INTRODUCTION TO QUANTUM ANNEALING

Formulating and solve QUBO Problems

Daniele Ottaviani

CINECA QUANTUM COMPUTING LAB

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- **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 conspecific 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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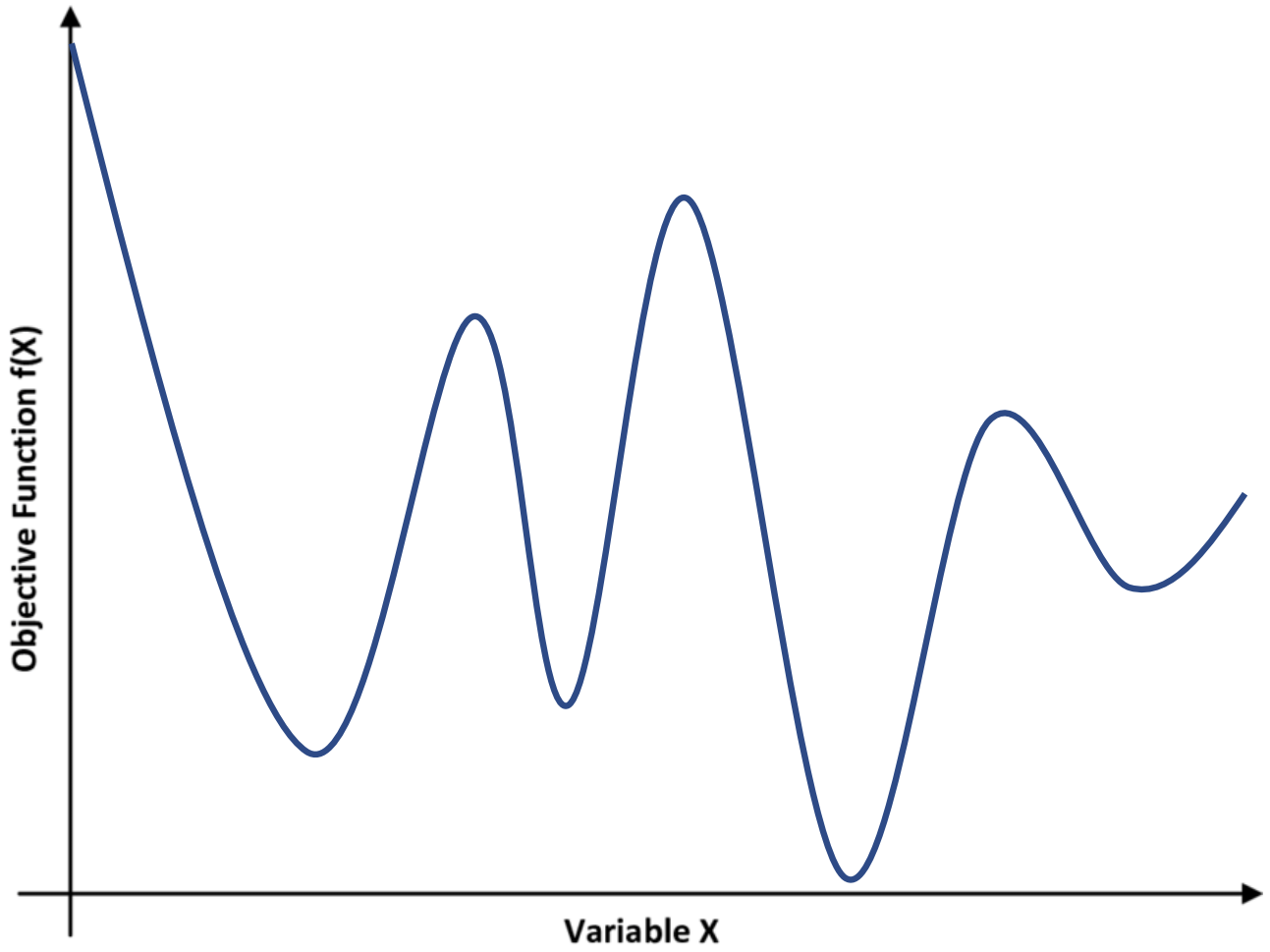

