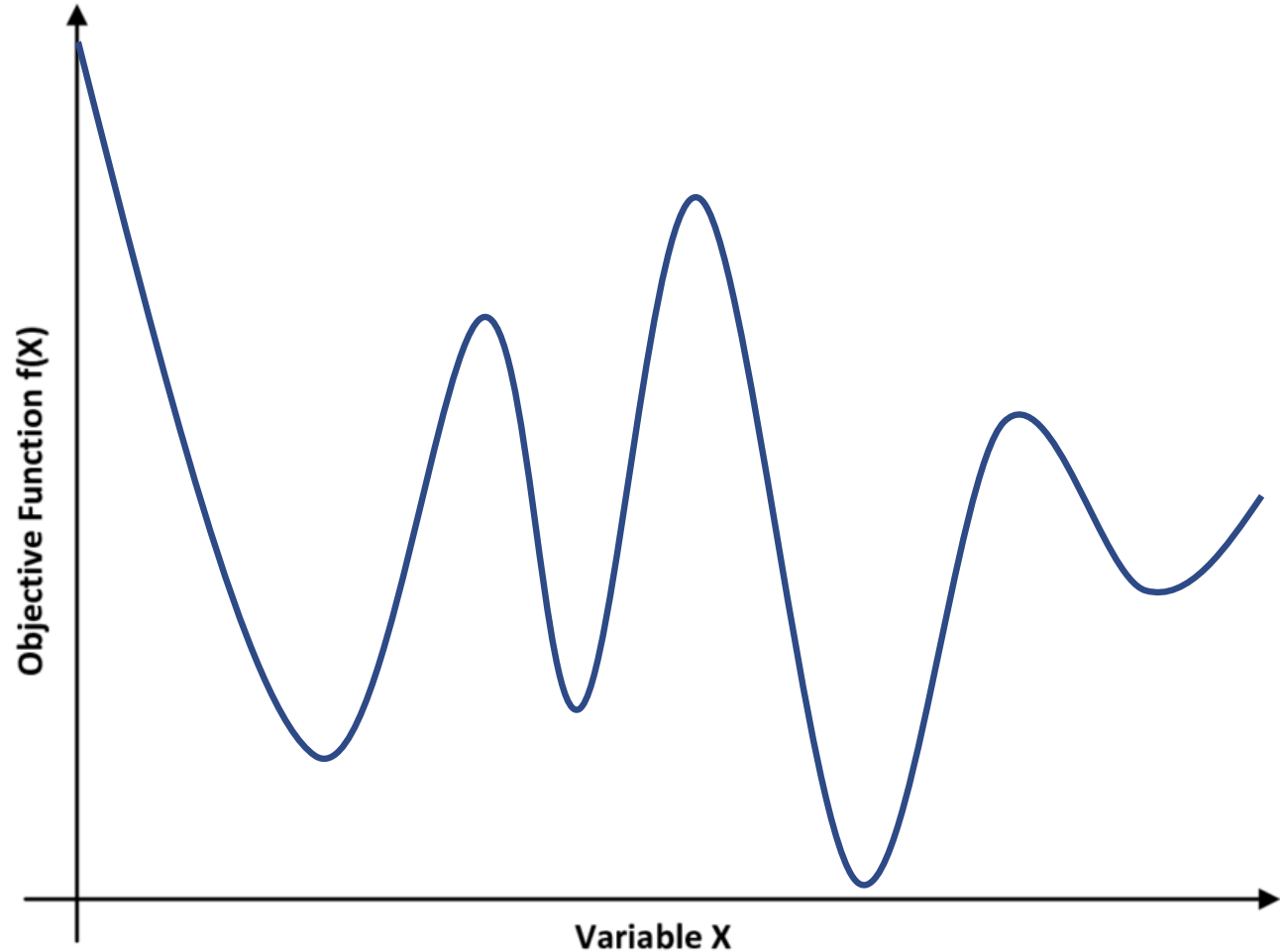
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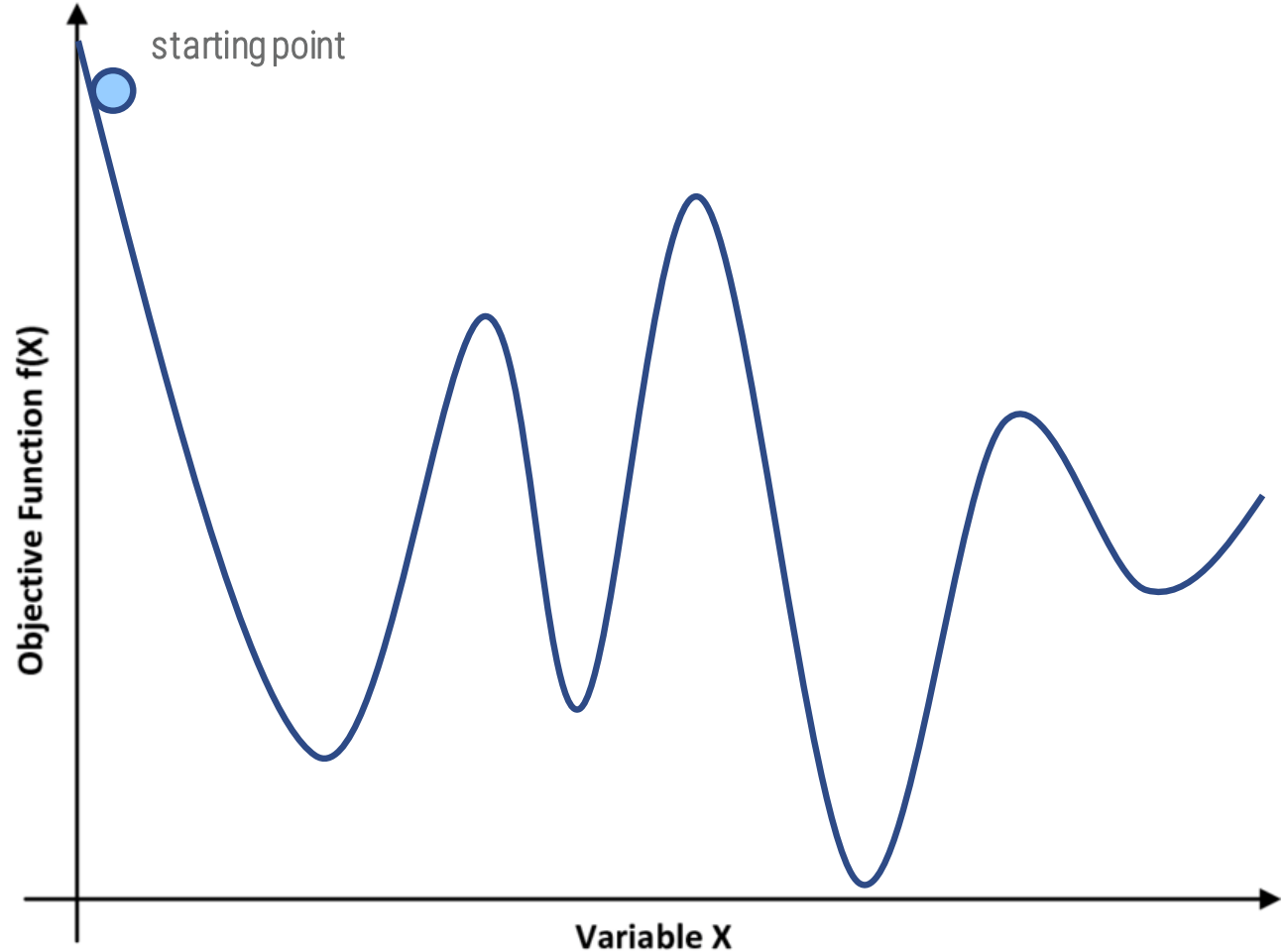
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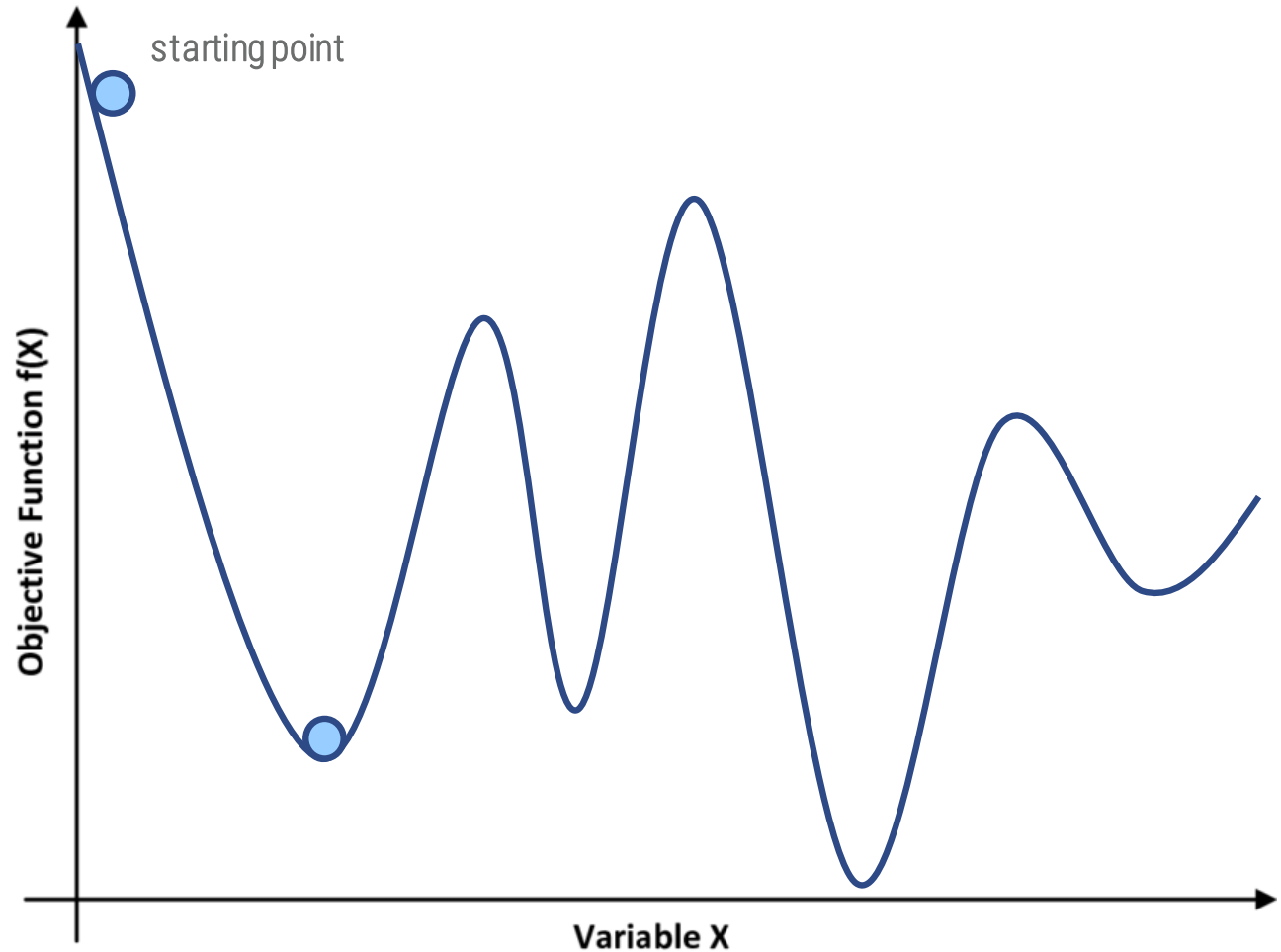
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- Simulated annealing is a probabilistic strategy used to solve optimization problems
- Without going into too much detail of the algorithm, we can explain the idea behind it by thinking of a **ball that rolls along the graph of a function, falling into the holes defined by the minima.**



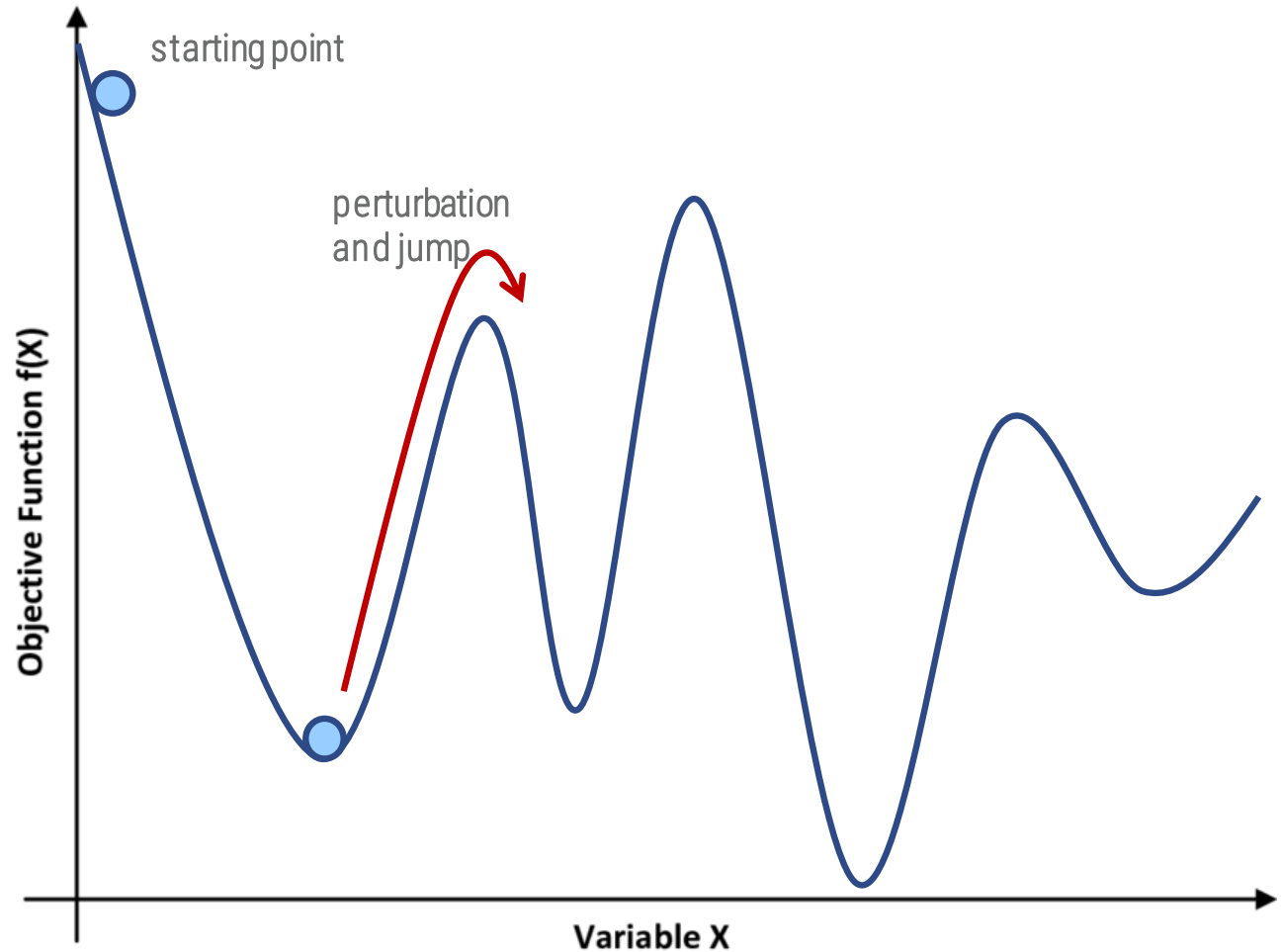
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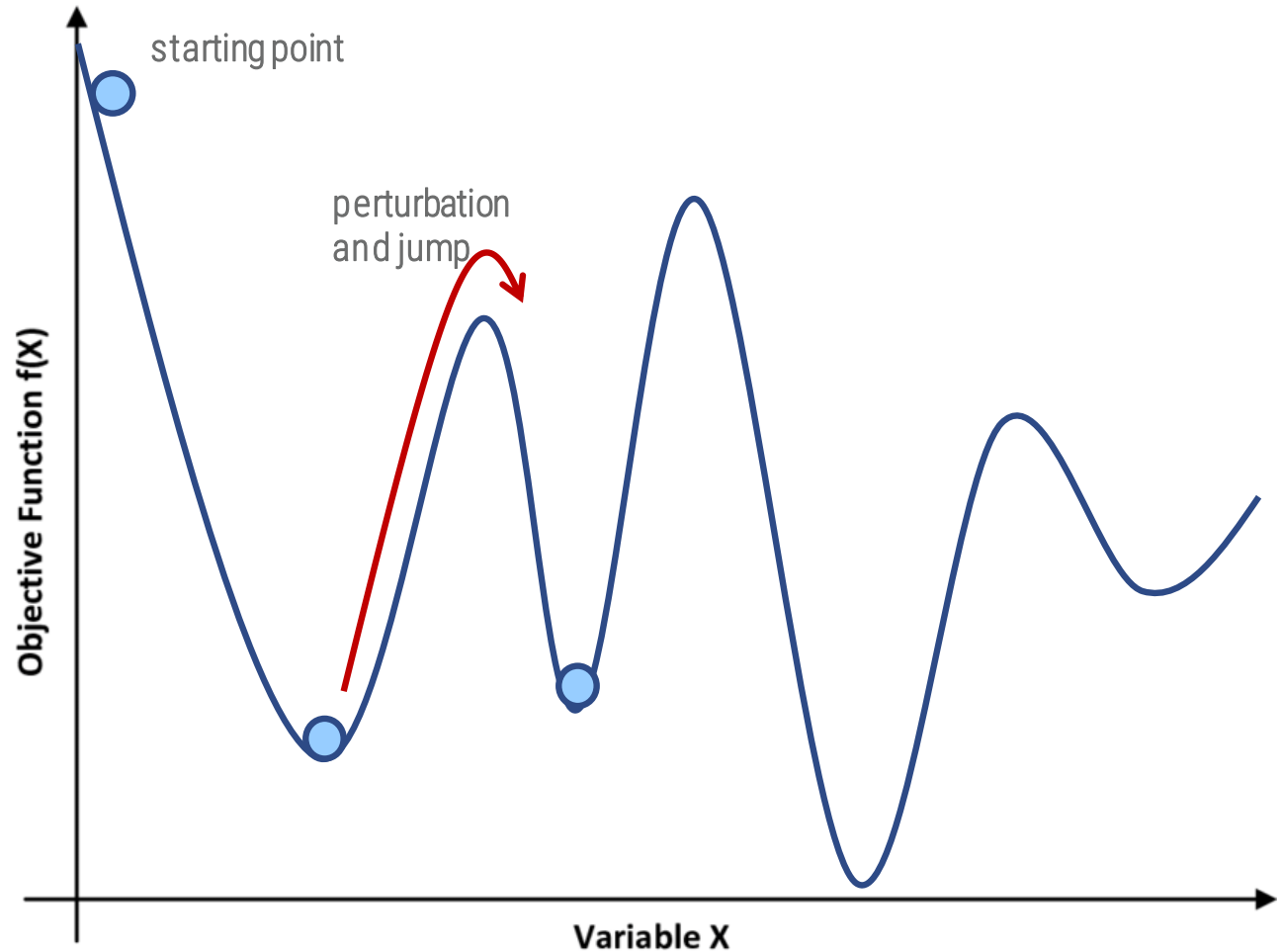
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- Every time a ball lands in a hole it receives a certain amount of energy, enough to make it jump over another piece of graph, looking for deeper minima points.



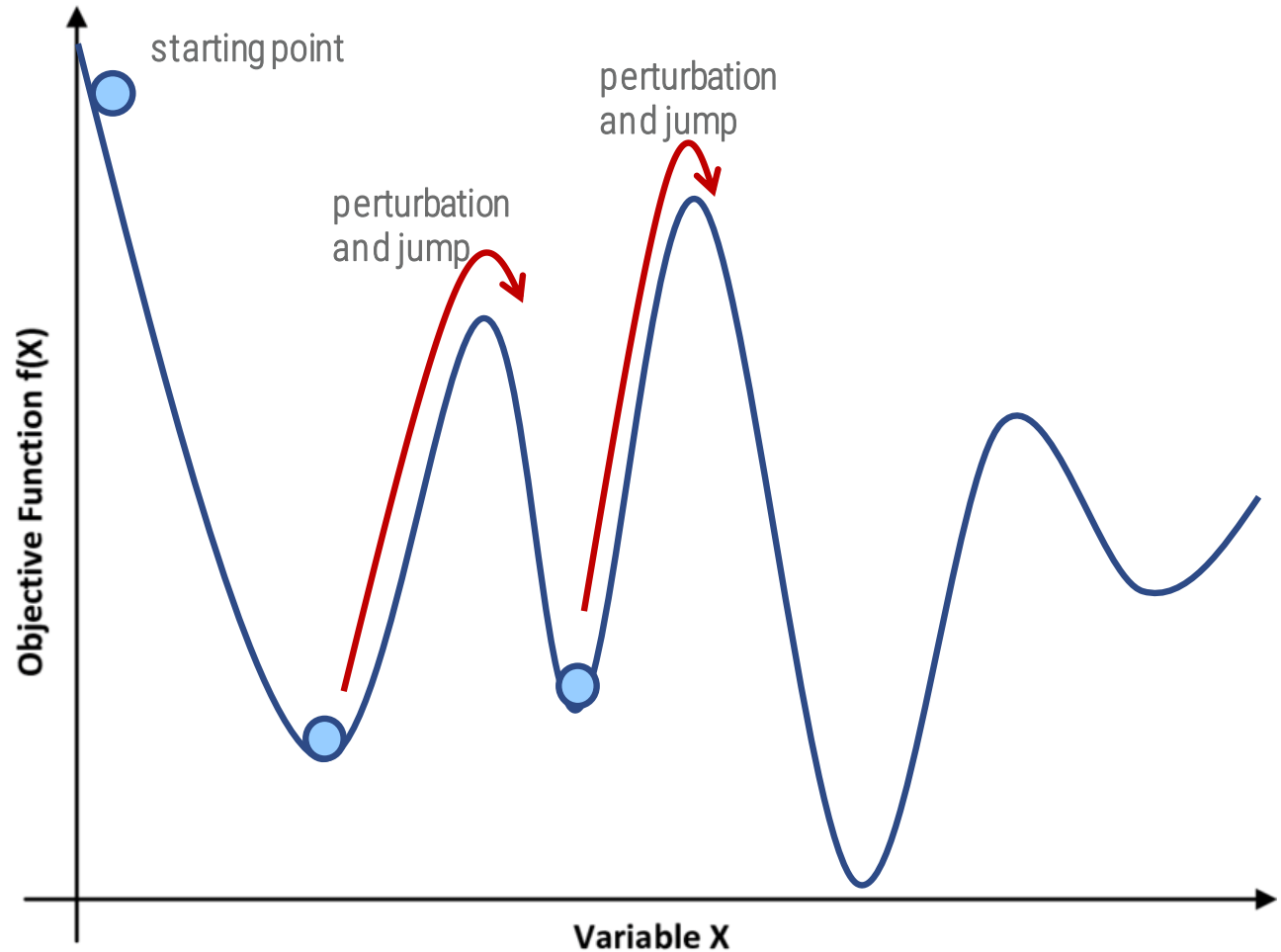
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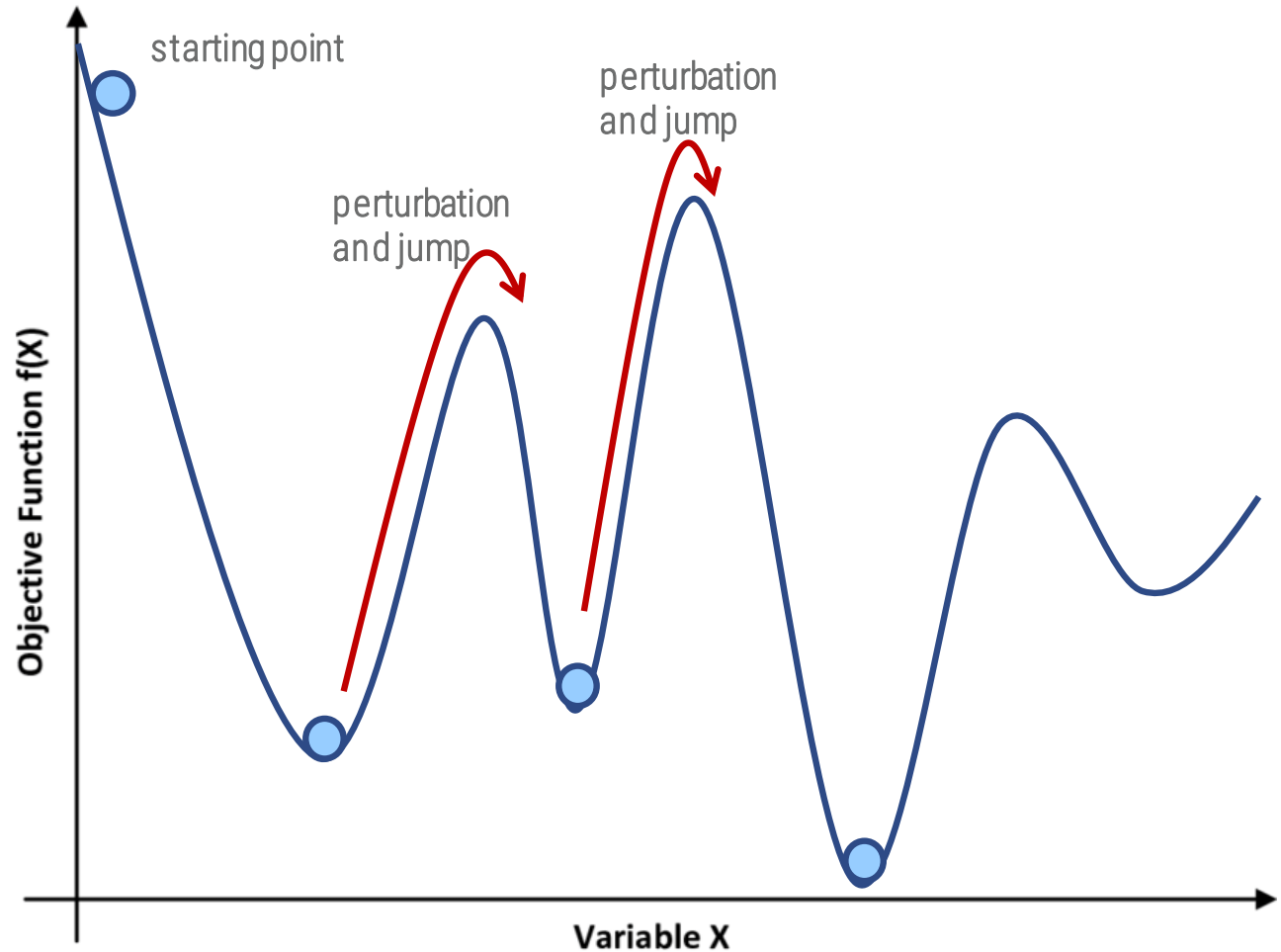
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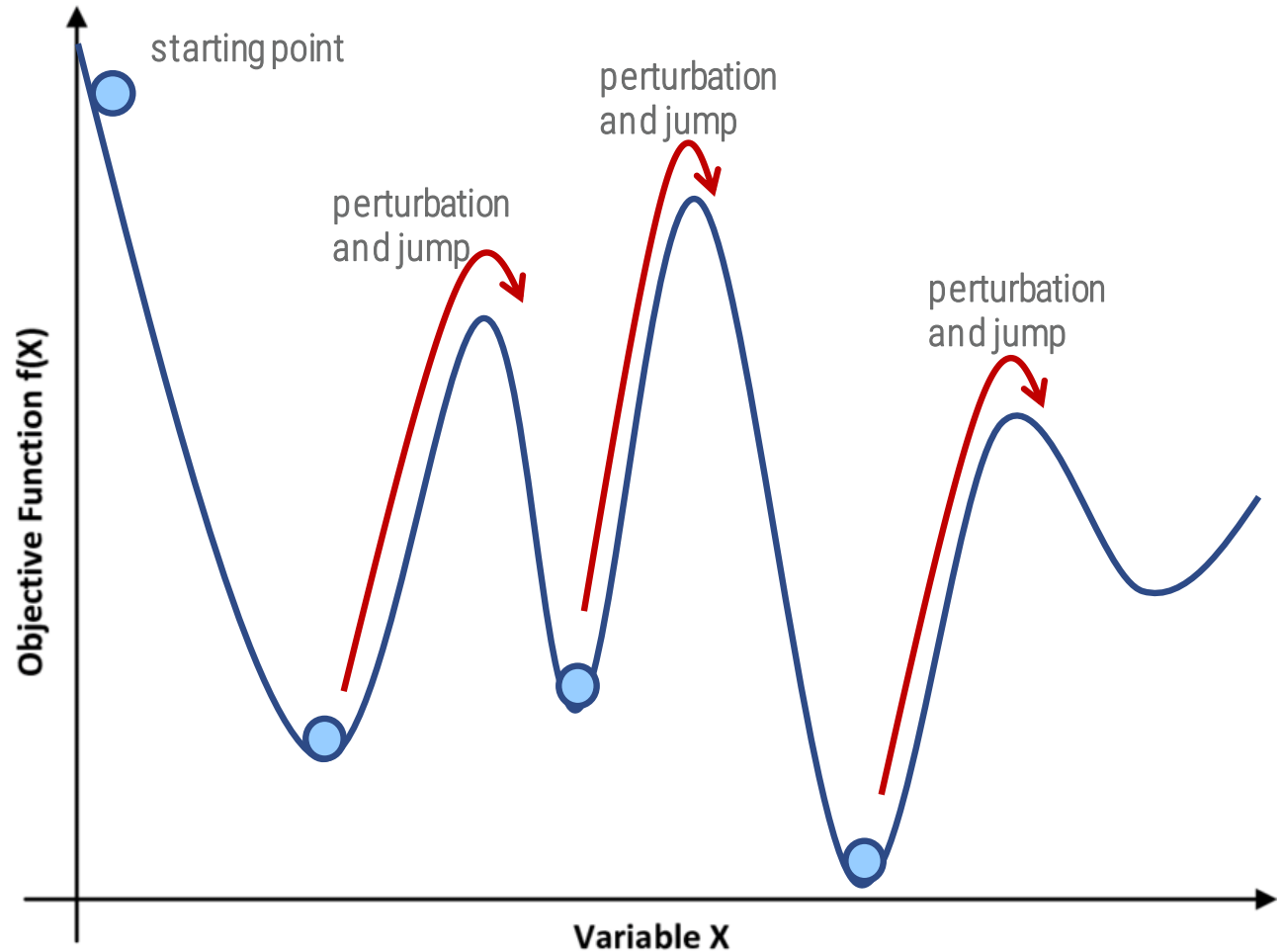
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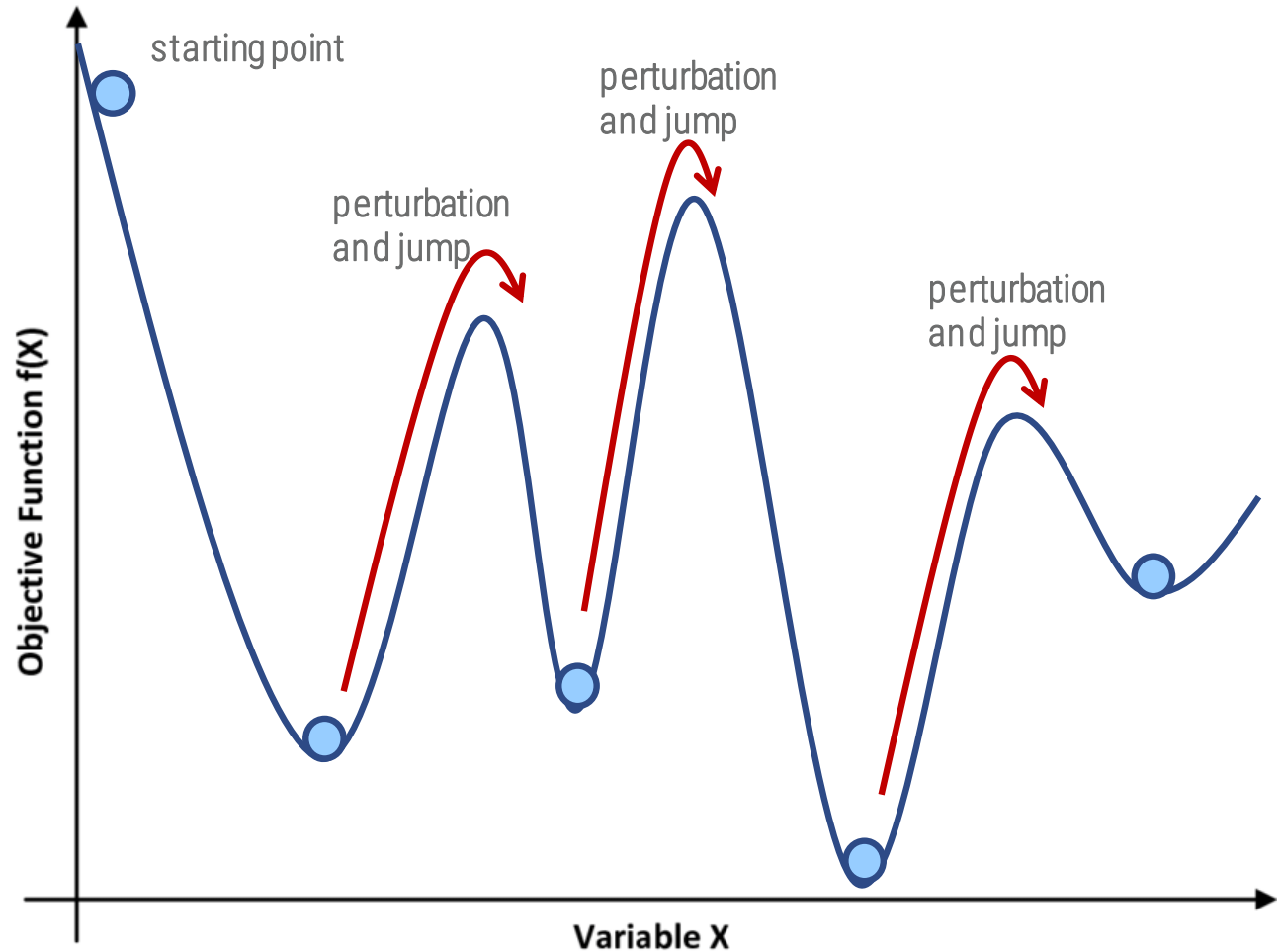
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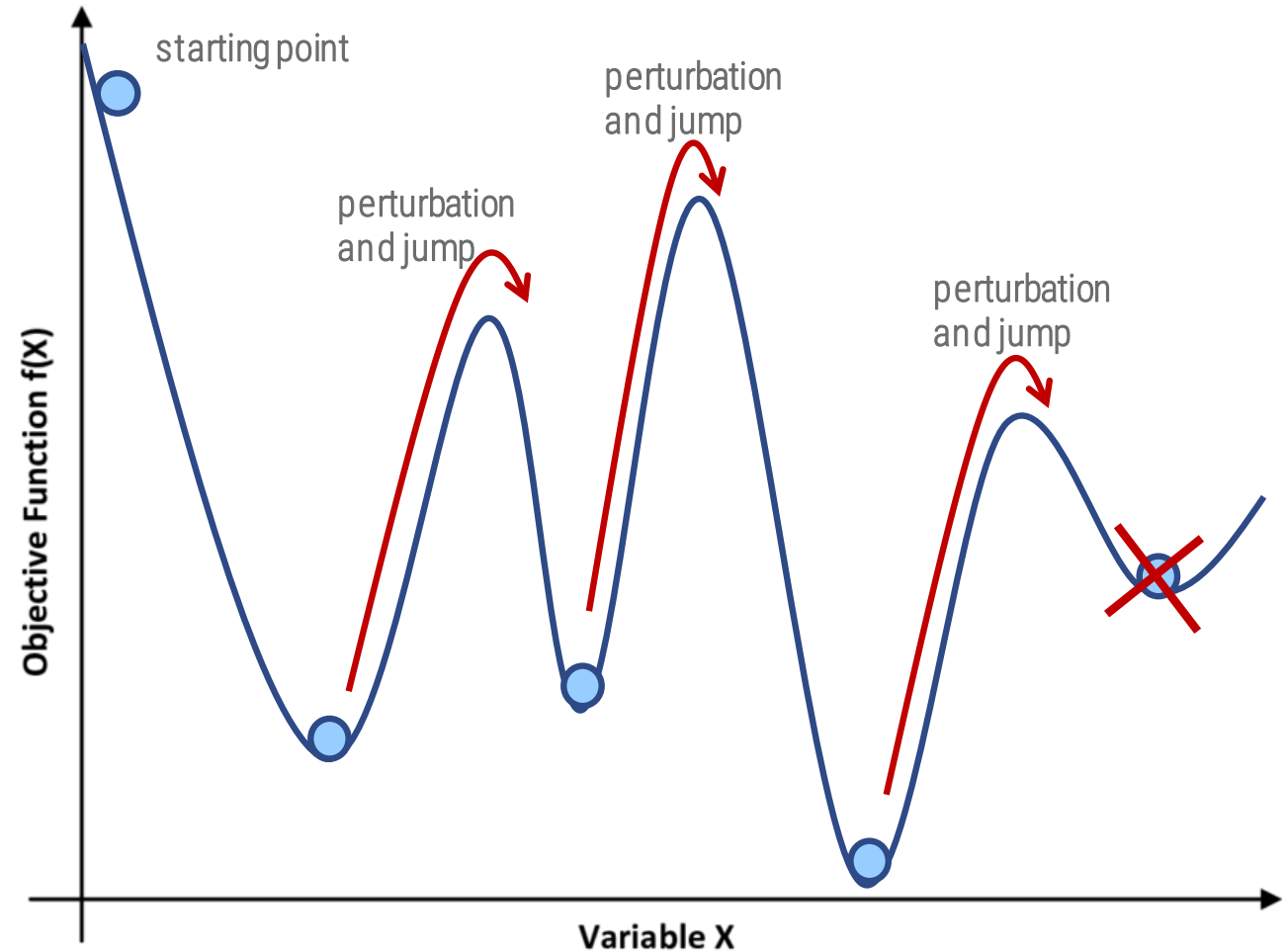
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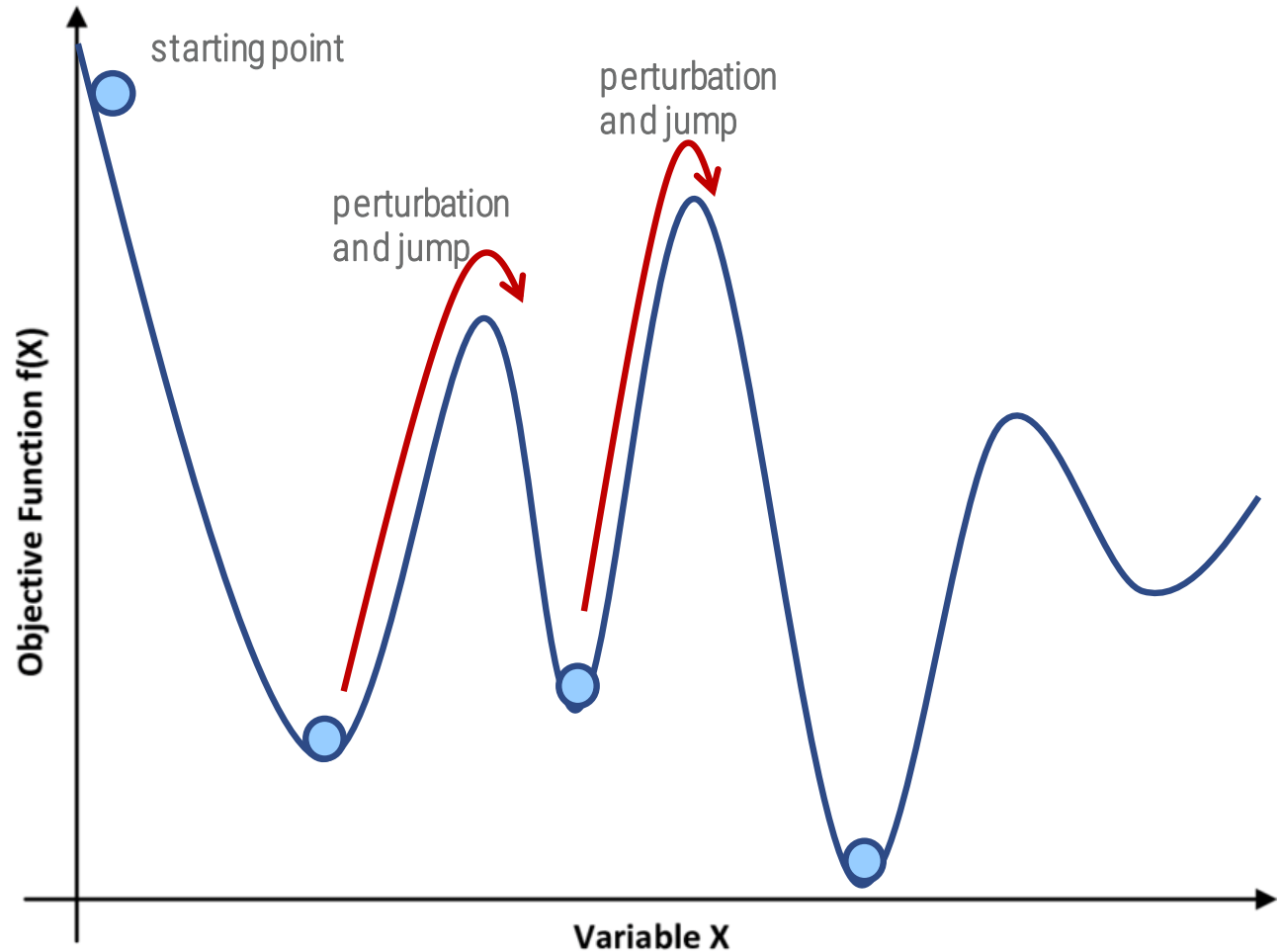
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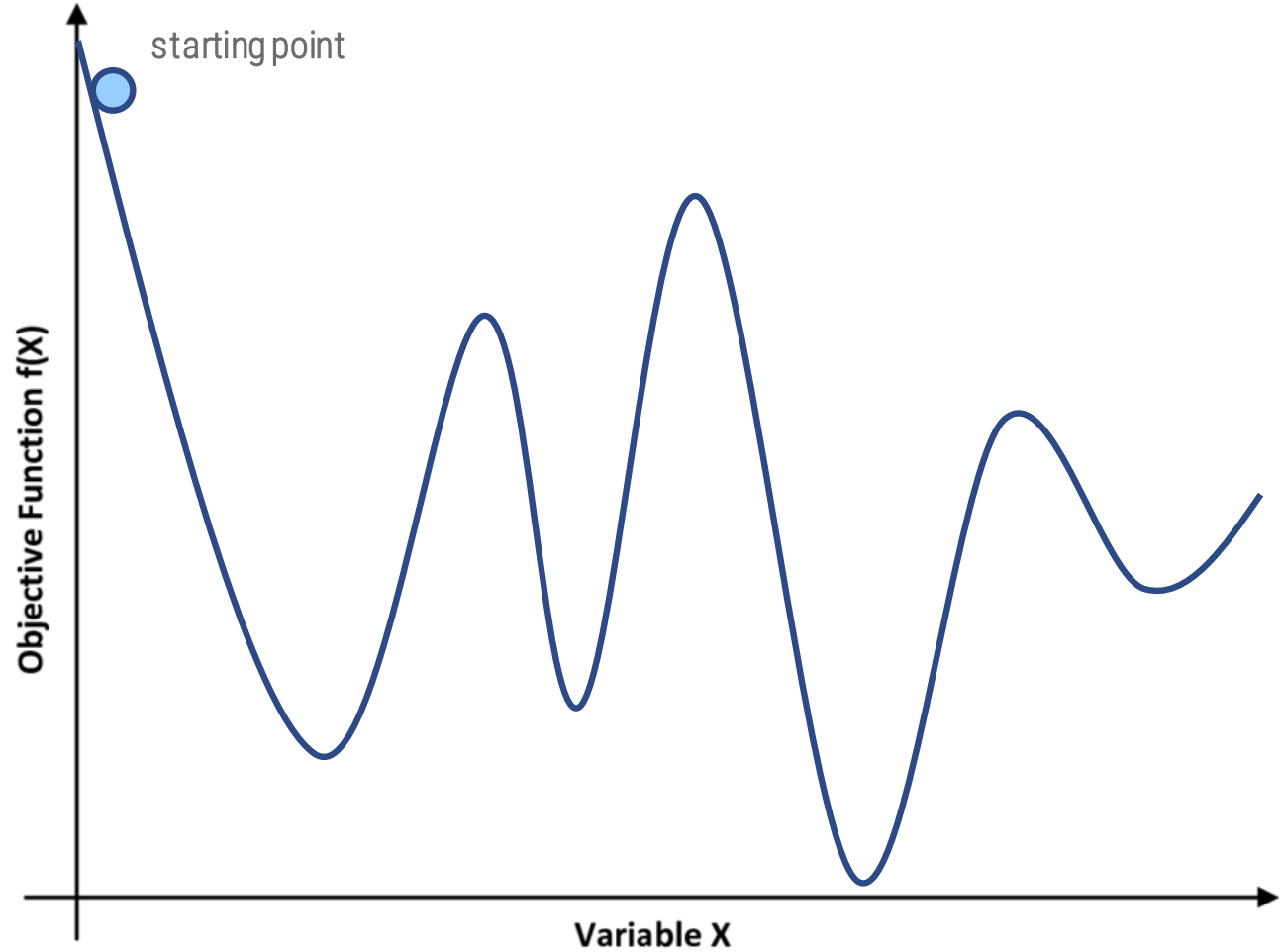
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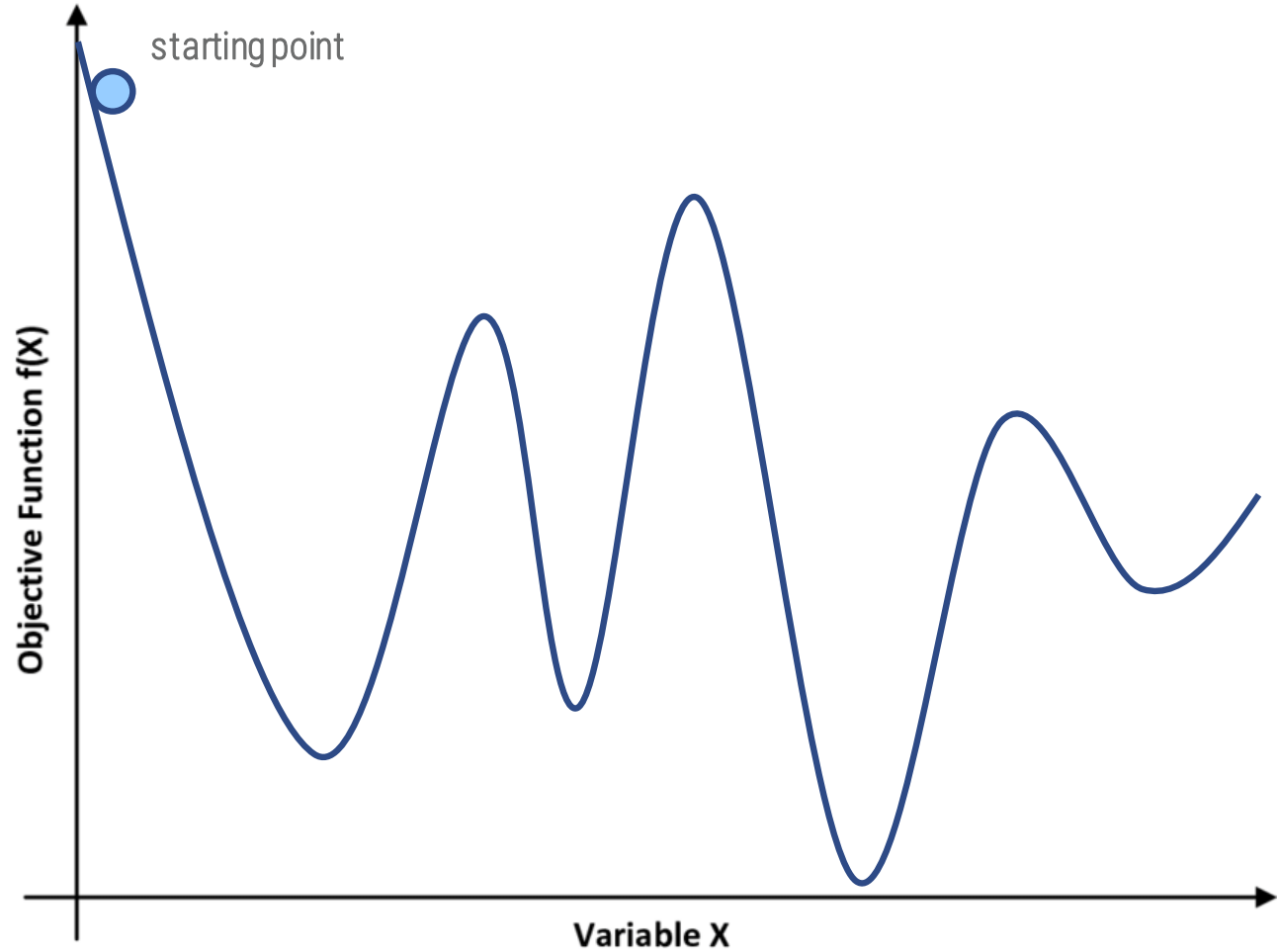
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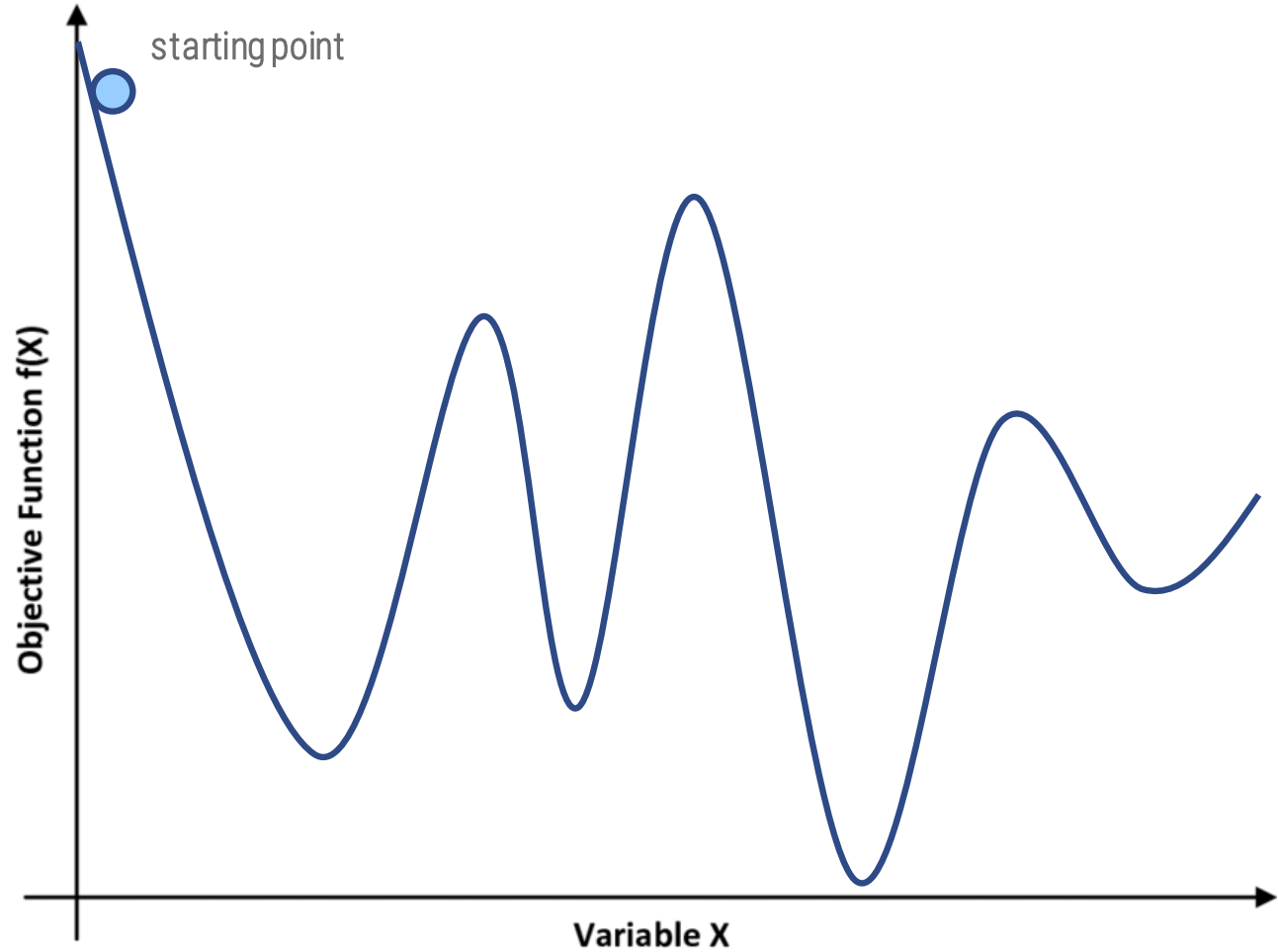
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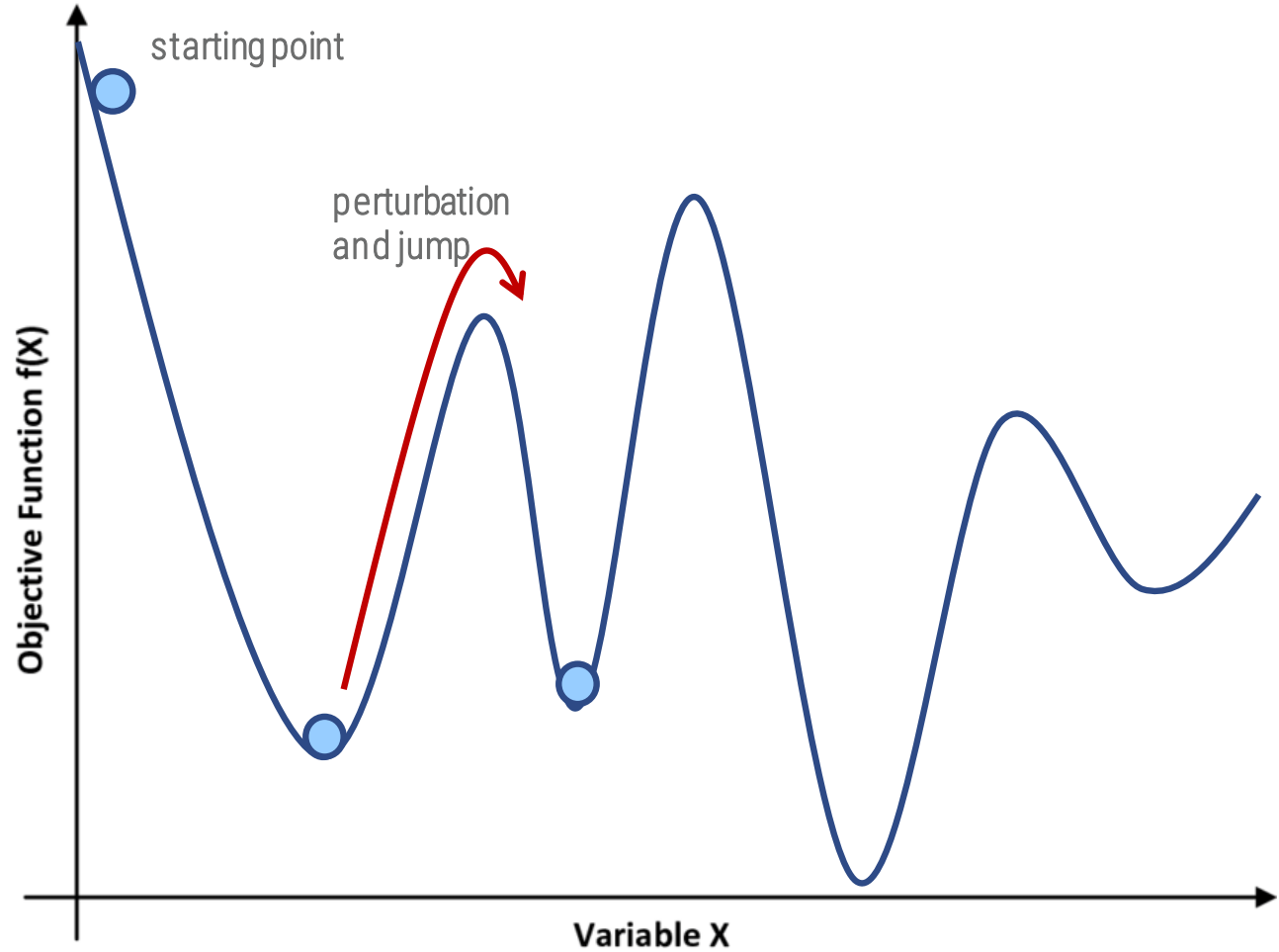
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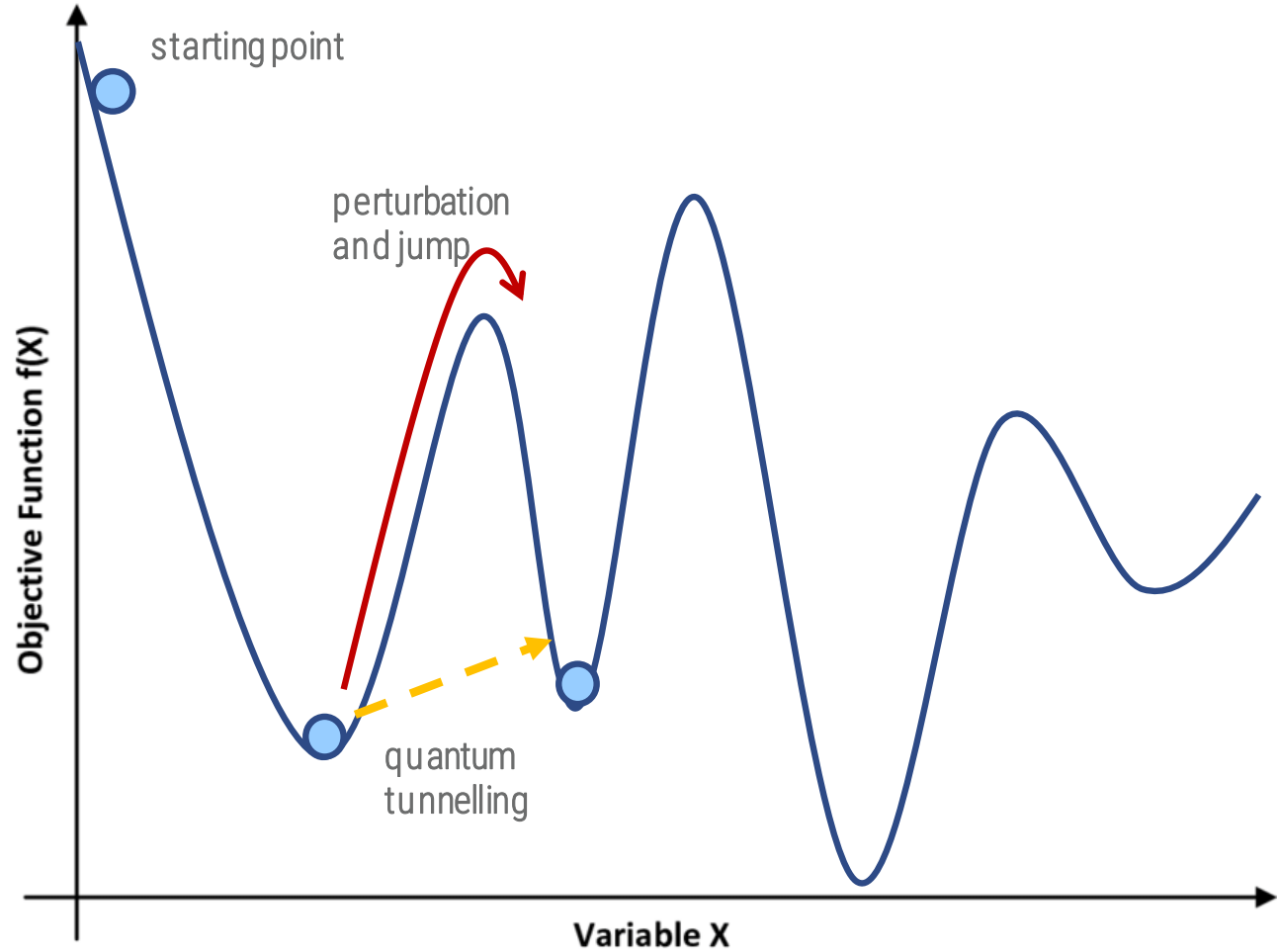
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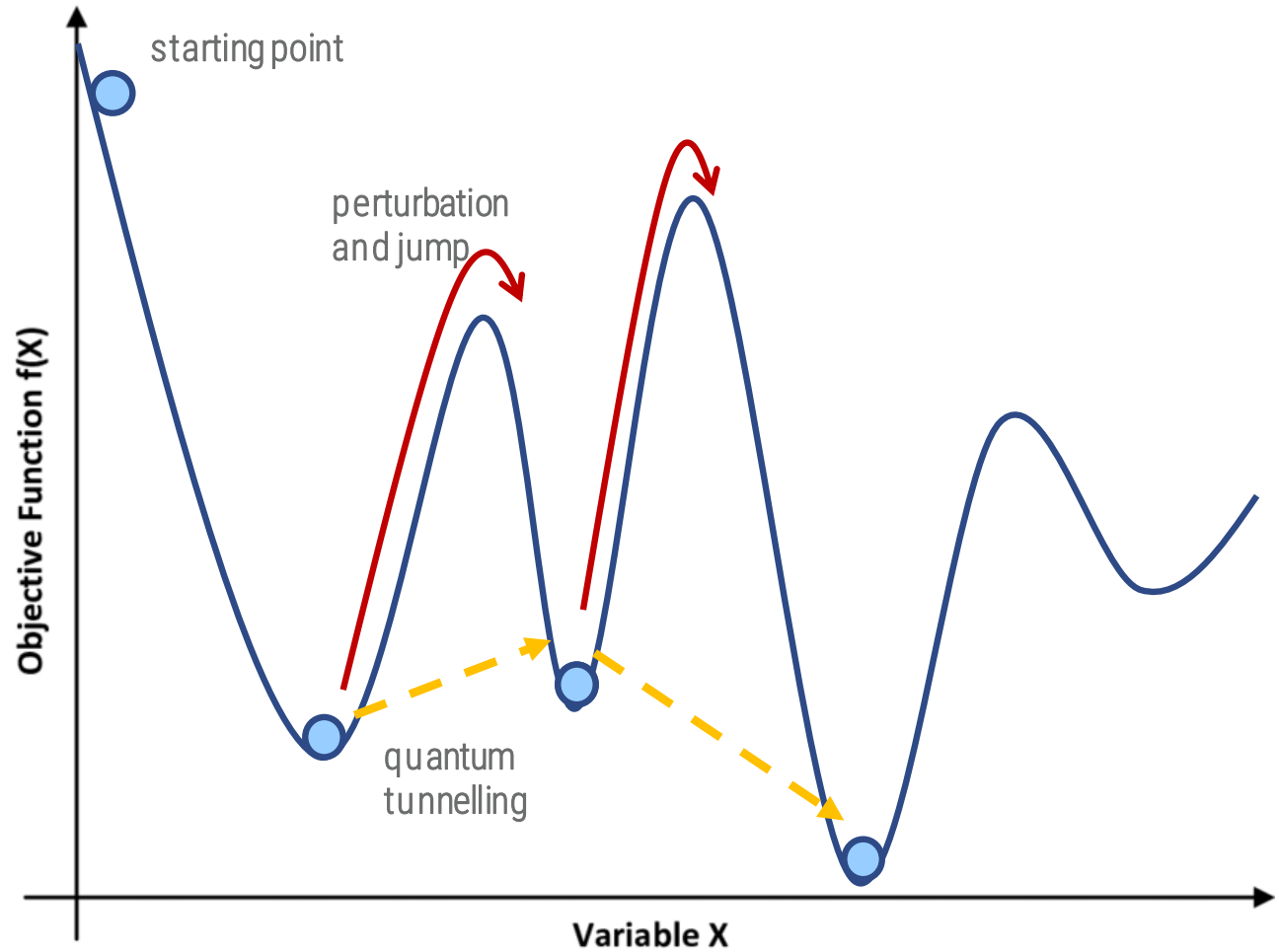
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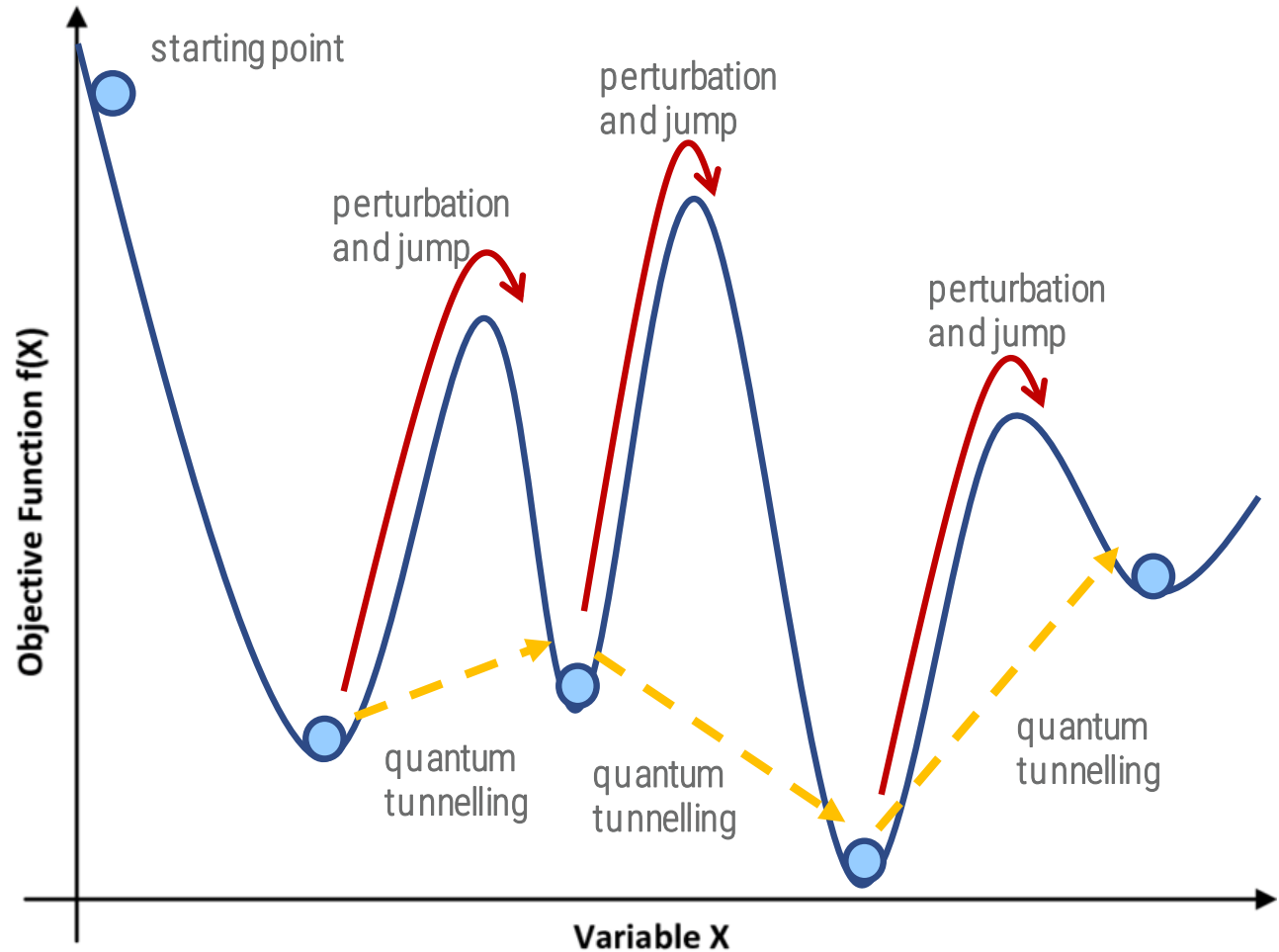
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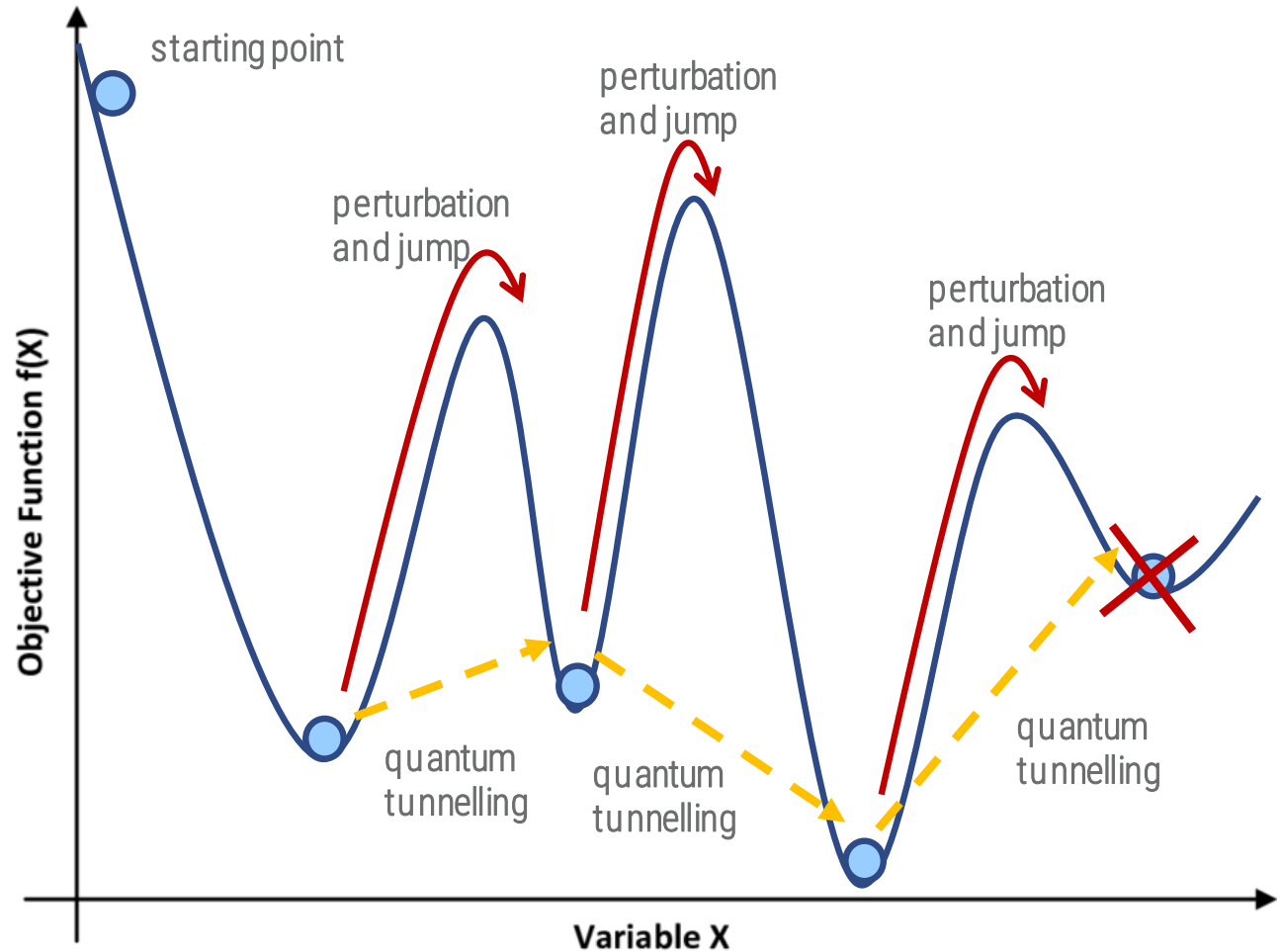
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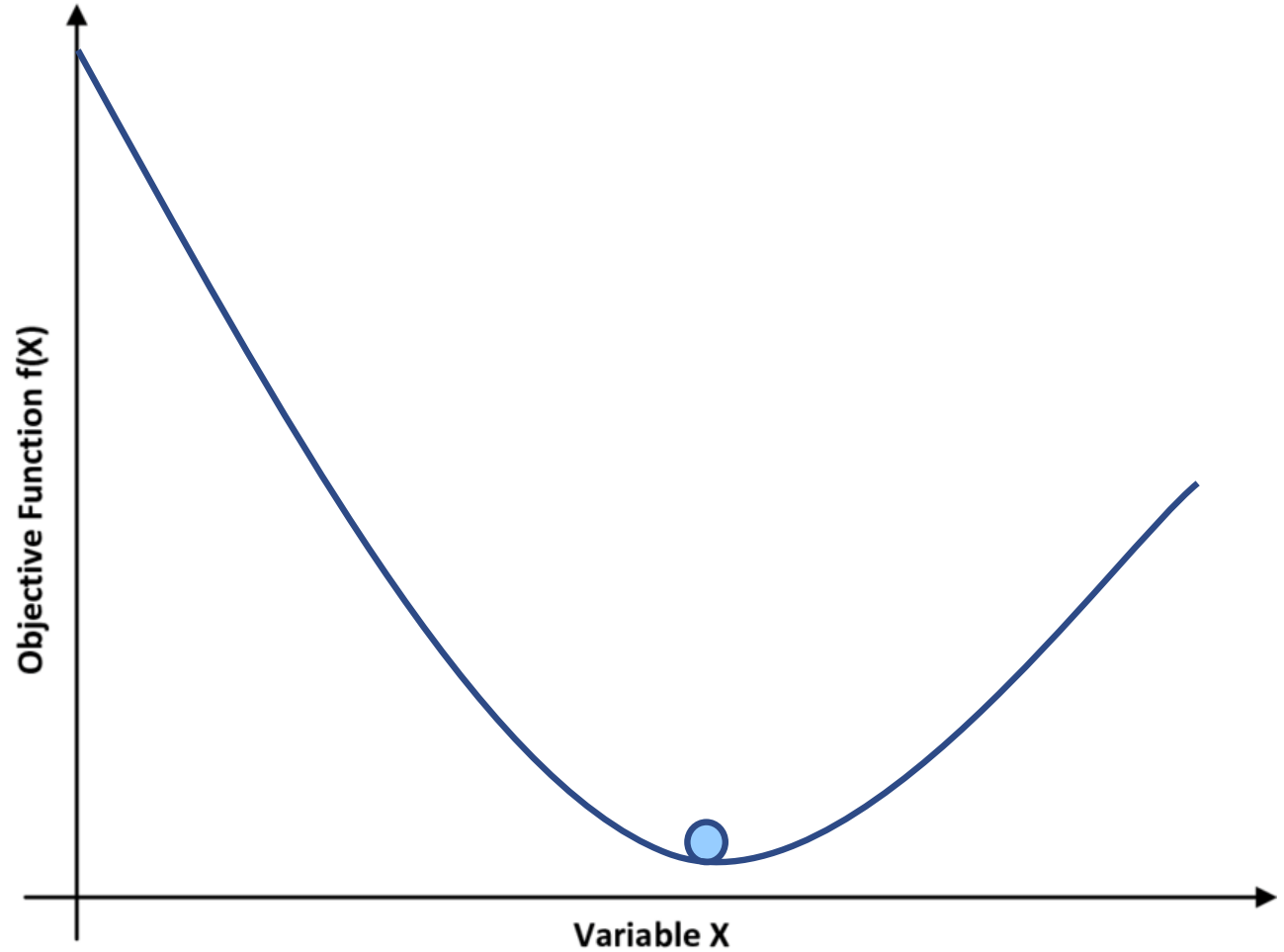
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A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum