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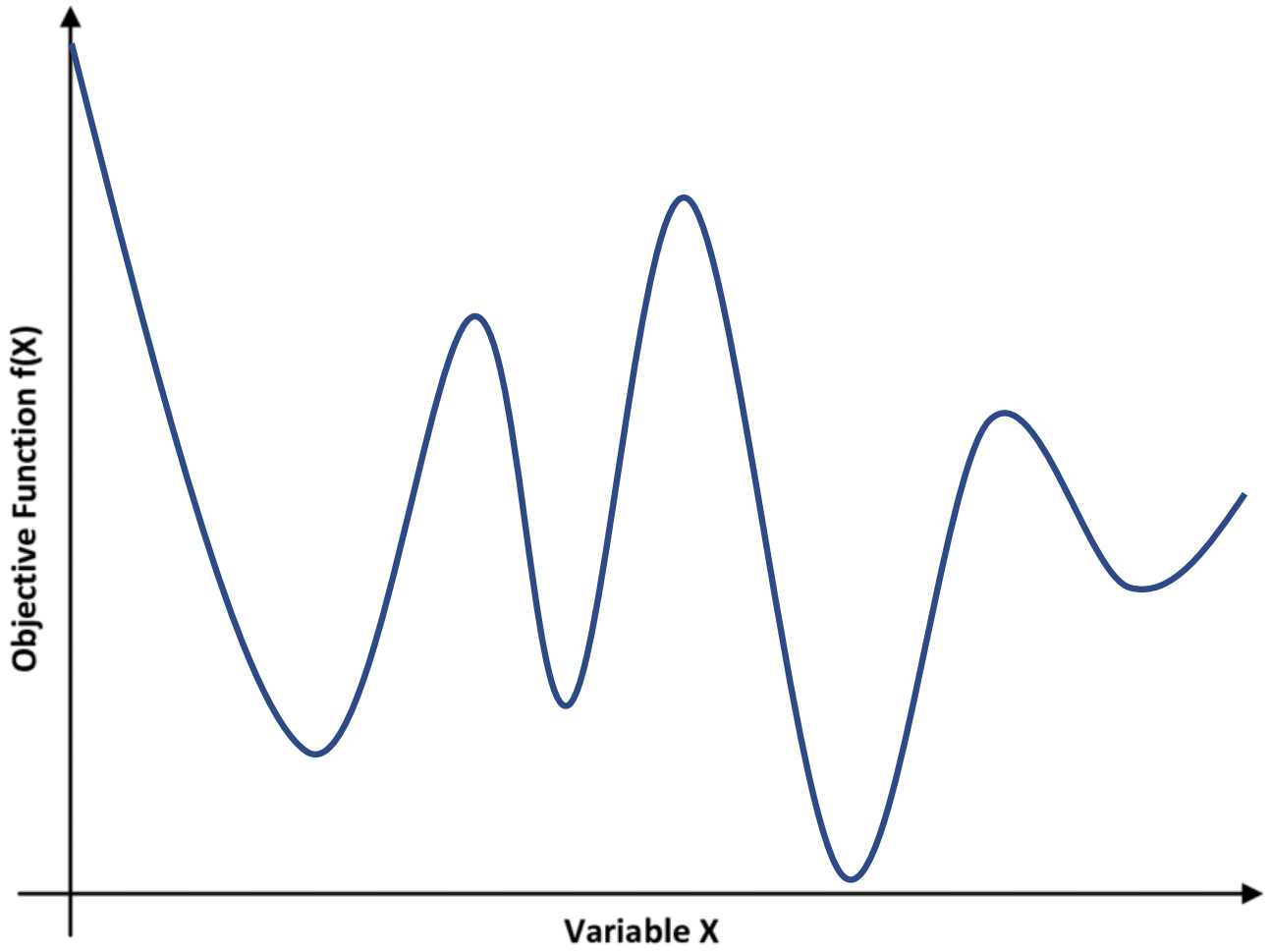

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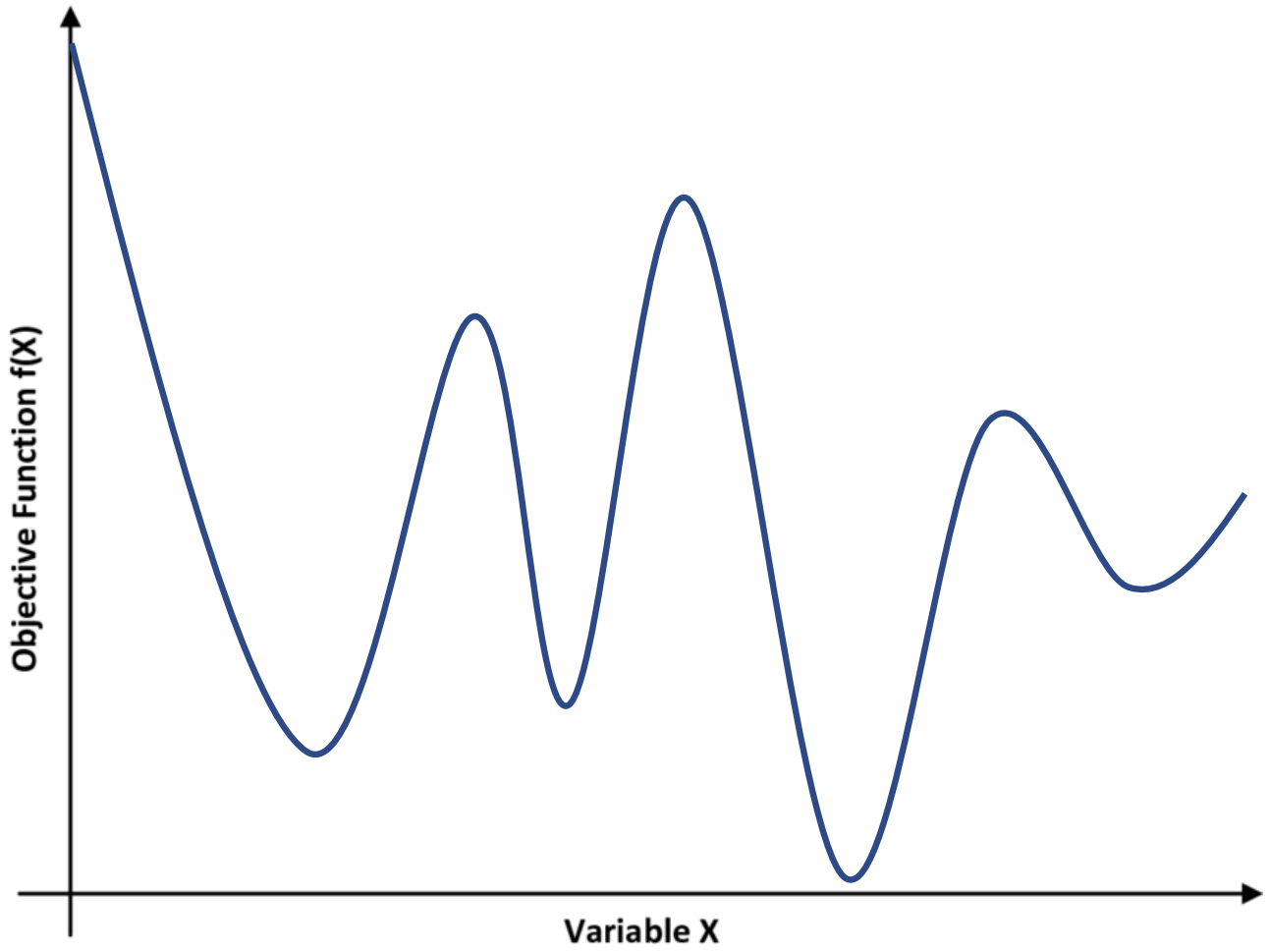