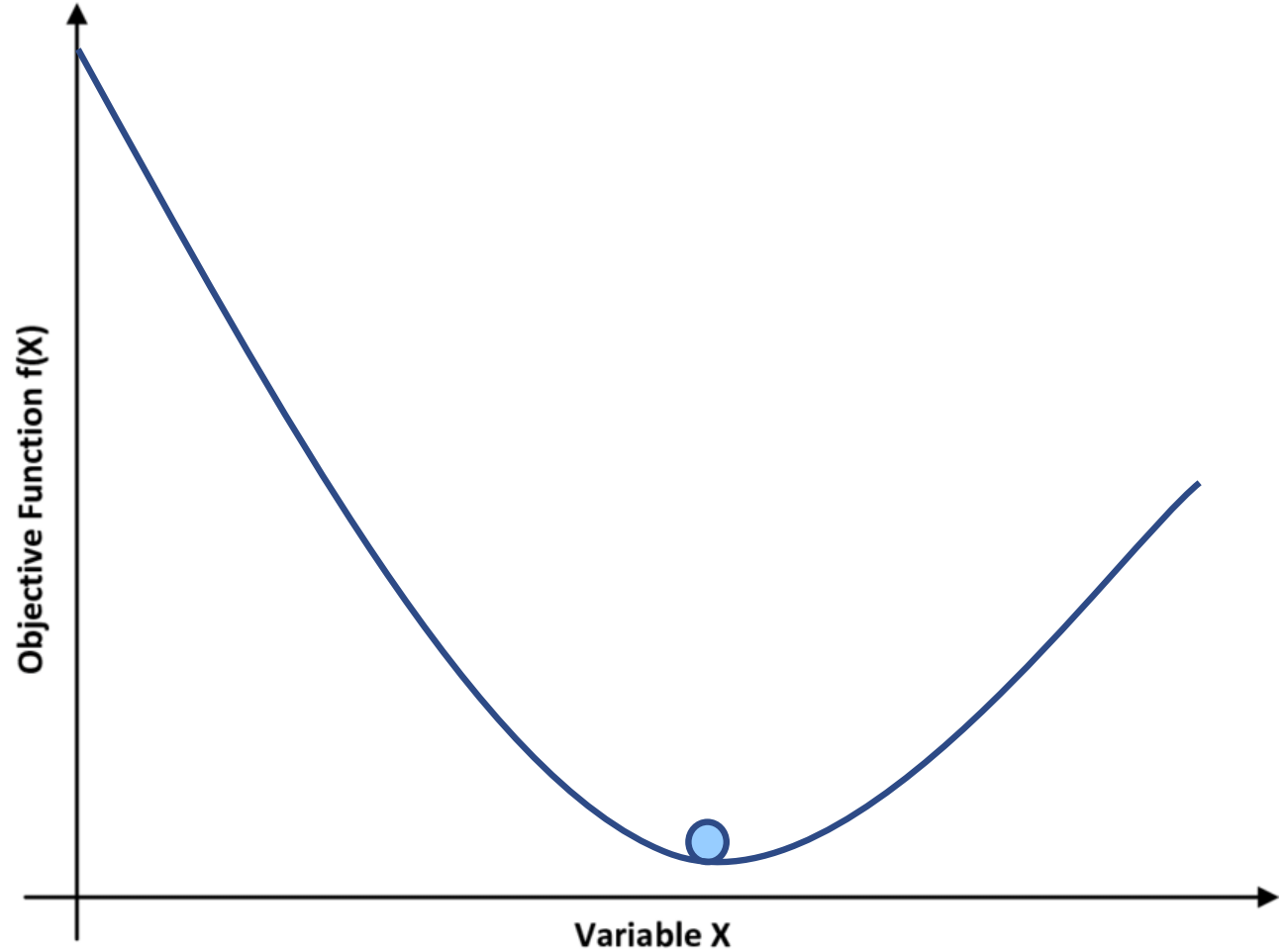
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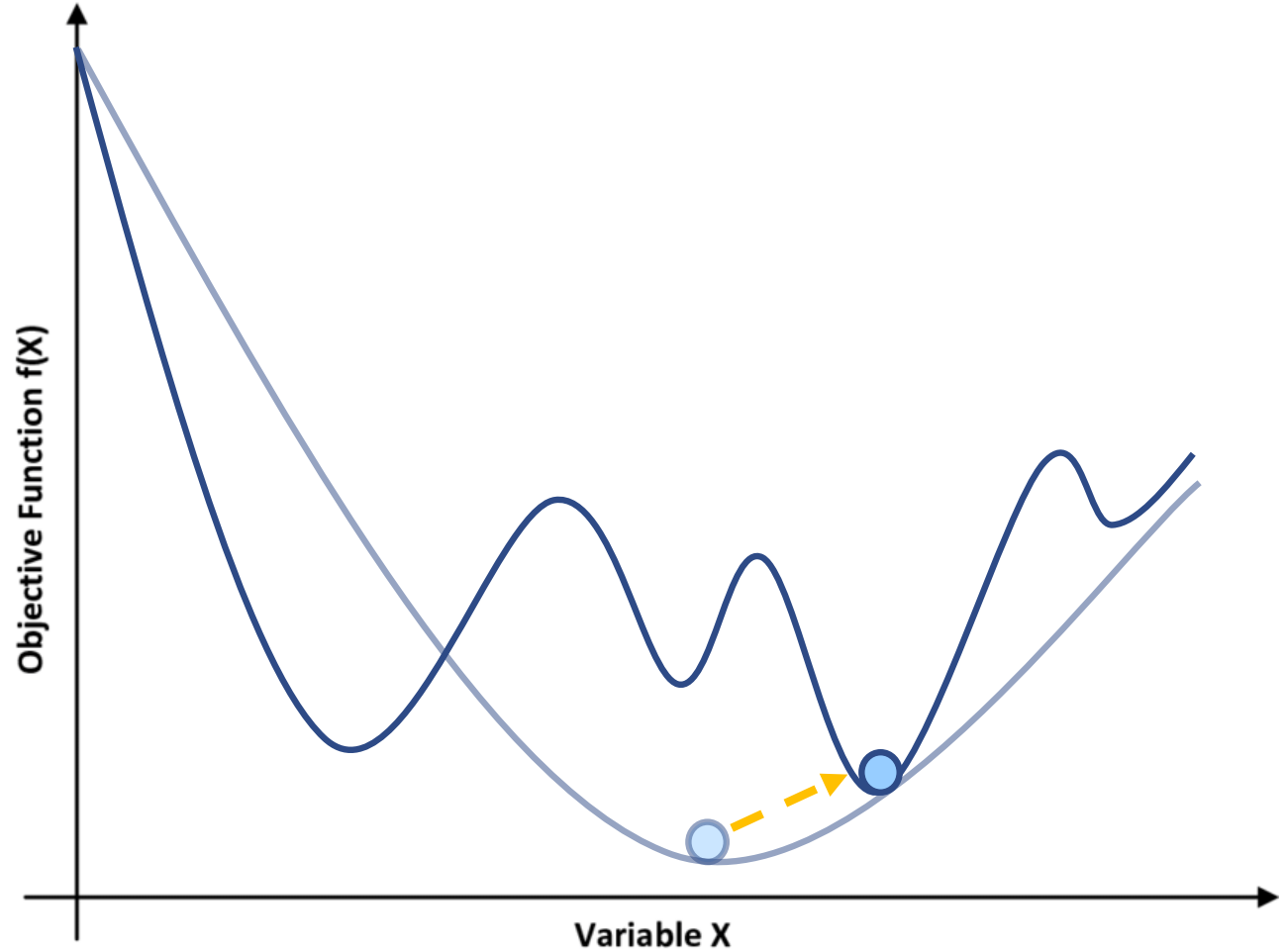
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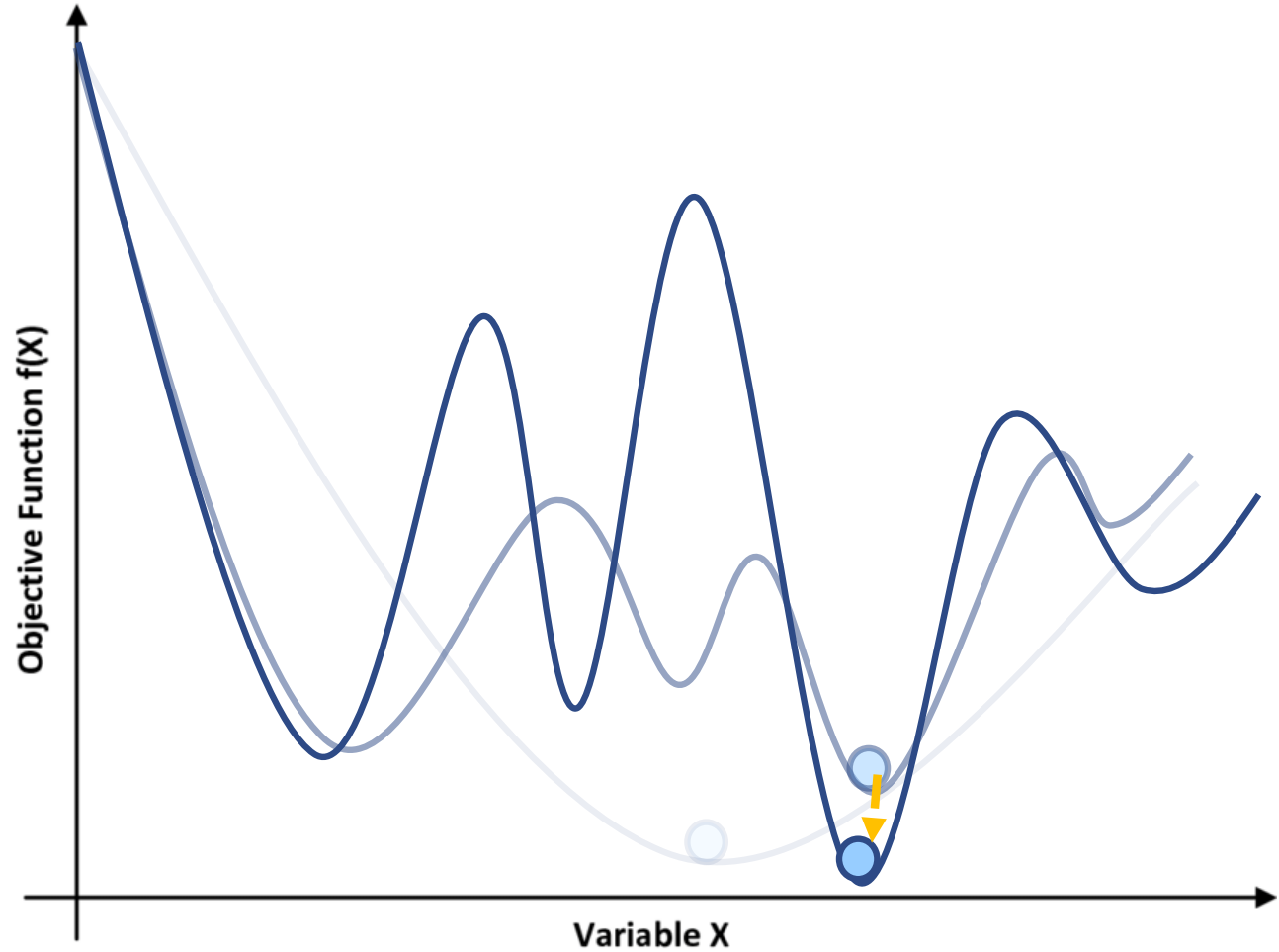
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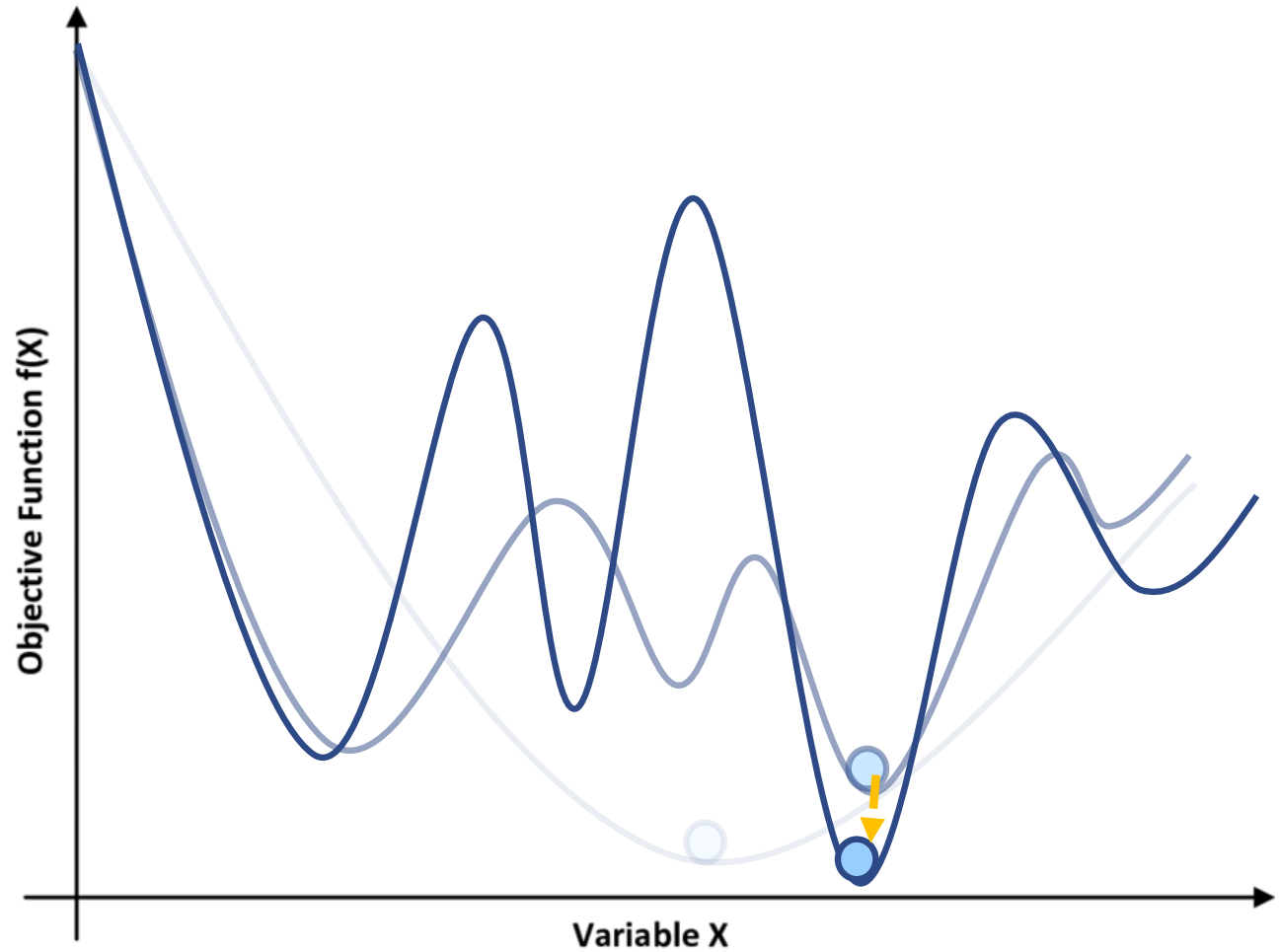
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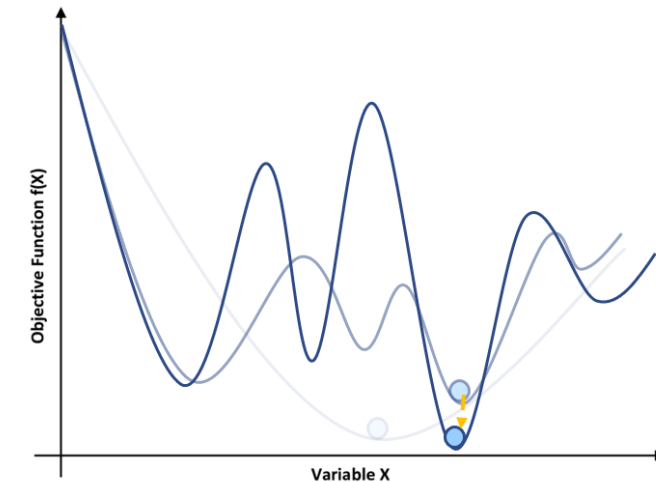
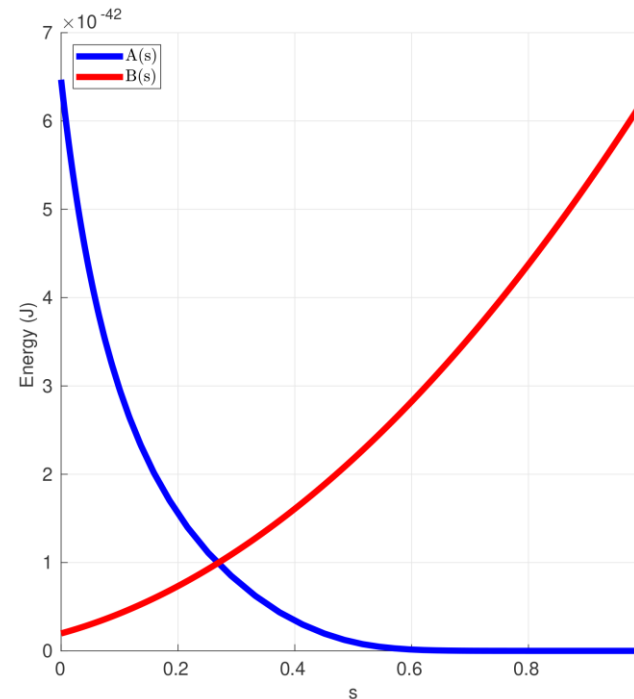
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$$\underbrace{-\frac{A(s)}{2} \left(\sum_i \hat{\sigma}_x^{(i)} \right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2} \left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \right)}_{\text{Final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



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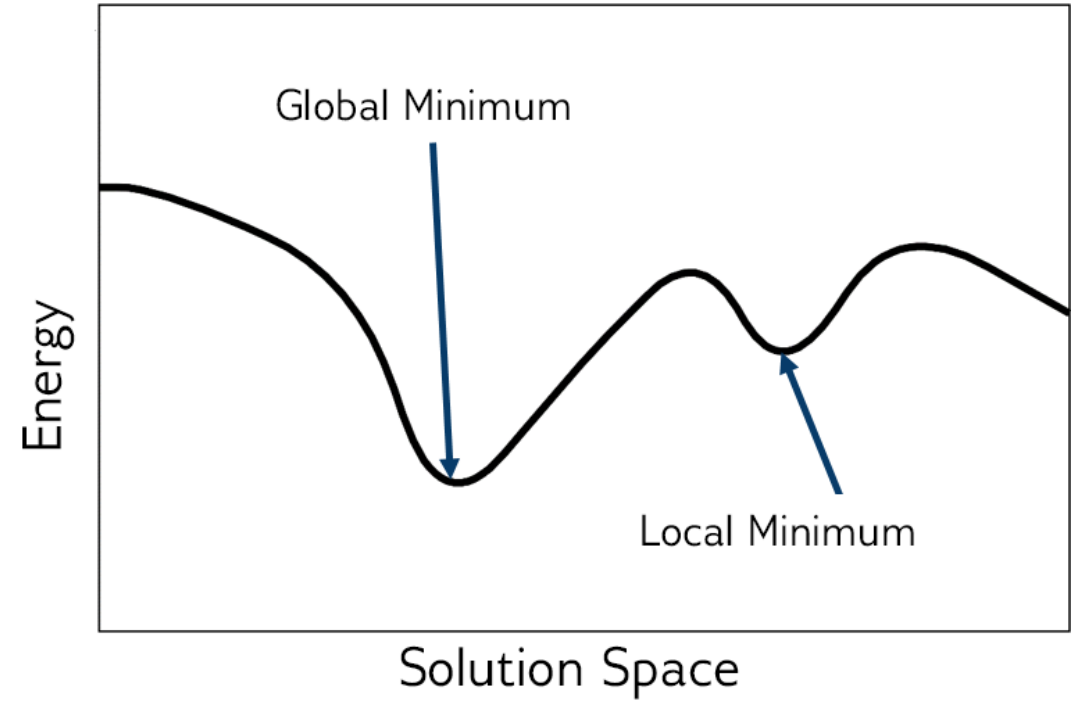
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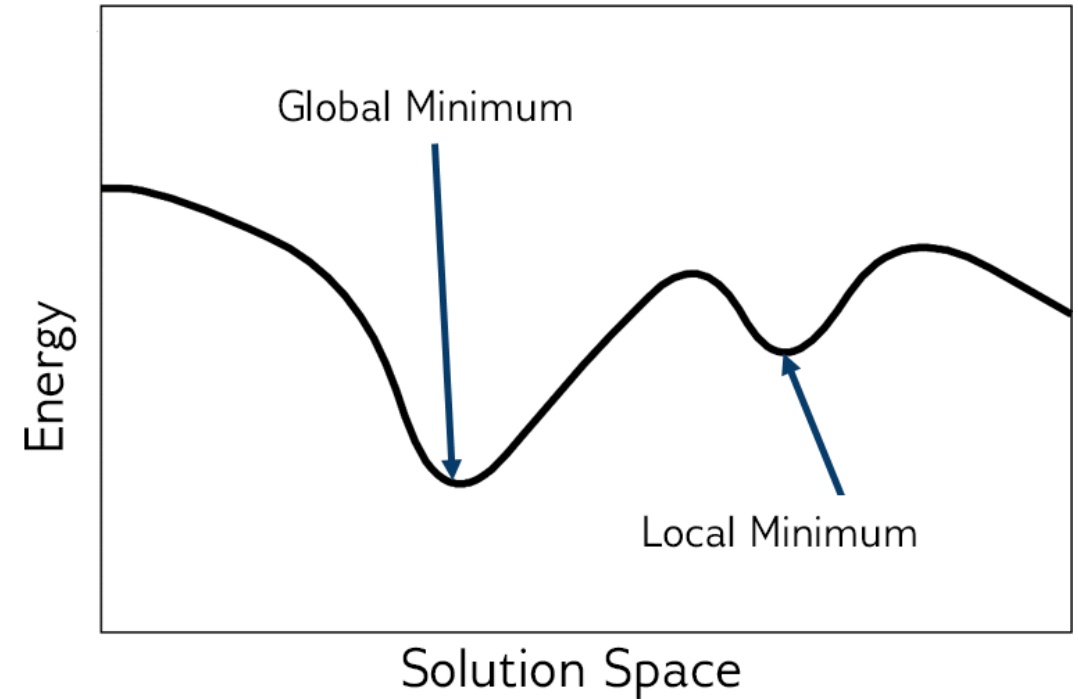
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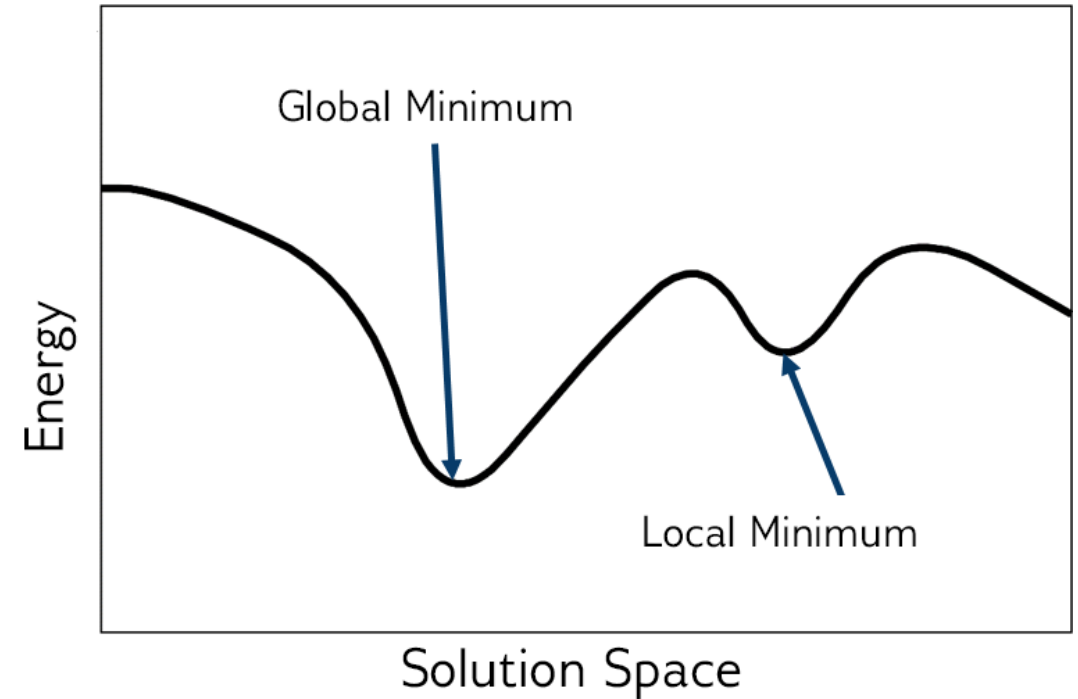
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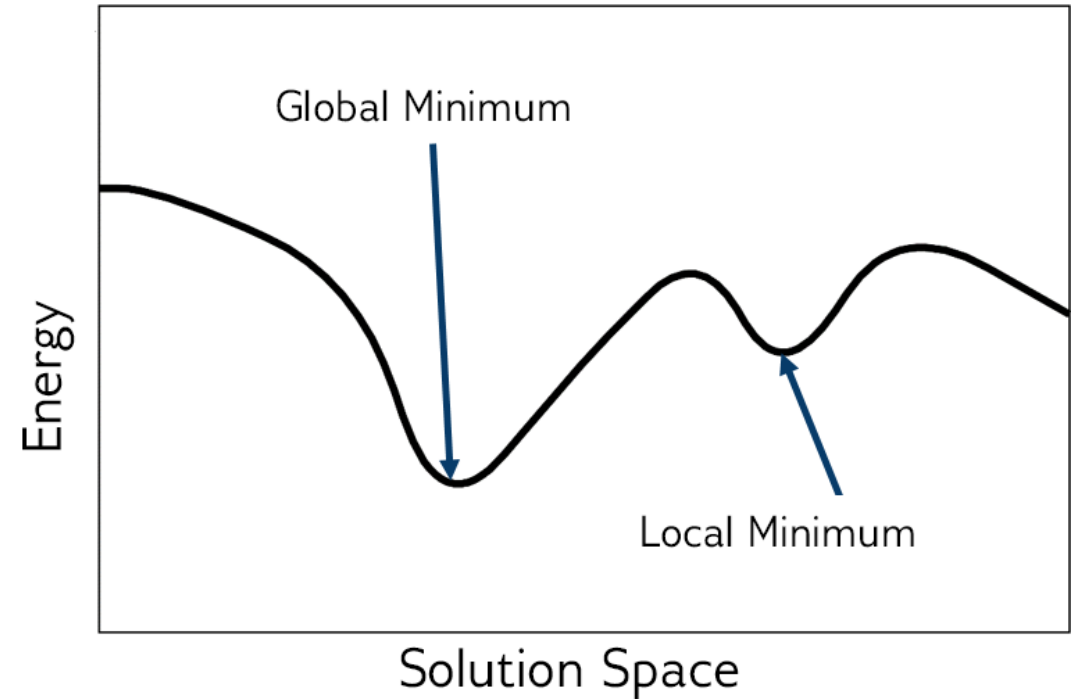
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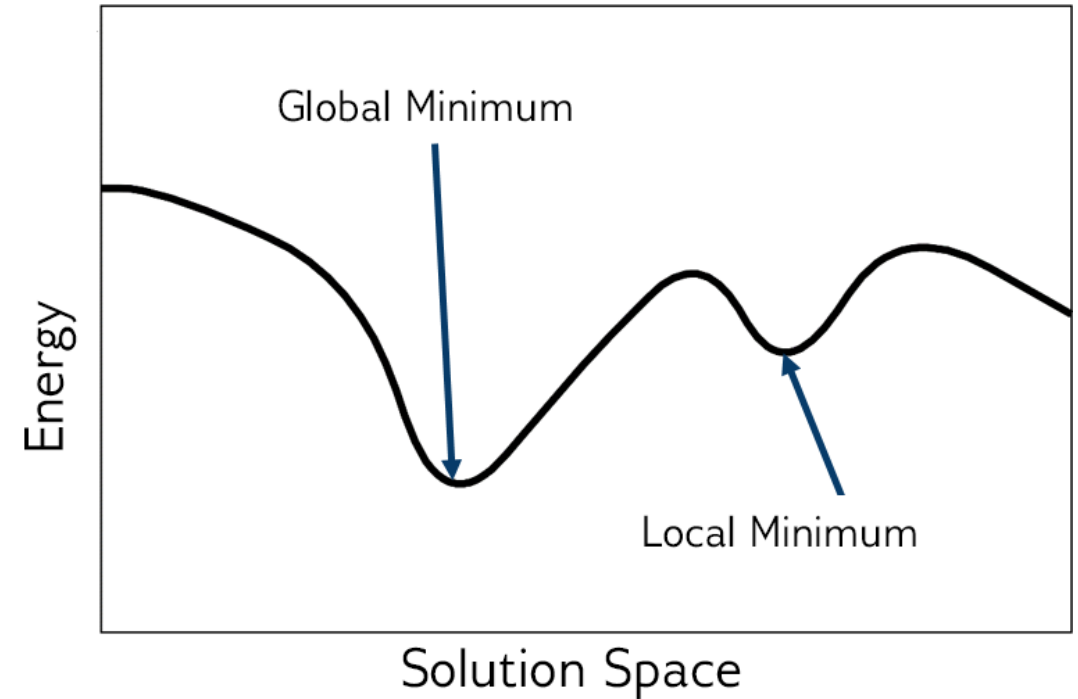
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- For most problems, the lower the energy of the objective function, the better the solution. Sometimes any state of local minimum for energy is an acceptable solution to the original problem; for other problems only optimal solutions are acceptable.



Objective Function

- Expressing a problem through a minimizable objective function means **thinking of every problem as a minimization problem**

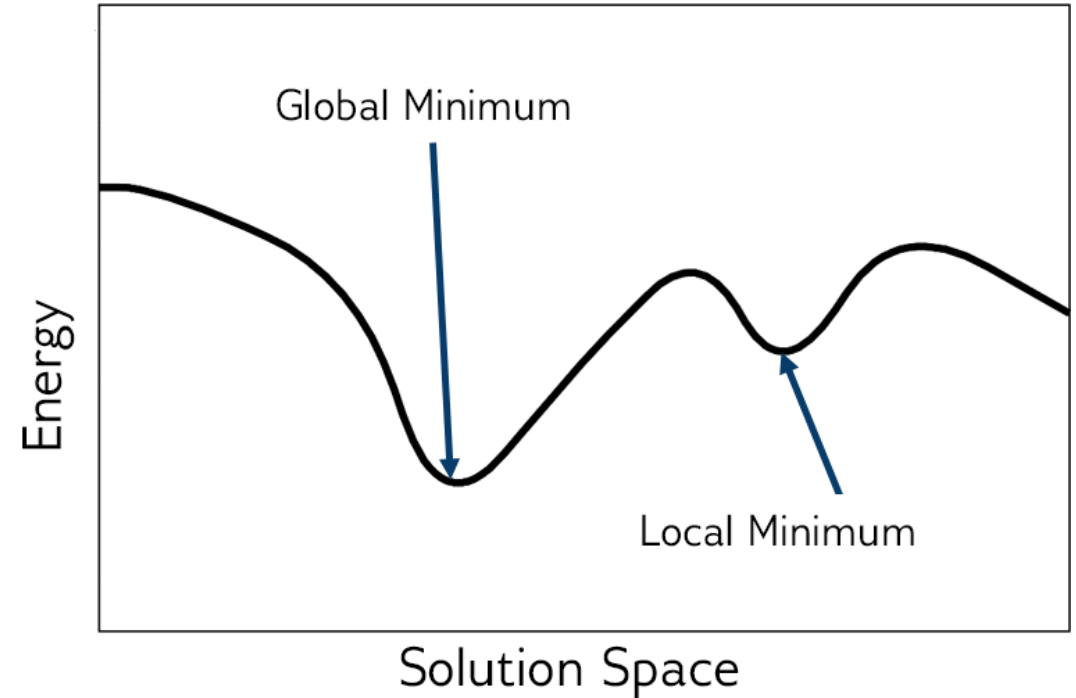


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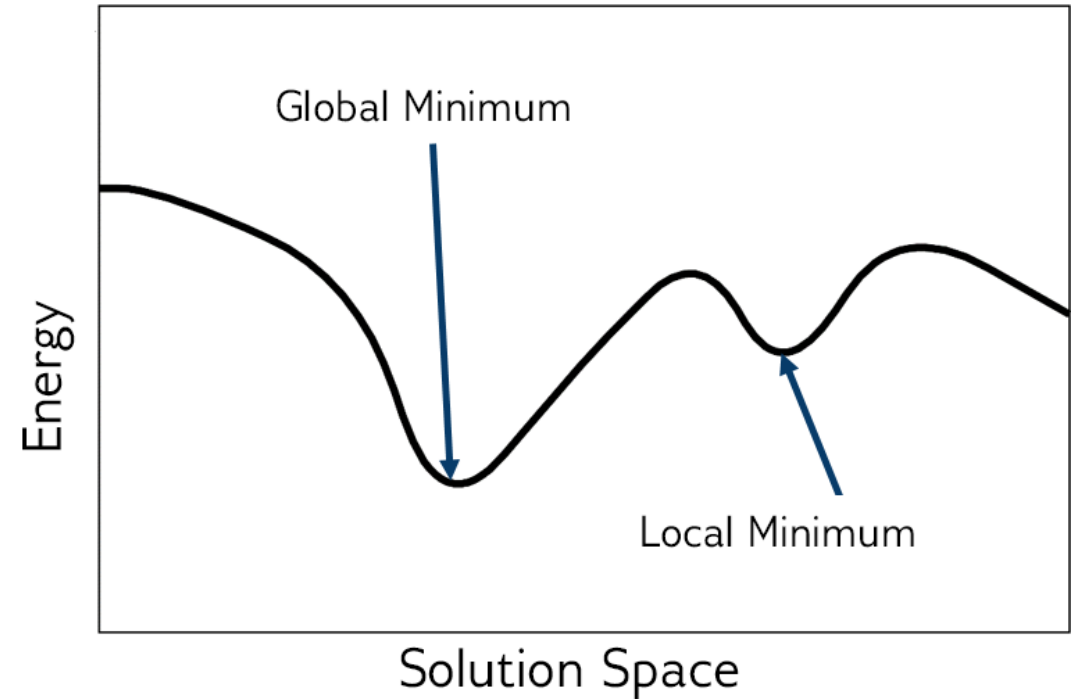


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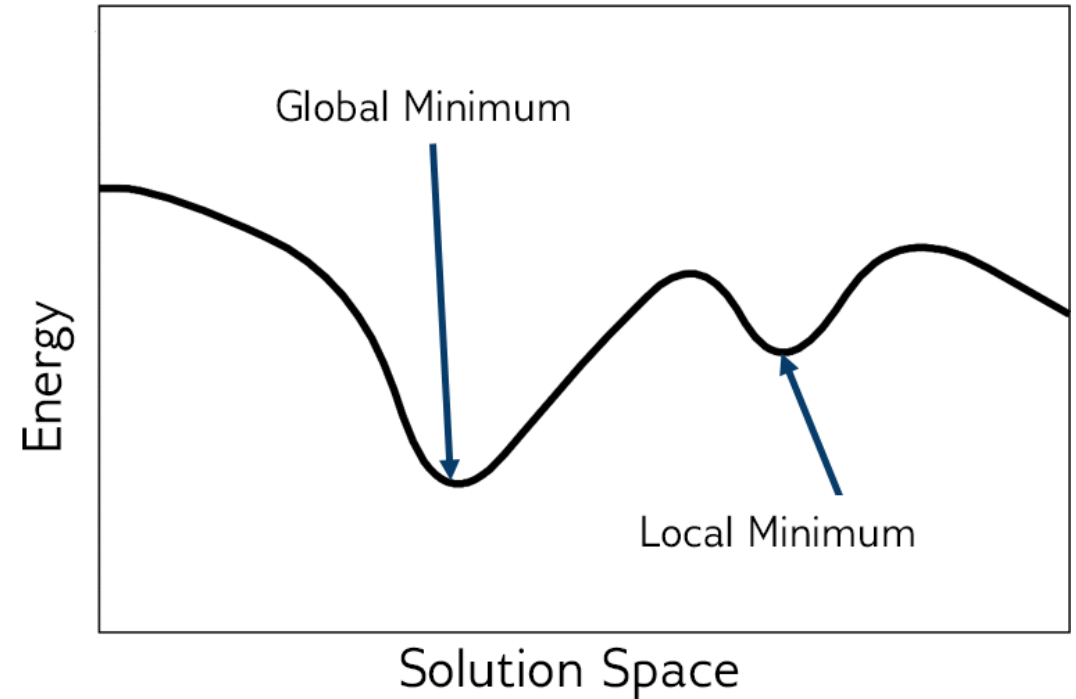


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- The objective functions accepted by the quantum annealer of D-Wave are of two types (equivalent to each other): **Ising Hamiltonians and QUBO formulations**



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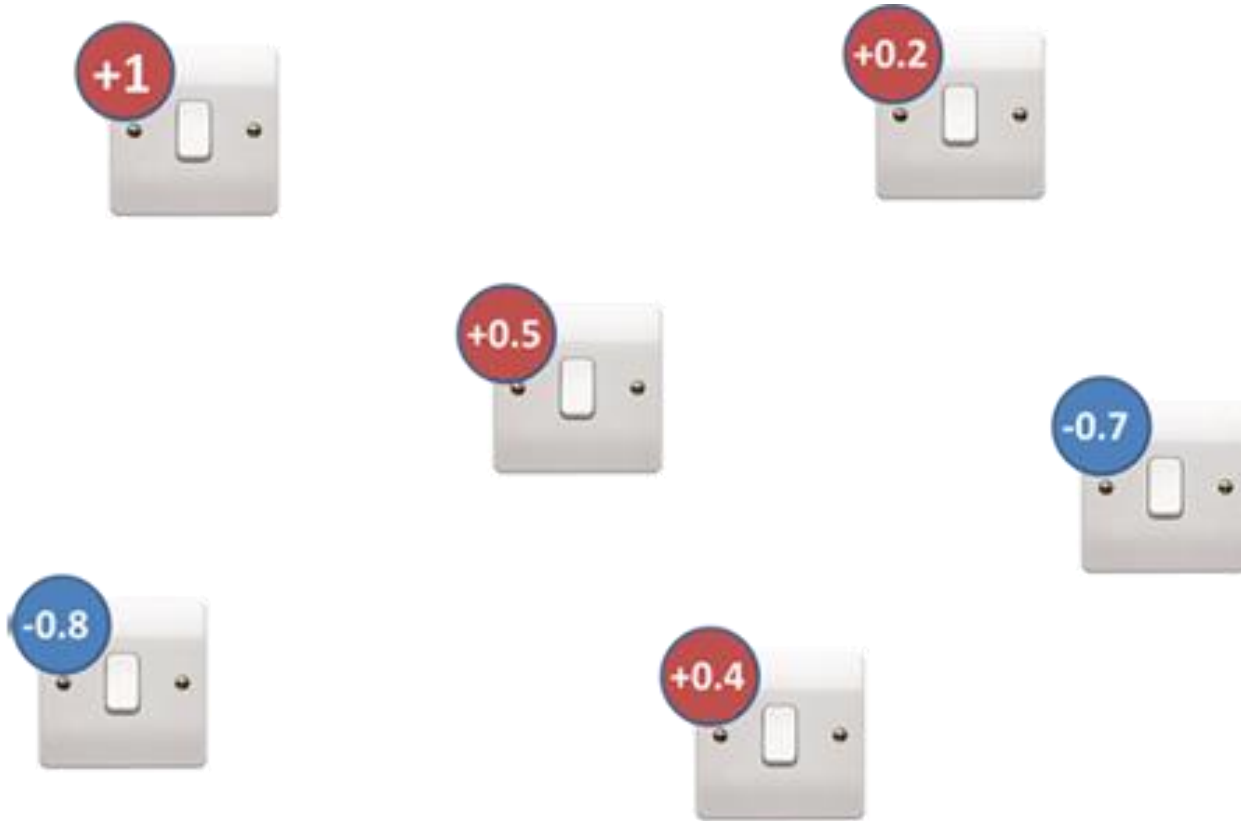
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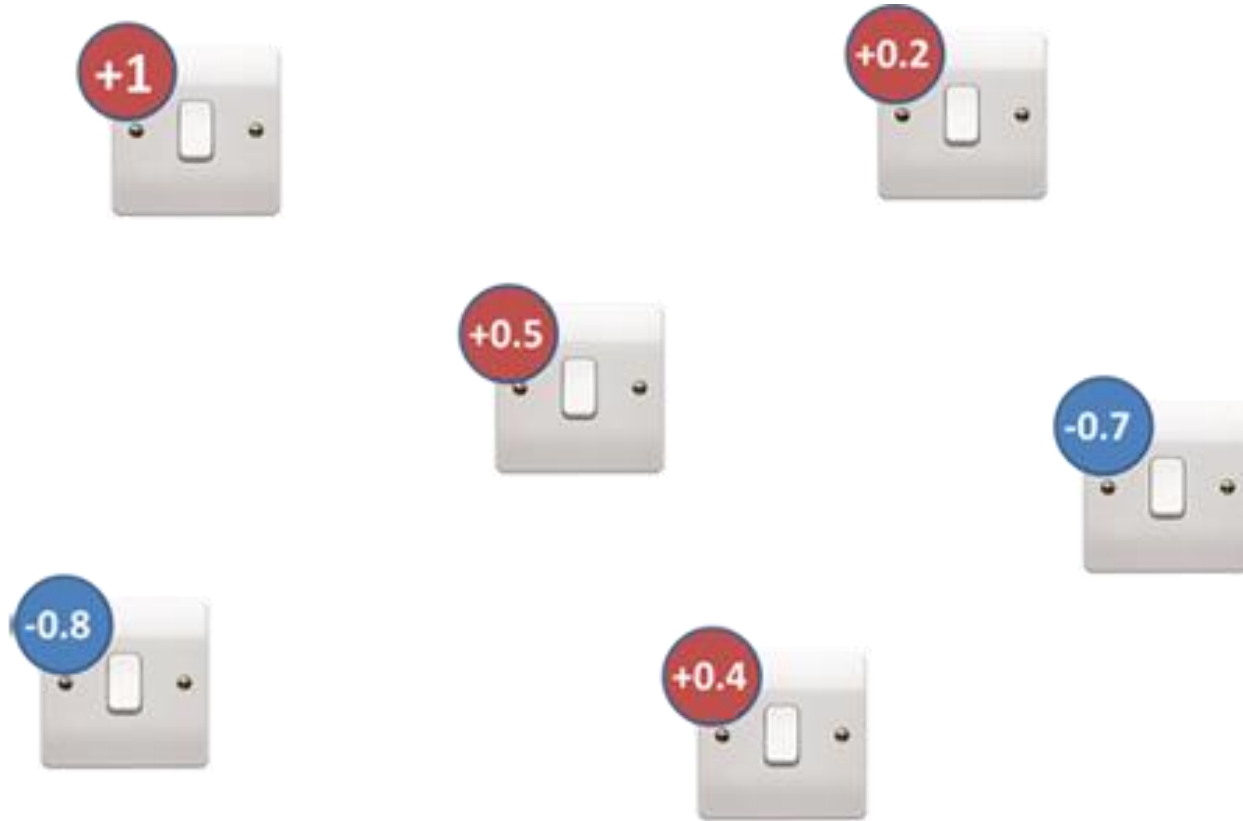
- Where the coefficients h represent the bias values associated with the qubits and the coefficients J represent the strength of the coupling bonds

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.

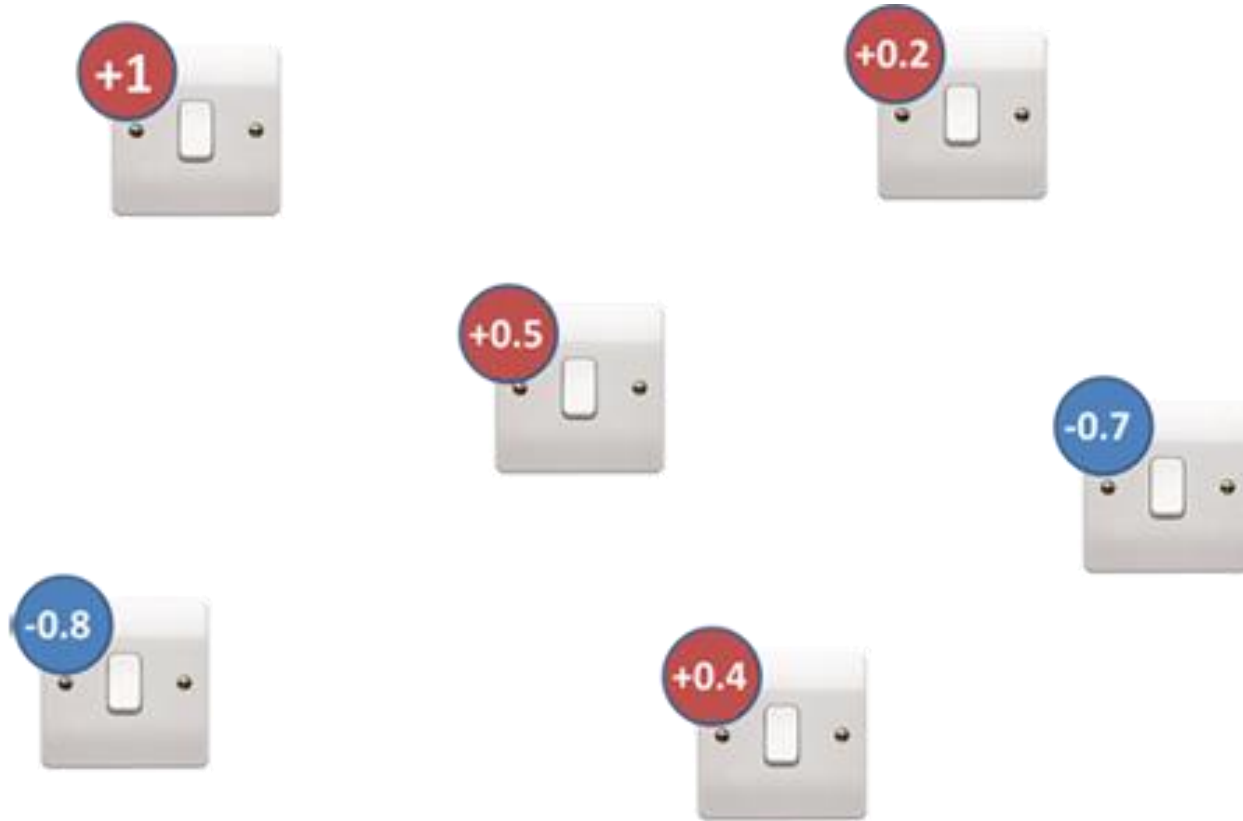


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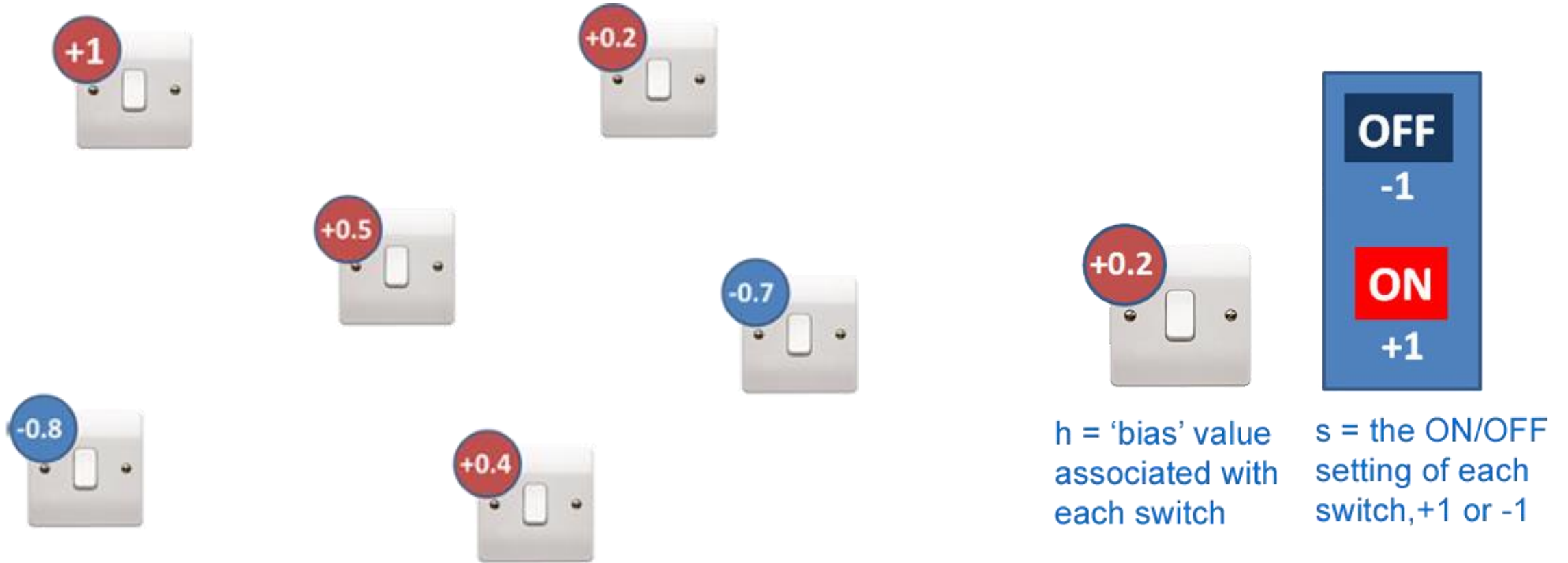
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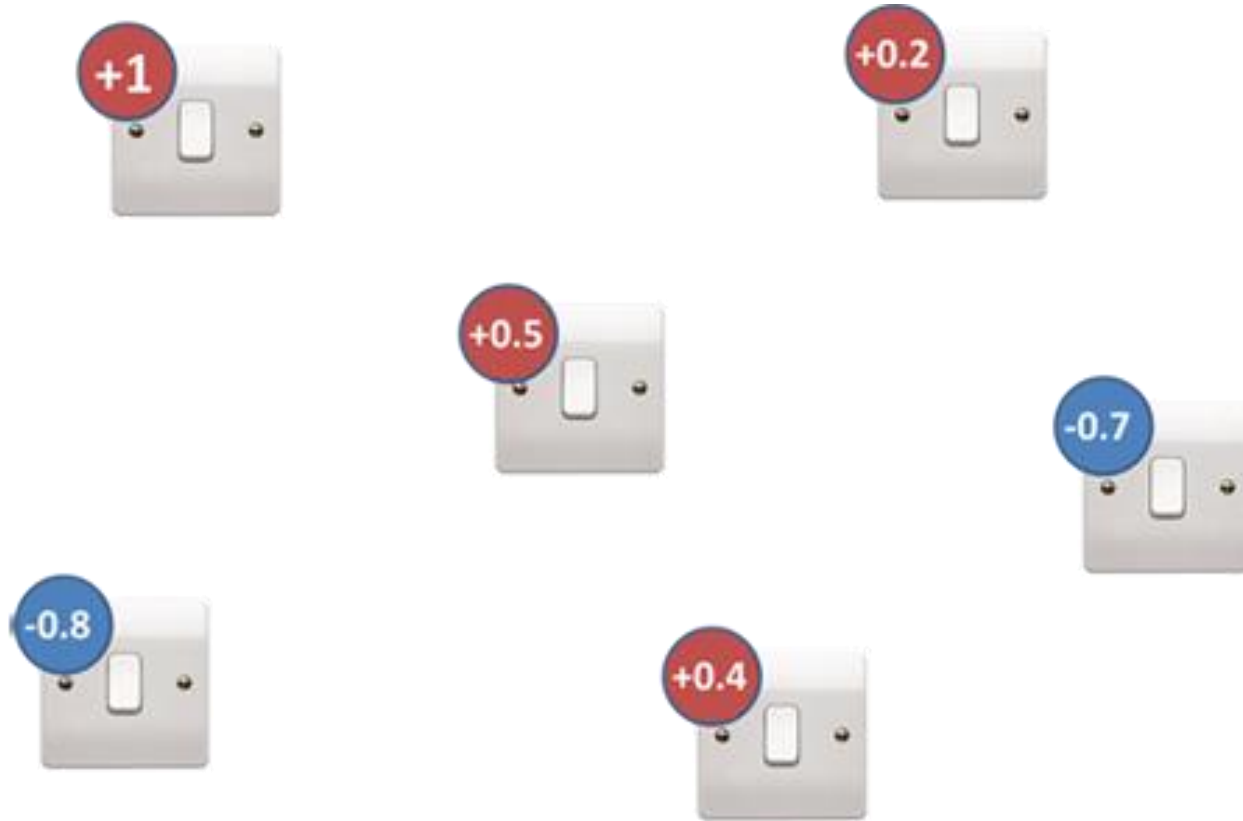


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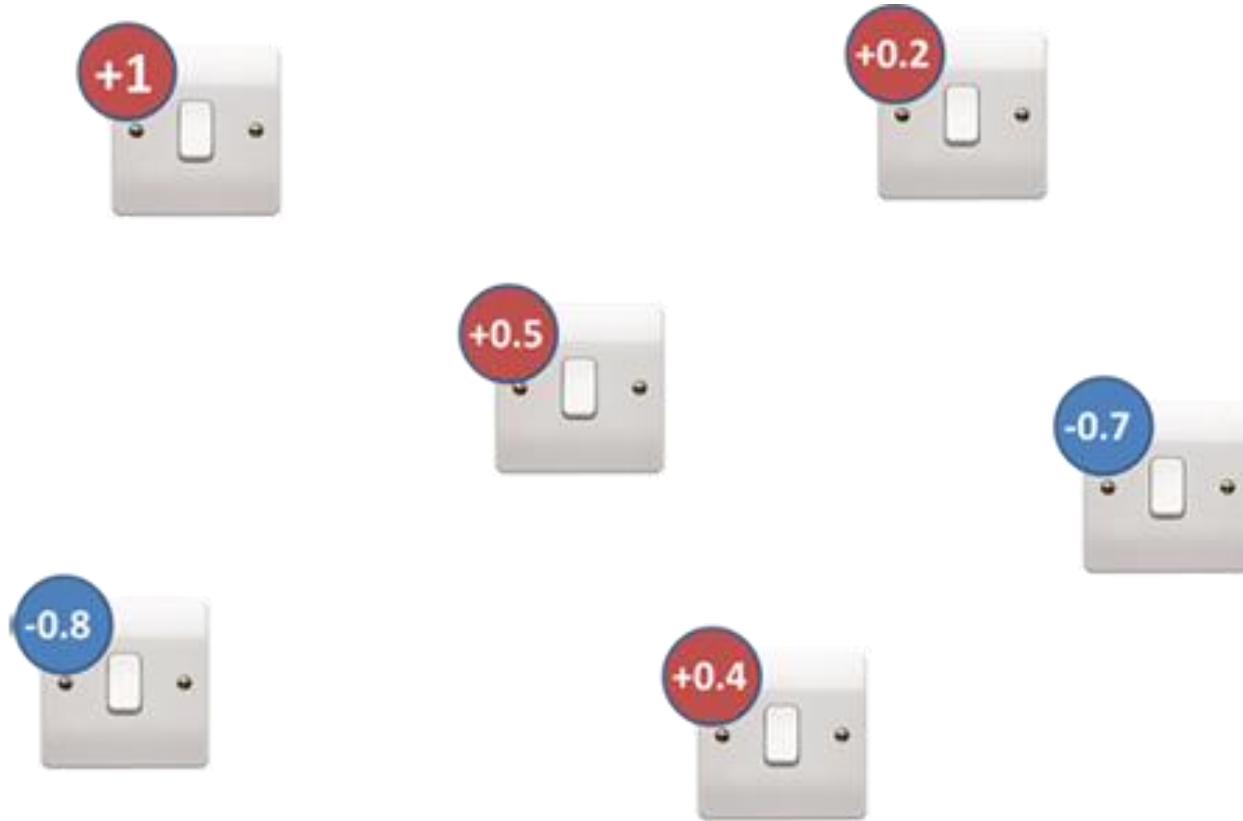


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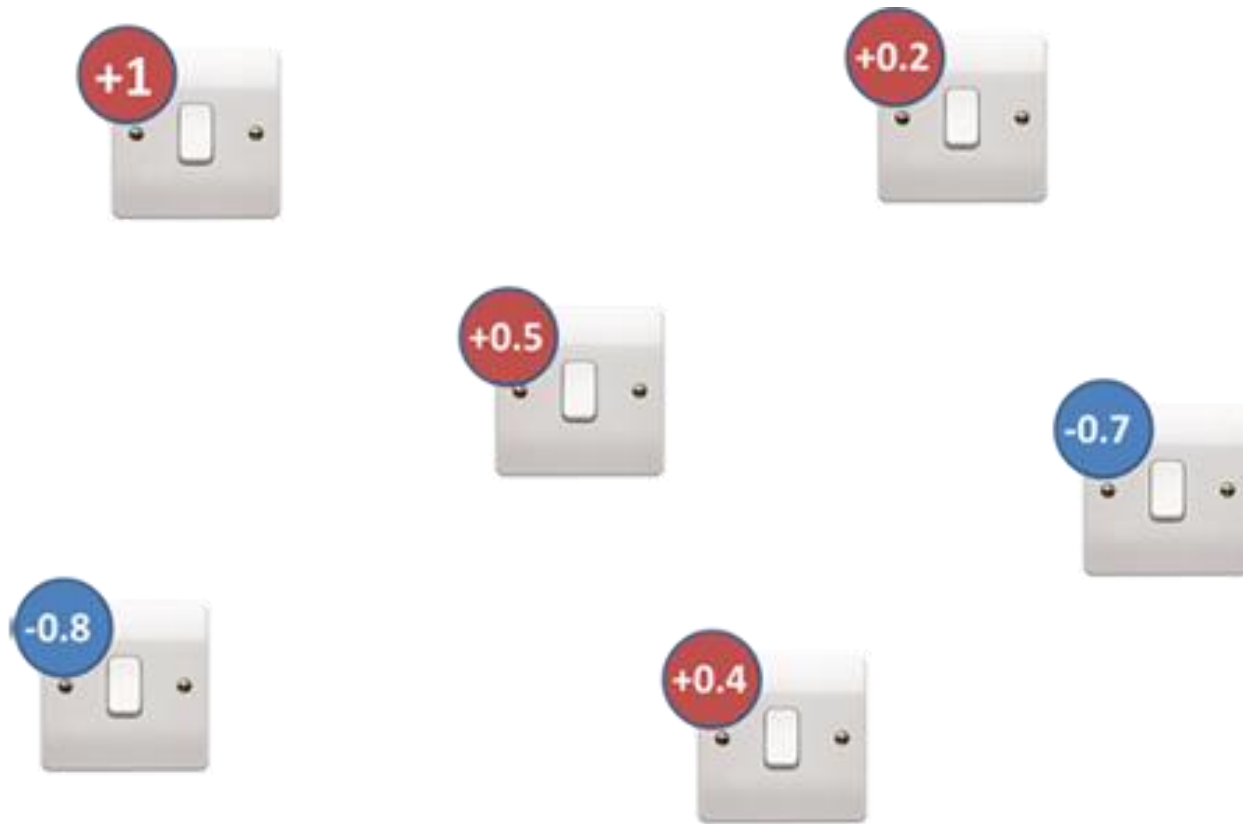
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- The value of a switch is calculated by multiplying its weight by its state
- The game consists in finding the combination of states for the switches such that the sum of their values is as low as possible

Game of Switches



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

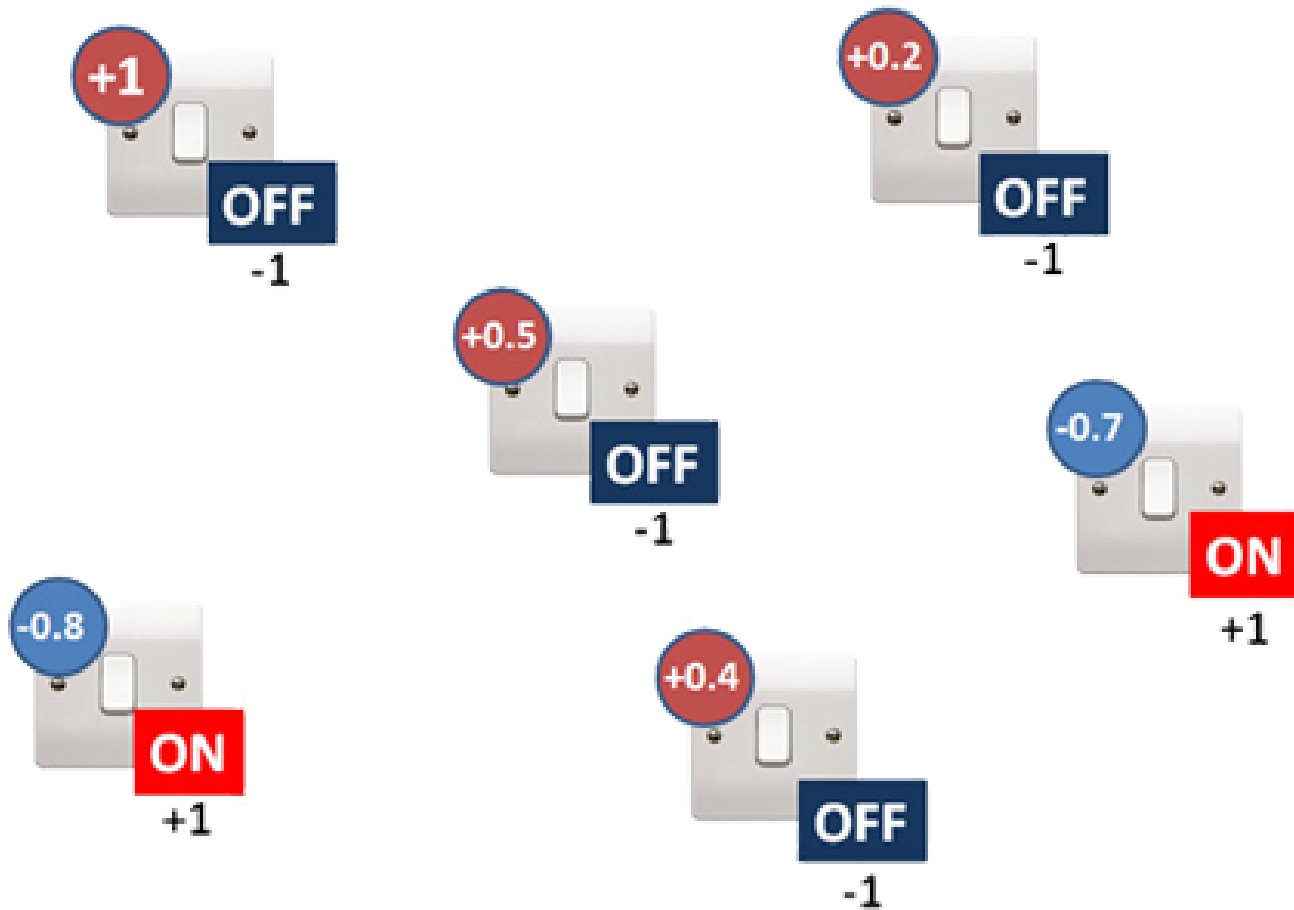


h = 'bias' value associated with each switch



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

Game of Switches

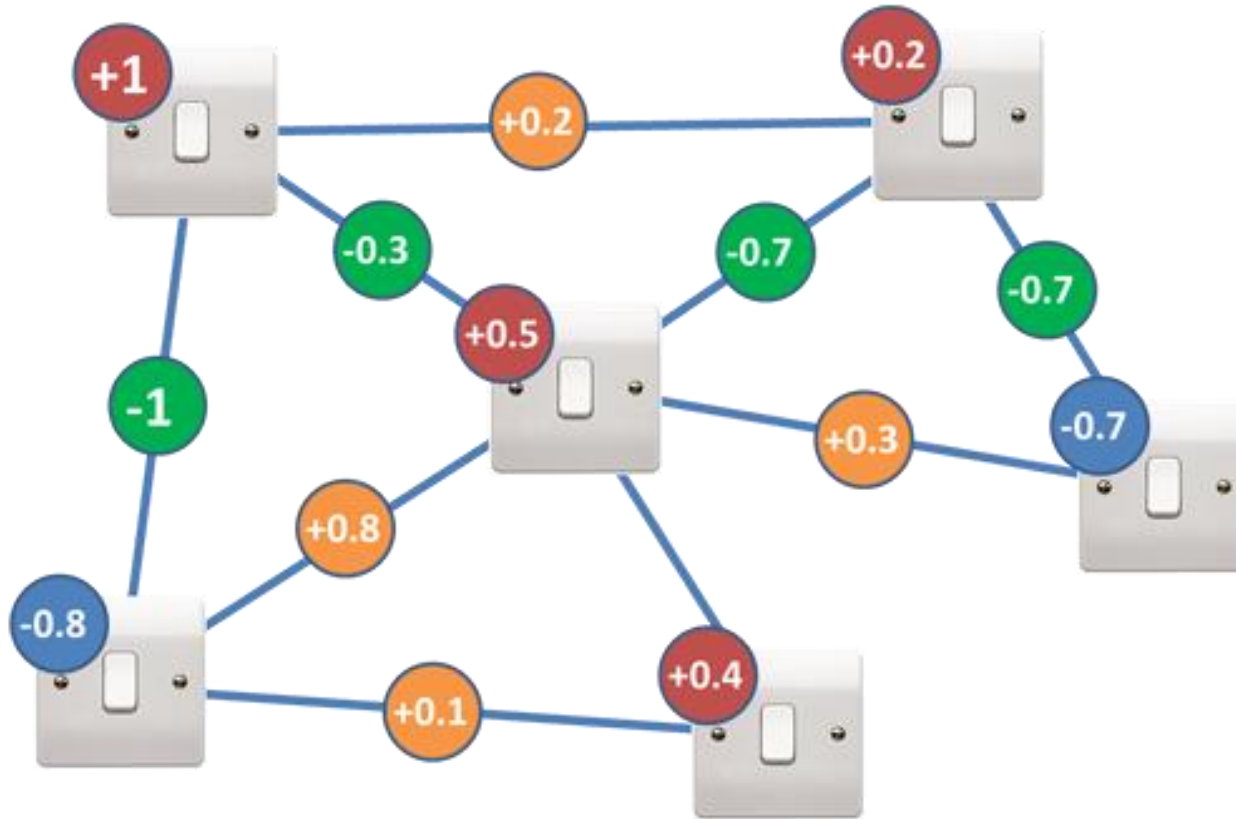


$$\begin{array}{rclcl} +1 & \times & -1 & = & -1 \\ +0.2 & \times & -1 & = & -0.2 \\ +0.5 & \times & -1 & = & -0.5 \\ -0.8 & \times & +1 & = & -0.8 \\ +0.4 & \times & -1 & = & -0.4 \\ -0.7 & \times & +1 & = & -0.7 \end{array}$$