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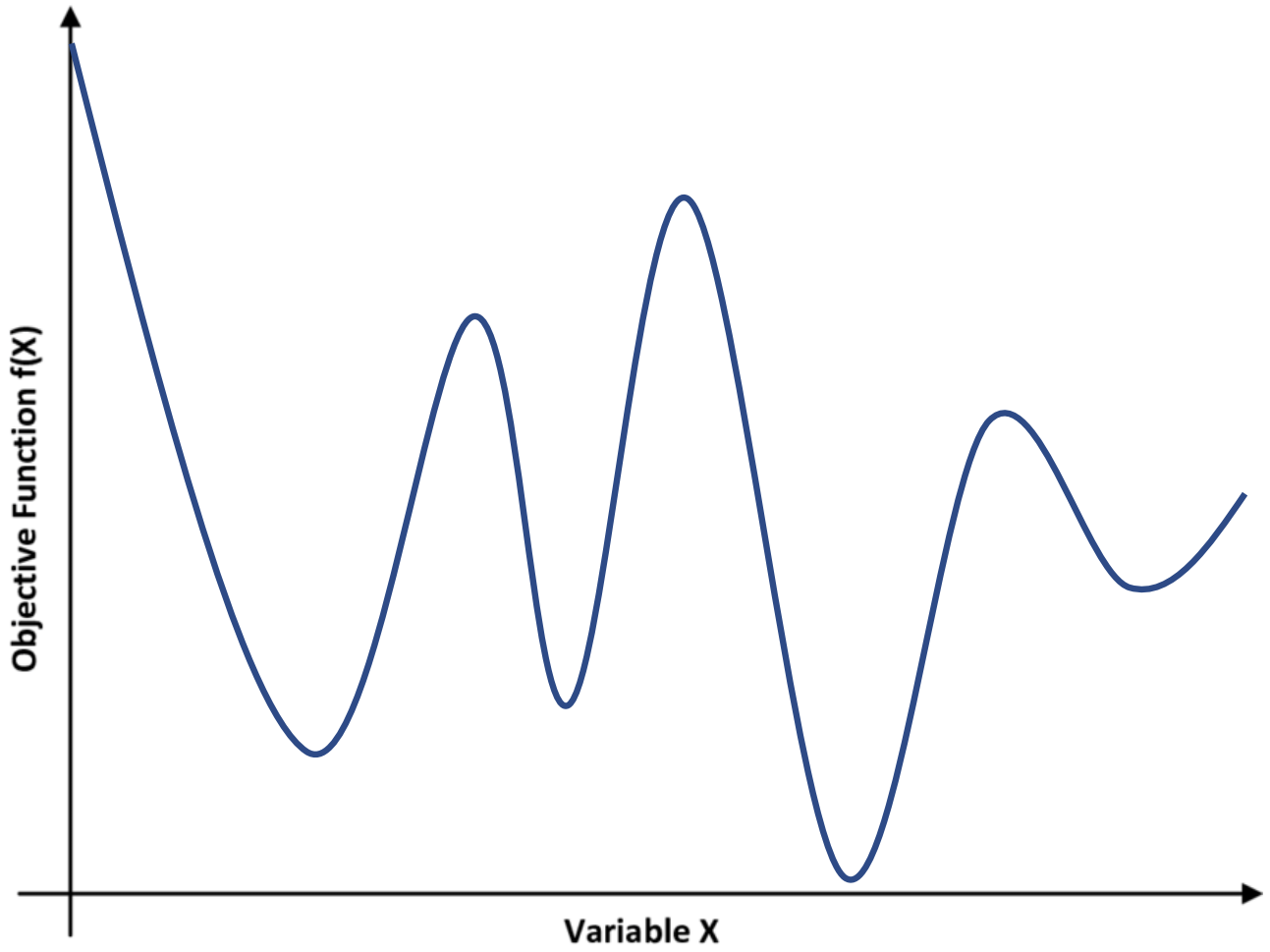
- Let's imagine for example the case of a function with **N** binary variables: the number of possible combinations is $\mathbf{2^N}$…