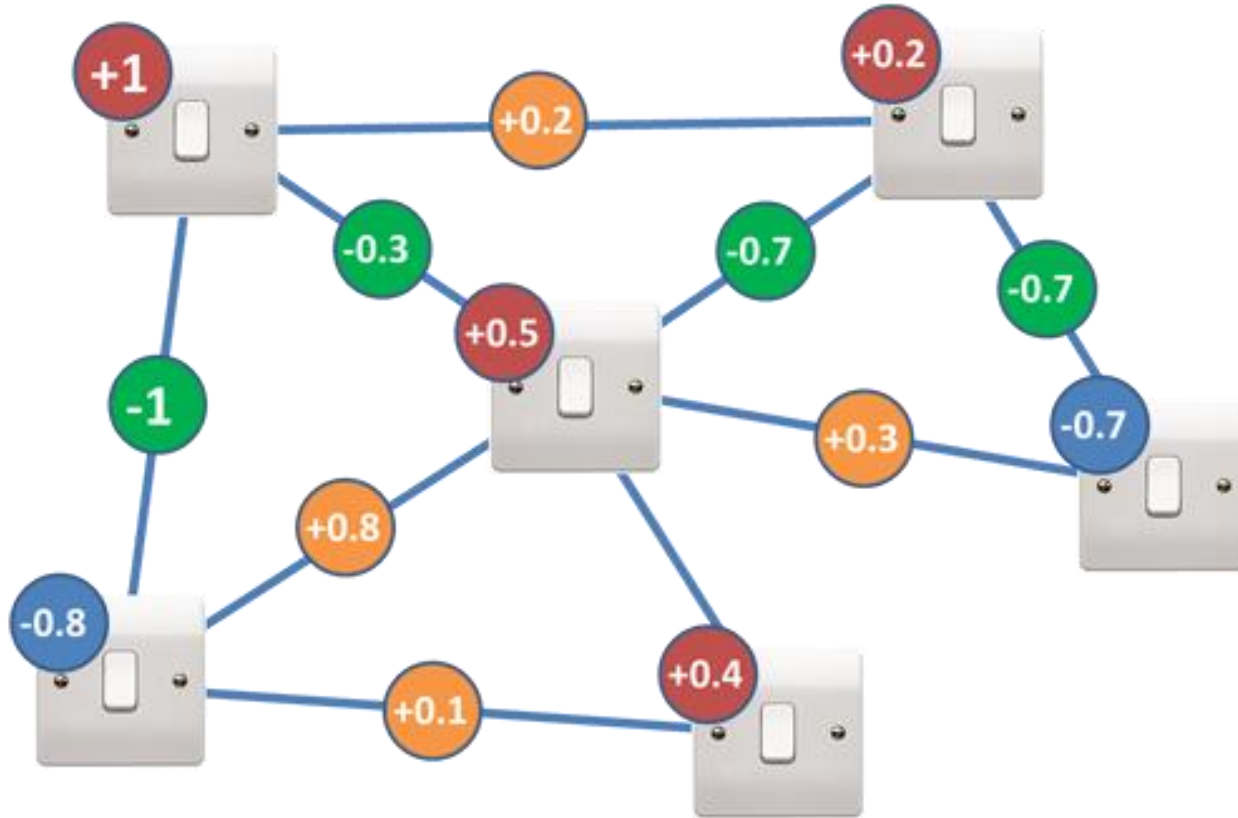
Total: -3.6

Game of Switches

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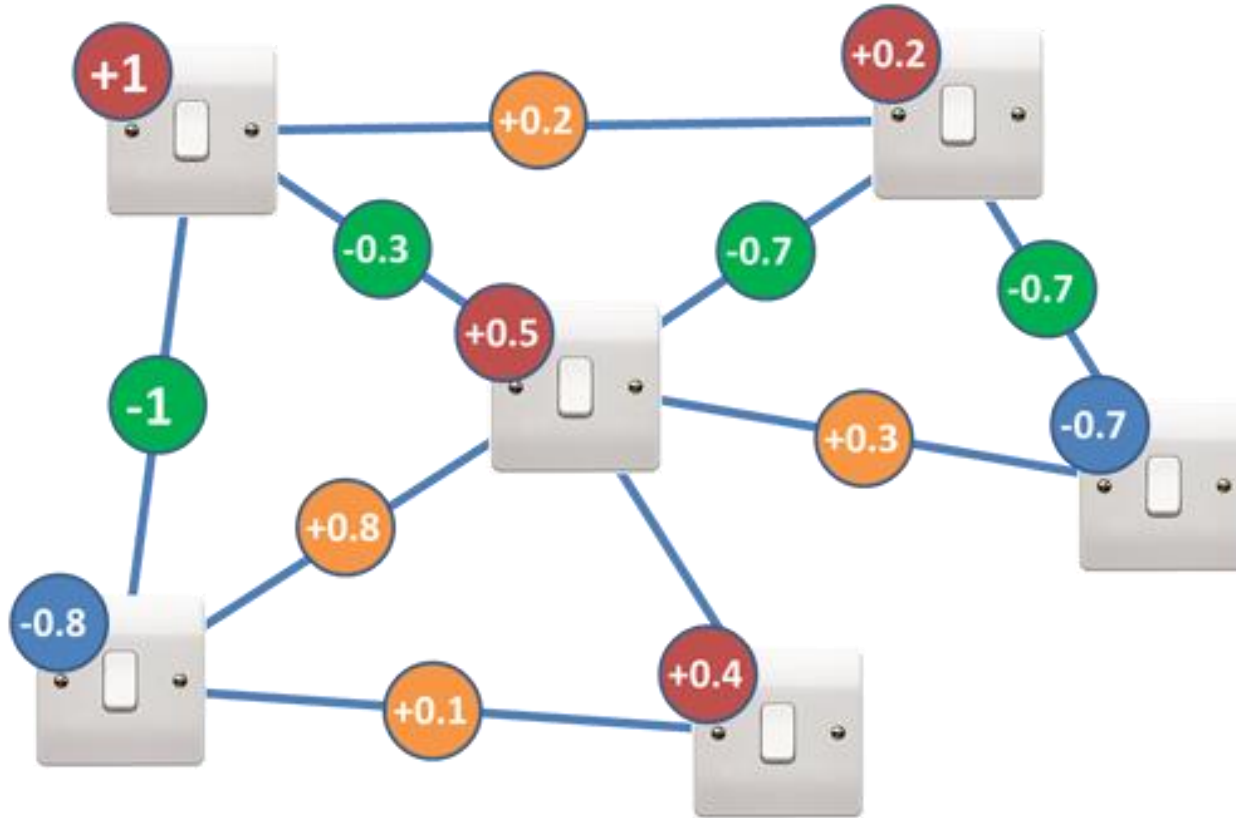


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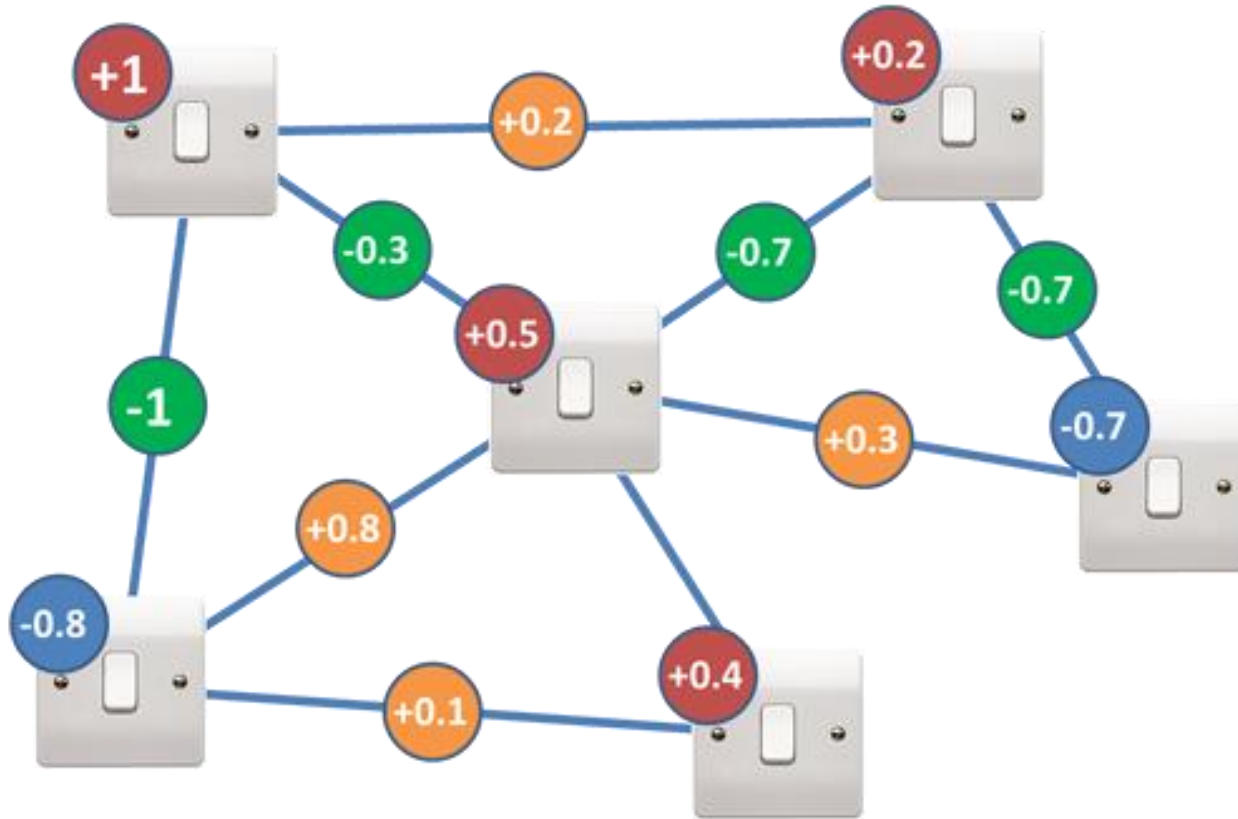
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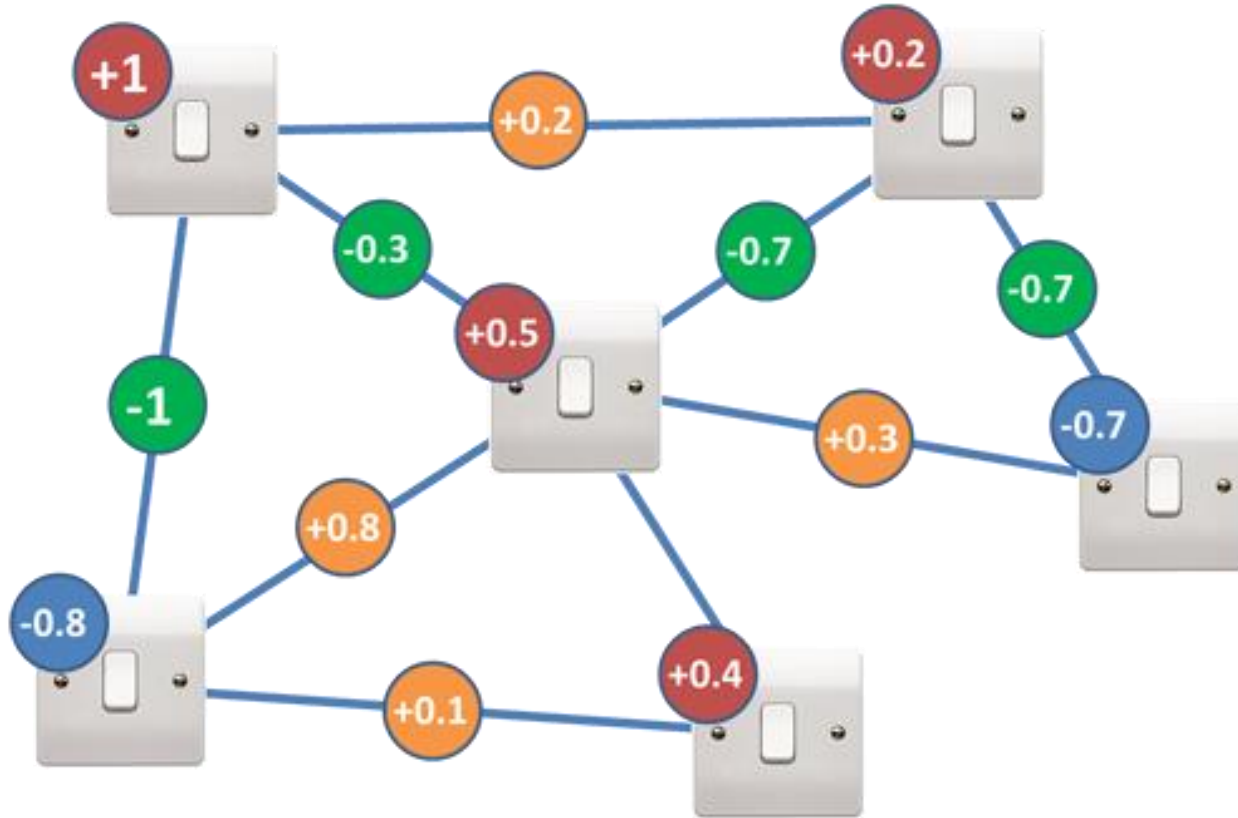
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Game of Switches



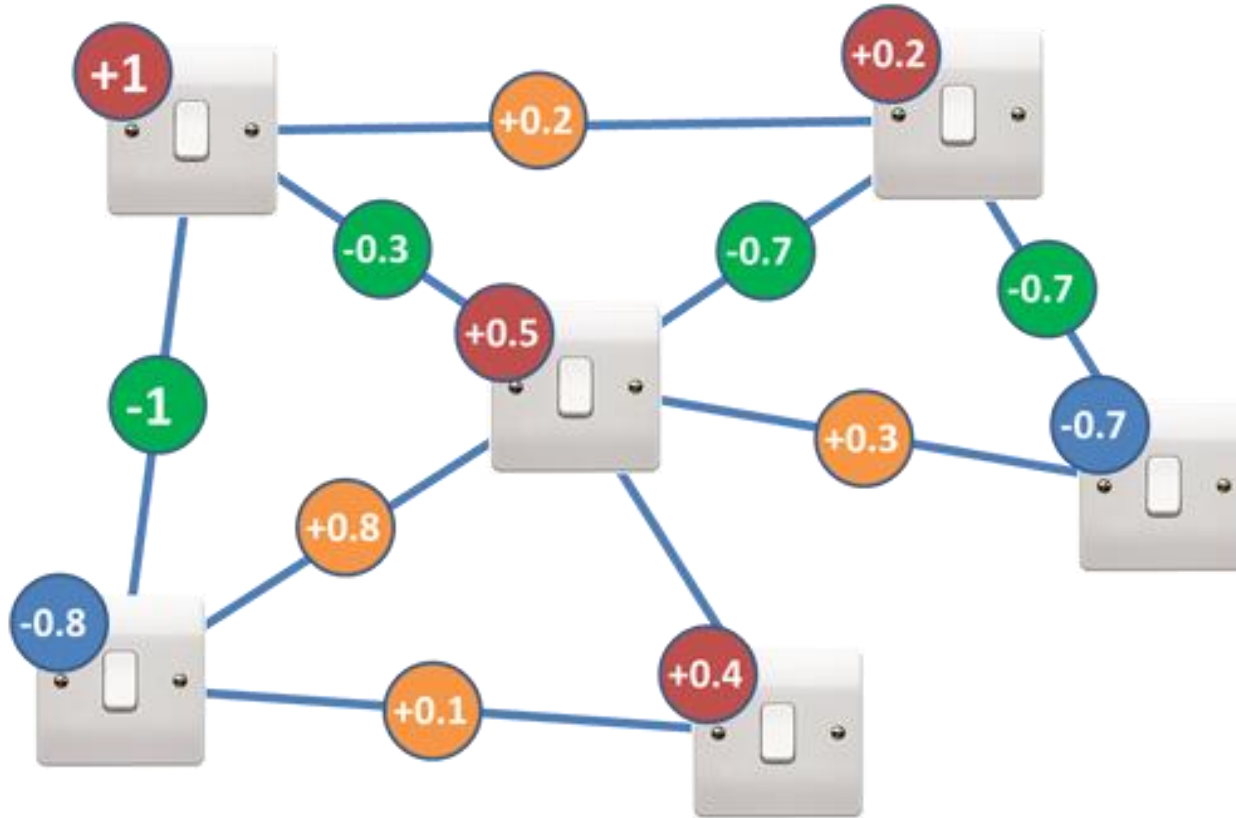
Adding another weight, J , which multiplies the product of the two switch settings.

Game of Switches



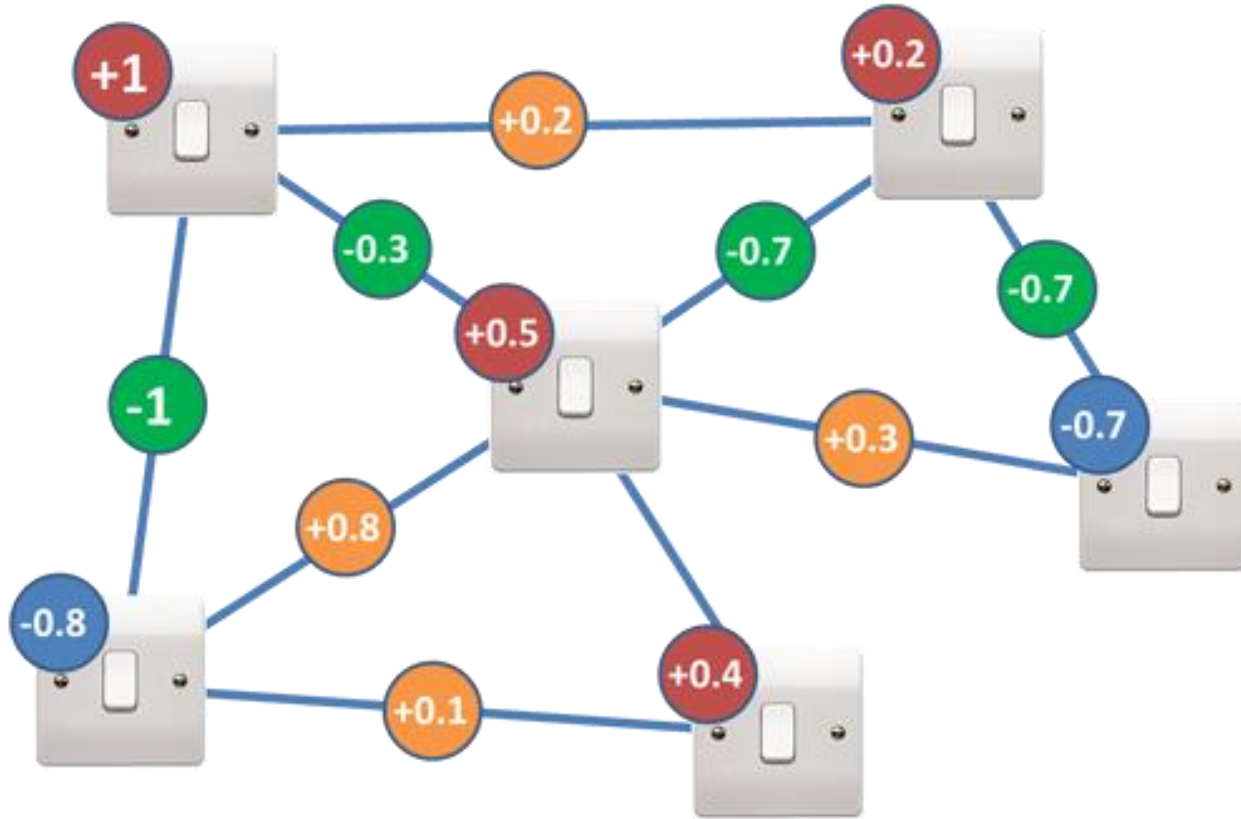
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Game of Switches

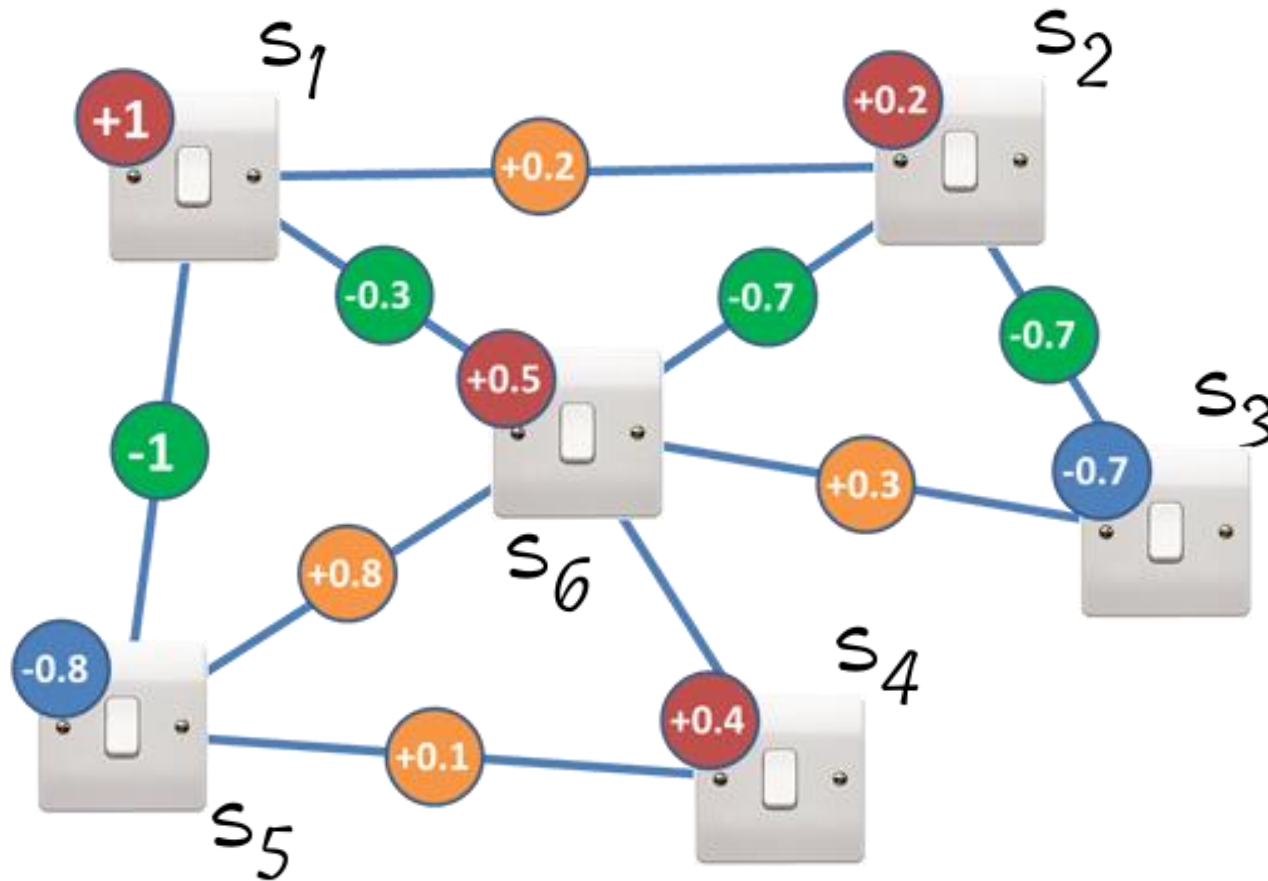


A simplified network of 3 switches (represented by light gray rectangular icons) connected by weighted edges (represented by blue lines). The switches have circular labels: +1 (red), -1 (green), and -0.8 (blue). The edge between the top and middle switches has a weight of -1 (green circle). The edge between the middle and bottom switches has a weight of -0.8 (blue circle). An arrow points from the -1 weight label to the $J_{i,j}$ term in the equation below.

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

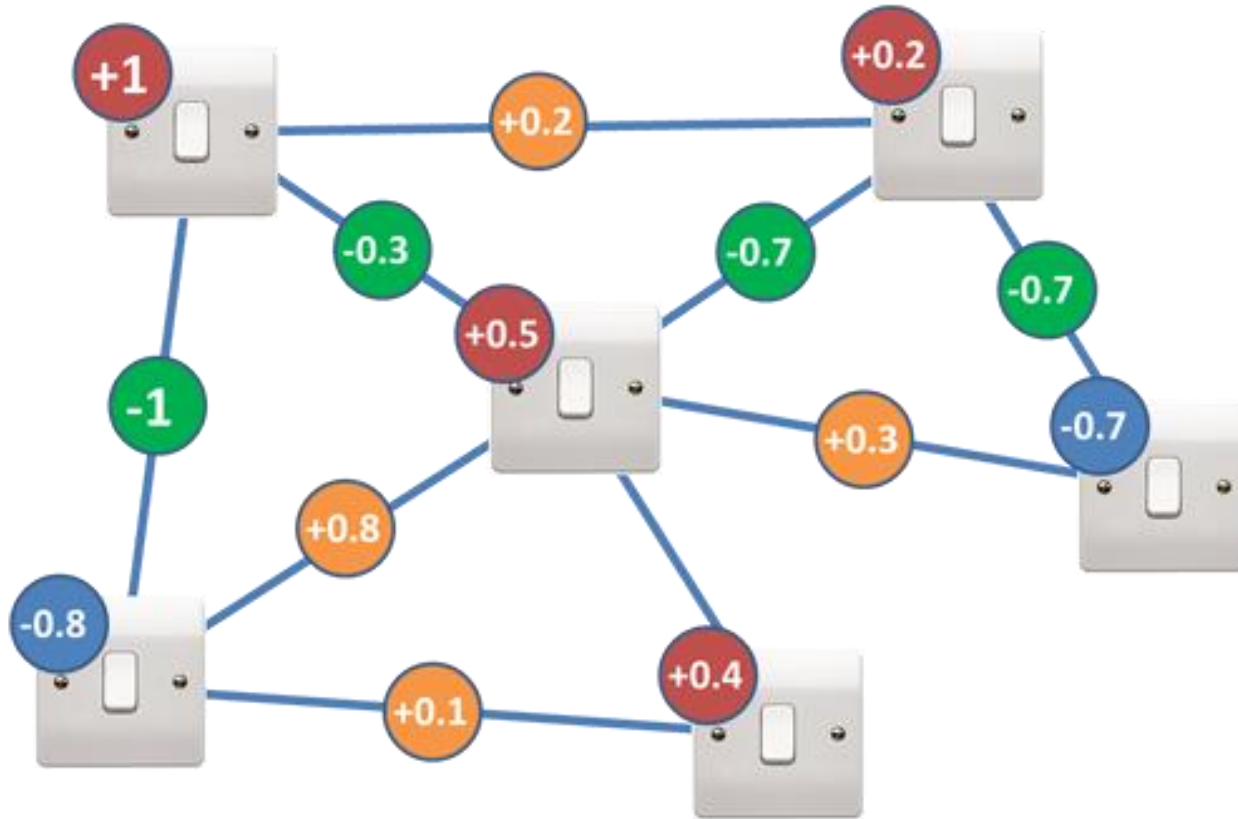
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Game of Switches



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

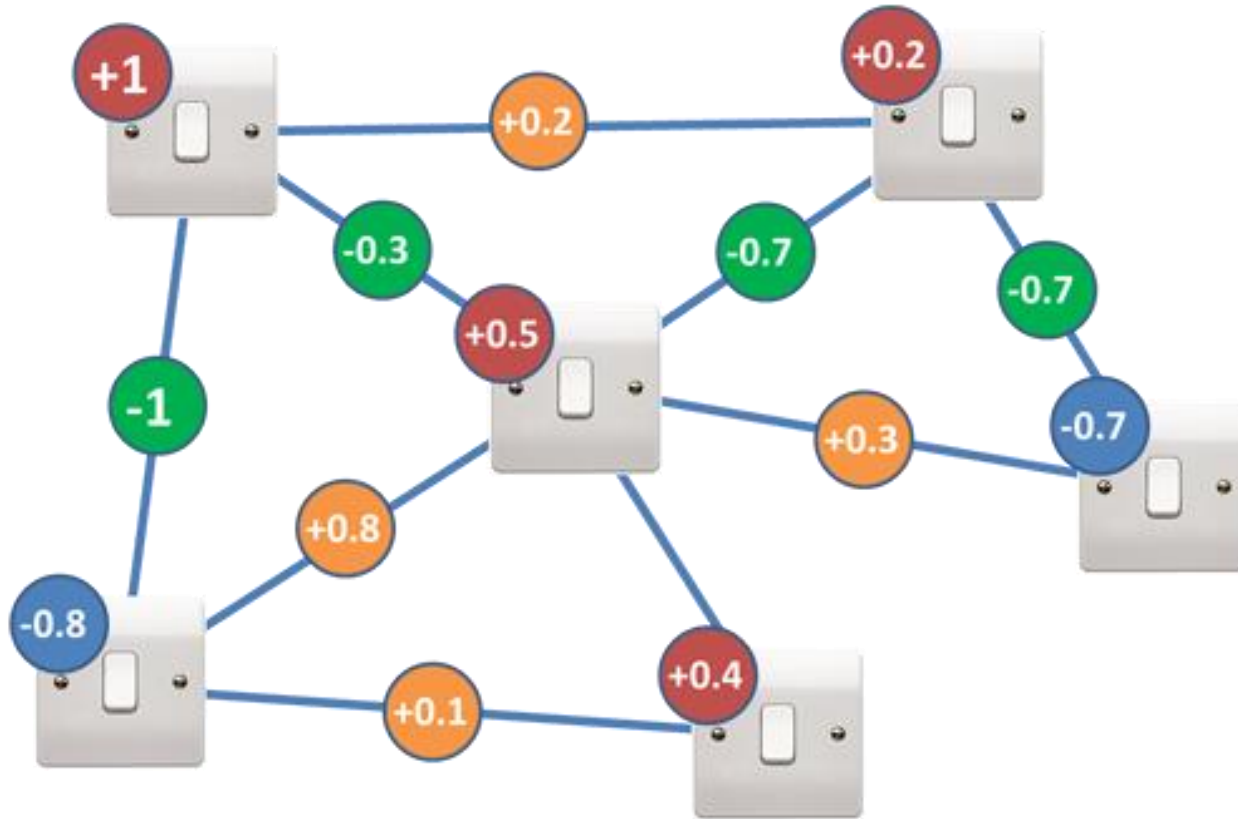
Game of Switches



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



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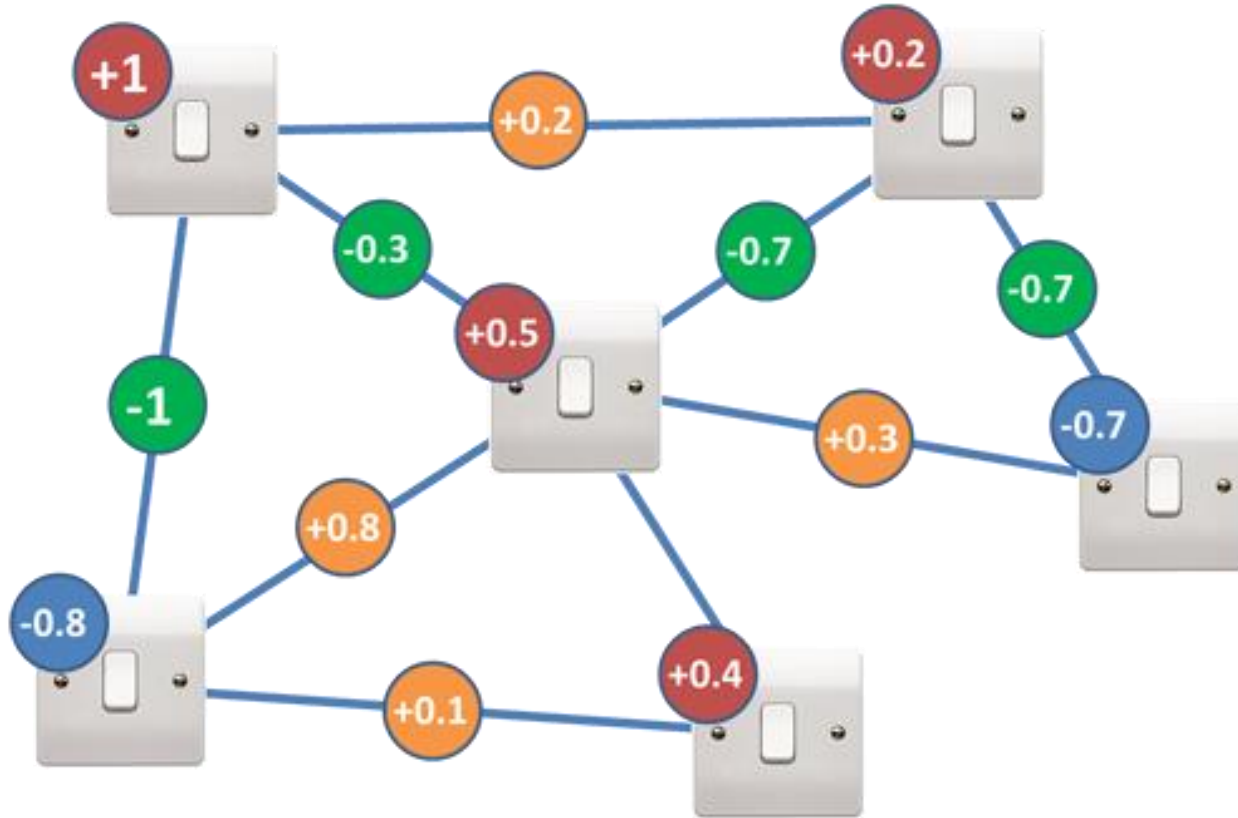


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Game of Switches



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



QUBO Problems

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

QUBO Problems

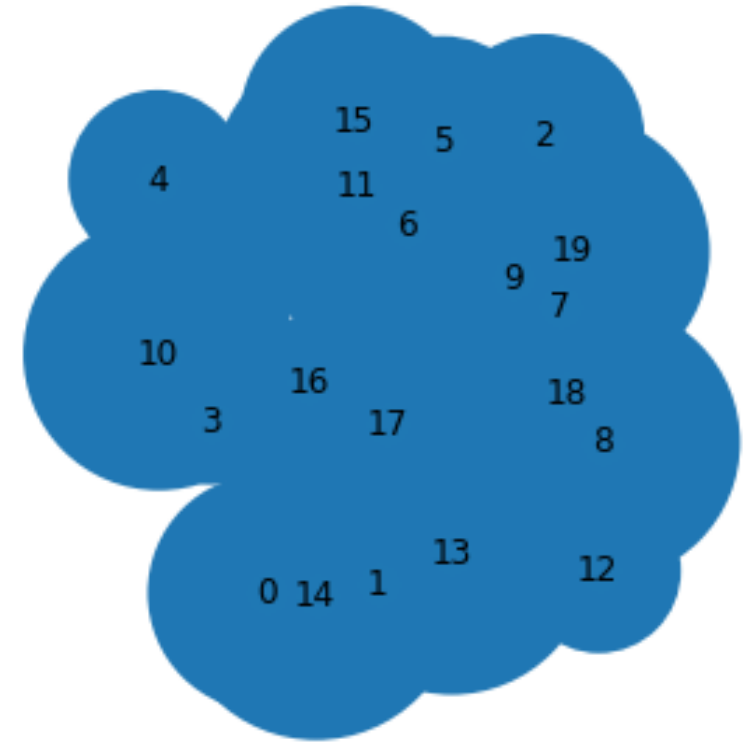
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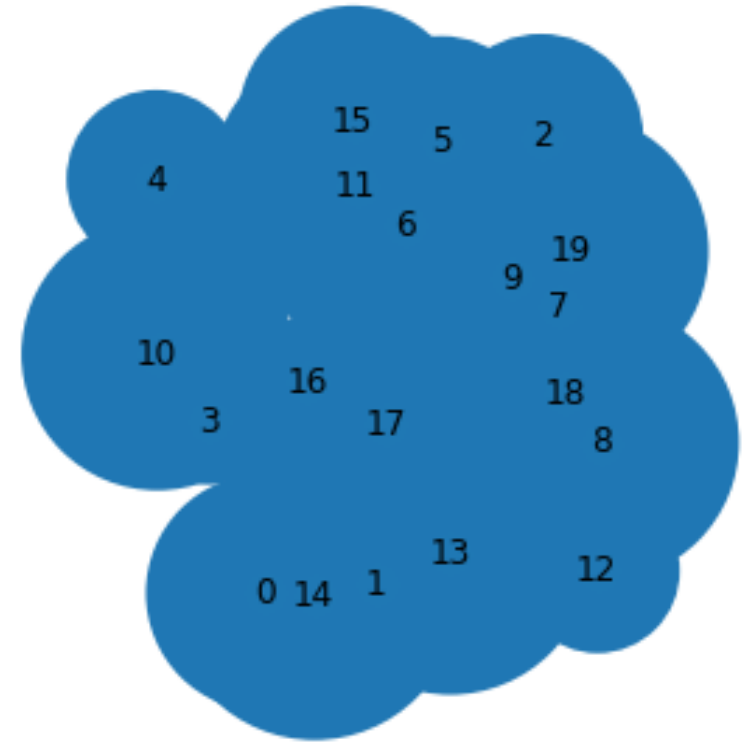
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- Suppose we have a certain number of antennas and a certain number of possible sites to place these antennas.
- Each antenna with its signal can cover a certain area. When multiple signals overlap, however, unpleasant interference is generated
- Our 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)

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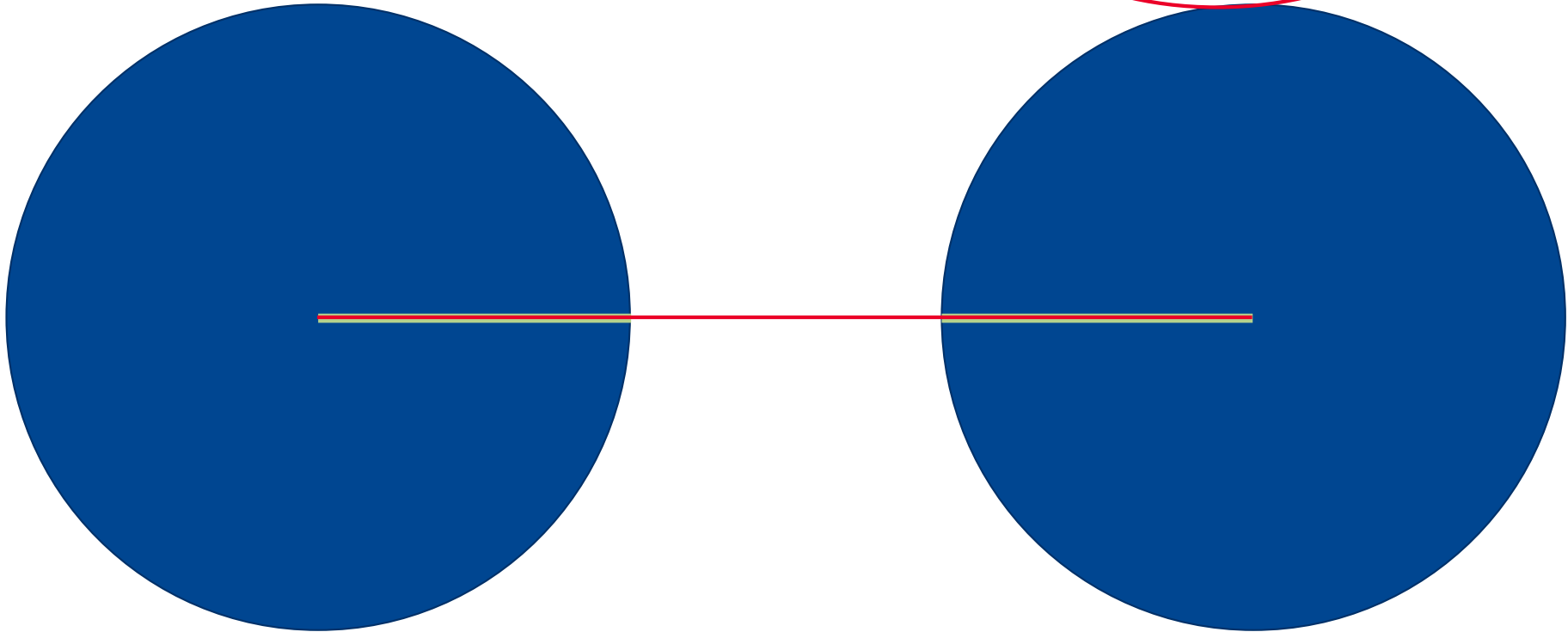
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- where r_i and r_j are the parameters relating to the range of action of the antennas i and j and $\text{dist}(c_i, c_j)$ is the distance between the points where the antennas are positioned

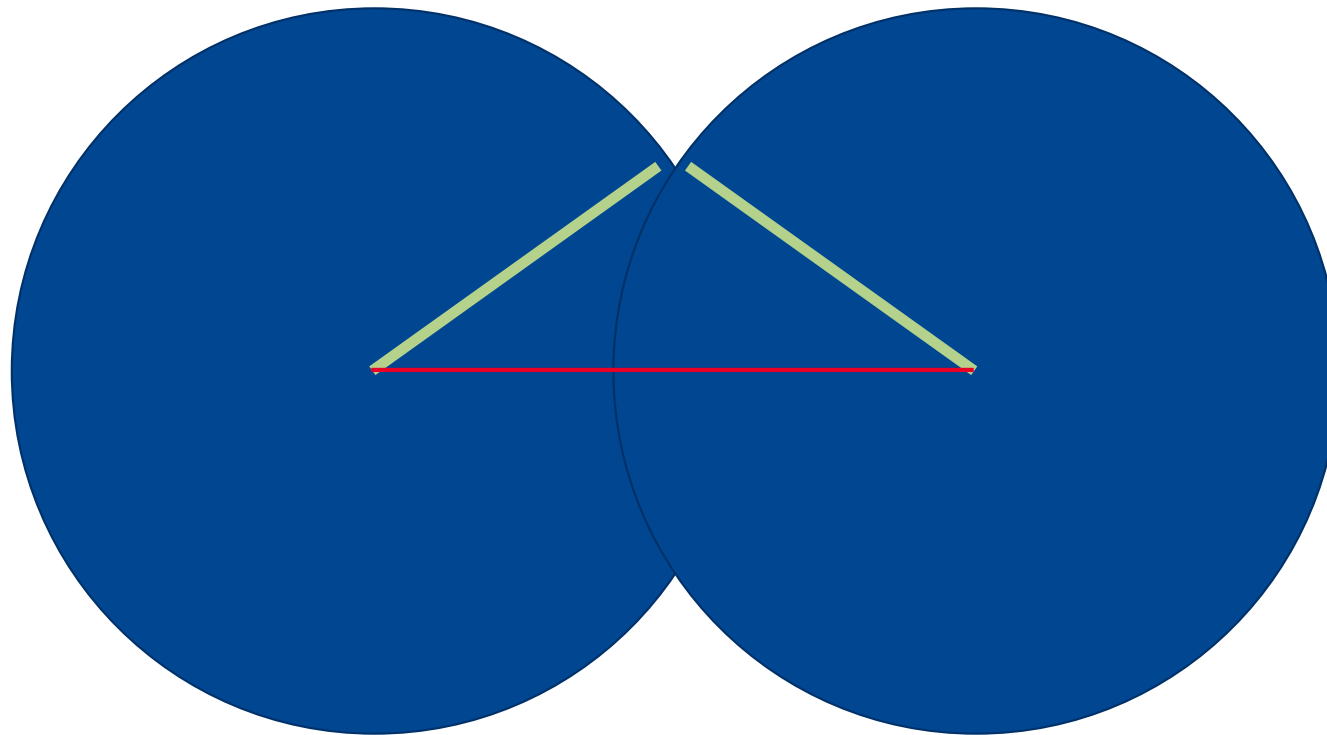
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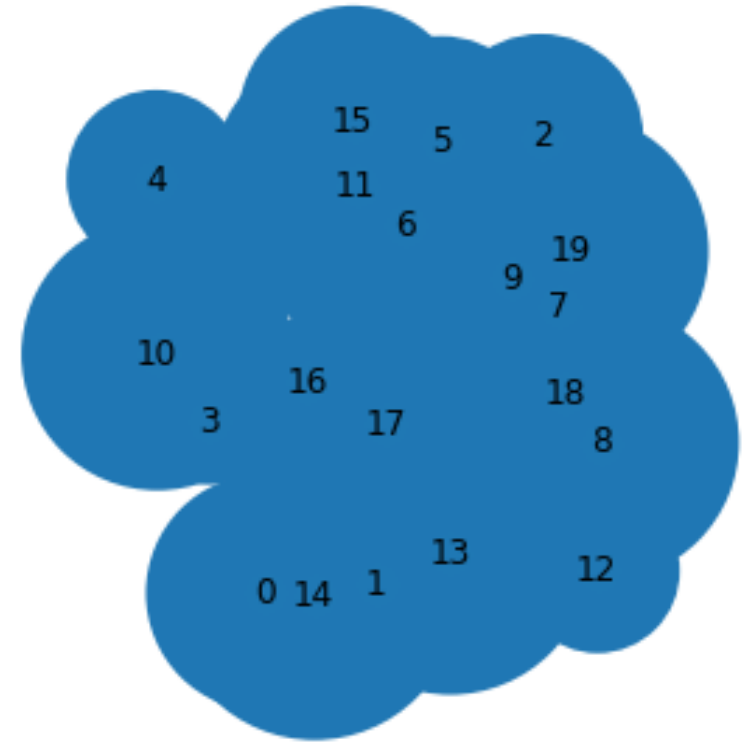
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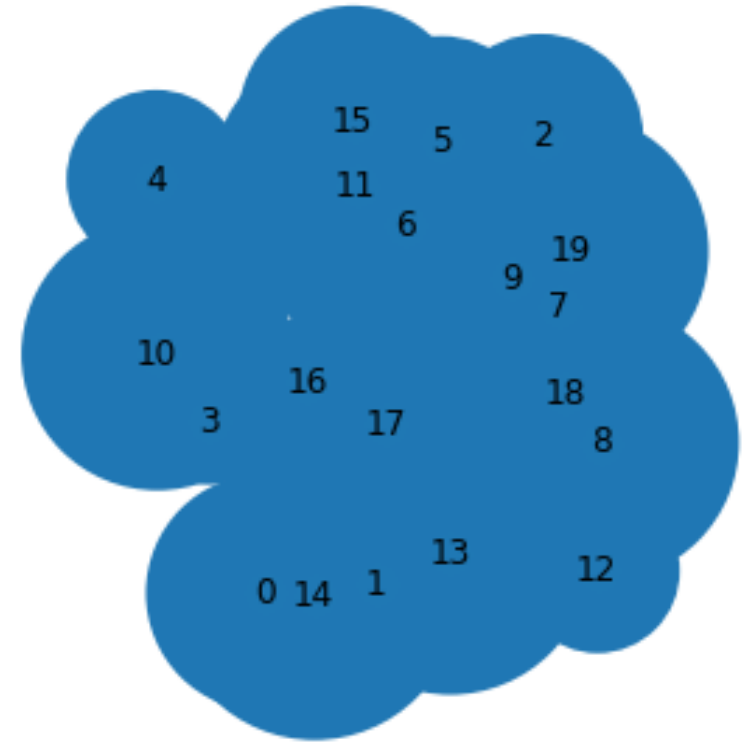
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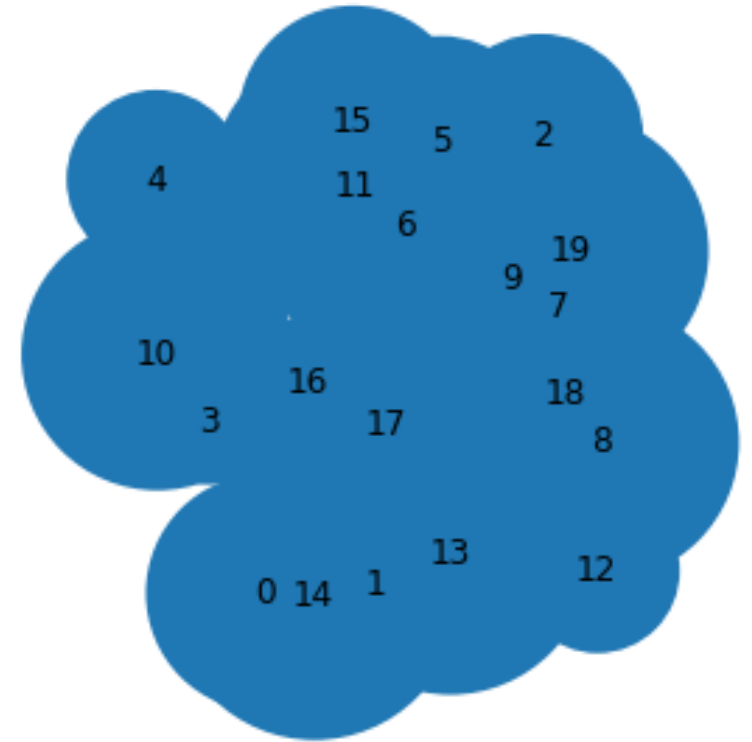
$$[q_0, \dots, q_{19}]$$



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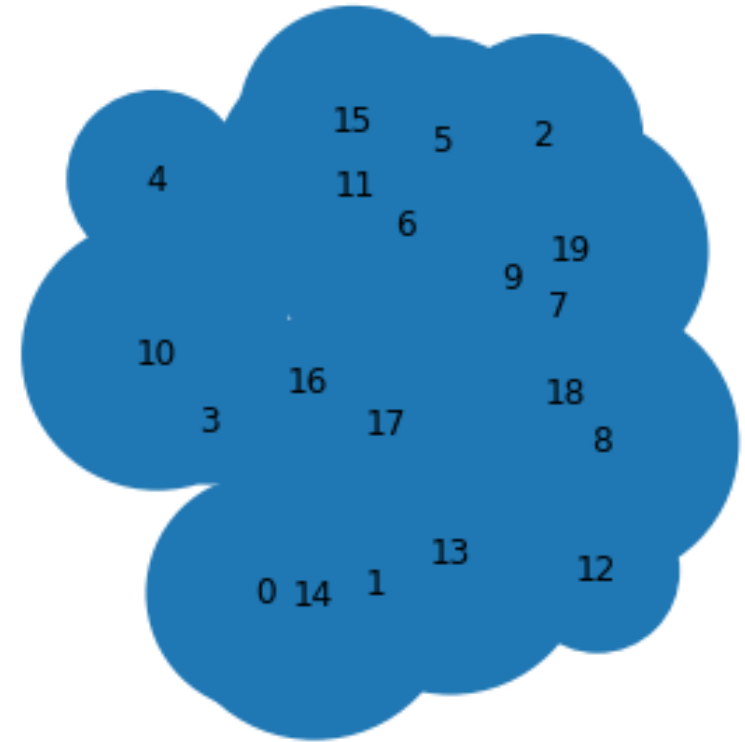