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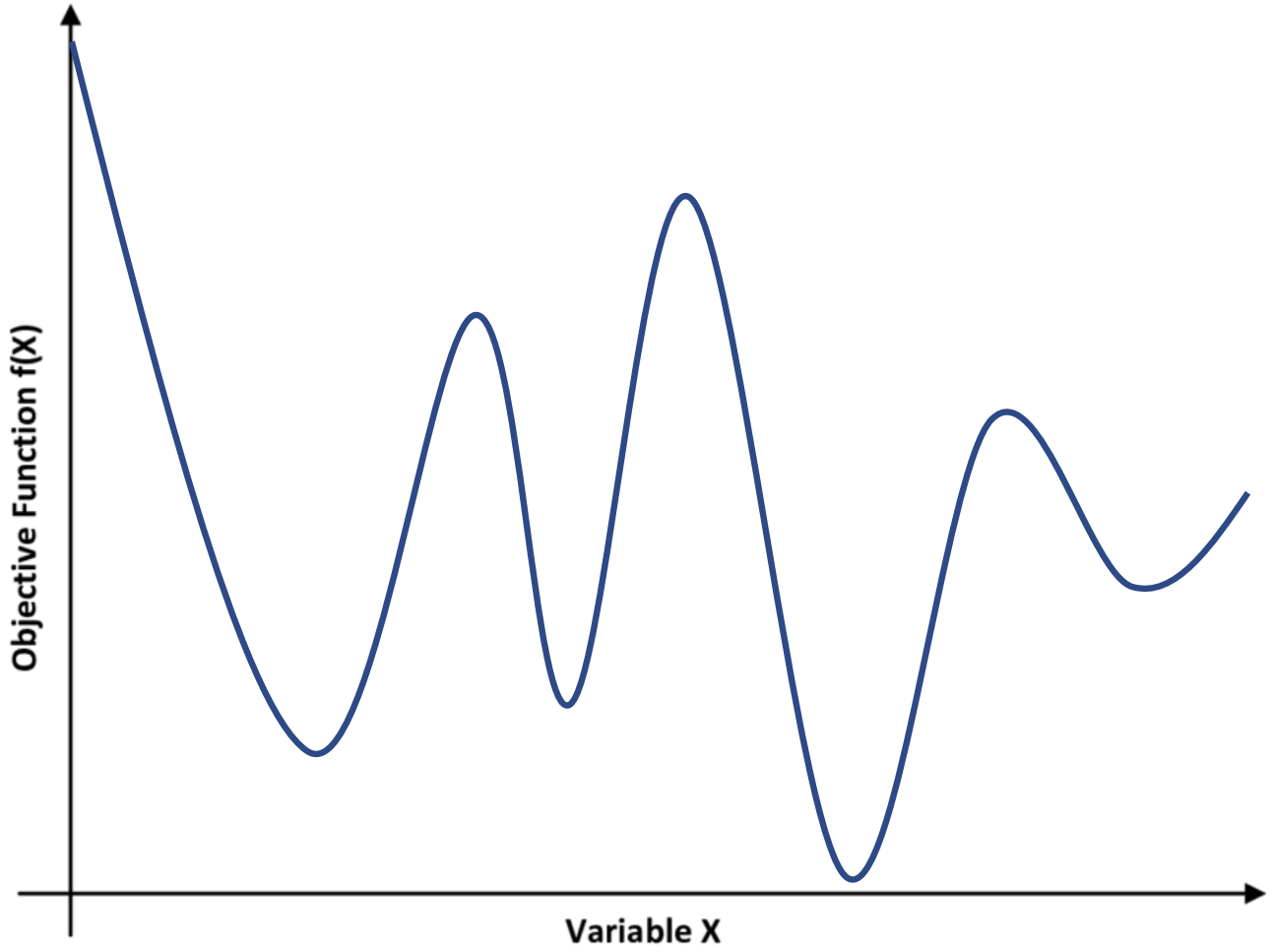

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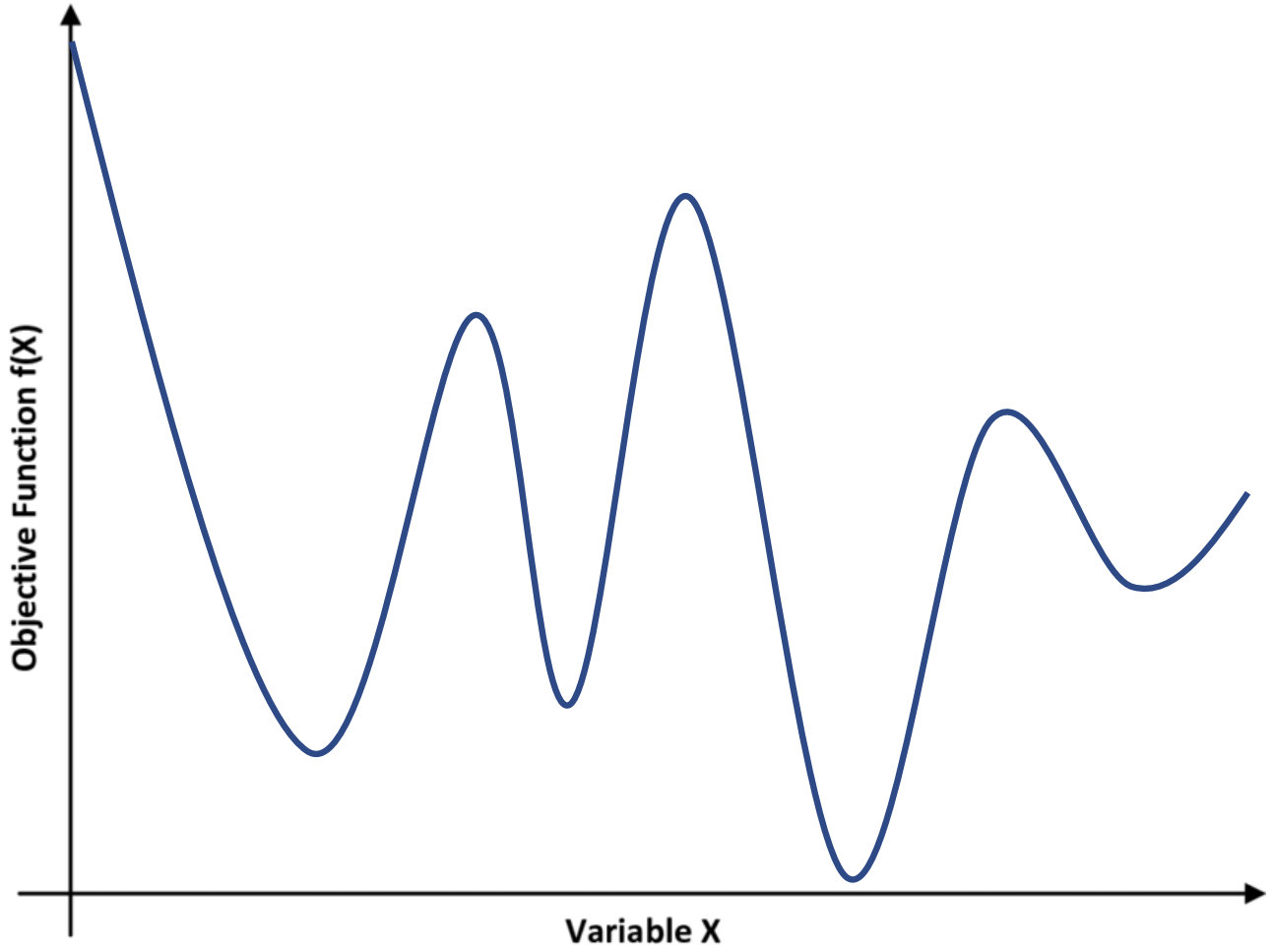

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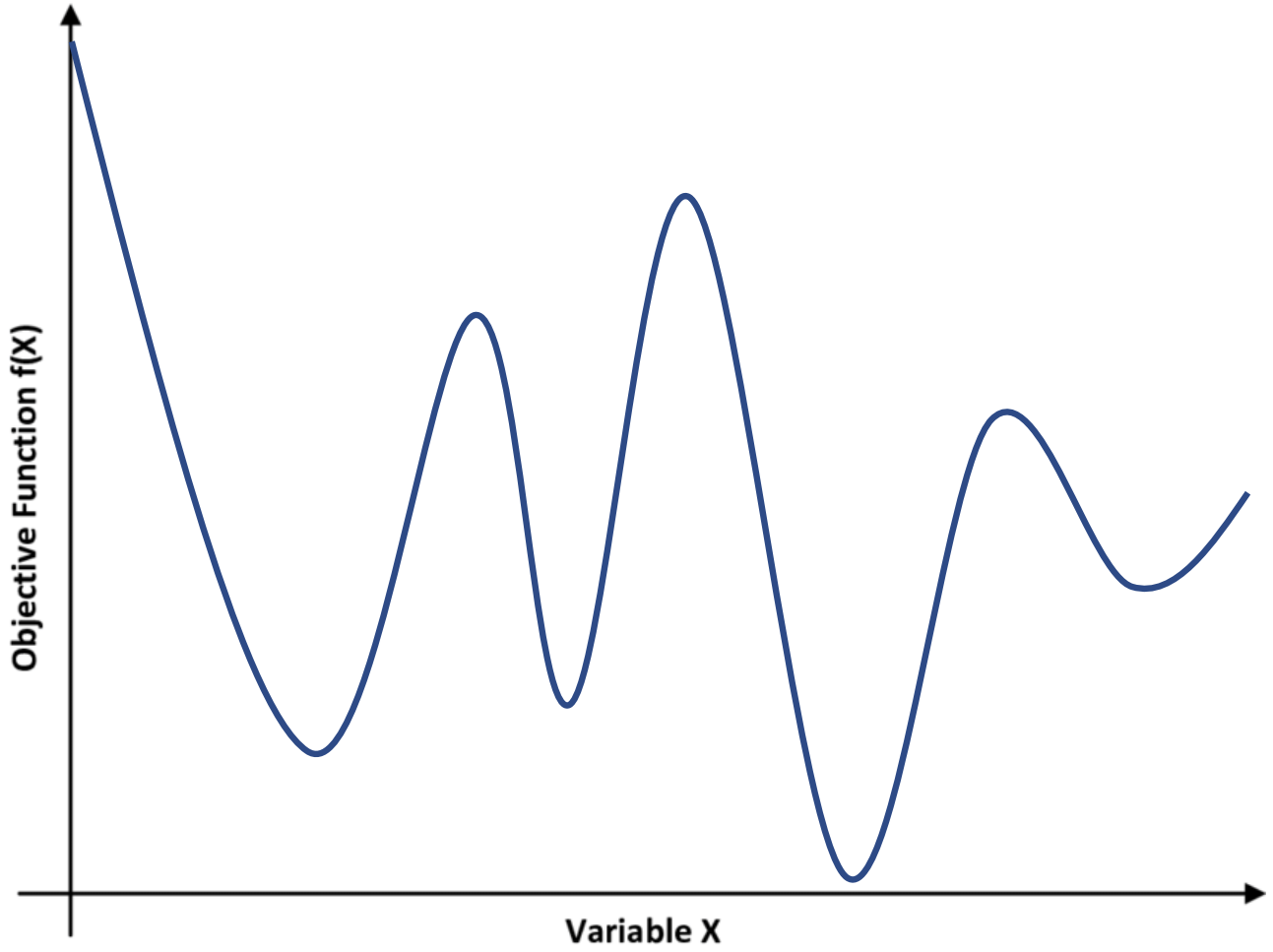