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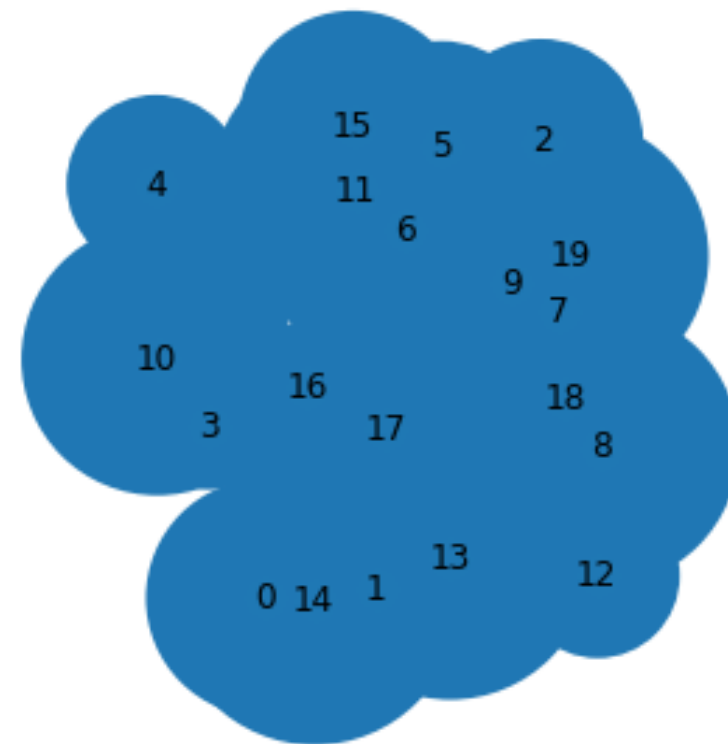
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QUBO Problems

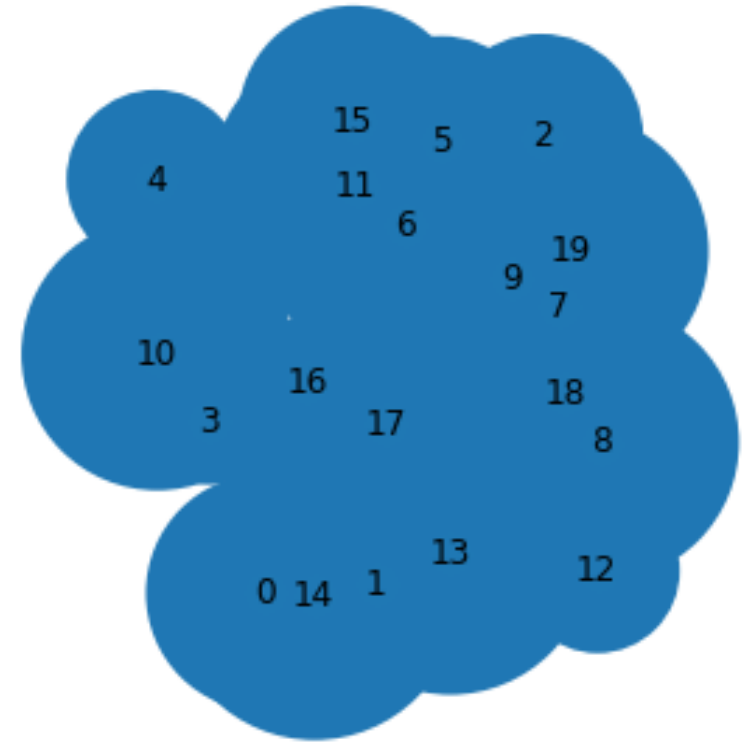
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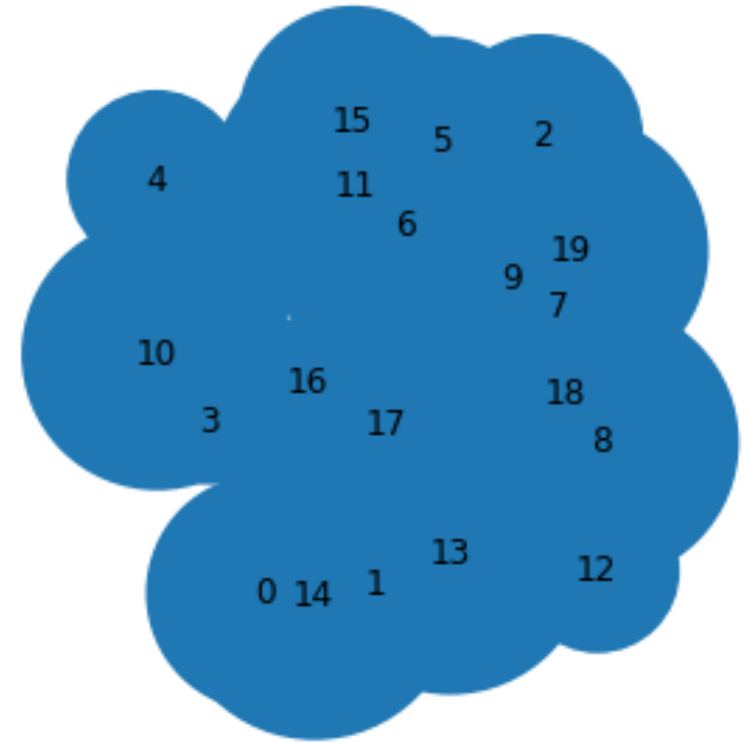
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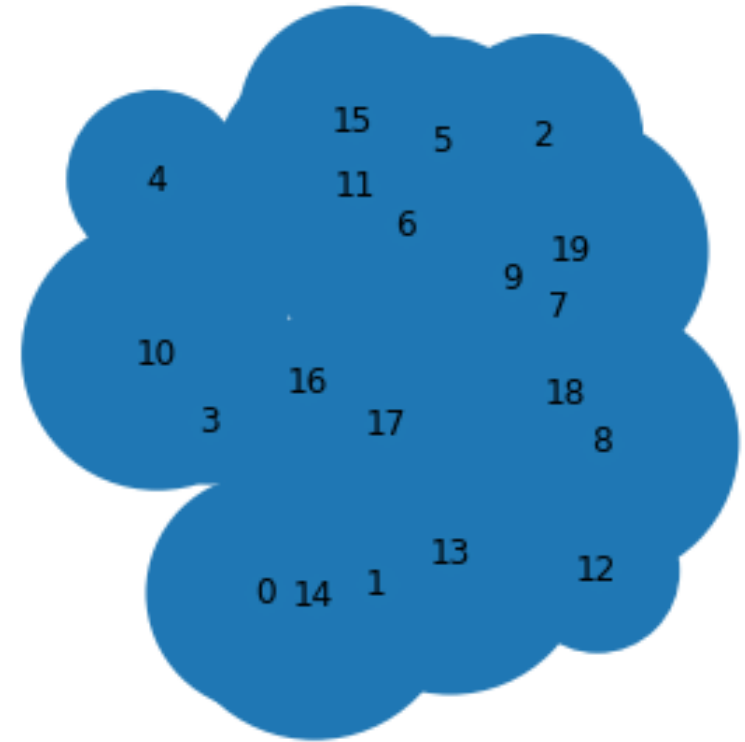
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$$E_{\text{QUBO}}(x) = \sum_i Q_{i,i} x_i + \sum_{i < j} Q_{i,j} x_i x_j$$

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- More generally, any mathematical problem can be mapped into a QUBO problem
- You just have to understand if it's worth it :)

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- 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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- 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

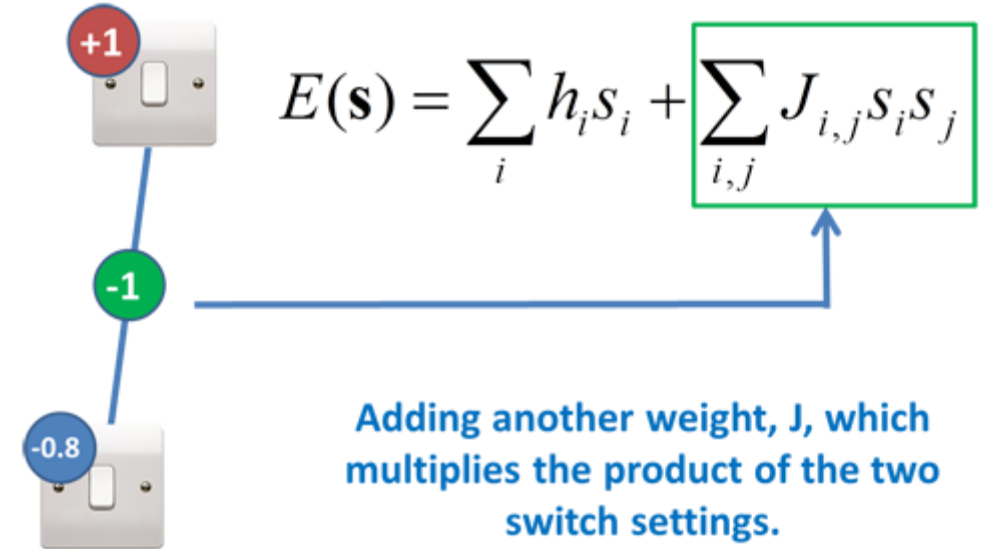
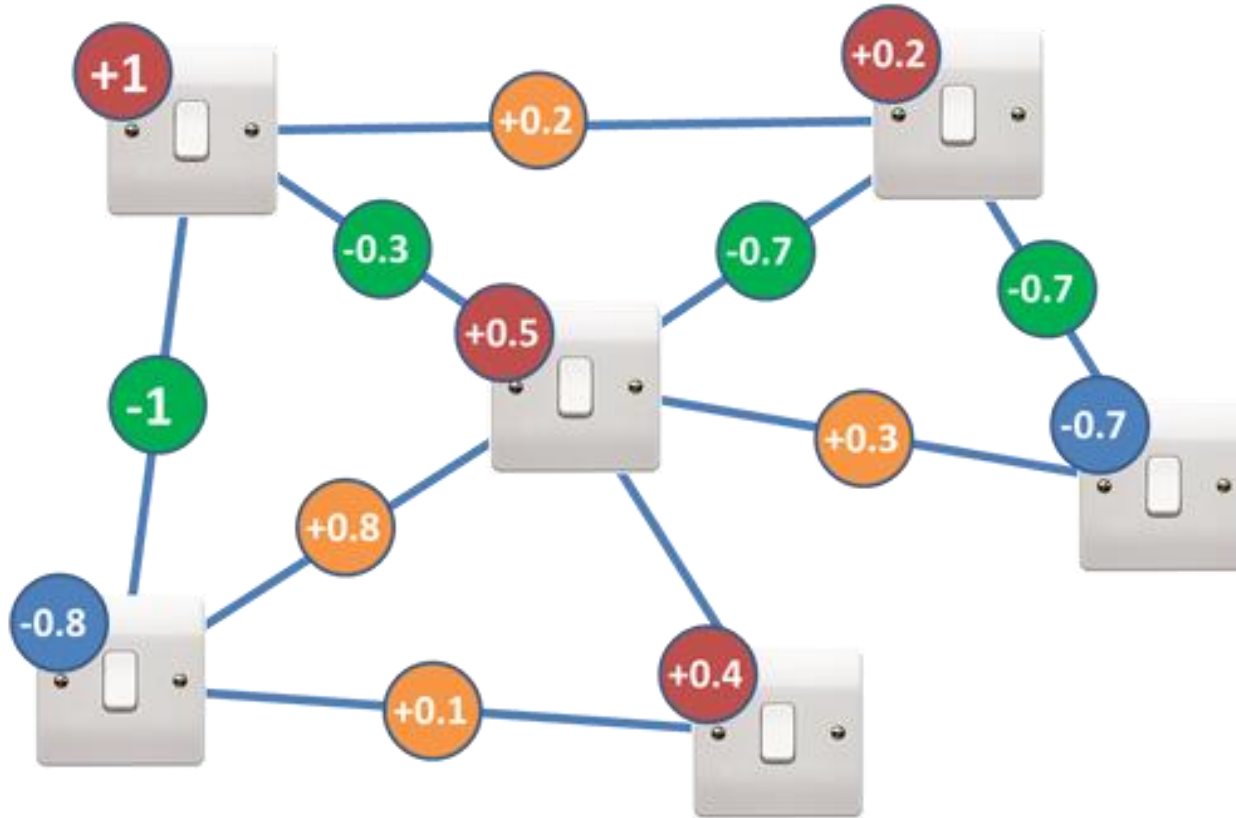
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```

```
>>> 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



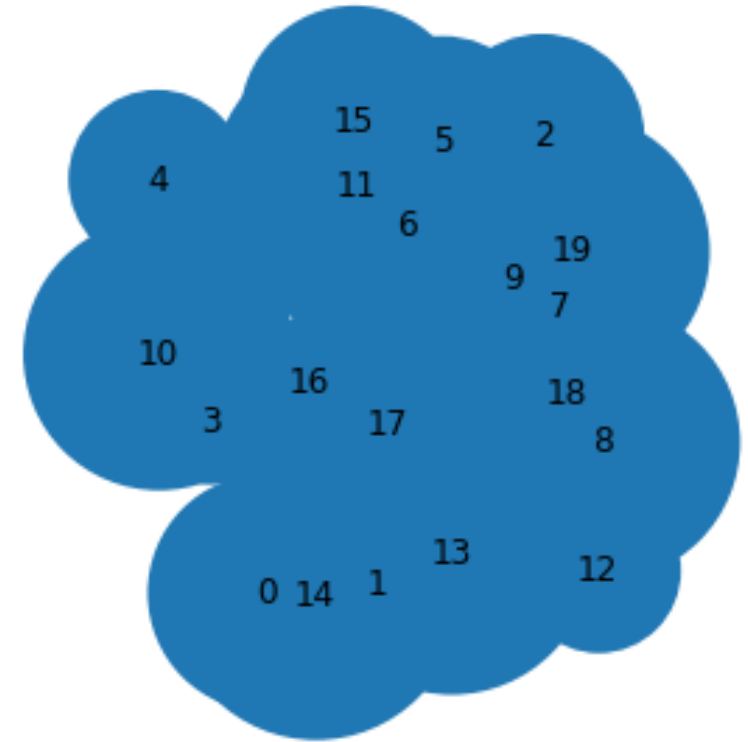
Exercise 2: Antenna Placement

- Try to implement the Antenna Placement Problem

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



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

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- 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

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

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

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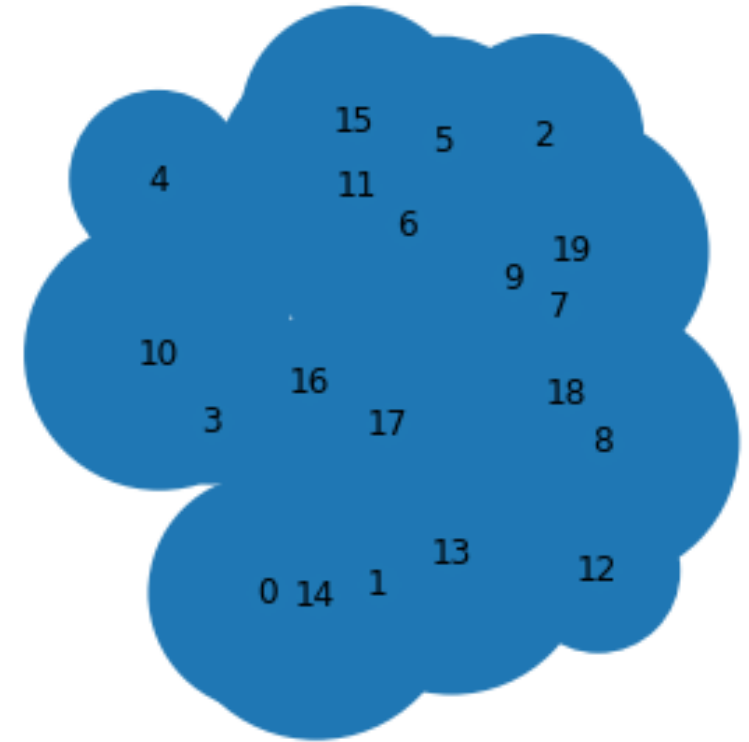
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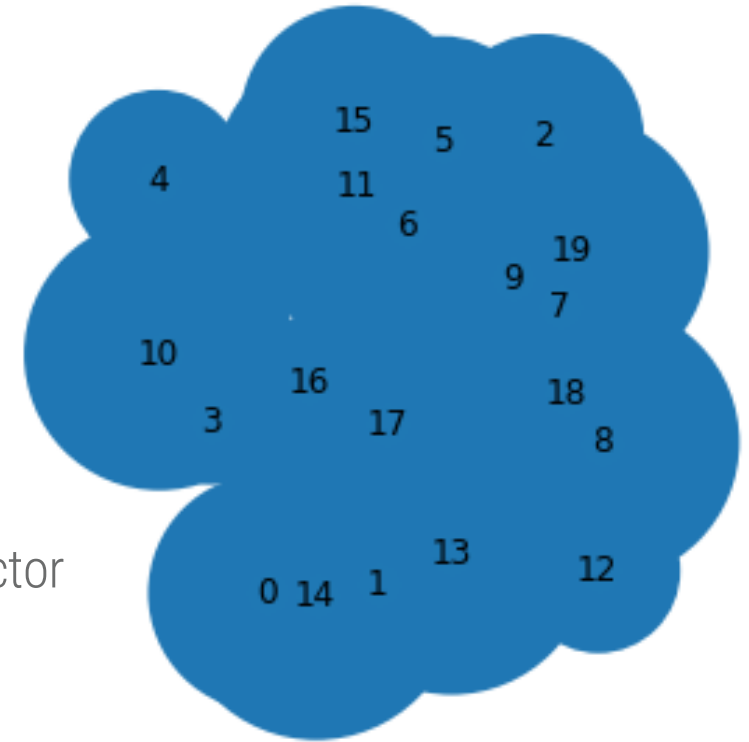
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- Implement and configure L vector
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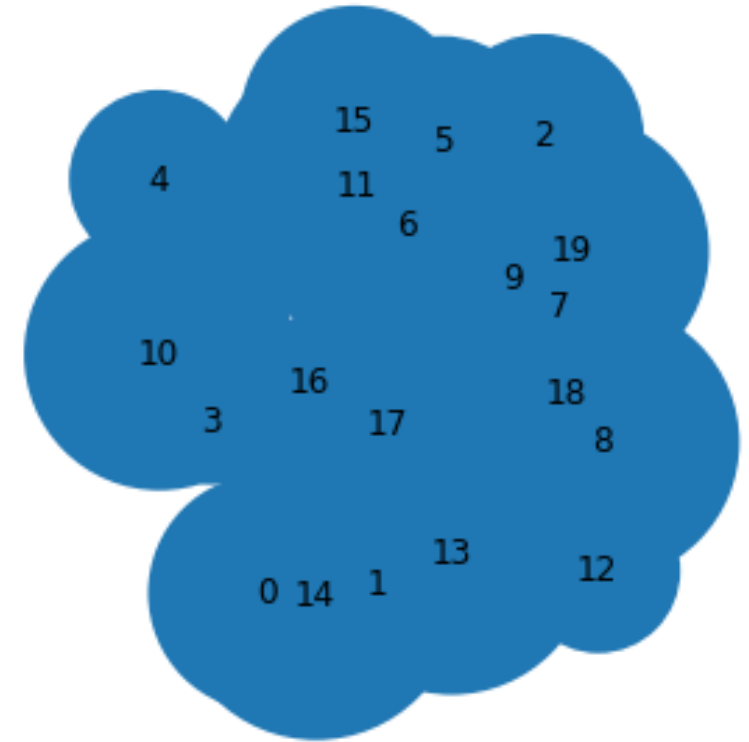
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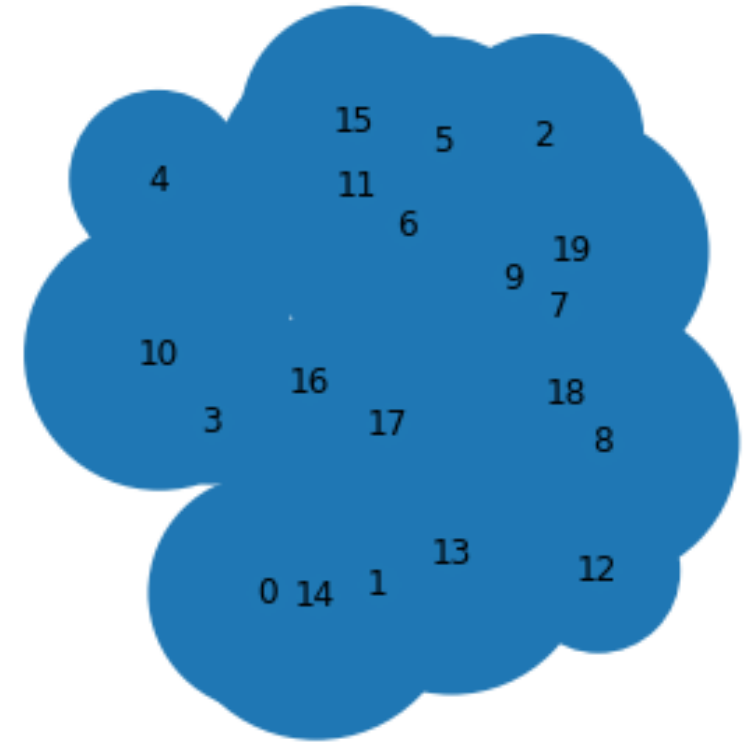
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x, y, z	xyz	$x + y + z - 2$	$\max_w \{w(x + y + z - 2)\}$
0, 0, 0	0	-2	$0 _{w=0}$
0, 0, 1	0	-1	$0 _{w=0}$
0, 1, 0	0	-1	$0 _{w=0}$
0, 1, 1	0	0	$0 _{w=0,1}$
1, 0, 0	0	-1	$0 _{w=0}$
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1, 1, 1	1	1	$1 _{w=1}$

Exercise 2: Antenna Placement

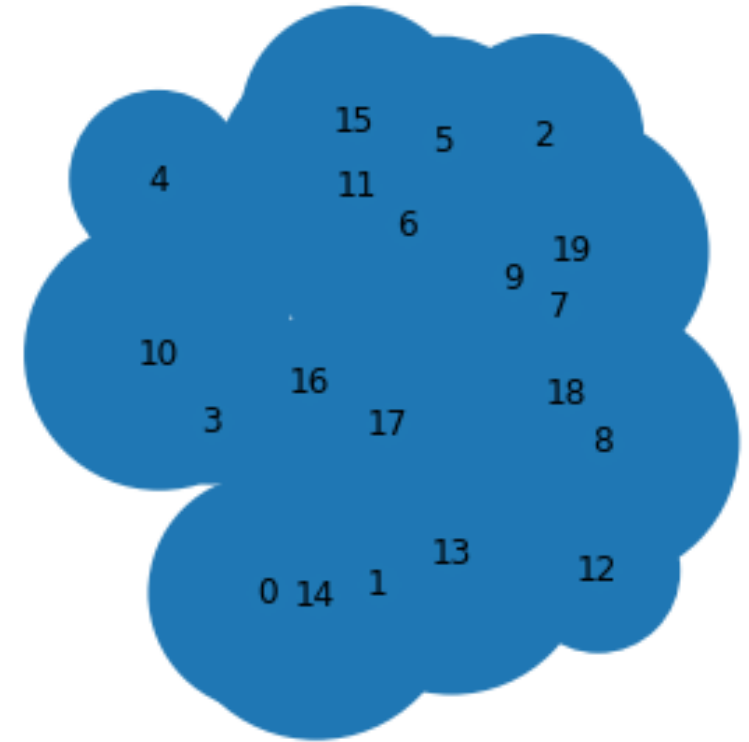
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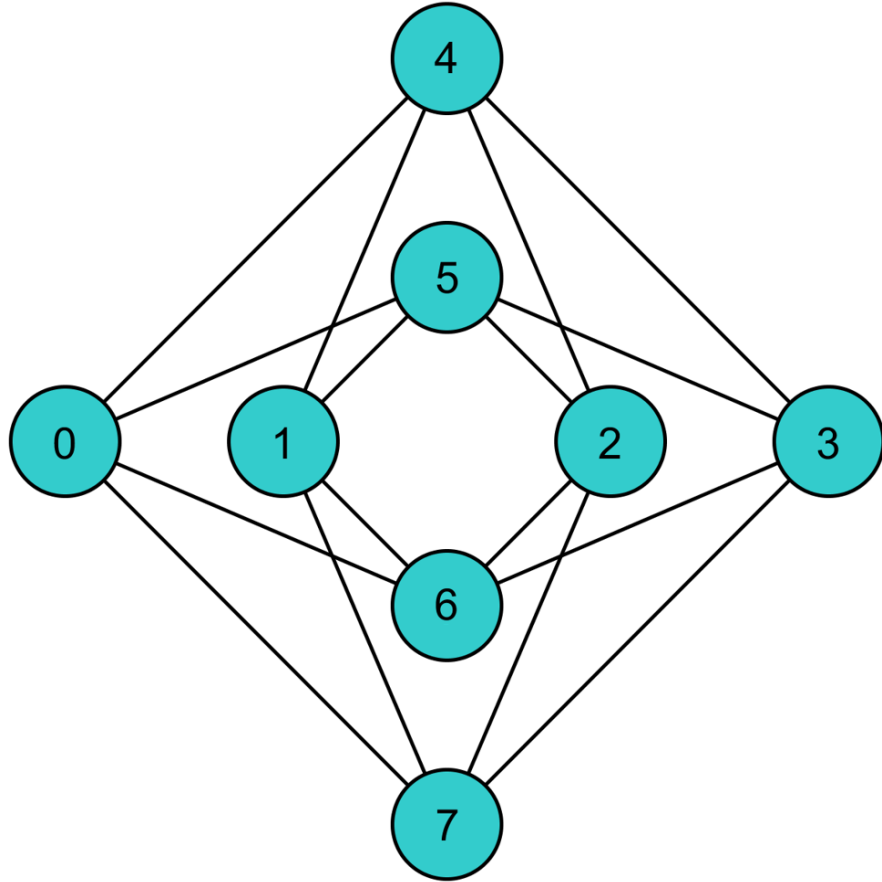
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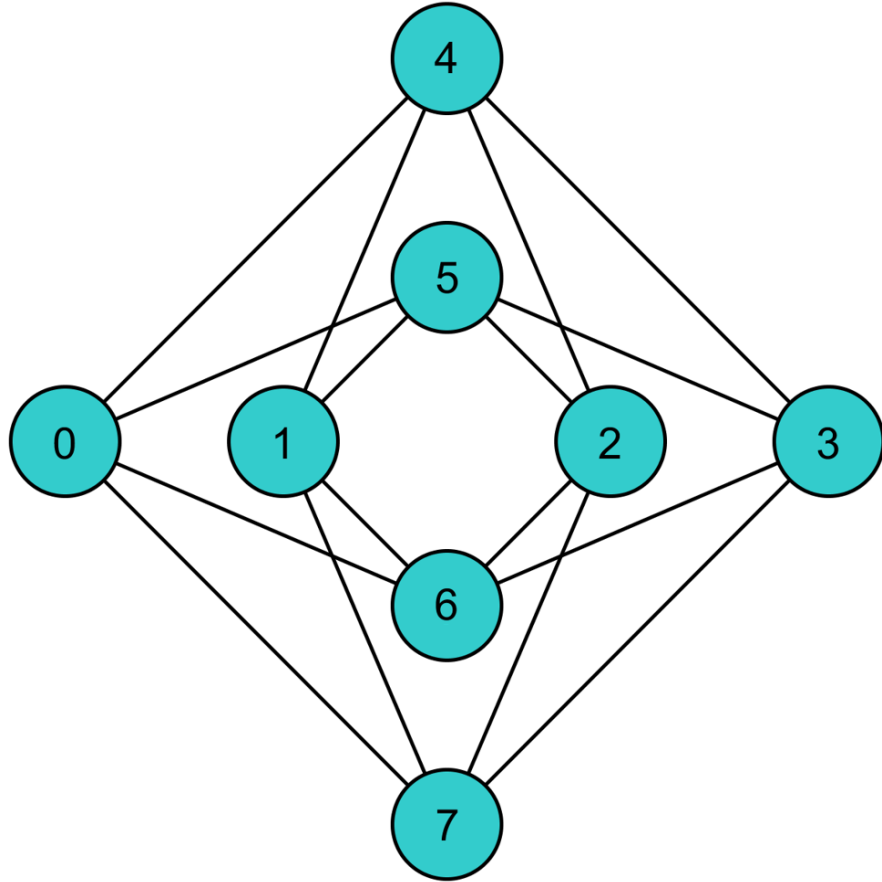
- Add High Order Terms to QUBO problem with pyqubo

Graphs



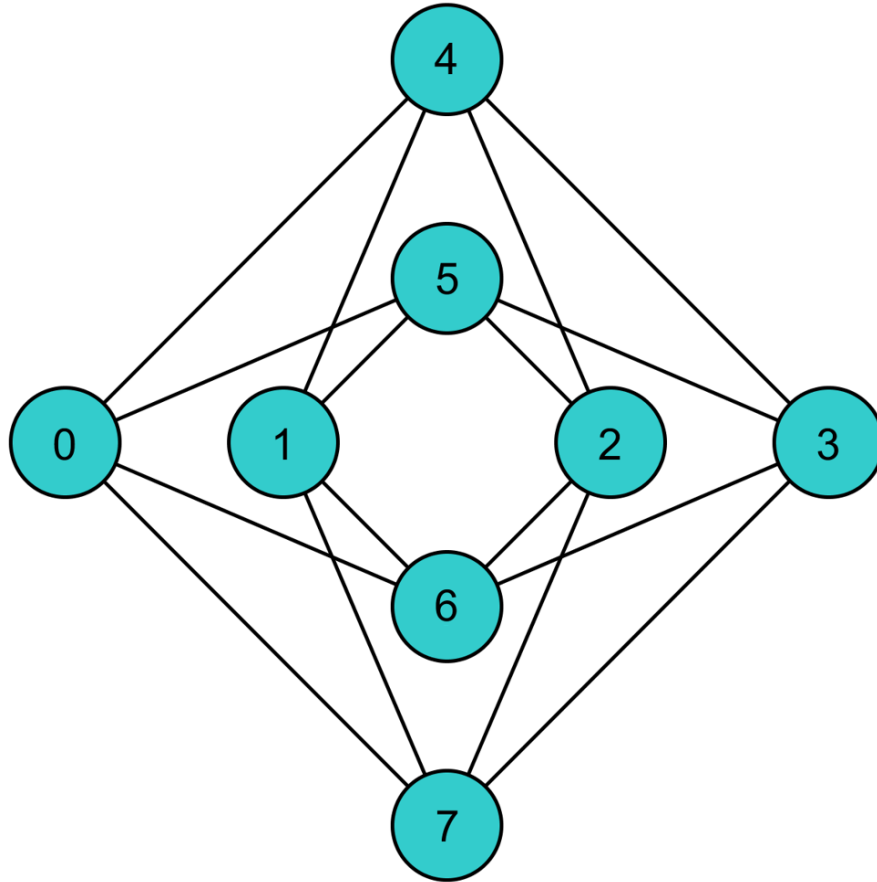
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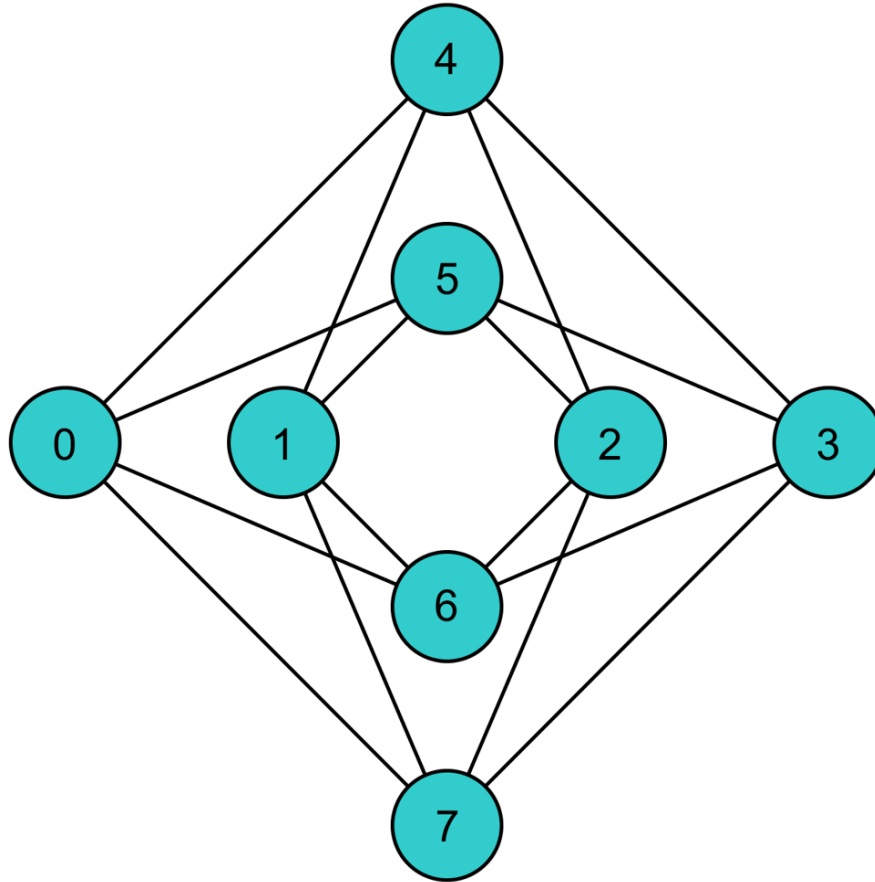
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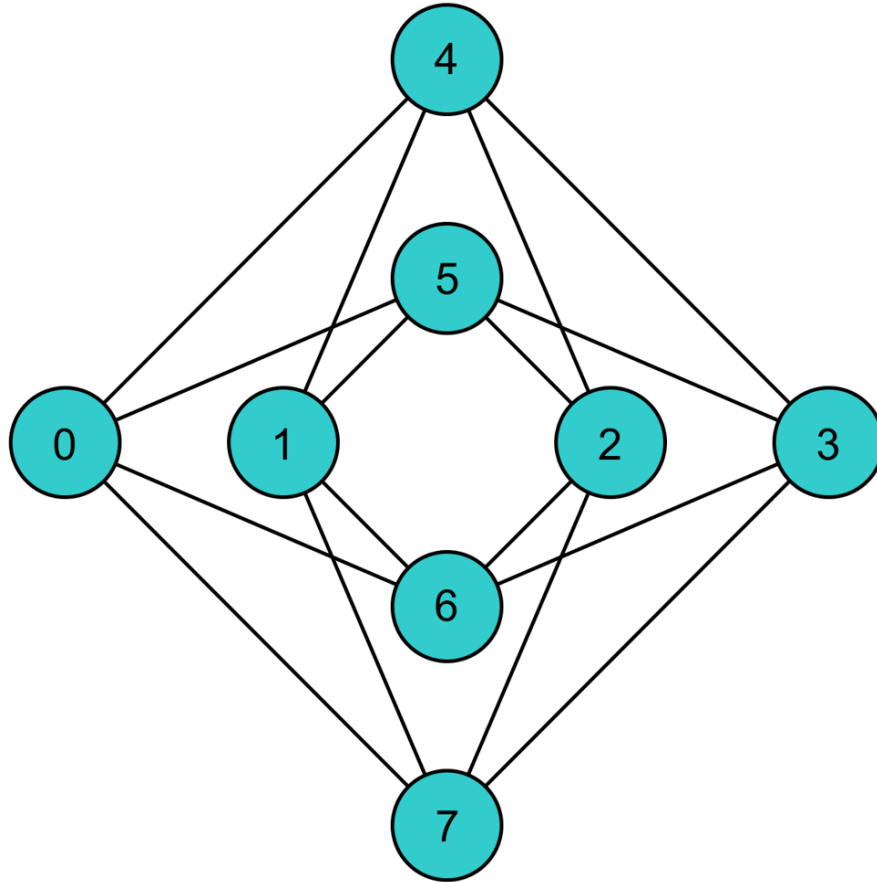
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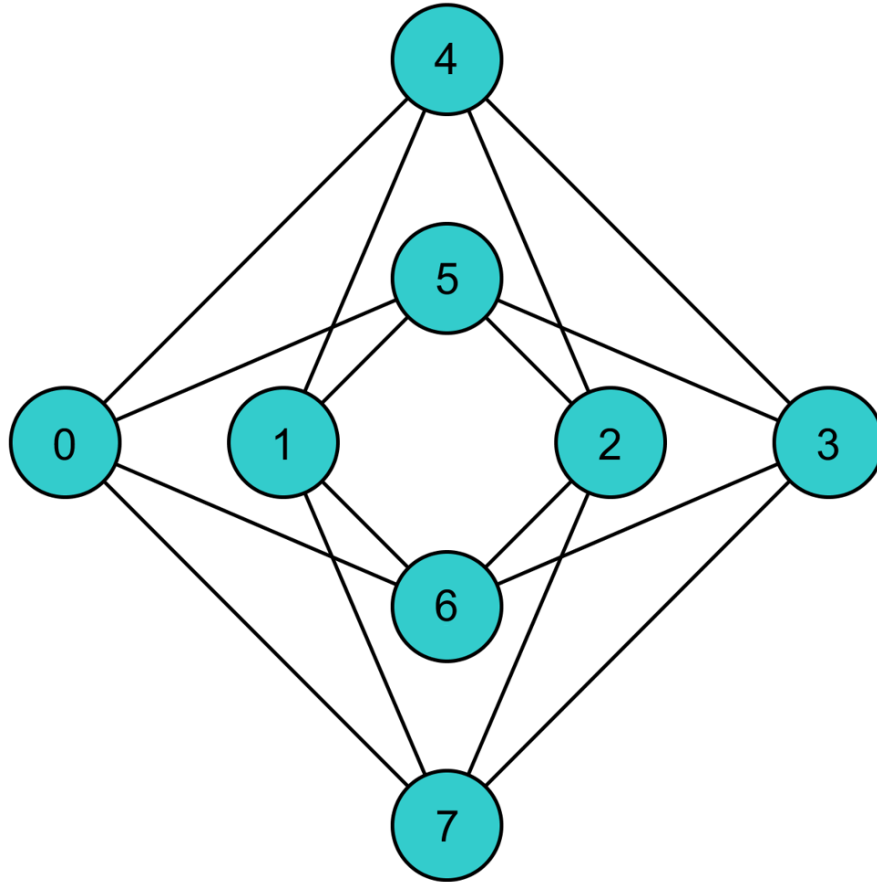
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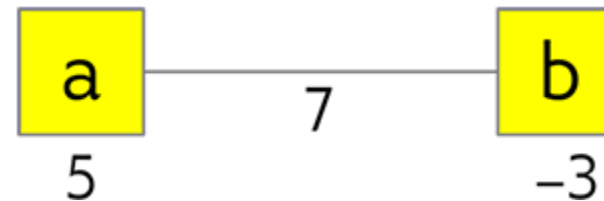
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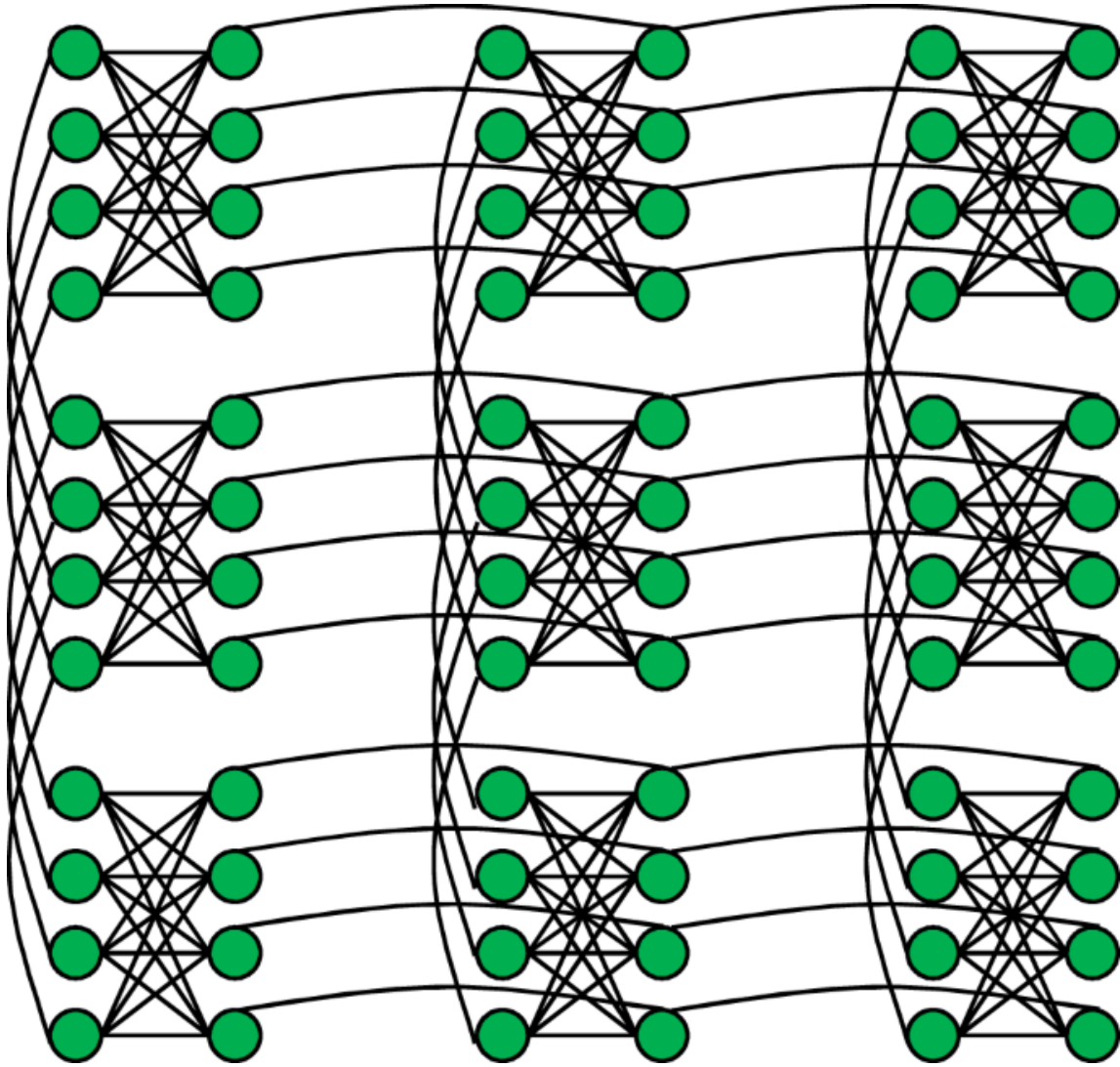


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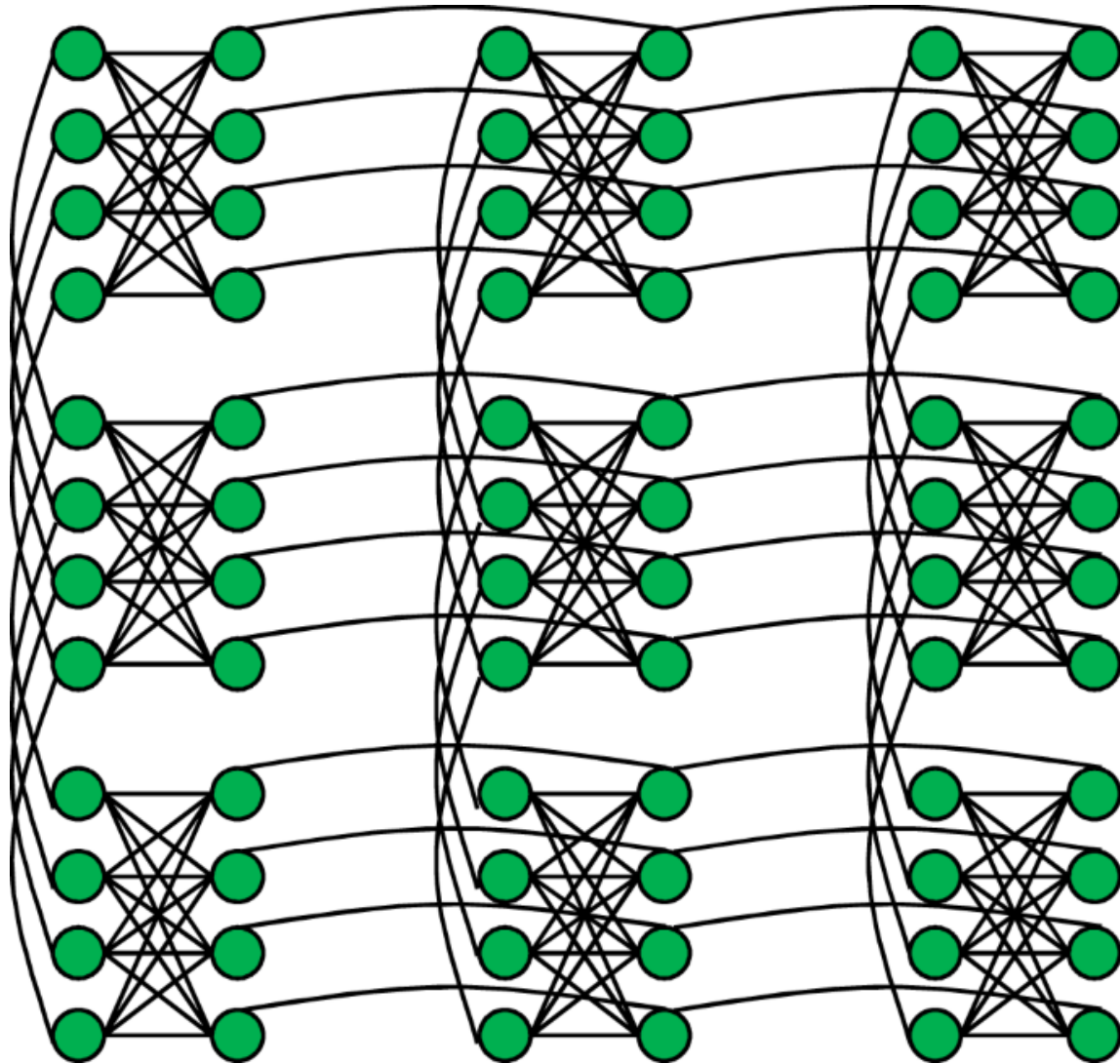


Embedding a problem on a graph



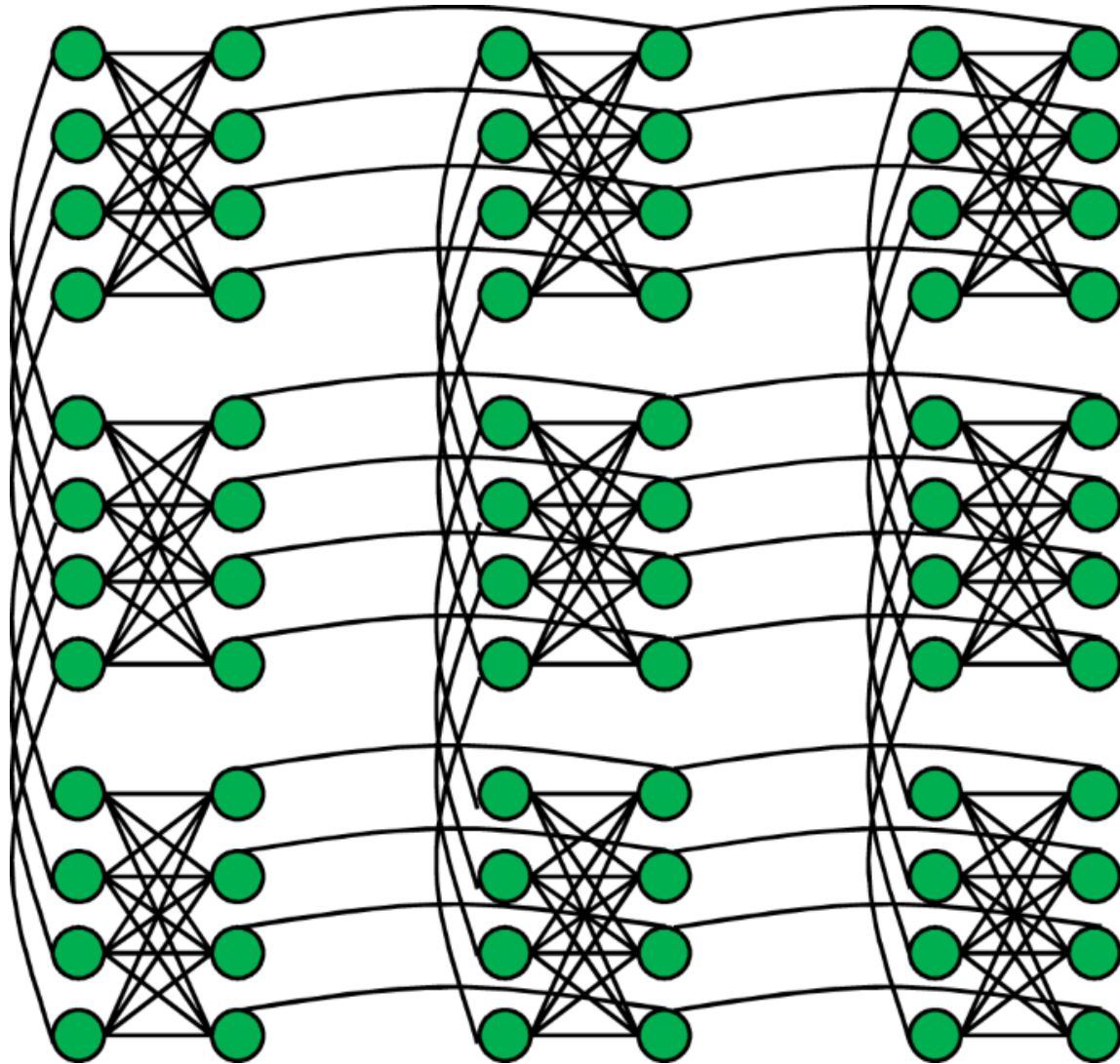
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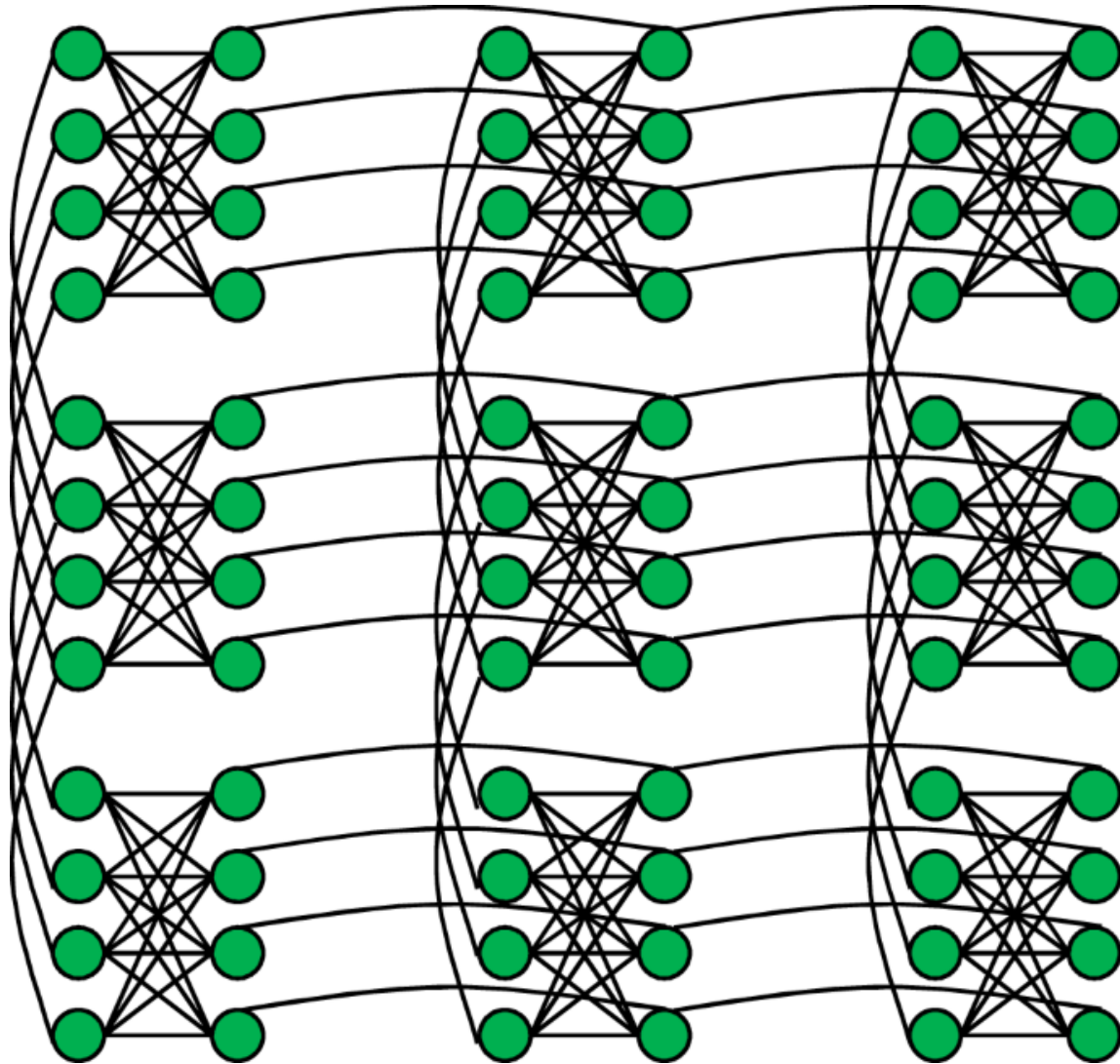
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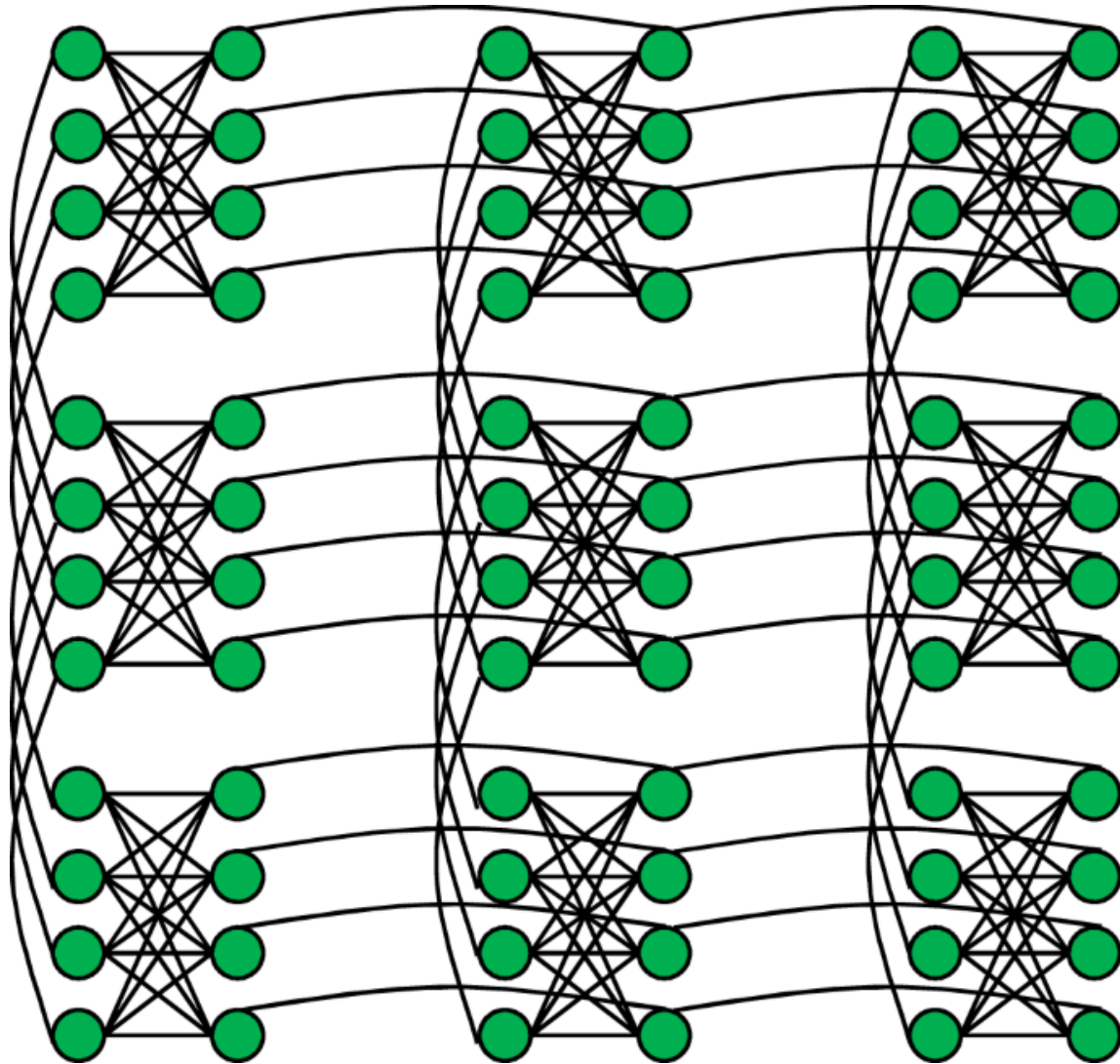
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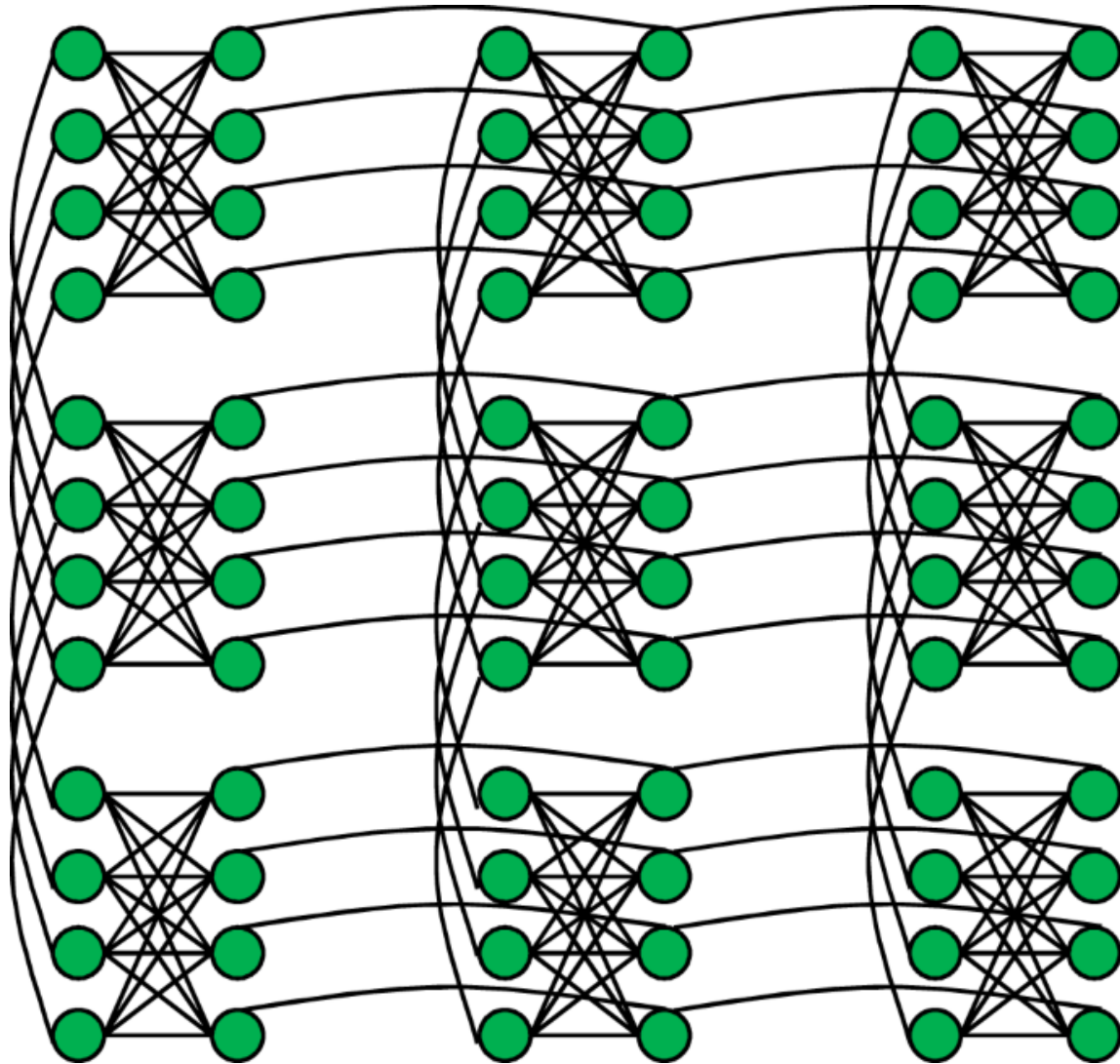
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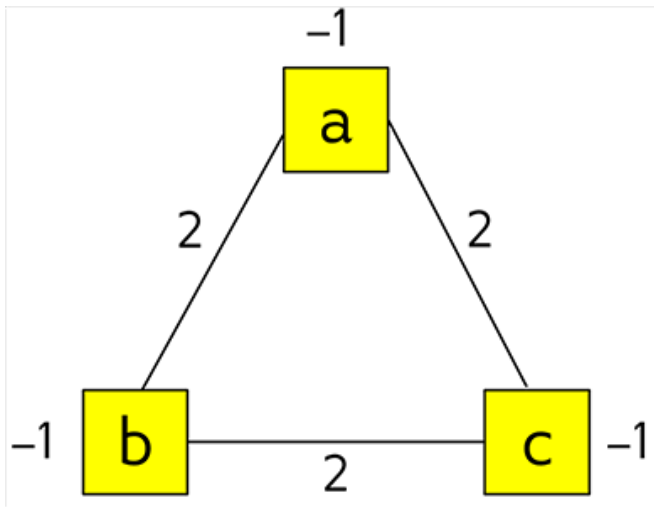
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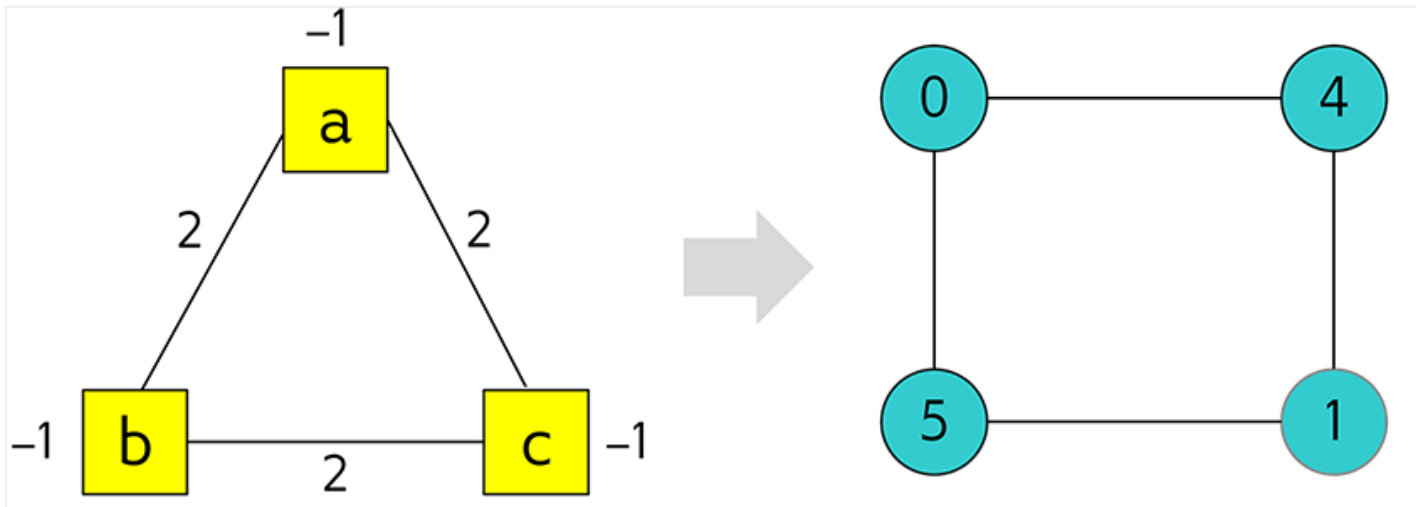
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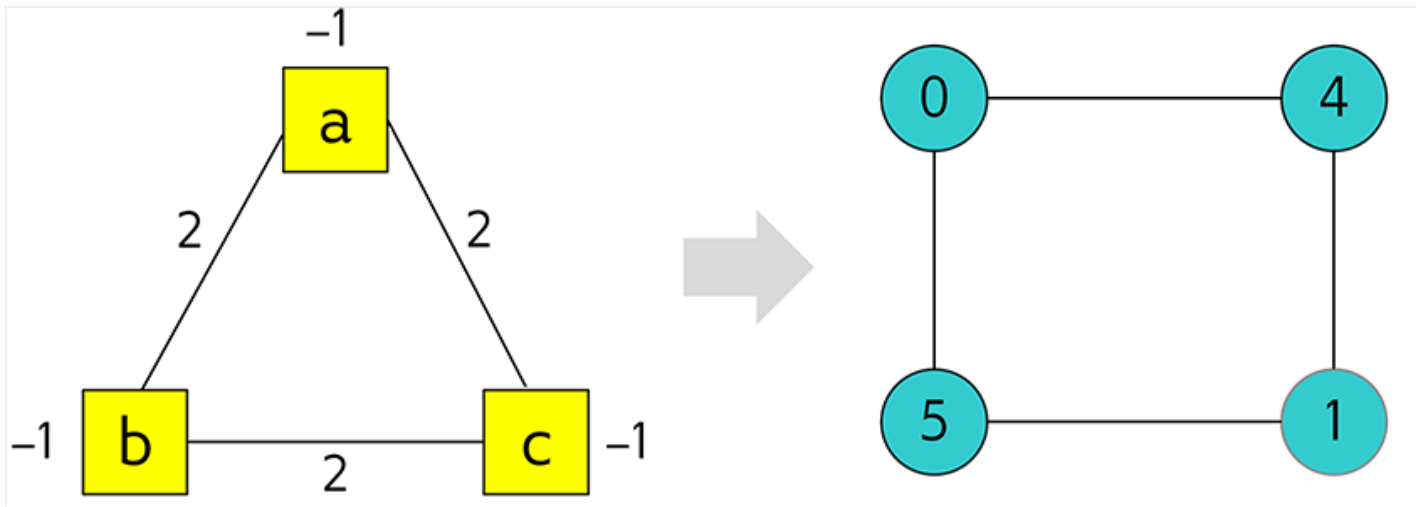
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- Suppose we have a QUBO problem that can be translated with the following graph
- Suppose we also have a quantum annealer with a graph of this shape



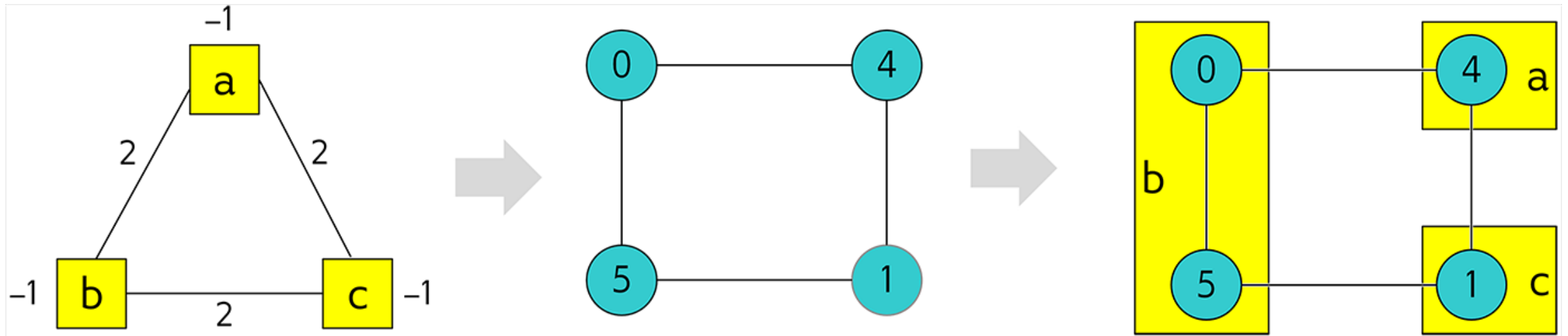
Embedding a problem on a graph

- 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



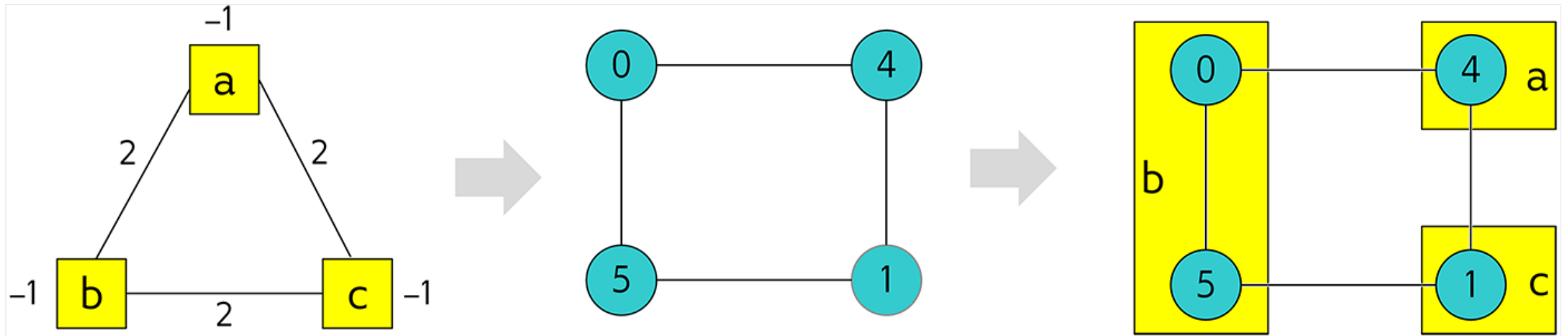
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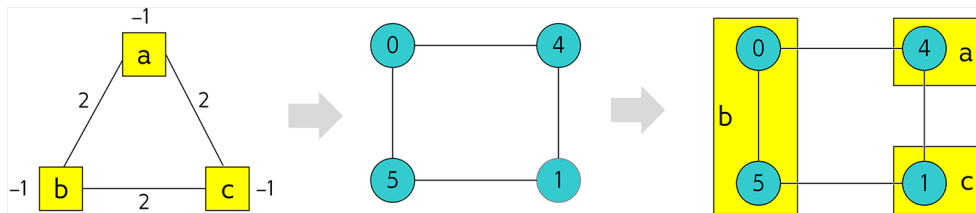
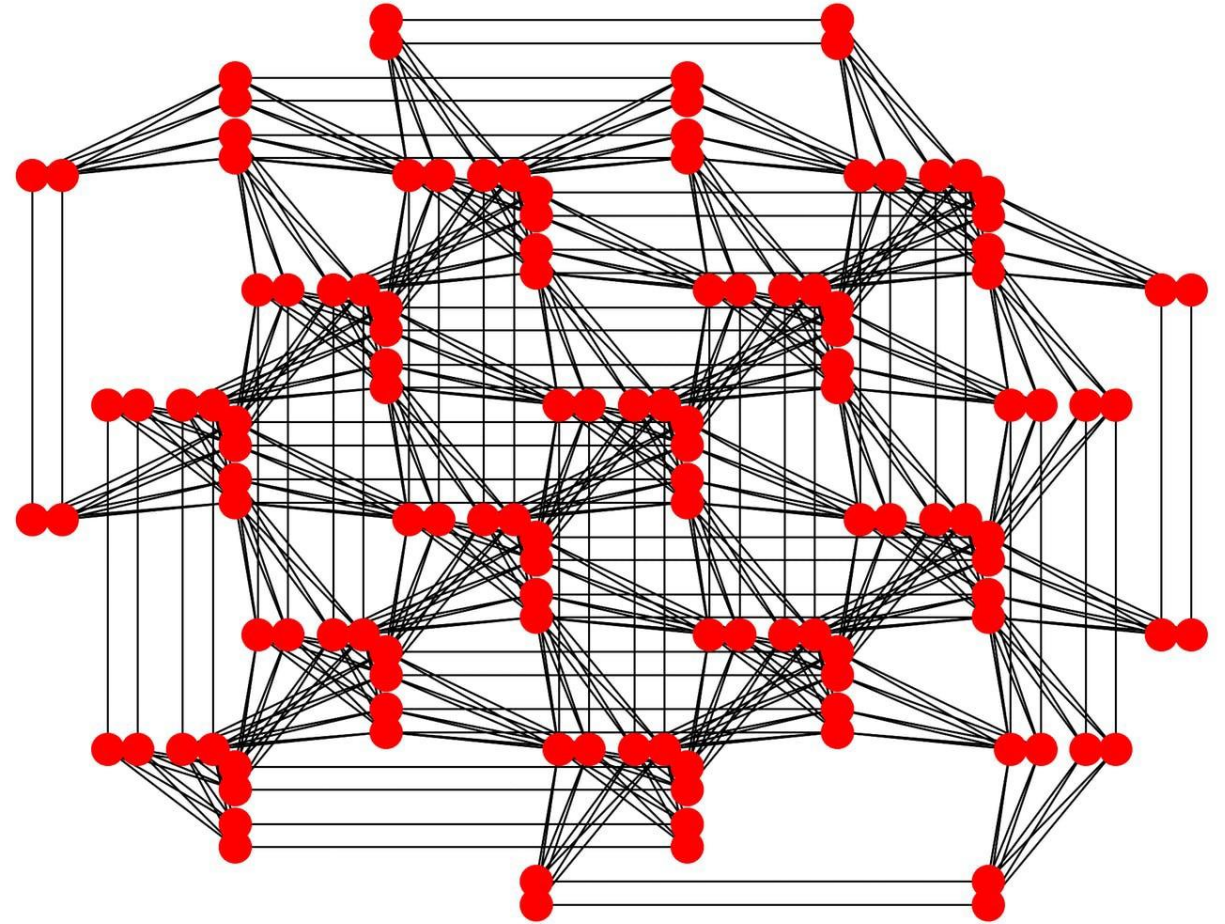
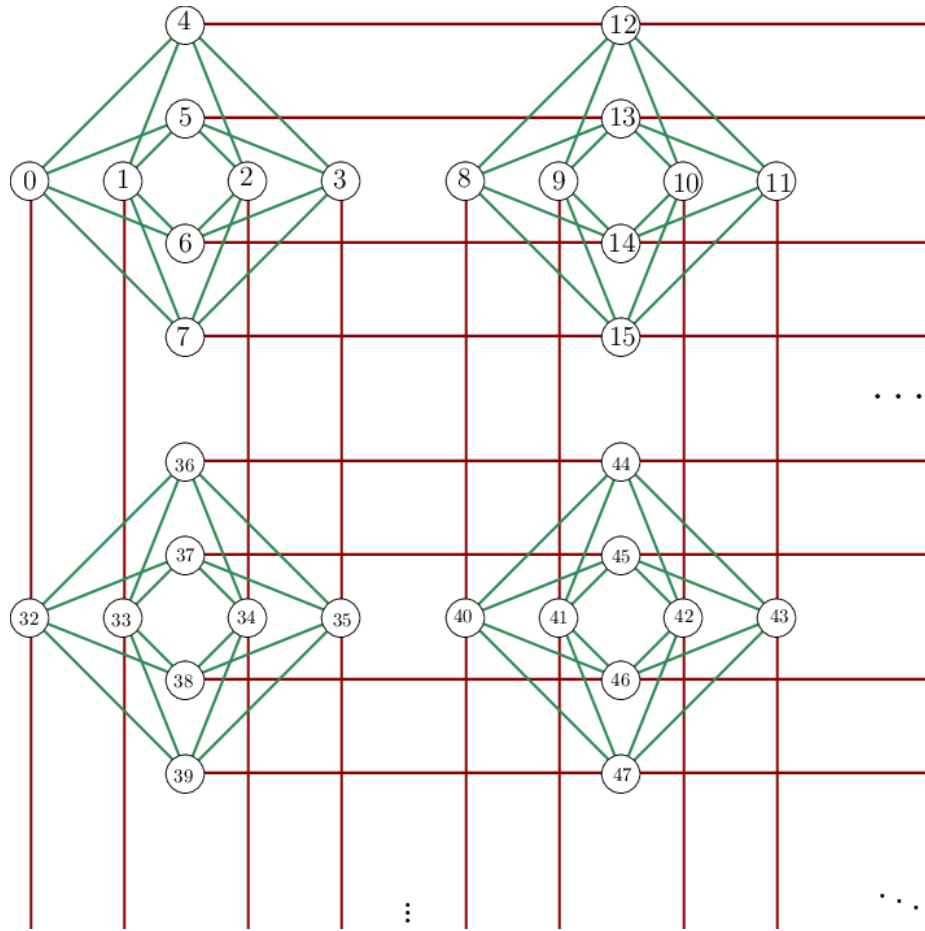


Embedding a problem on a graph

- 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

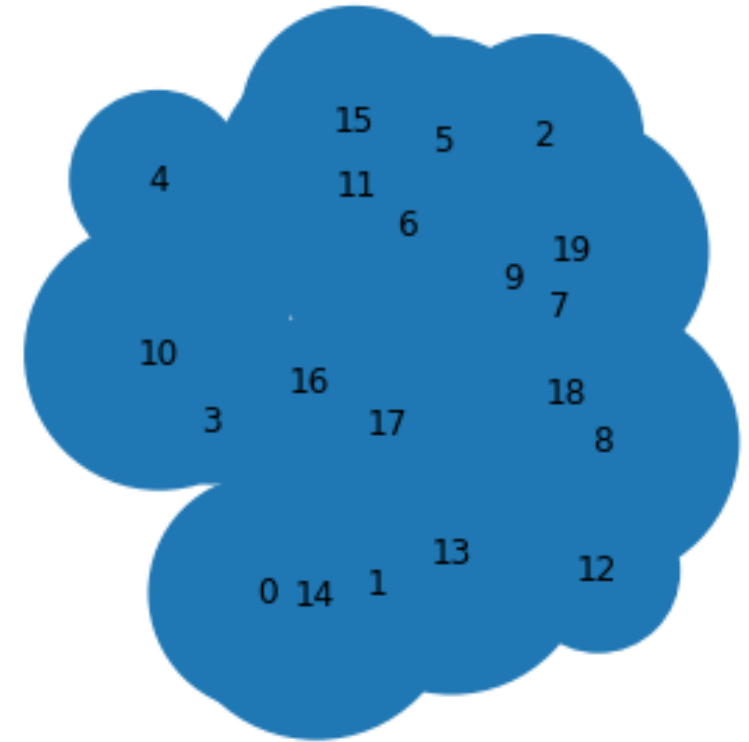
- Implement constraint into the Antenna Placement Problem

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

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

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

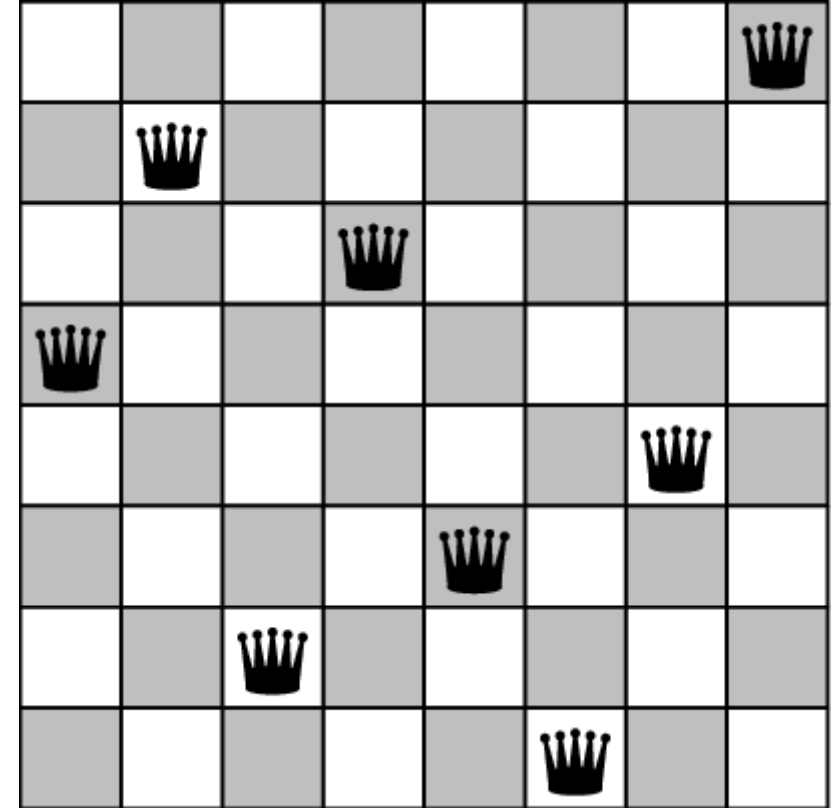
$$\sum_{i=1}^{2N} C_i A_i q_i = A_m$$



- Try the embedding on Pegasus and Chimera

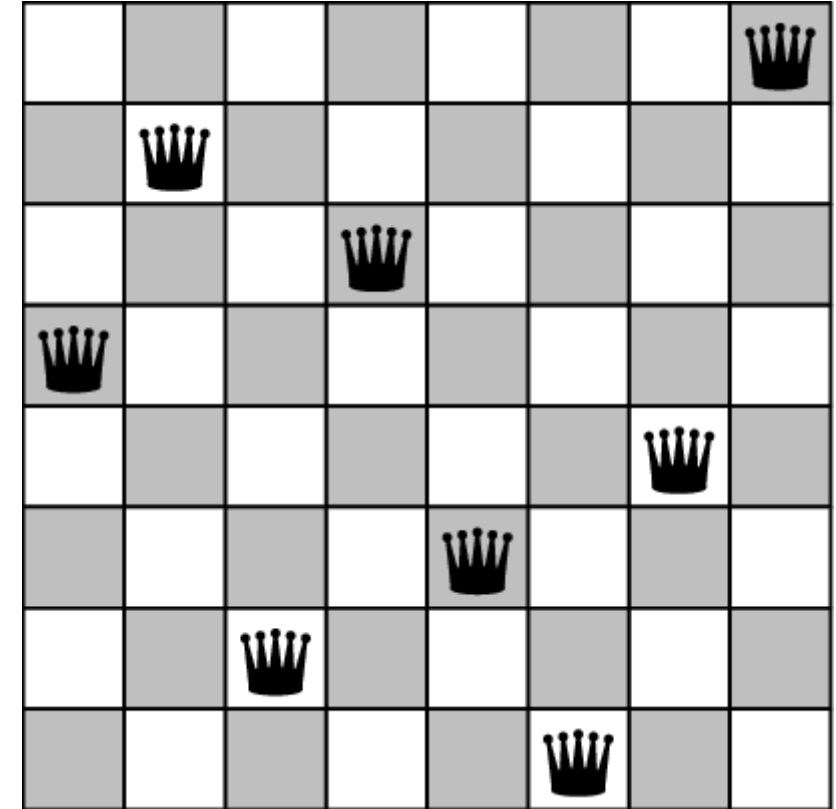
Exercise 3: N-Queens Puzzle

- Let us now turn to another problem: the N-queens puzzle



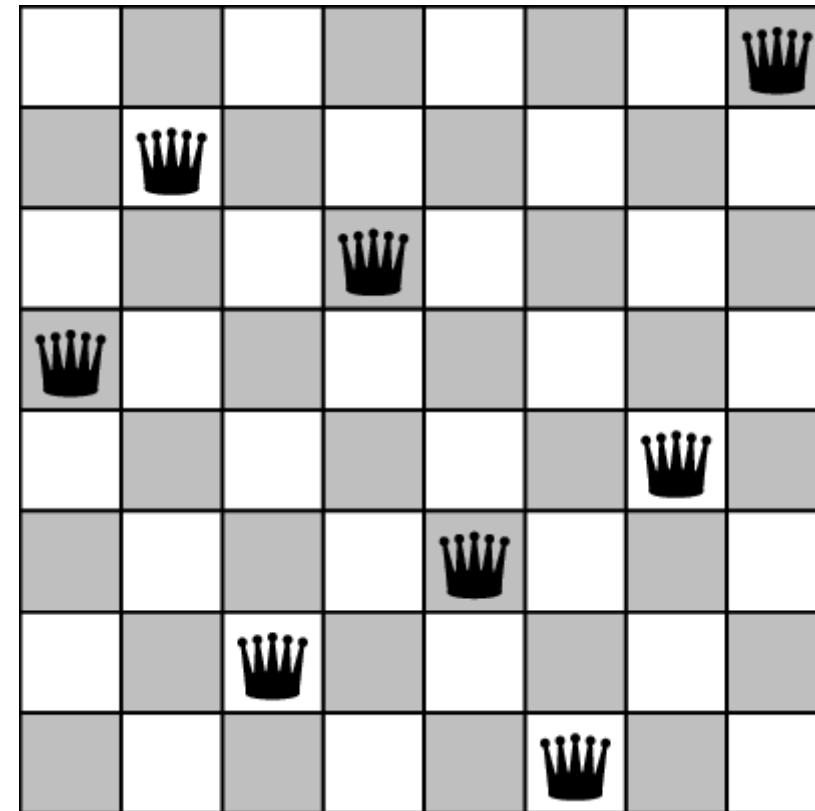
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- Let us now turn to another problem: the N-queens puzzle
- The N-queens puzzle is a generalization of the better known 8-queens puzzle



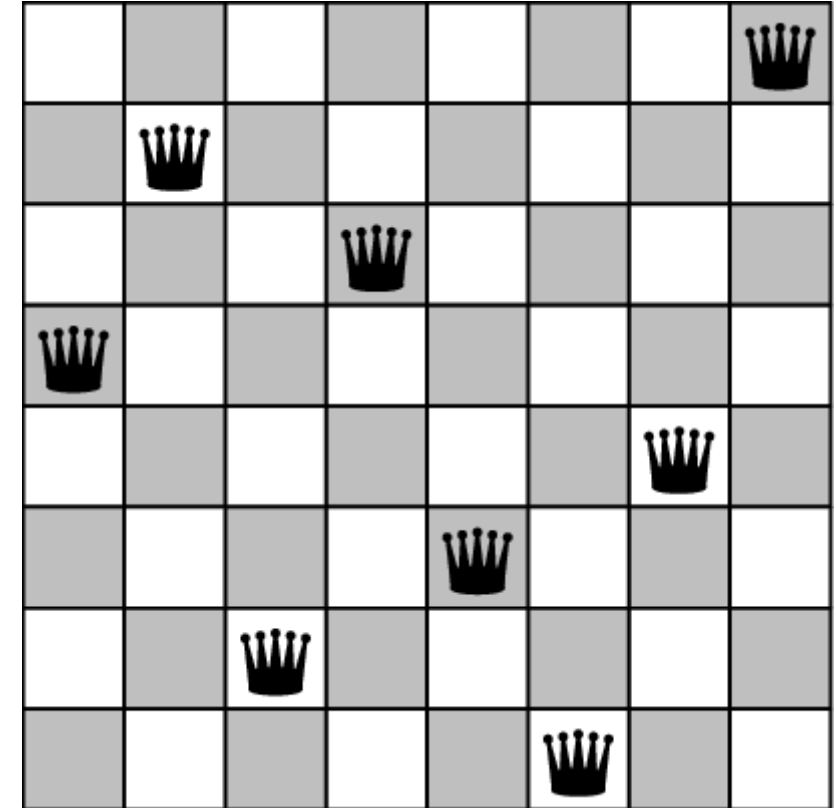
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- Let us now turn to another problem: the N-queens puzzle
- The N-queens puzzle is a generalization of the better known 8-queens puzzle
- The 8-queens puzzle can be described in the following way: let's consider a chessboard. Find a way to arrange 8 queens on the chessboard so that **none of them are in check** by any of the other queens



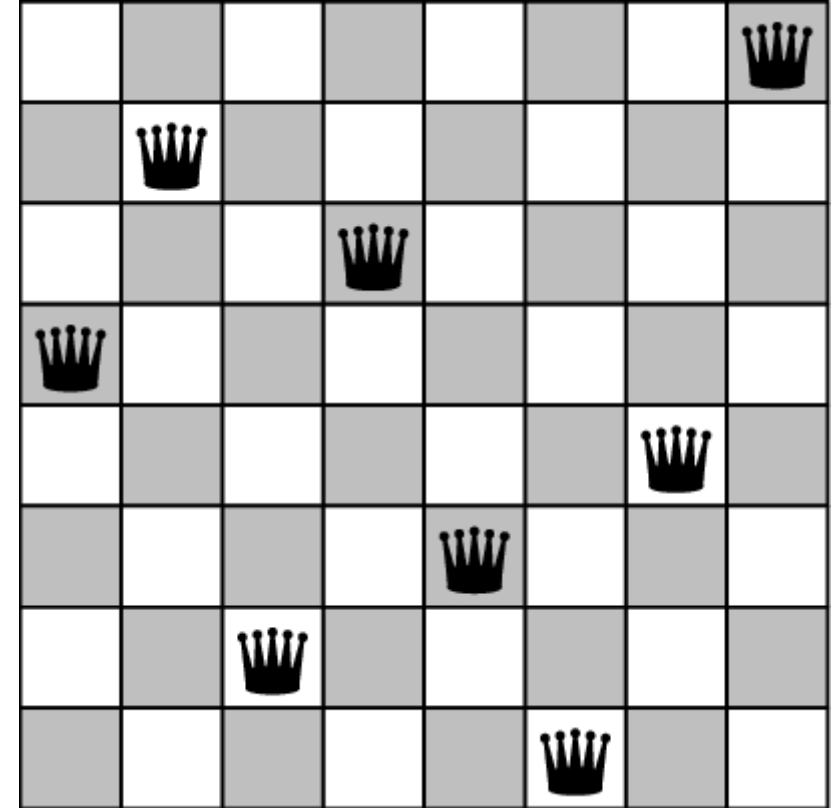
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- The 8-queens puzzle can be described in the following way: let's consider a chessboard. Find a way to arrange 8 queens on the chessboard so that **none of them are in check** by any of the other queens
- The game is generalized as follows: let's consider a chessboard of dimension $N \times N$. Find a way to arrange **N queens** on the chessboard so that none of them are in check by any of the other queens



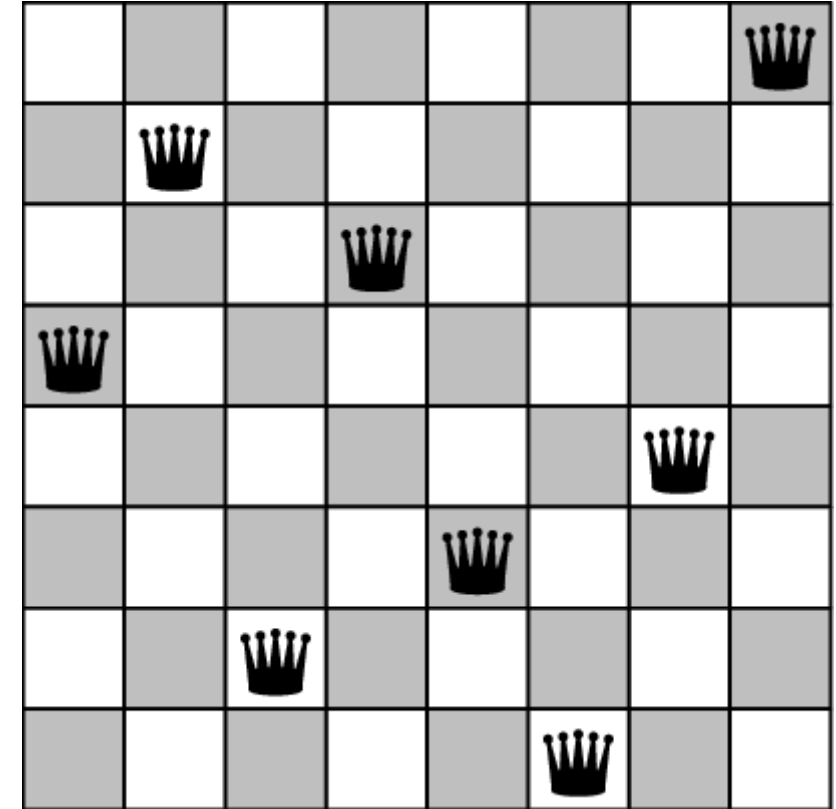
Exercise 3: N-Queens Puzzle

- Let's think about how to turn the problem into a QUBO problem



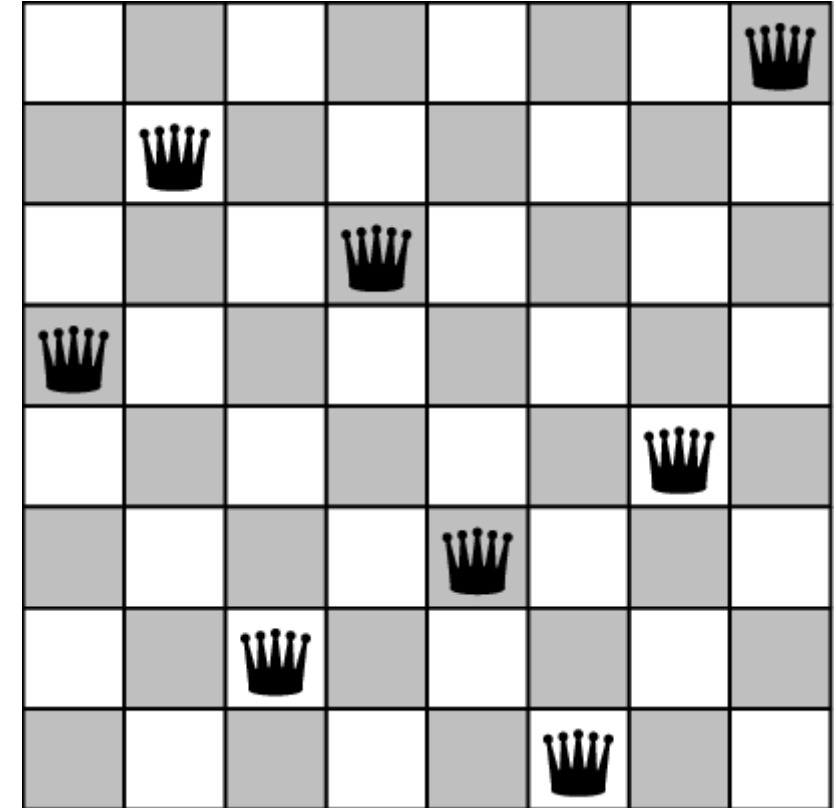
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- Let's think about how to turn the problem into a QUBO problem
- We therefore consider a **vector of binary variables**. We will take **one for each square** of the board we are considering.



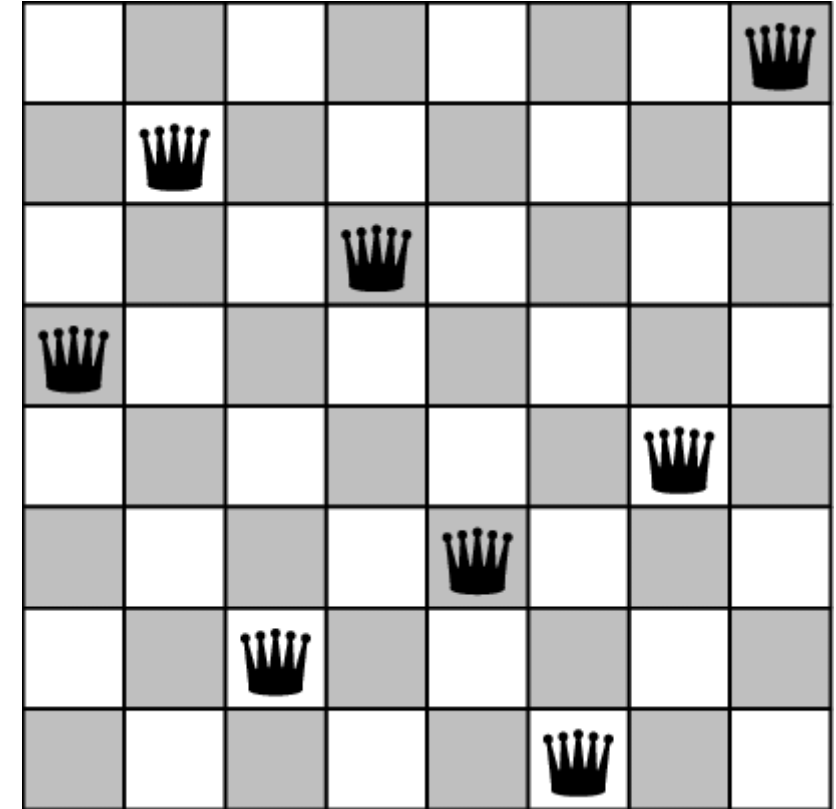
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- Each binary variable is therefore associated with a square on the chessboard



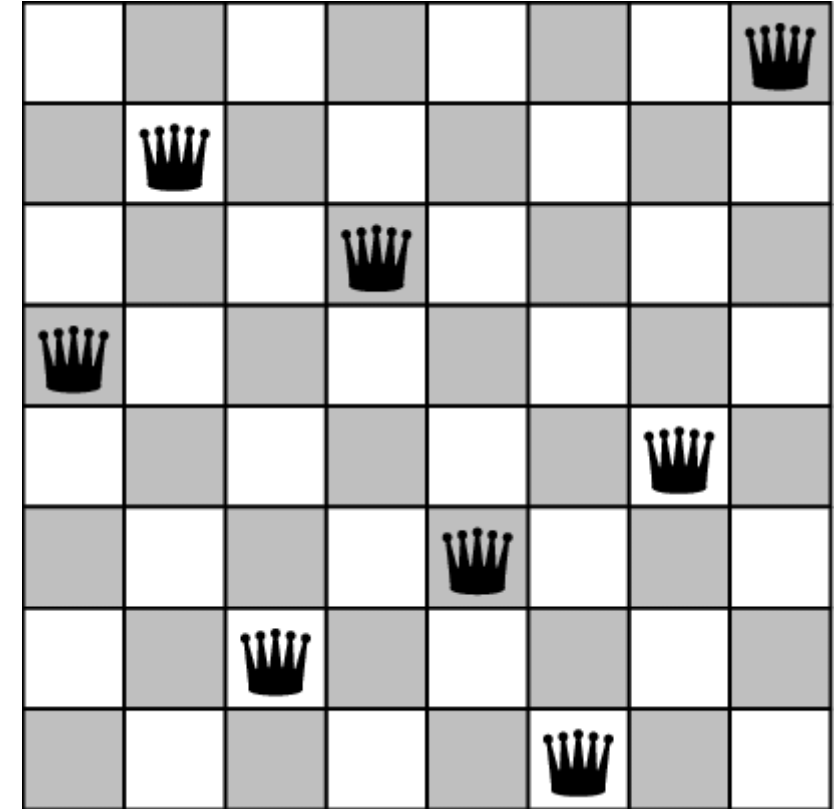
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Exercise 3: N-Queens Puzzle

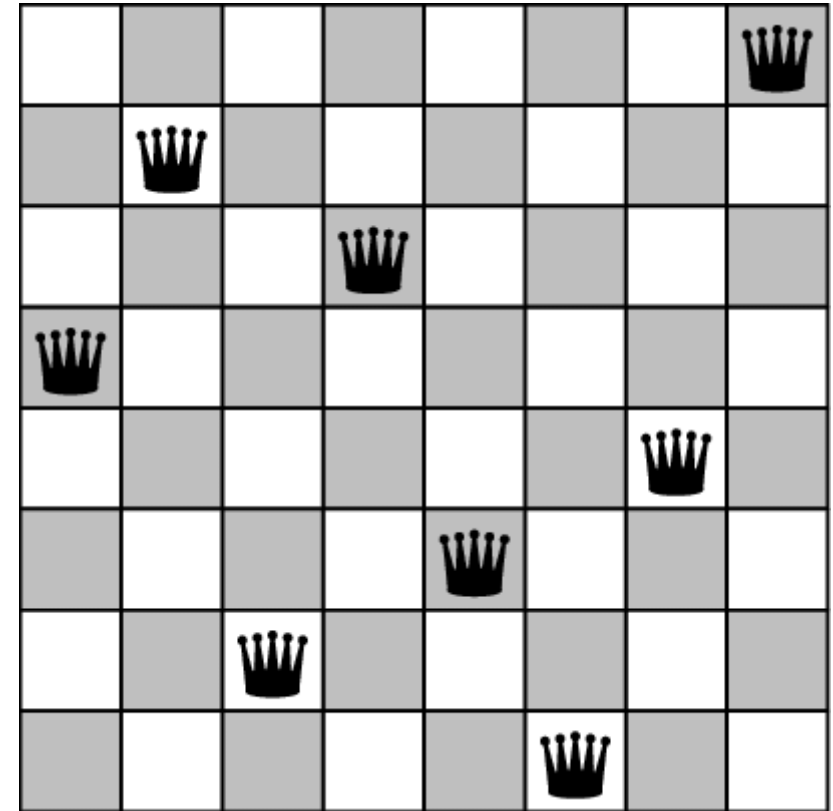
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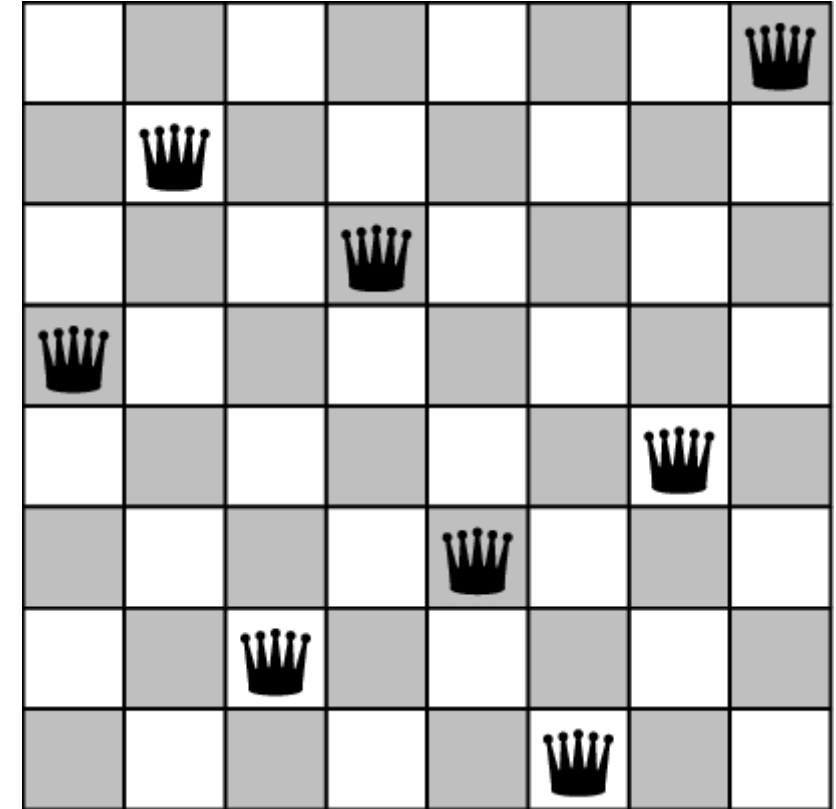
$$\sum_{i=1}^N q_i = N$$



Exercise 3: N-Queens Puzzle

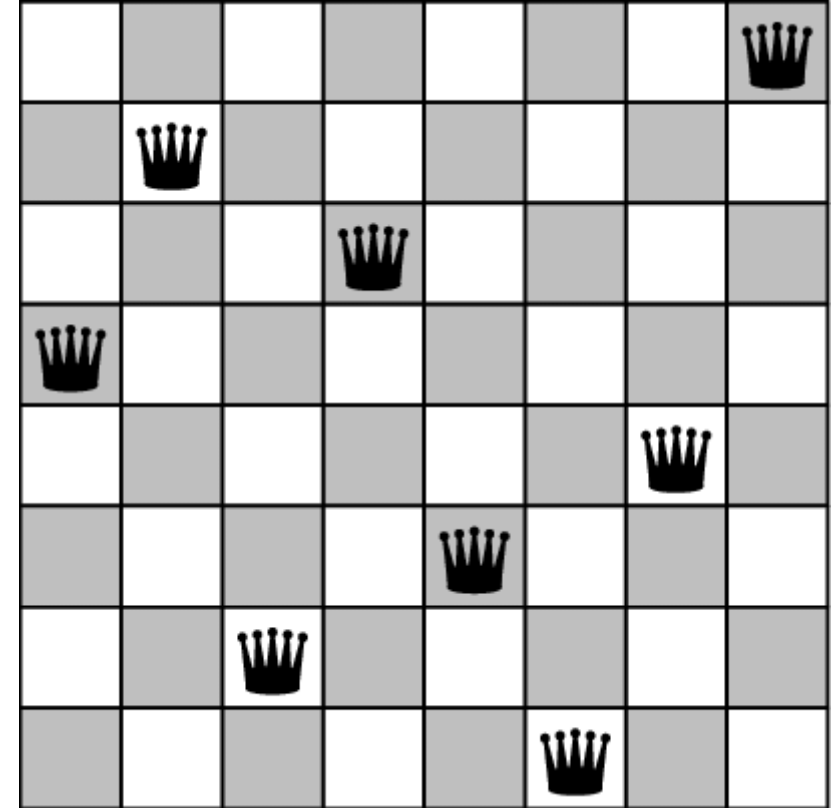
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$$\sum_{i=1}^N q_i = N \Rightarrow \min \left(\sum_{i=1}^N q_i - N \right)^2$$



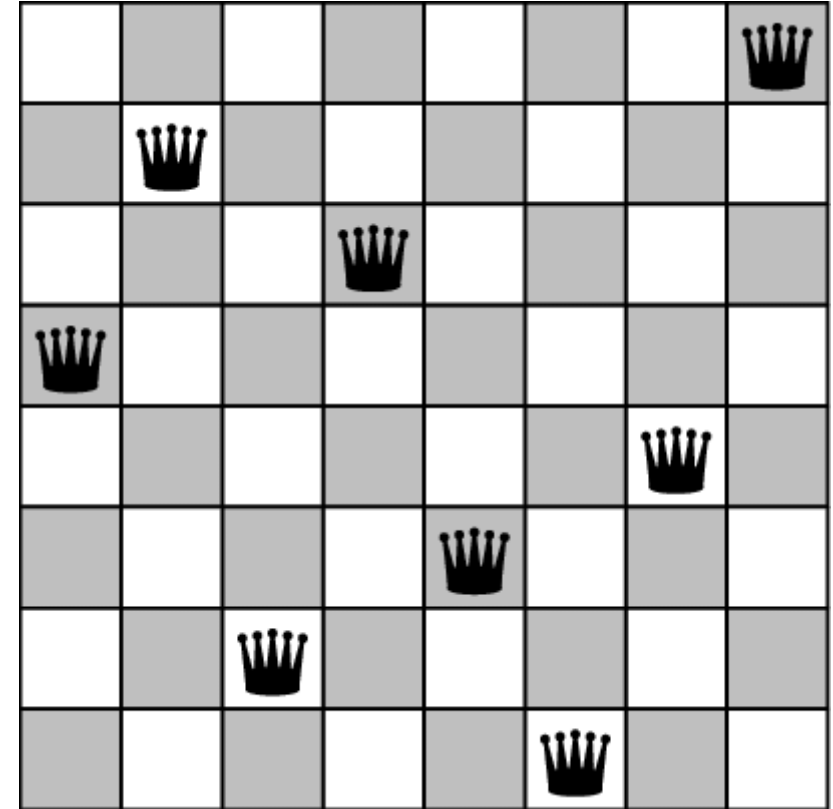
Exercise 3: N-Queens Puzzle

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



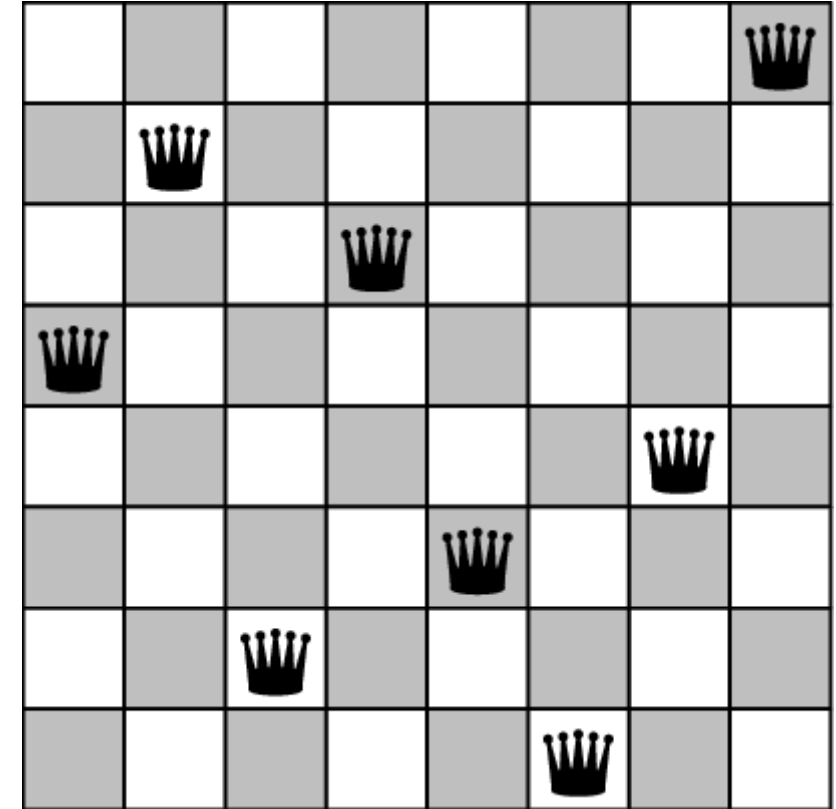
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$$\left(\sum_{i=1}^N q_i - N \right)^2 = \left(\sum_{i=1}^N q_i \right)^2 - 2 \sum_{i=1}^N q_i$$



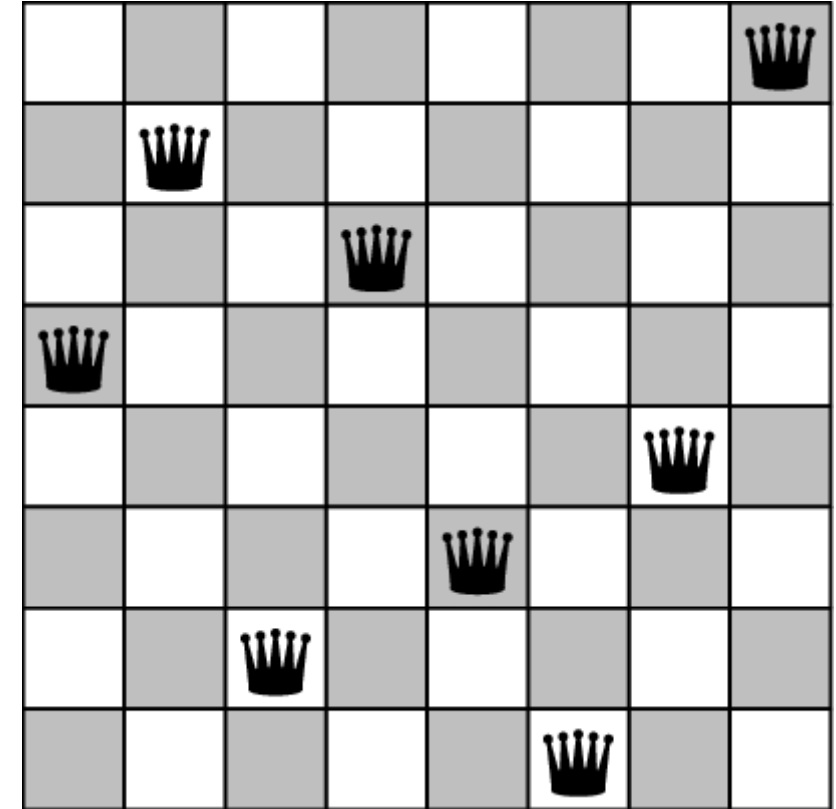
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$$\begin{aligned}\left(\sum_{i=1}^N q_i - N\right)^2 &= \left(\sum_{i=1}^N q_i\right)^2 - 2\sum_{i=1}^N q_i \\ &= \sum_{i=1}^N q_i + 2\sum_{i < j} q_i q_j - 2\sum_{i=1}^N q_i\end{aligned}$$



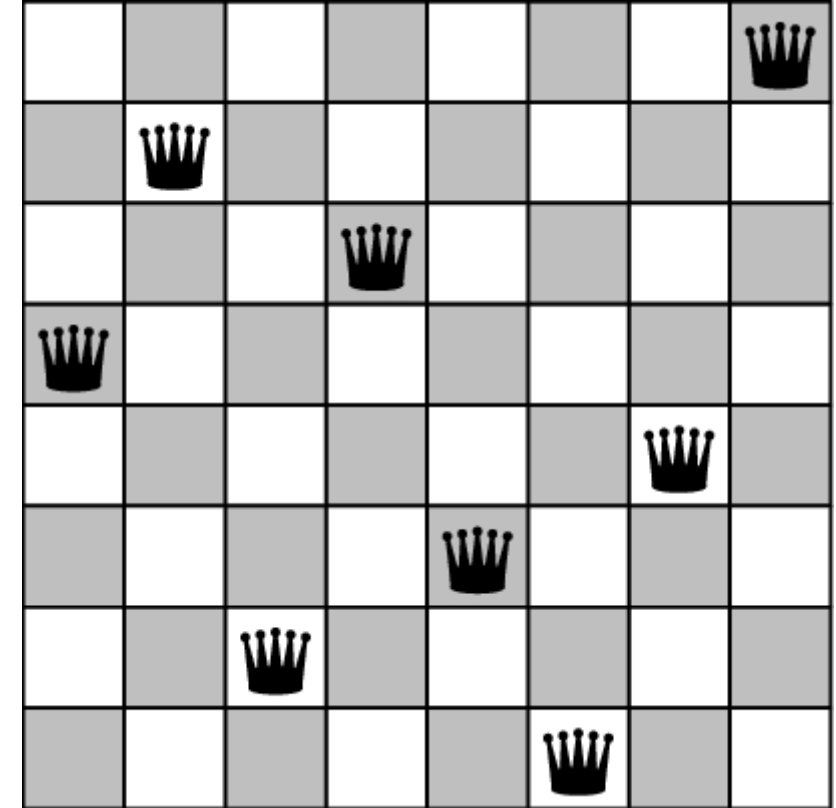
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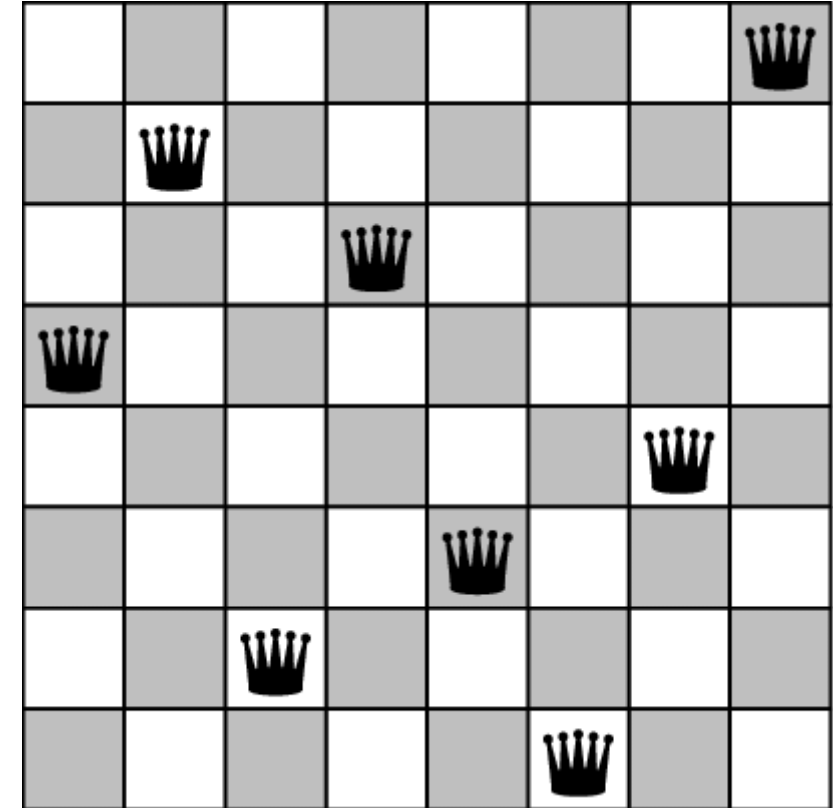
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- Ok, what we have just found can be a good starting point for the construction of the QUBO problem



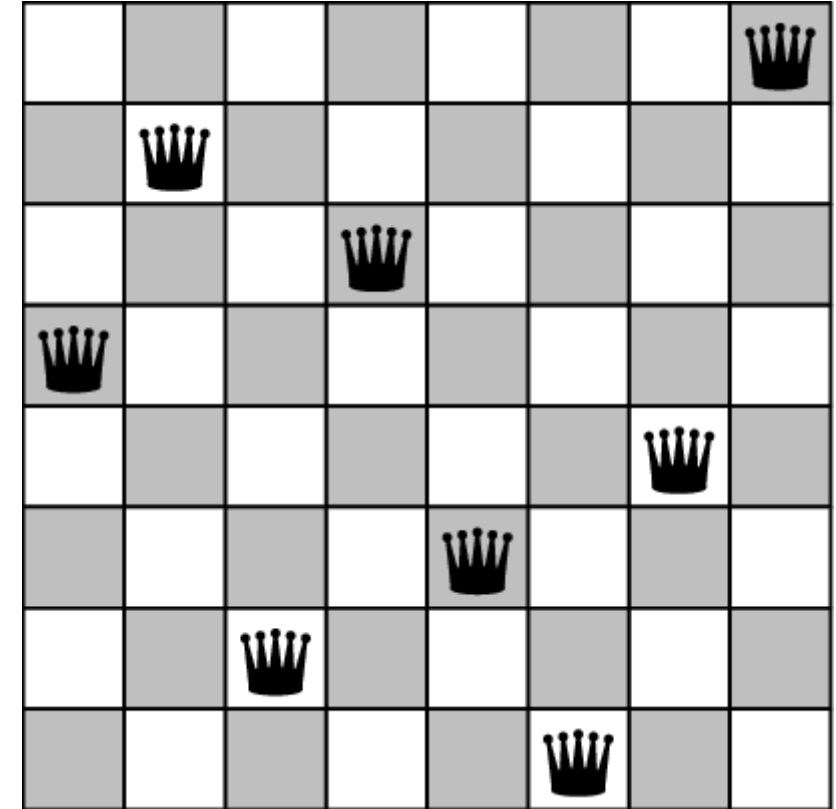
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- Ok, what we have just found can be a good starting point for the construction of the QUBO problem
- Now we have to put some constraints



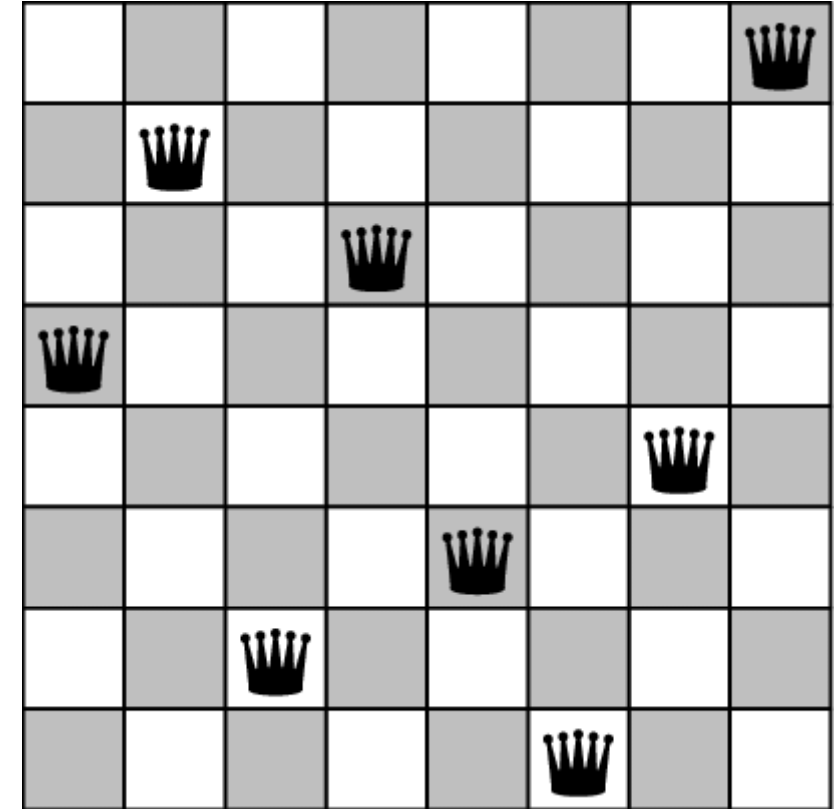
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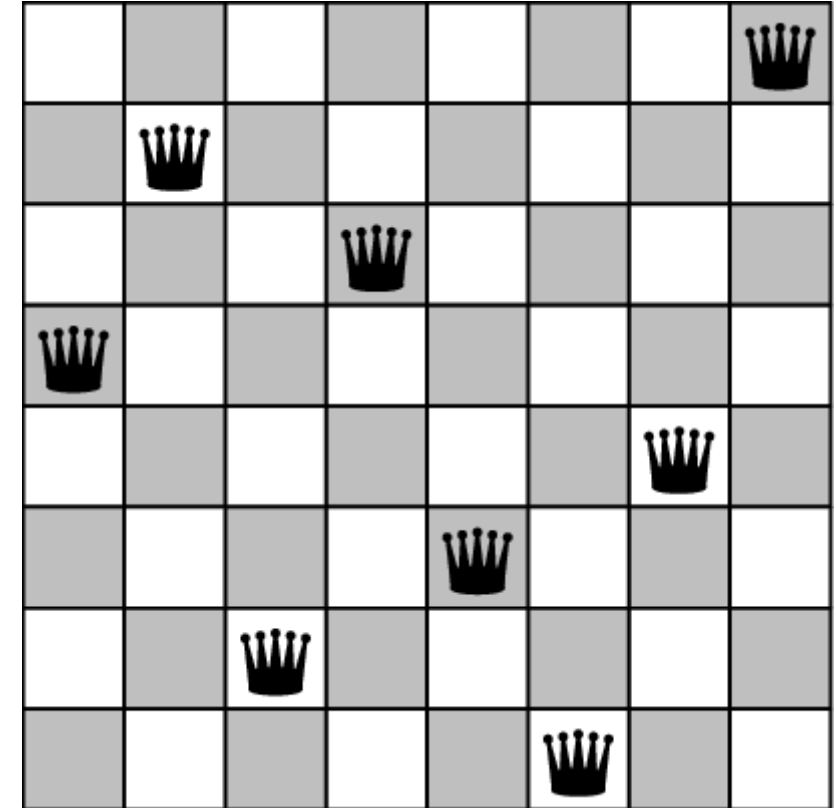
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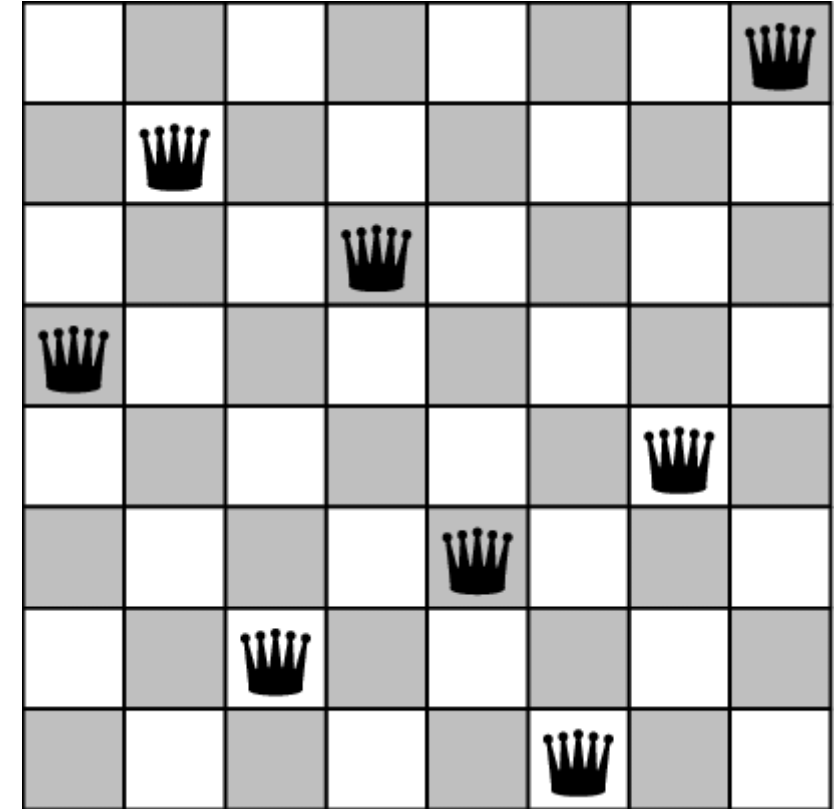
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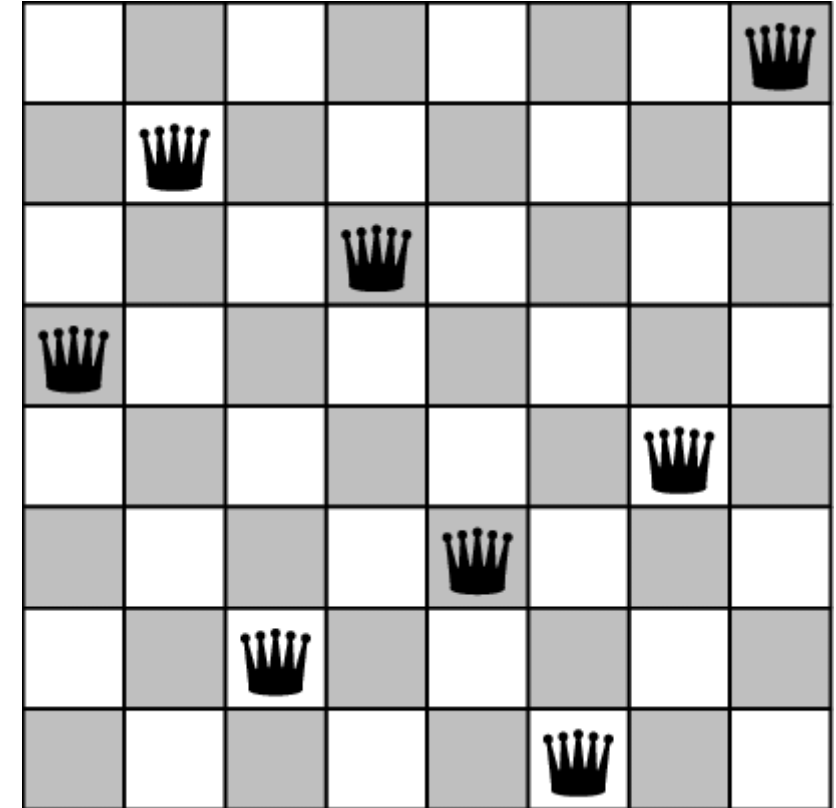
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- At most one queen for each diagonal (both directions)



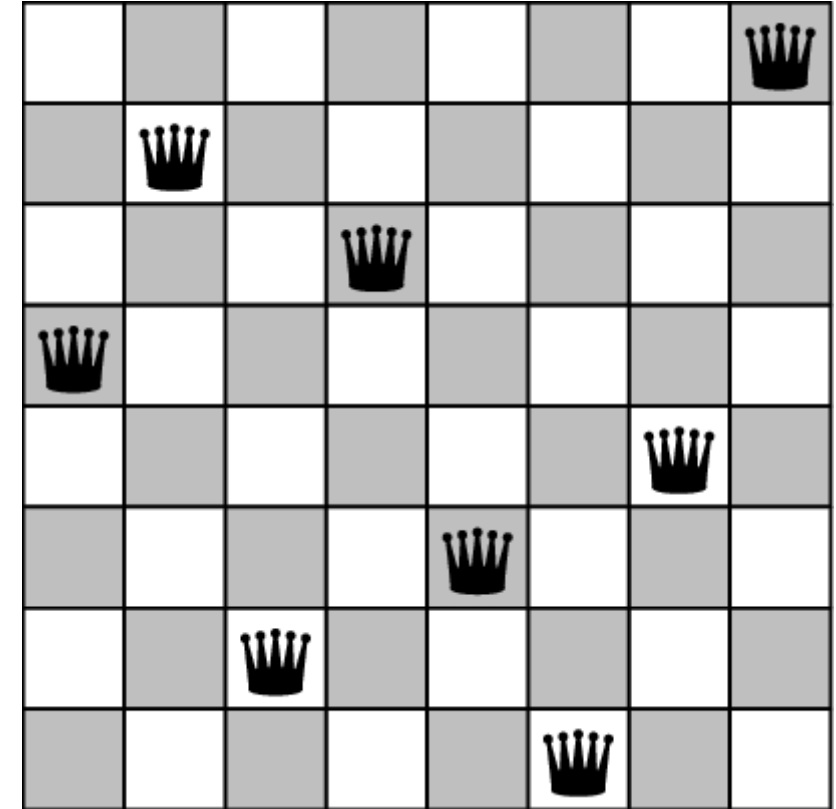
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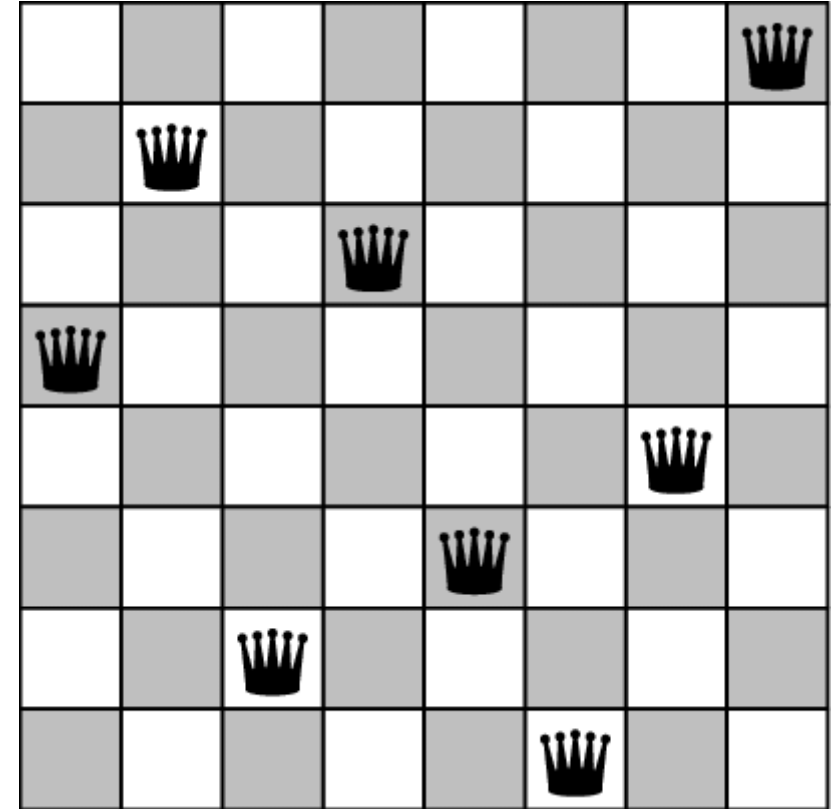
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- The only problem is the large amount of math!



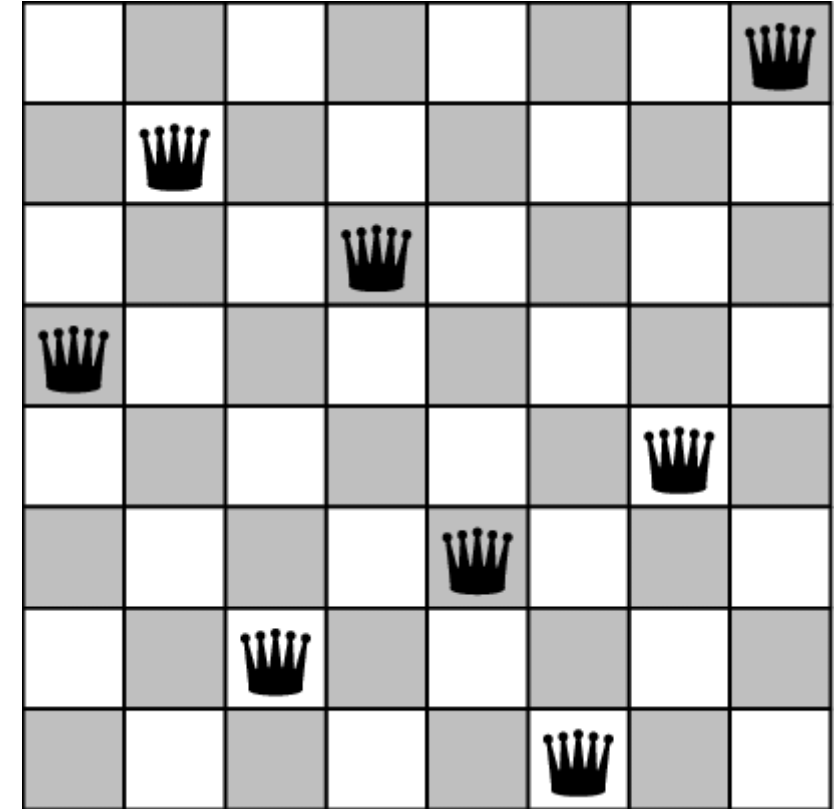
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- Let us then consider the problem from another point of view.



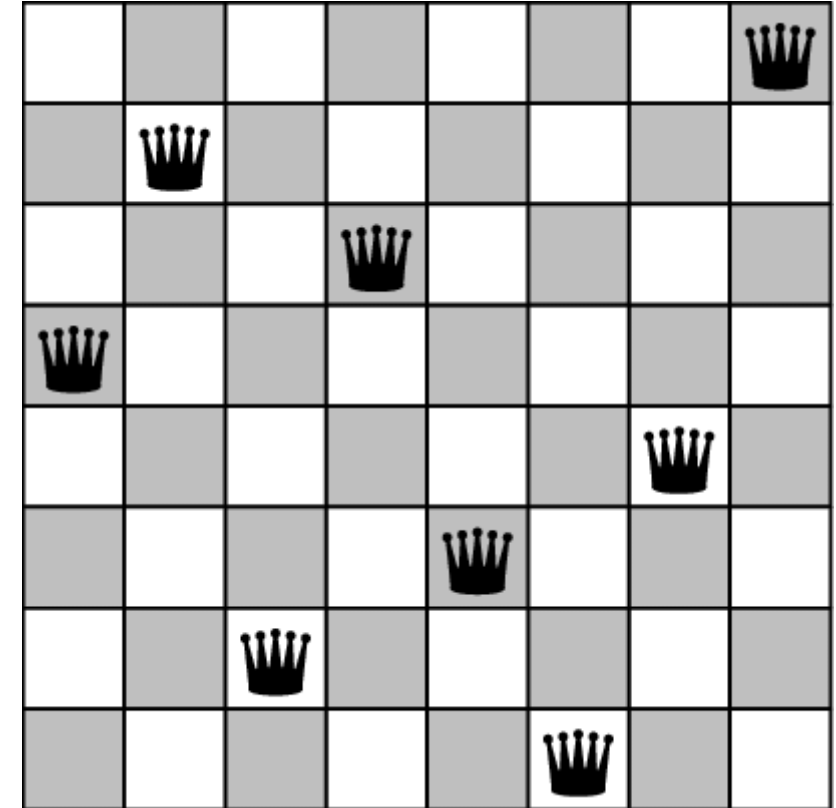
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- Let us then consider the problem from another point of view.
- Instead of mathematically calculating all the constraints, let's do something else



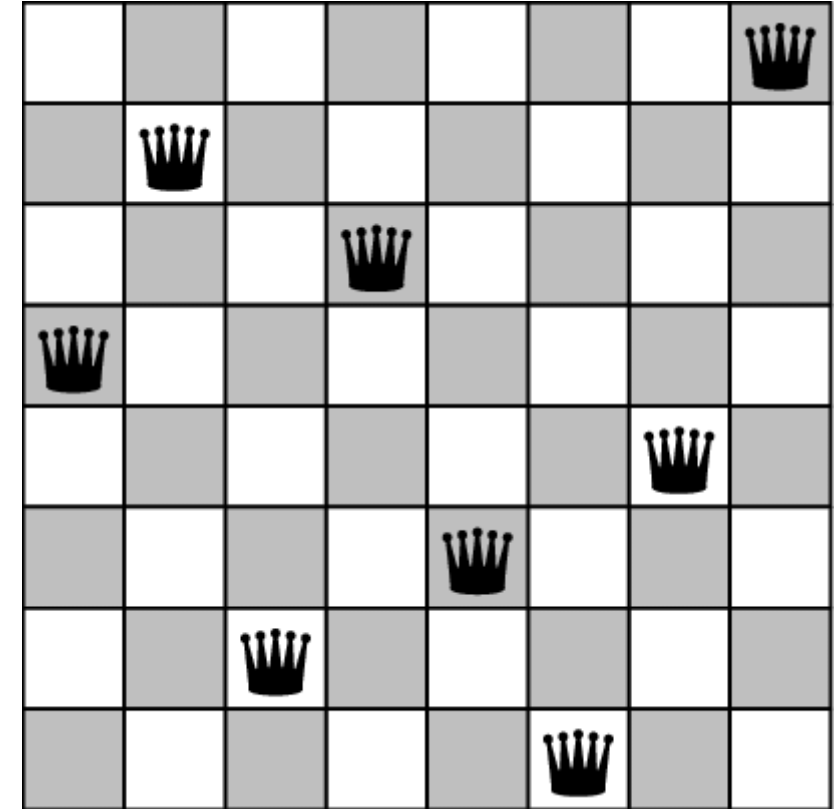
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- Let us then consider the problem from another point of view.
- Instead of mathematically calculating all the constraints, let's do something else
- Let us consider the matrix of the quadratic contributions of the QUBO problem



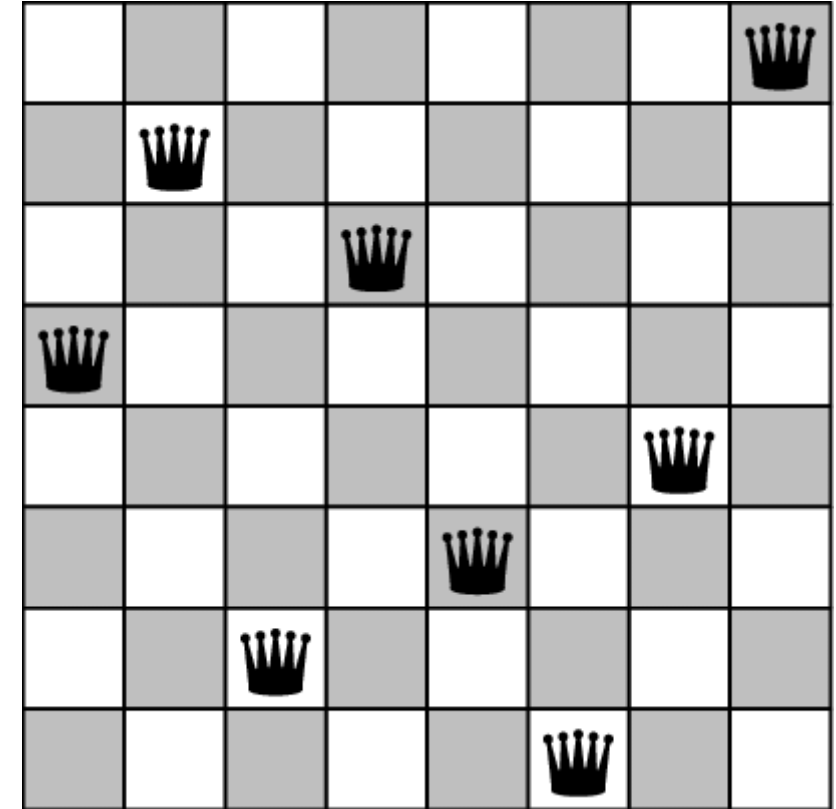
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- Let us then consider the problem from another point of view.
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- Let us consider the matrix of the quadratic contributions of the QUBO problem
- This matrix has as elements all the possible pairs of squares on the chessboard ($N \times N \times N$)



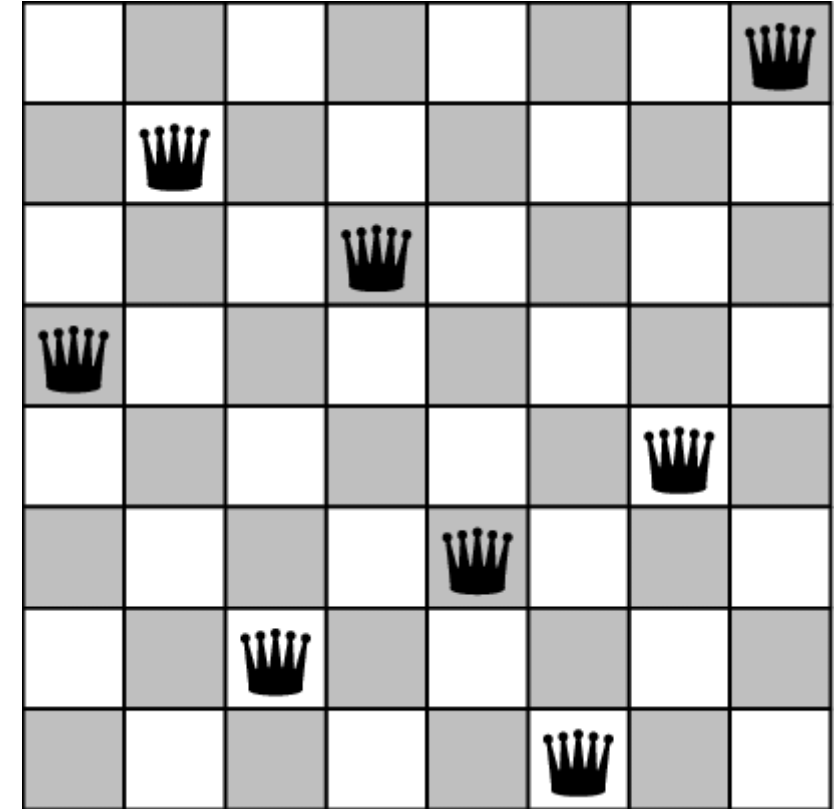
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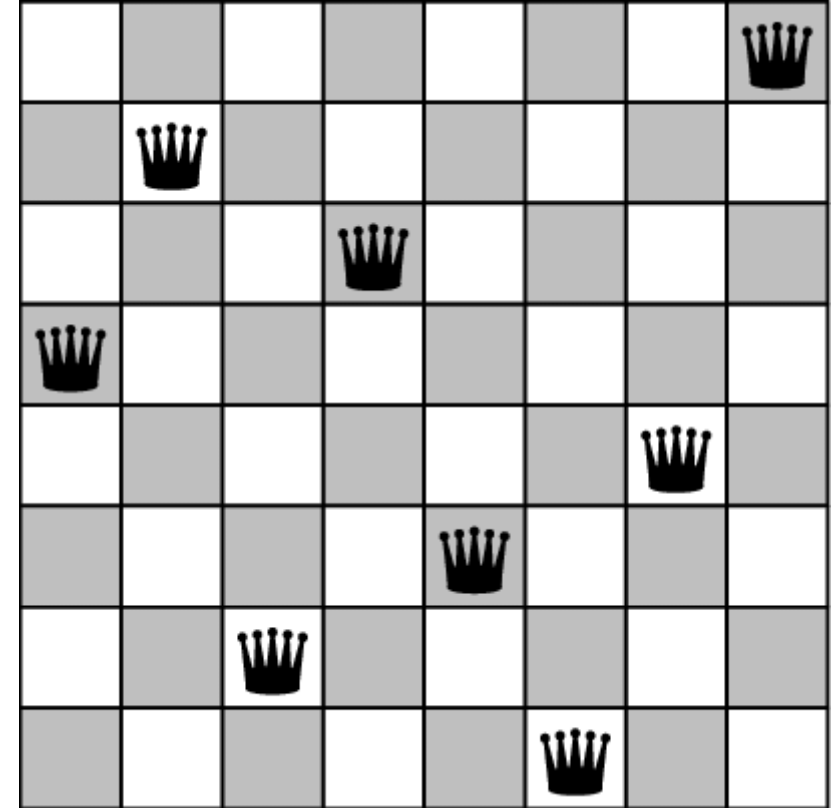
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- To implement our constraints, we do the following: we analyze the matrix of the quadratic contributions and, for each pair that is "forbidden", we increase the value of its weight
- The weight, by definition, is activated only if both qubits, or squares, are in state 1, i.e. both host a queen



Exercise 3: N-Queens Puzzle

- One way to do this, is to define a function in this way