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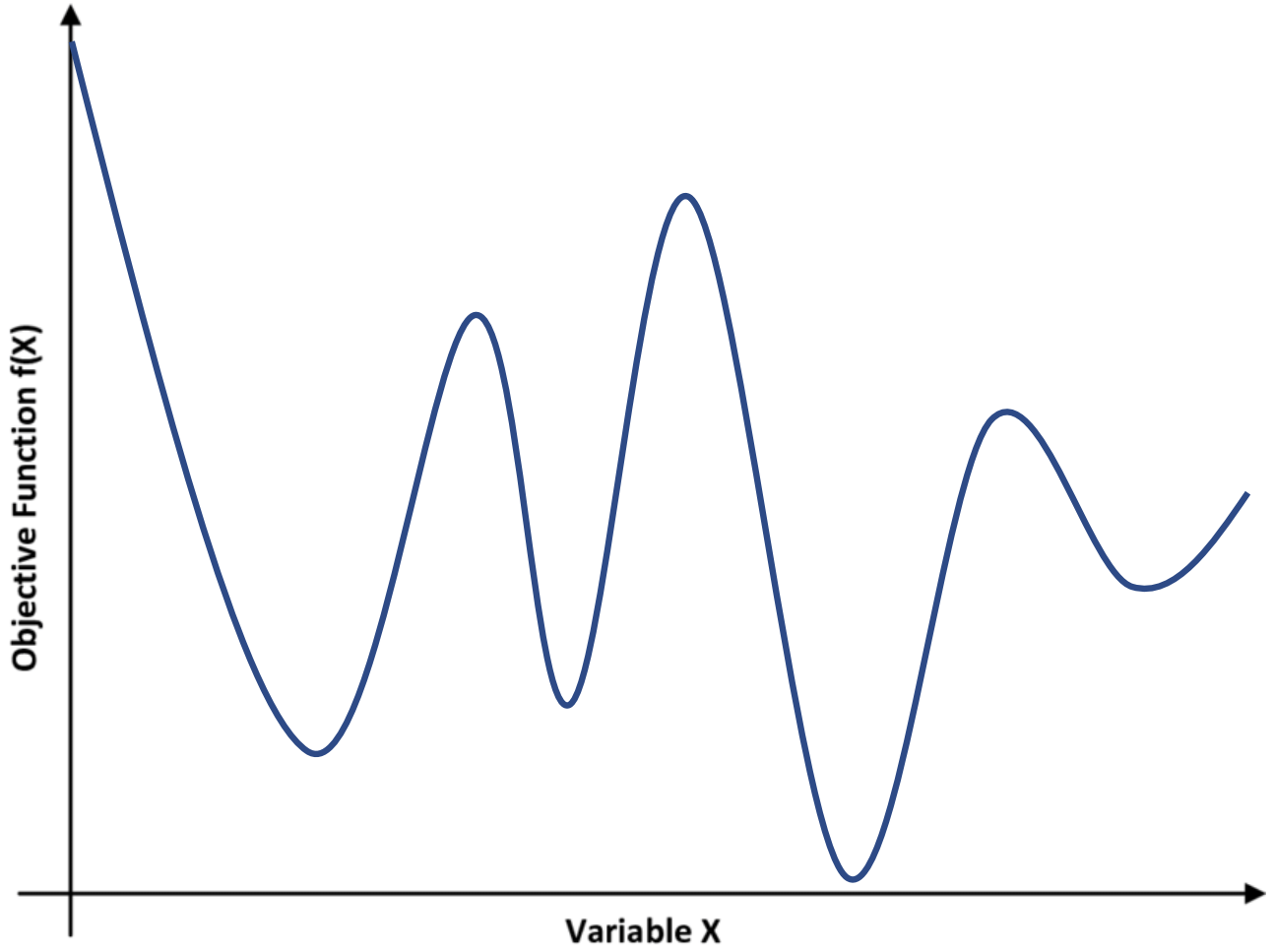

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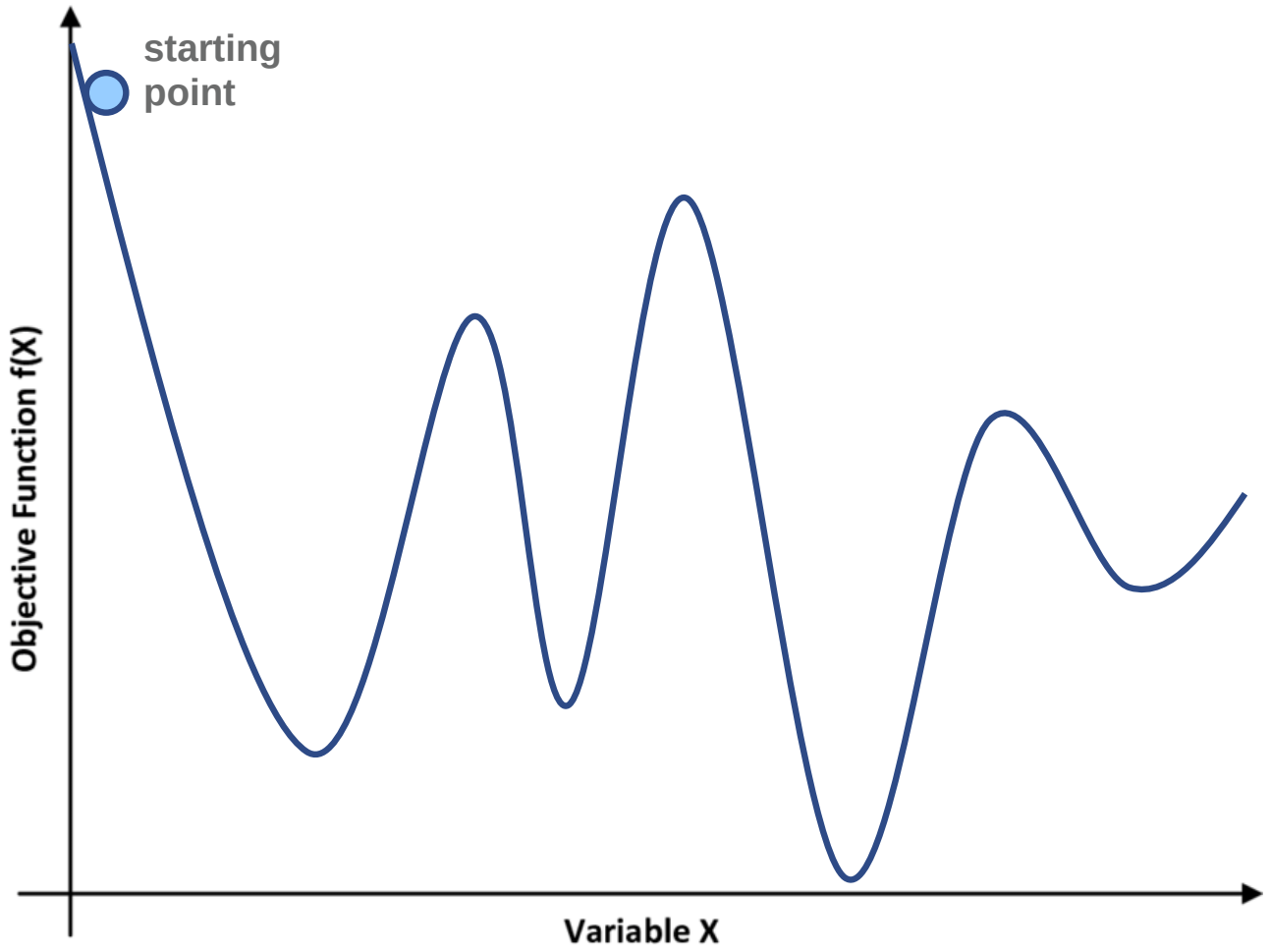

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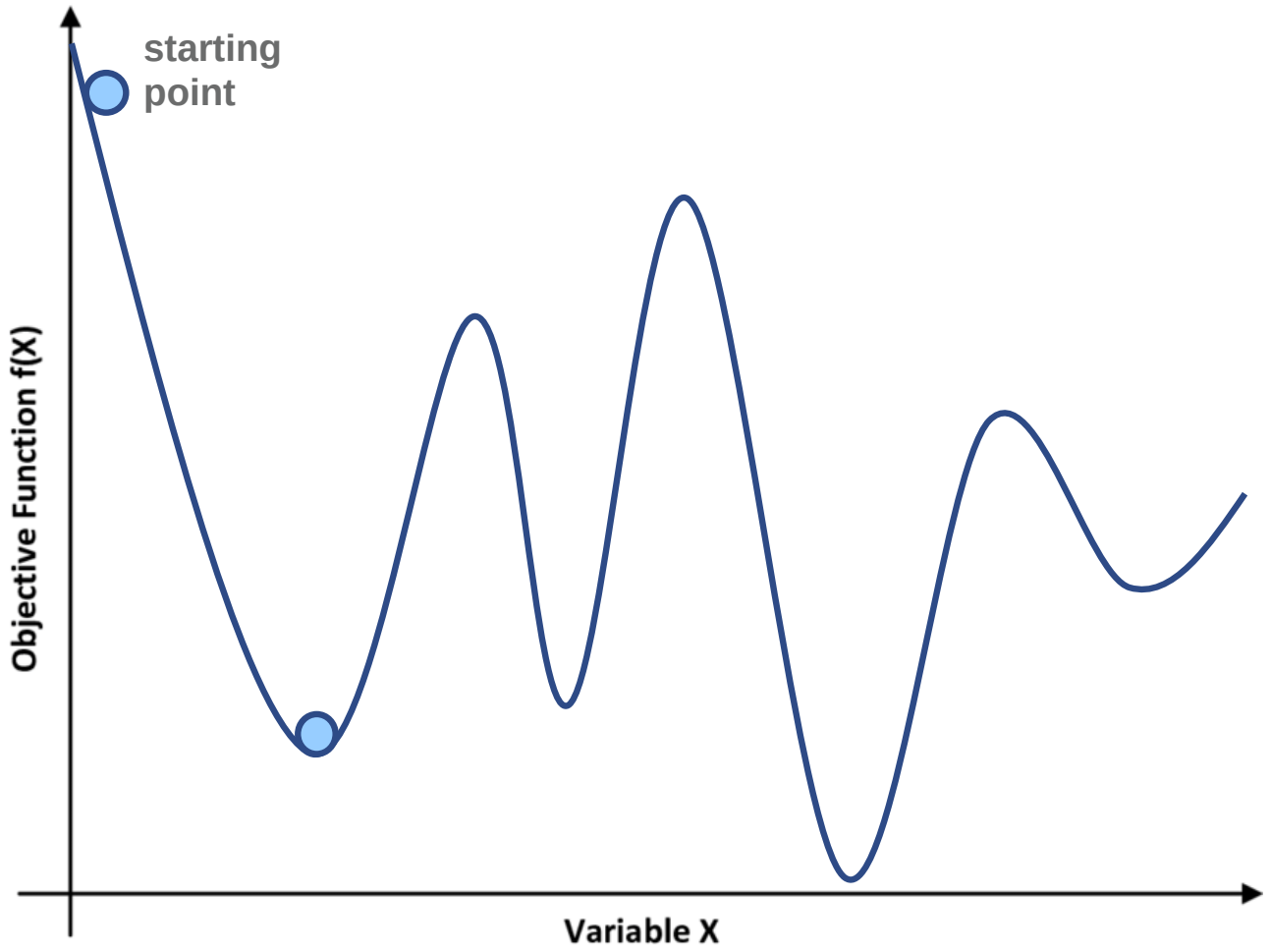