```
def ROW(row,dim):  
    C=np.zeros((dim,dim), dtype=int)  
    C[row,:] = 1  
    return C.flatten()
```

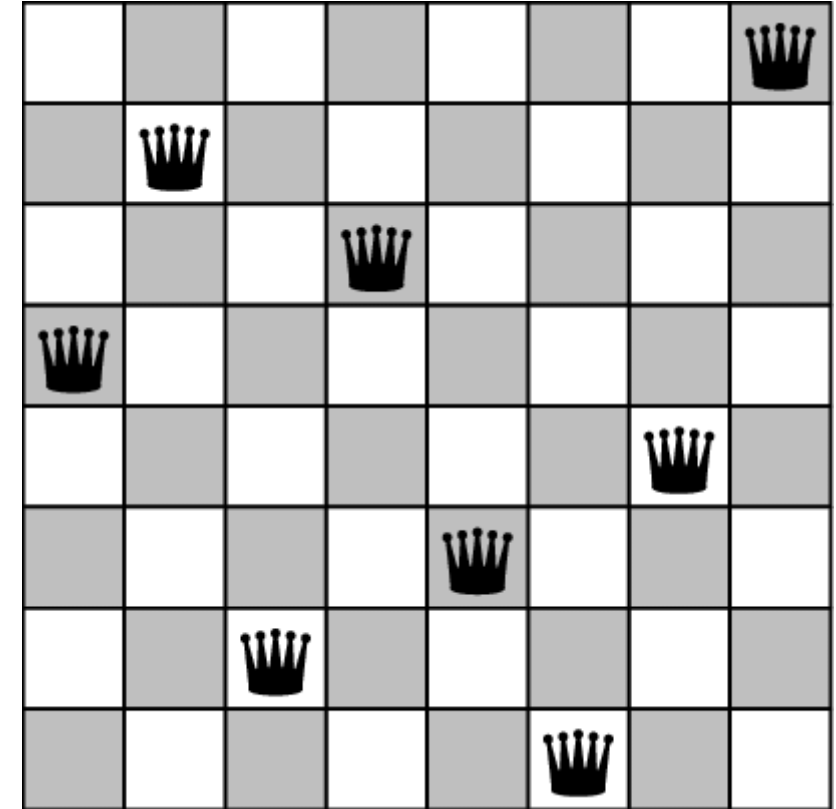


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- This function calculates a linearized vector containing all the possible pairs of squares on the board

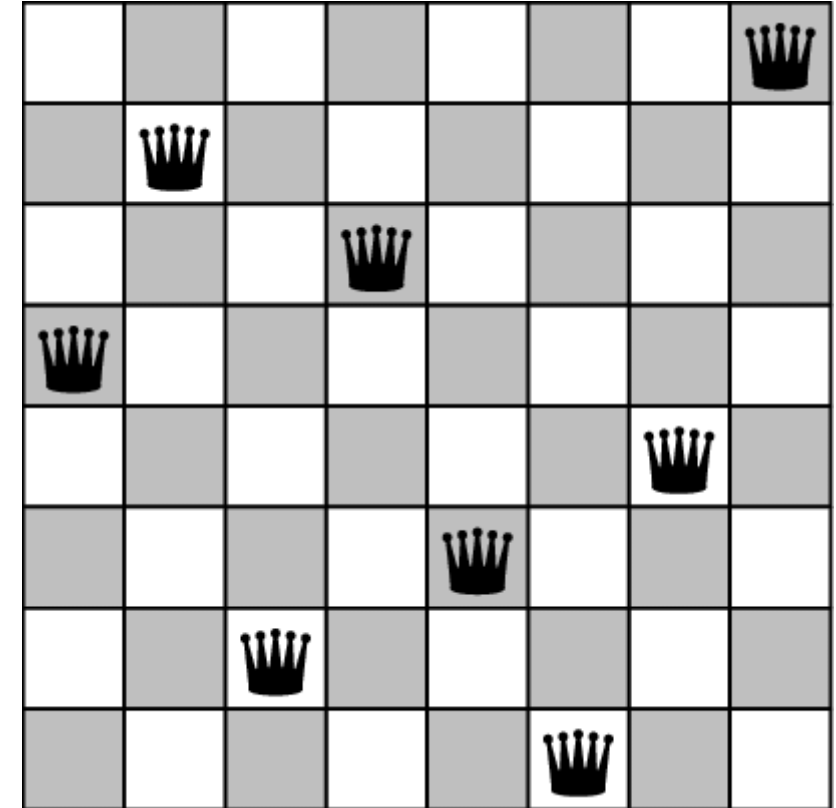


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- Once a specific row has been chosen, the vector will have the value 1 if the pair of squares belongs to the same row, 0 otherwise
- With this definition, I can start building the penalty matrix like this

```
N=4
w=1
B=np.zeros((N*N,N*N), dtype=float)
for row in range(N):
    R=ROW(row,N)
    for i in range(N*N):
        for j in range(i+1,N*N):
            B[i][j]=B[i][j]+R[i]*R[j]*w
print(B)
```

```
[
[0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
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- With this definition, I can start building the penalty matrix like this
- Basically I'm saying: if two squares are part of the same row, it increases their weight by a factor w

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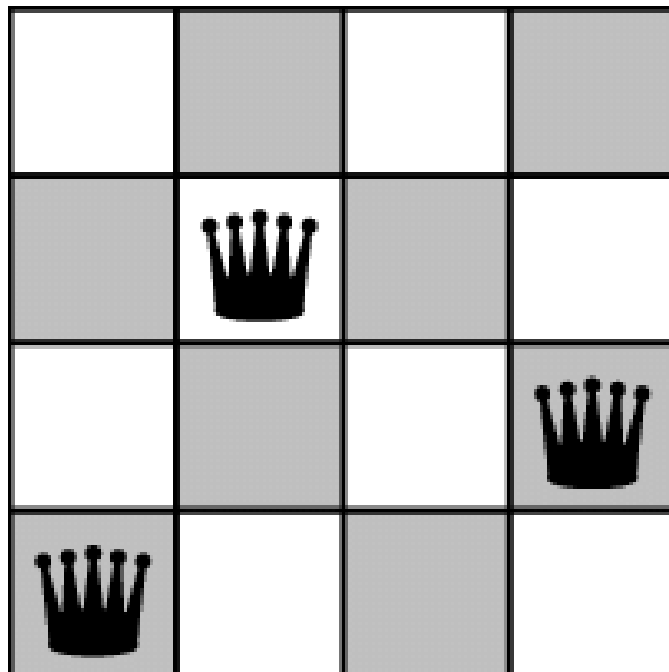
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[
[0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
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[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
]
```

Exercise 3: N-Queens Puzzle

- One way to do this, is to define a function in this way

```
def ROW(row,dim):
    C=np.zeros((dim,dim), dtype=int)
    C[row,:]=1
    return C.flatten()
```

```
R=ROW(0,4)
```

$$\begin{bmatrix} [1 & 1 & 1 & 1] \\ [0 & 0 & 0 & 0] \\ [0 & 0 & 0 & 0] \\ [0 & 0 & 0 & 0] \end{bmatrix}$$


```
N=4
w=1
B=np.zeros((N*N,N*N), dtype=float)
for row in range(N):
    R=ROW(row,N)
    for i in range(N*N):
        for j in range(i+1,N*N):
            B[i][j]=B[i][j]+R[i]*R[j]*w
print(B)
```

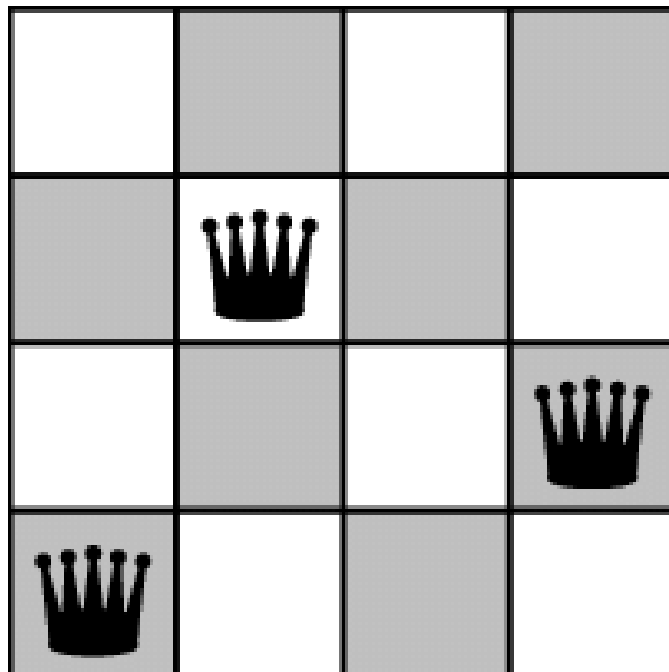
```
[
[0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
]
```

Exercise 3: N-Queens Puzzle

- One way to do this, is to define a function in this way

```
def ROW(row,dim):
    C=np.zeros((dim,dim), dtype=int)
    C[row,:]=1
    return C.flatten()
```

```
R=ROW(0,4)
```

$$\begin{bmatrix} [1 & 1 & 1 & 1] \\ [0 & 0 & 0 & 0] \\ [0 & 0 & 0 & 0] \\ [0 & 0 & 0 & 0] \end{bmatrix}$$
$$[1 \ 1 \ 1 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]$$


```
N=4
w=1
B=np.zeros((N*N,N*N), dtype=float)
for row in range(N):
    R=ROW(row,N)
    for i in range(N*N):
        for j in range(i+1,N*N):
            B[i][j]=B[i][j]+R[i]*R[j]*w
print(B)
```

```
[
[0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
]
```

Exercise 3: N-Queens Puzzle

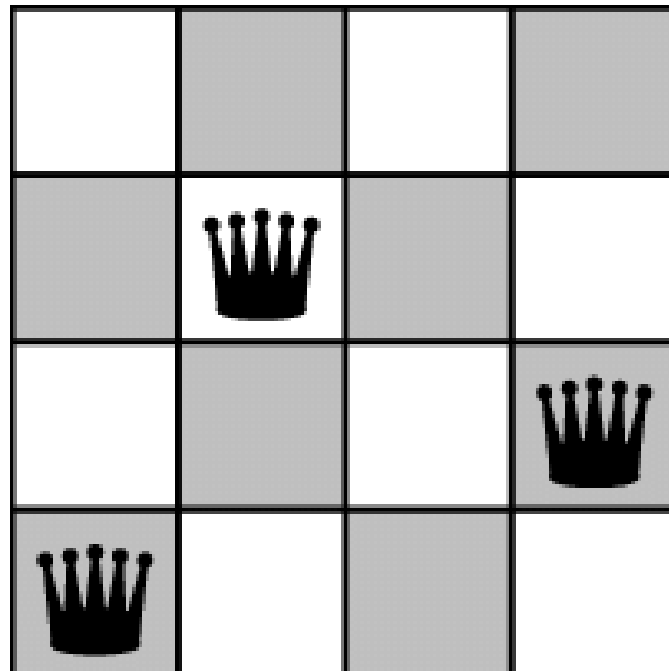
- One way to do this, is to define a function in this way

```
def ROW(row,dim):  
    C=np.zeros((dim,dim), dtype=int)  
    C[row,:]=1  
    return C.flatten()
```

```
R=ROW(1,4)
```

```
[[0 0 0 0]  
 [1 1 1 1]  
 [0 0 0 0]  
 [0 0 0 0]]
```

```
[0 0 0 0 1 1 1 1 0 0 0 0 0 0 0 0]
```



```
N=4  
  
w=1  
  
B=np.zeros((N*N,N*N), dtype=float)  
for row in range(N):  
    R=ROW(row,N)  
    for i in range(N*N):  
        for j in range(i+1,N*N):  
            B[i][j]=B[i][j]+R[i]*R[j]*w  
print(B)
```

```
[[0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
```

Exercise 3: N-Queens Puzzle

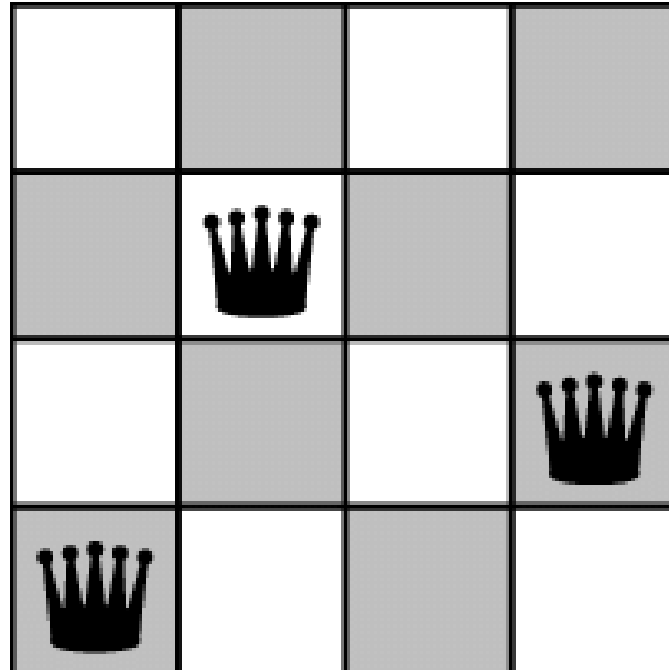
- Same thing for columns

```
def COL(col,dim):  
    C=np.zeros((dim,dim), dtype=int)  
    C[:,col] = 1  
    return C.flatten()
```

```
C=COL(0,4)
```

```
[[1 0 0 0]  
 [1 0 0 0]  
 [1 0 0 0]  
 [1 0 0 0]]
```

```
[1 0 0 0 1 0 0 0 1 0 0 0 1 0 0 0]
```



```
for col in range(N):  
    C=COL(col,N)  
    for i in range(N*N):  
        for j in range(i+1,N*N):  
            B[i][j]=B[i][j]+C[i]*C[j]*w  
  
print(B)
```

```
[[0. 1. 1. 1. 1. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0.]  
 [0. 0. 1. 1. 0. 1. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0.]  
 [0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 0. 1. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
```

Exercise 3: N-Queens Puzzle

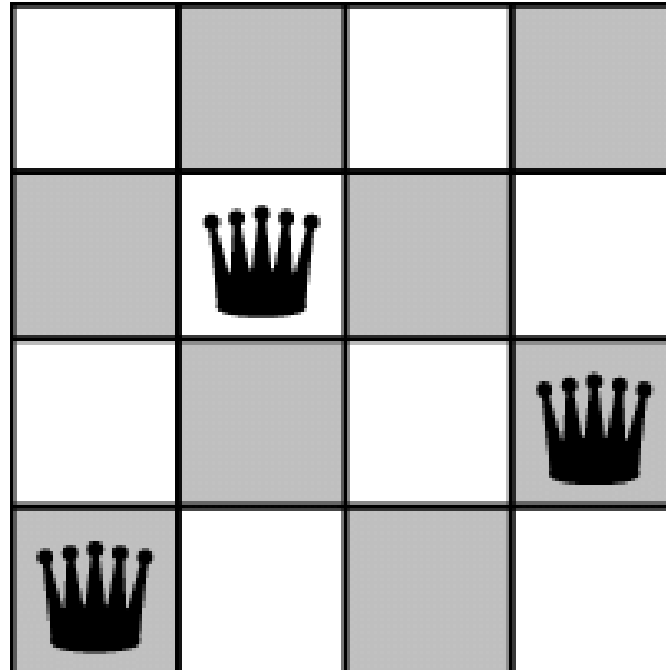
- Same thing for columns

```
def COL(col,dim):  
    C=np.zeros((dim,dim), dtype=int)  
    C[:,col] = 1  
    return C.flatten()
```

```
C=COL(1,4)
```

```
[[0 1 0 0]  
 [0 1 0 0]  
 [0 1 0 0]  
 [0 1 0 0]]
```

```
[0 1 0 0 0 1 0 0 0 1 0 0 0 1 0 0]
```



```
for col in range(N):  
    C=COL(col,N)  
    for i in range(N*N):  
        for j in range(i+1,N*N):  
            B[i][j]=B[i][j]+C[i]*C[j]*w  
  
print(B)
```

```
[[0. 1. 1. 1. 1. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0.]  
 [0. 0. 1. 1. 0. 1. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0.]  
 [0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 0. 1. 0. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
```

Exercise 3: N-Queens Puzzle

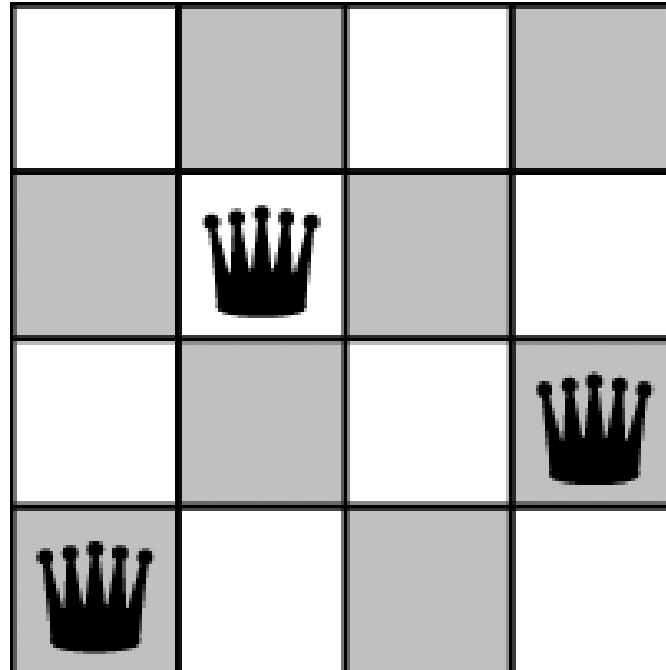
- Same thing for diagonals

```
def DIAG1(k,dim):  
    d=np.ones(dim-abs(k), dtype=int)  
    C=np.diag(d,k=k)  
    return C.flatten()
```

```
D=DIAG1(0,4)
```

```
[[1 0 0 0]  
 [0 1 0 0]  
 [0 0 1 0]  
 [0 0 0 1]]
```

```
[1 0 0 0 0 1 0 0 0 0 1 0 0 0 0 1]
```



```
for diag1 in range(-(N-2),N-1):  
    D1=DIAG1(diag1,N)  
    for i in range(N*N):  
        for j in range(i+1,N*N):  
            B[i][j]=B[i][j]+D1[i]*D1[j]*w  
  
print(B)
```

```
[[0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0. 1.]  
 [0. 0. 1. 1. 0. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0.]  
 [0. 0. 0. 1. 0. 0. 1. 1. 0. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 1. 0. 0. 1. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
```


Exercise 3: N-Queens Puzzle

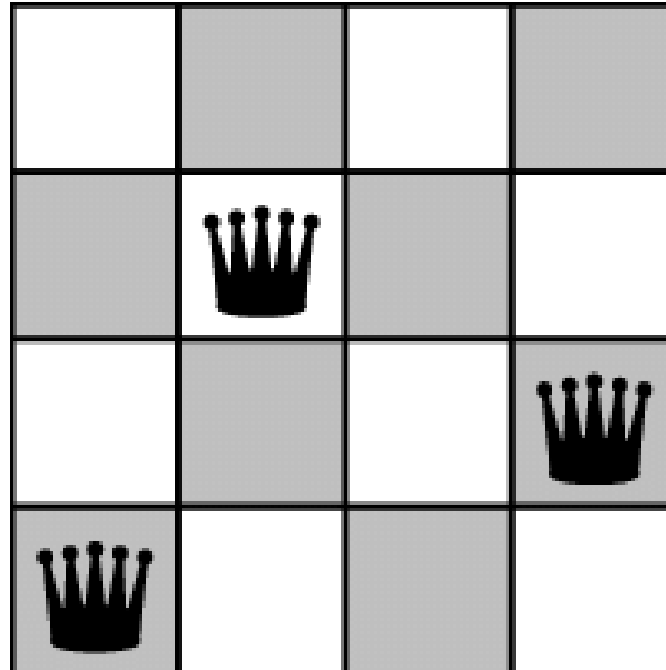
- Same thing for diagonals

```
def DIAG1(k,dim):  
    d=np.ones(dim-abs(k), dtype=int)  
    C=np.diag(d,k=k)  
    return C.flatten()
```

```
D=DIAG1(1,4)
```

```
[[0 1 0 0]  
 [0 0 1 0]  
 [0 0 0 1]  
 [0 0 0 0]]
```

```
[0 1 0 0 0 0 1 0 0 0 0 1 0 0 0 0]
```



```
for diag1 in range(-(N-2),N-1):  
    D1=DIAG1(diag1,N)  
    for i in range(N*N):  
        for j in range(i+1,N*N):  
            B[i][j]=B[i][j]+D1[i]*D1[j]*w  
  
print(B)
```

```
[[0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0. 1.]  
 [0. 0. 1. 1. 0. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0.]  
 [0. 0. 0. 1. 0. 0. 1. 1. 0. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 1. 0. 0. 1. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 1. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
```


Exercise 3: N-Queens Puzzle

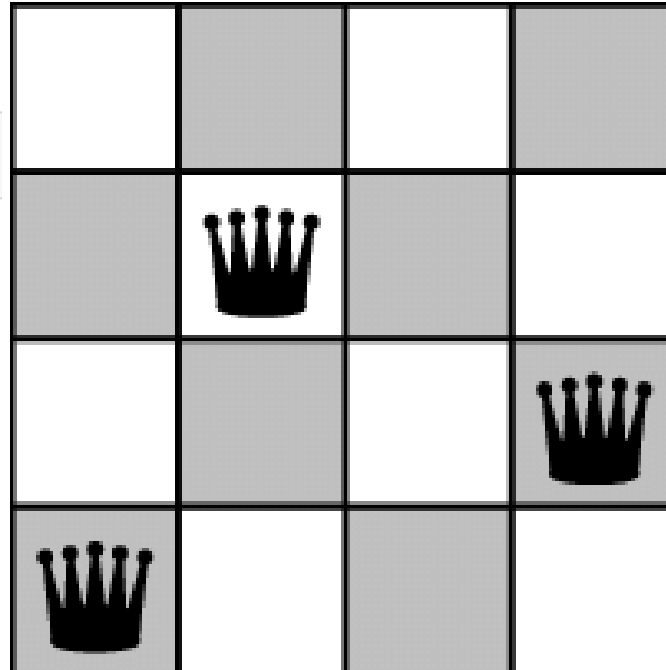
- Same thing for diagonals

```
def DIAG1(k,dim):  
    d=np.ones(dim-abs(k), dtype=int)  
    C=np.diag(d,k=k)  
    return C.flatten()
```

```
D=DIAG1(-1,4)
```

```
[[0 0 0 0]  
 [1 0 0 0]  
 [0 1 0 0]  
 [0 0 1 0]]
```

```
[0 0 0 0 1 0 0 0 0 1 0 0 0 0 1 0]
```



```
for diag1 in range(-(N-2),N-1):  
    D1=DIAG1(diag1,N)  
    for i in range(N*N):  
        for j in range(i+1,N*N):  
            B[i][j]=B[i][j]+D1[i]*D1[j]*w  
  
print(B)
```

```
[[0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0. 1.]  
 [0. 0. 1. 1. 0. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0.]  
 [0. 0. 0. 1. 0. 0. 1. 1. 0. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 1. 0. 0. 1. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 1. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
```

Exercise 3: N-Queens Puzzle

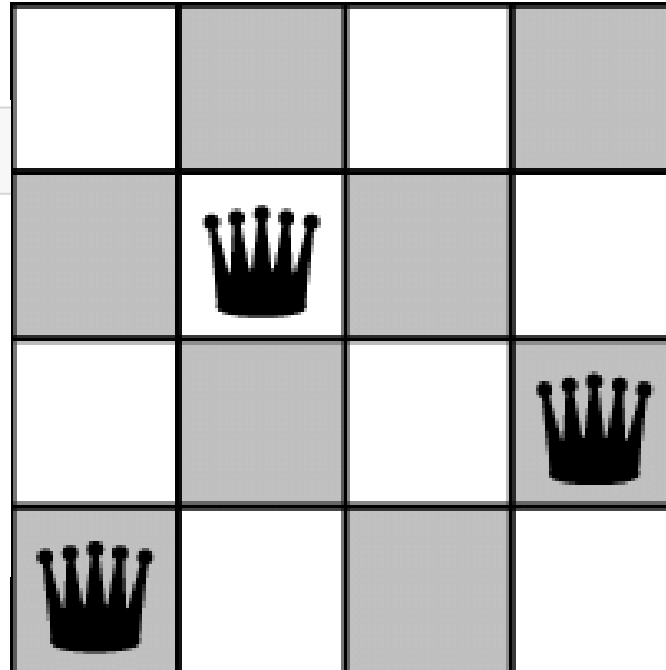
- Same thing for diagonals

```
def DIAG2(k,dim):  
    d=np.ones(dim-abs(k), dtype=int)  
    C=np.fliplr(np.diag(d,k=k))  
    return C.flatten()
```

```
D=DIAG2(0,4)
```

```
[[0 0 0 1]  
 [0 0 1 0]  
 [0 1 0 0]  
 [1 0 0 0]]
```

```
[0 0 0 1 0 0 1 0 0 1 0 0 1 0 0 0]
```



```
for diag2 in range(-(N-2),N-1):  
    D2=DIAG2(diag2,N)  
    for i in range(N*N):  
        for j in range(i+1,N*N):  
            B[i][j]=B[i][j]+D2[i]*D2[j]*w  
  
print(B)
```

```
[[0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0. 1.]  
 [0. 0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 0.]  
 [0. 0. 0. 1. 0. 1. 1. 1. 1. 0. 1. 0. 0. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 0. 1. 1. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0. 1. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 1. 1. 1. 0. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 1. 0.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]  
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
```

Advanced Annealing Techniques



Quantum Annealing with continuous variables: Low-Rank Matrix Factorization

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Quantum Computing and High Performance Computing
CINECA Casalecchio di Reno, Bologna, 18-12-2018

Advanced Annealing Techniques

QUBO Problems with real variables

We define a QUBO problem with real variables as a Quadratic Unconstrained Optimization problem with unknown variables expressed as:

$$x = c \cdot \sum_{e=0}^{N-1} 2^e q_e, \quad c = 10^{-a}, \text{ for some } a \in \mathbb{N}$$

For example, the QUBO problem associated with the simple equation $x - b = 0$ is:

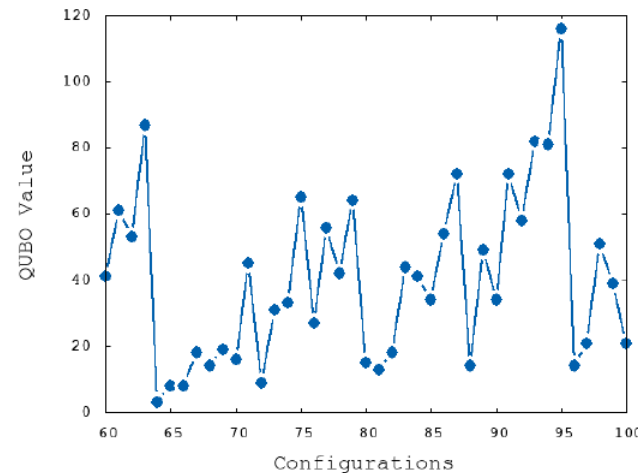
$$\min_{\mathbf{q}=(q_0, \dots, q_{N-1})} \left(\sum_{e=0}^{N-1} (c^2 2^{2e} - bc 2^{e+1}) q_e + \sum_{e < f} (c^2 2^{e+f+1}) q_e q_f \right)$$

Considering $x - b = 0$ as $\min_{x \in \mathbb{R}} (x - b)^2$

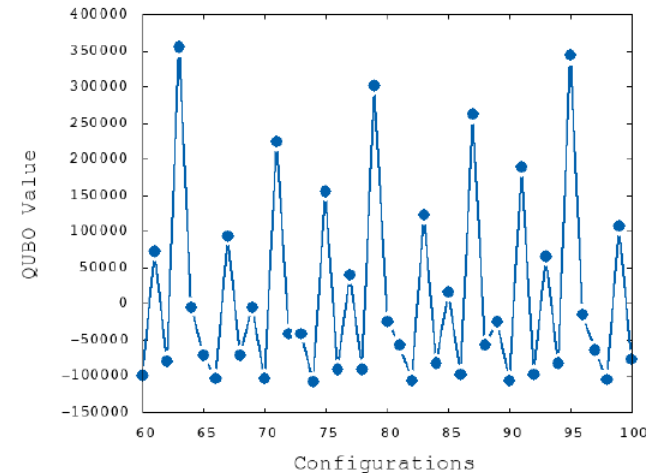
Graphical representation

**QUBO problems of this kind are particularly difficult to solve.
Especially with annealing techniques.**

This is due to the exponential dependence of the coefficients from the binary variable indices, which create numerous local minima very similar to the global minimum.



"Normal" QUBO landscape



"Real-variables" QUBO landscape

Advanced Annealing Techniques

Solving a linear system

We have chosen to solve a linear system $A\mathbf{x} = b$, where

$$\mathbf{x} = (x_1, x_2, x_3) \text{ and } x_i \in [0,1].$$

We represent $x_i = c \cdot \sum_{e=0}^9 2^e q_e$, $c = 10^{-3}$ ($N = 10$, $a = 3$).

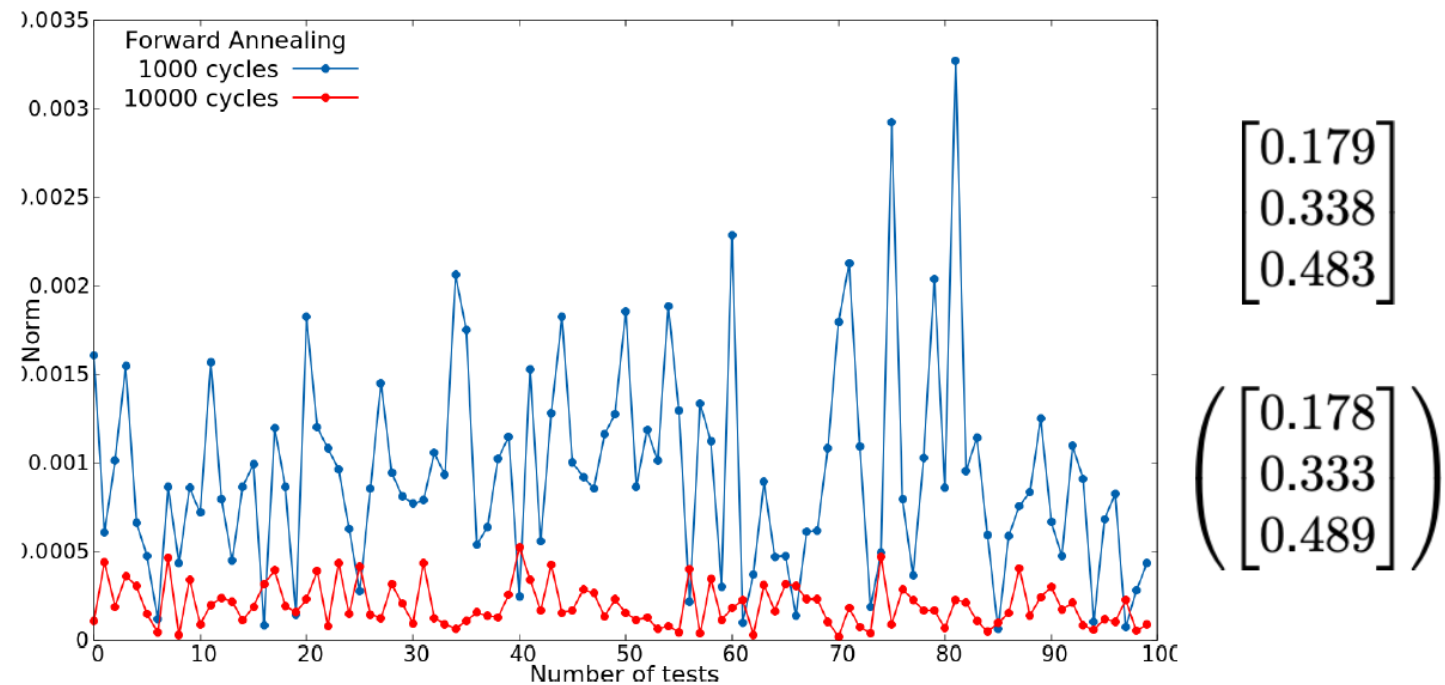
We will find \mathbf{x} solving $\min_{\mathbf{x} \in [0,1]^3} \|A\mathbf{x} - b\|_2^2$

$$\begin{bmatrix} 1.301 & 0.125 & 0.187 \\ 0.440 & 0.342 & 0.082 \\ 0.672 & 0.709 & 0.802 \\ 0.218 & 0.427 & 0.520 \\ 0.024 & 0.036 & 0.038 \end{bmatrix} \cdot \begin{bmatrix} 0.178 \\ 0.333 \\ 0.489 \end{bmatrix} = \begin{bmatrix} 0.365 \\ 0.232 \\ 0.748 \\ 0.435 \\ 0.035 \end{bmatrix}$$

Advanced Annealing Techniques

Attempt number 1: Forward Annealing

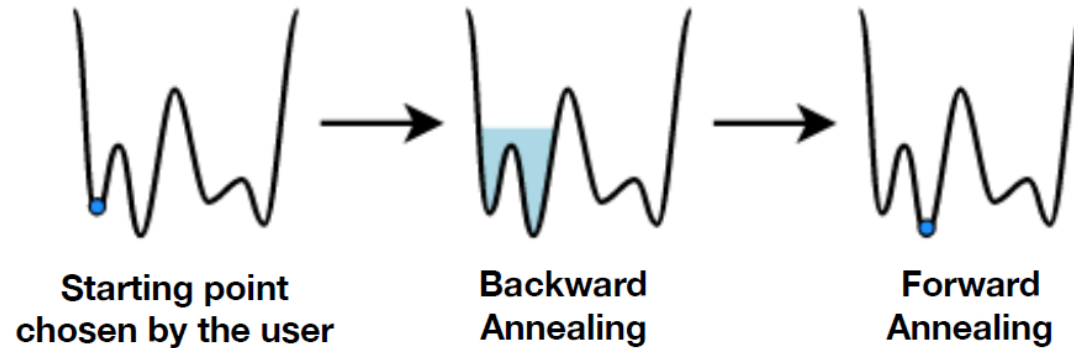
100 attempts with 1,000 and 10,000 annealing cycles



Advanced Annealing Techniques

Local refinement of solutions: Reverse Annealing

Introduced with the last D-Wave model, DWAVE2000Q



During the **Backward Annealing** phase, the transverse field slowly increases up to a value chosen by the user (*Reversal Distance*)

The last **Forward Annealing** phase is a **LOCAL** quantum annealing search:
how much local depends on the reversal distance value.

Image taken from *Reverse Quantum Annealing for Local Refinement of Solutions*, D-Wave White Papers, 2017

Advanced Annealing Techniques

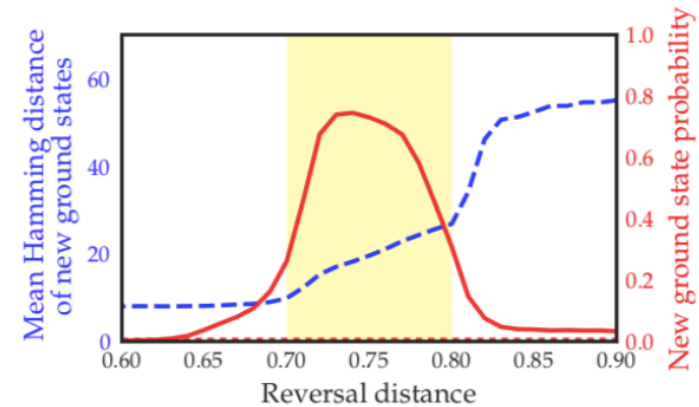
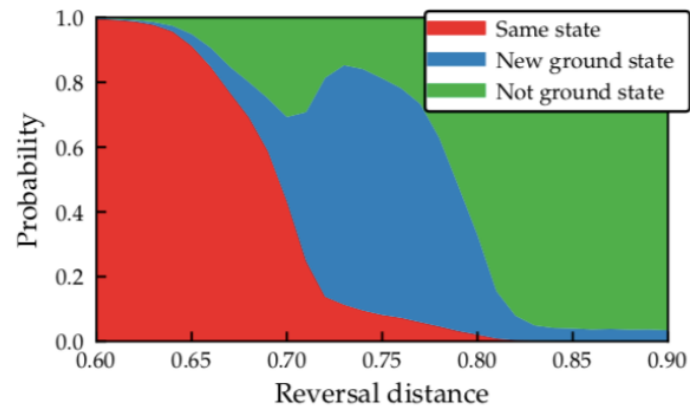
Tuning the reversal distance

D:WAVE

The Quantum Computing Company™

Reverse Quantum Annealing for Local Refinement of Solutions

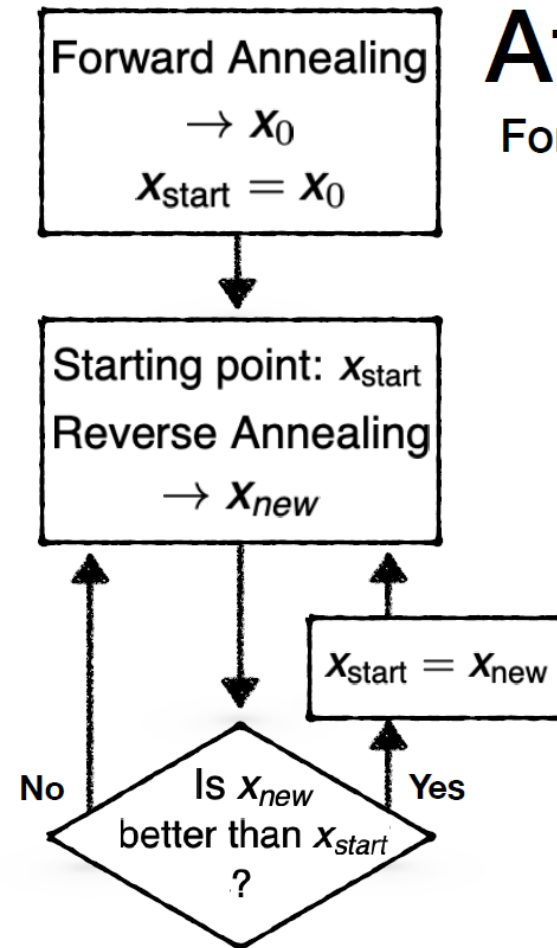
WHITEPAPER



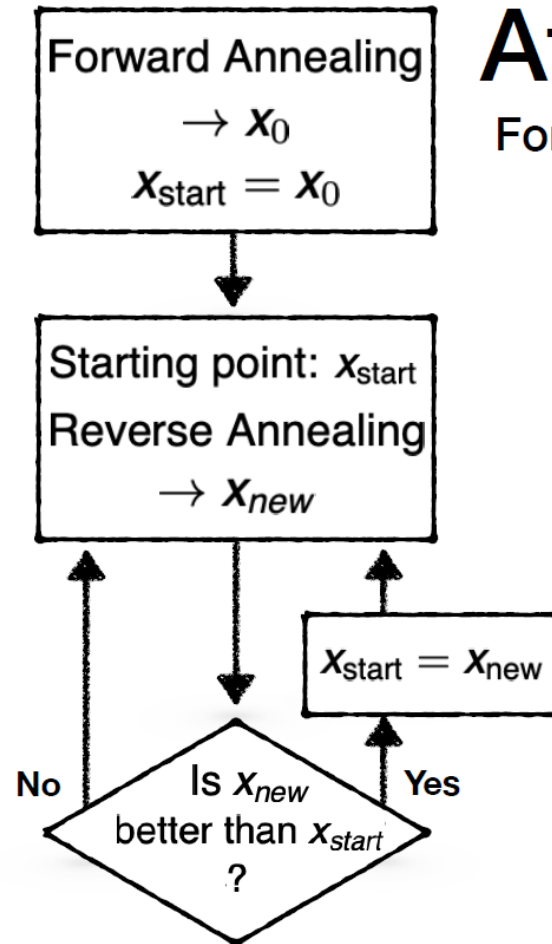
Advanced Annealing Techniques

Attempt number 2:

Forward Annealing + Reverse Annealing



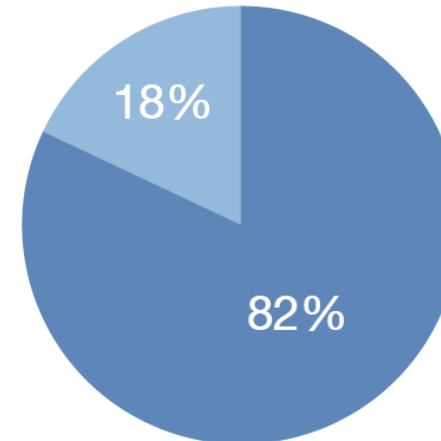
Advanced Annealing Techniques



Attempt number 2:

Forward Annealing + Reverse Annealing

● Not Solved ● Solved

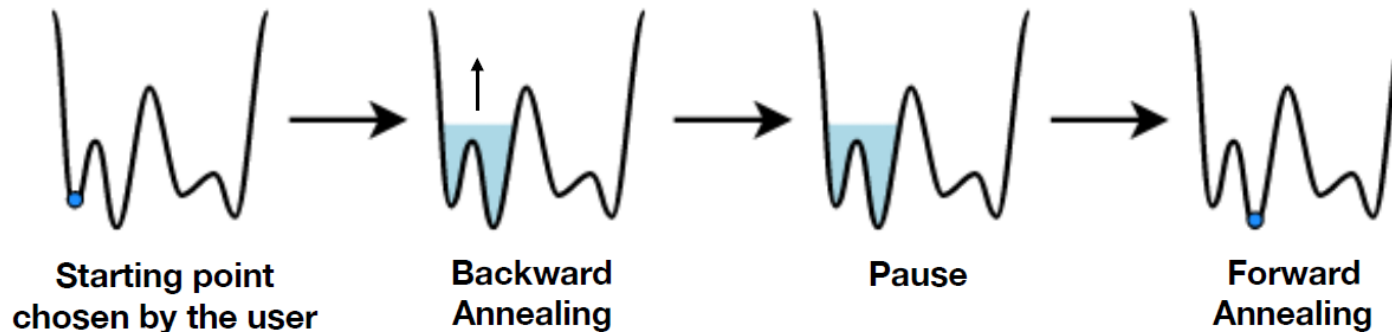


Advanced Annealing Techniques

Pausing the annealing process

Being able to pause the annealing process is another of the new features introduced with the latest D-WAVE quantum annealer.

We can use the pause during a Reverse Annealing search in this way:



Why pause? Because pausing the annealing process means better exploration of the selected zone, increasing the chances of obtaining a new global minimum.

But pay attention: pause can't be too long. For two main reasons:

- 1) it increase the computational time of each annealing cycle.
- 2) if it is too long, it may also risk to increase the search radius more than desired.

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Correlation between pause and search radius

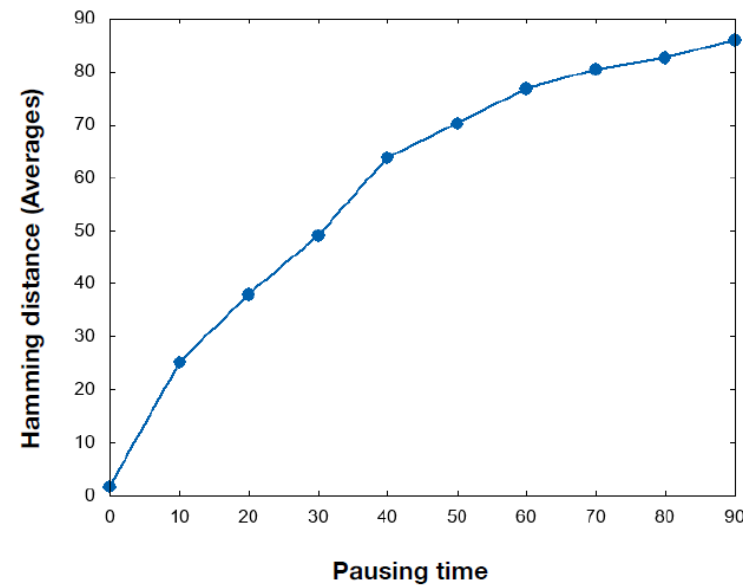
We can realize a posteriori the search radius of a reverse annealing search by analyzing the average distance between the solutions found by each cycle.

To do this, we choose the Hamming distance, a function written to calculate the distance between vectors of binary numbers.

We have observed that there is a correlation between the pause time and the average distance between the solutions obtained with each annealing cycle

As with the reversal distance, here too we have to be careful about the right break time:

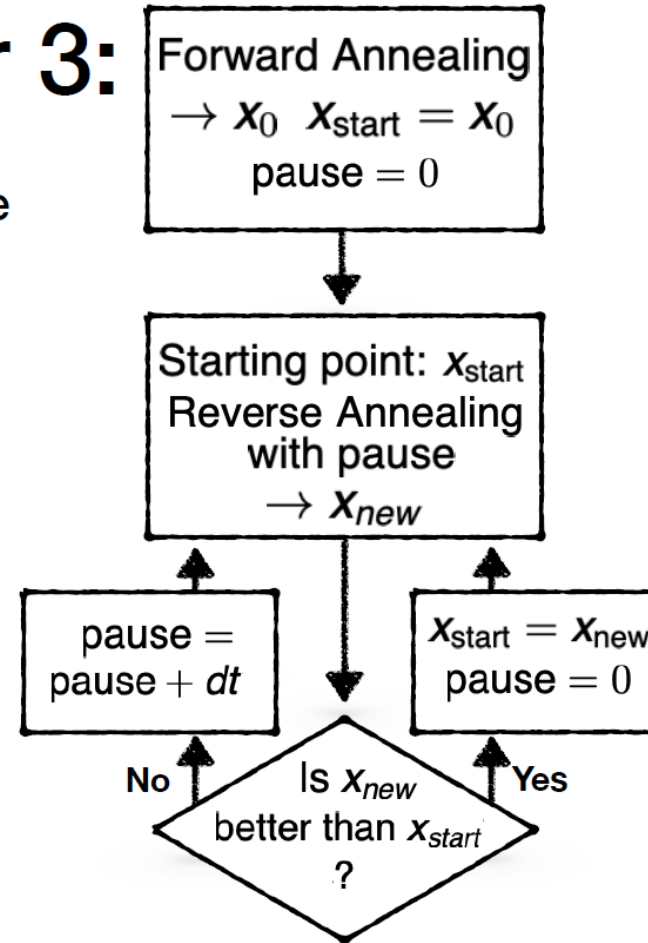
too little is not enough,
too much can lead to wrong
results



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Attempt number 3:

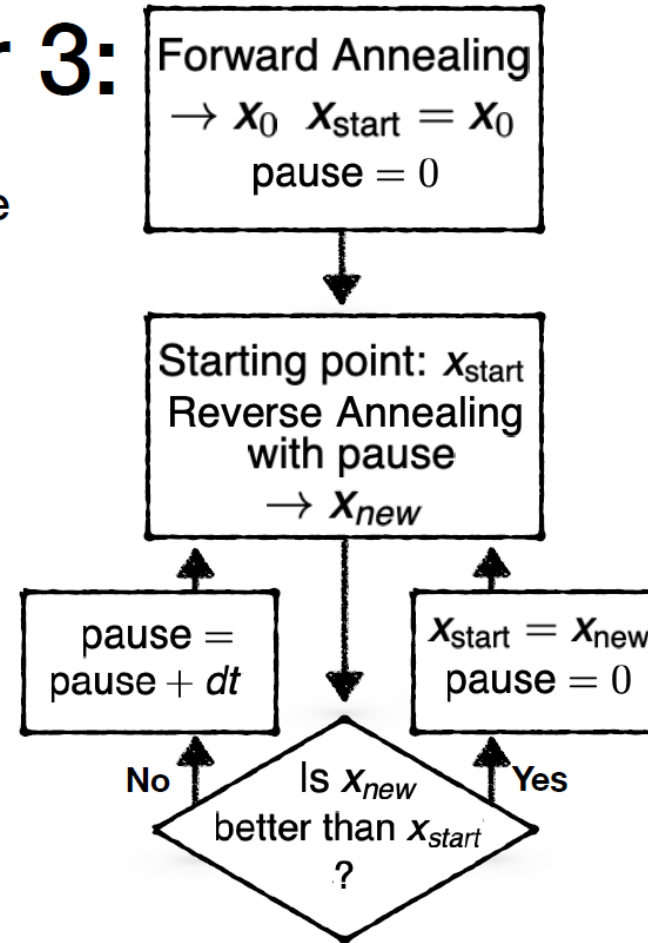
Forward Annealing +
Reverse Annealing with pause



Advanced Annealing Techniques

Attempt number 3:

Forward Annealing +
Reverse Annealing with pause



Advanced Annealing Techniques

Attempt number 3:

Forward Annealing +
Reverse Annealing with pause

● Not Solved ● Solved