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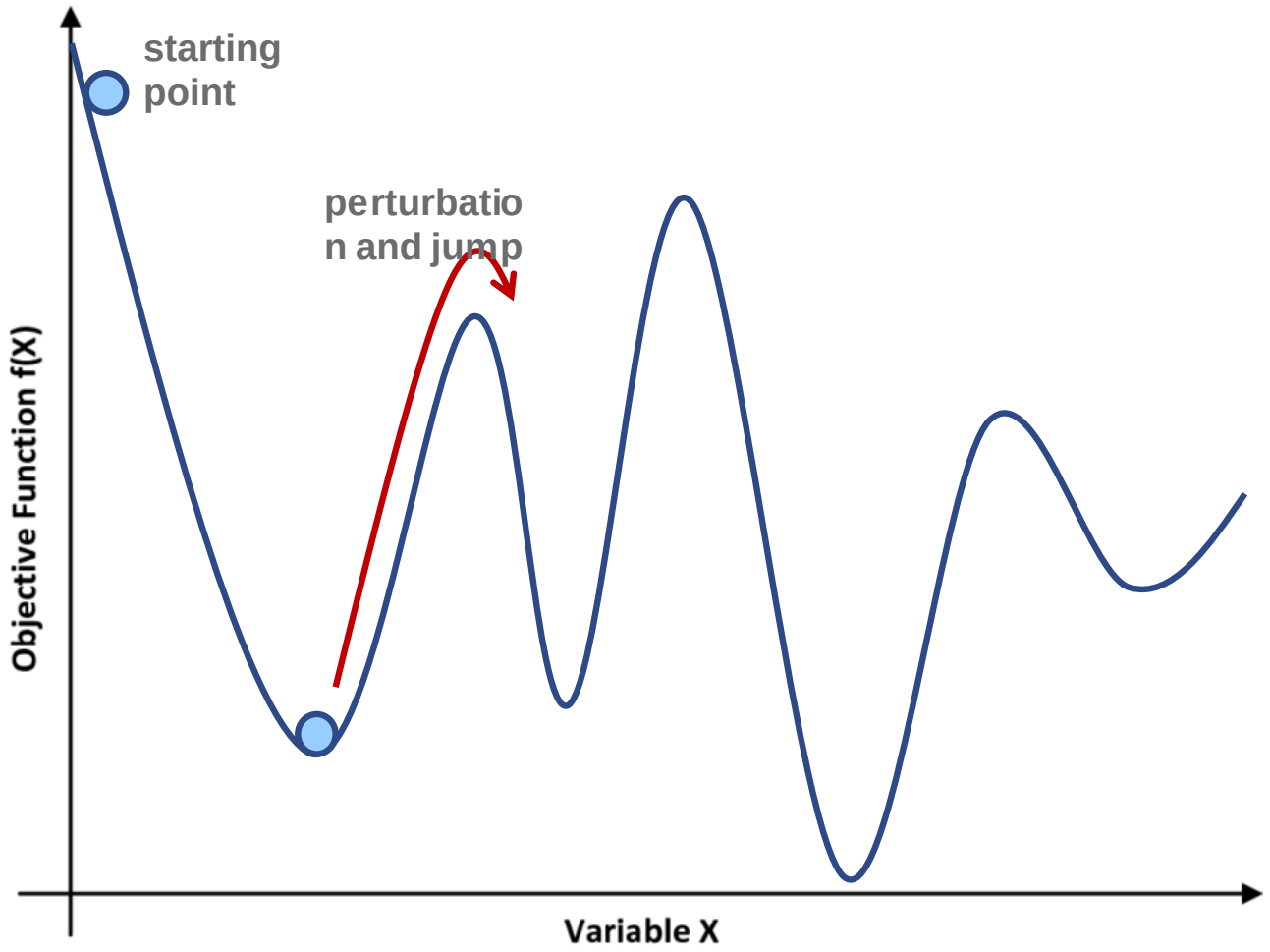

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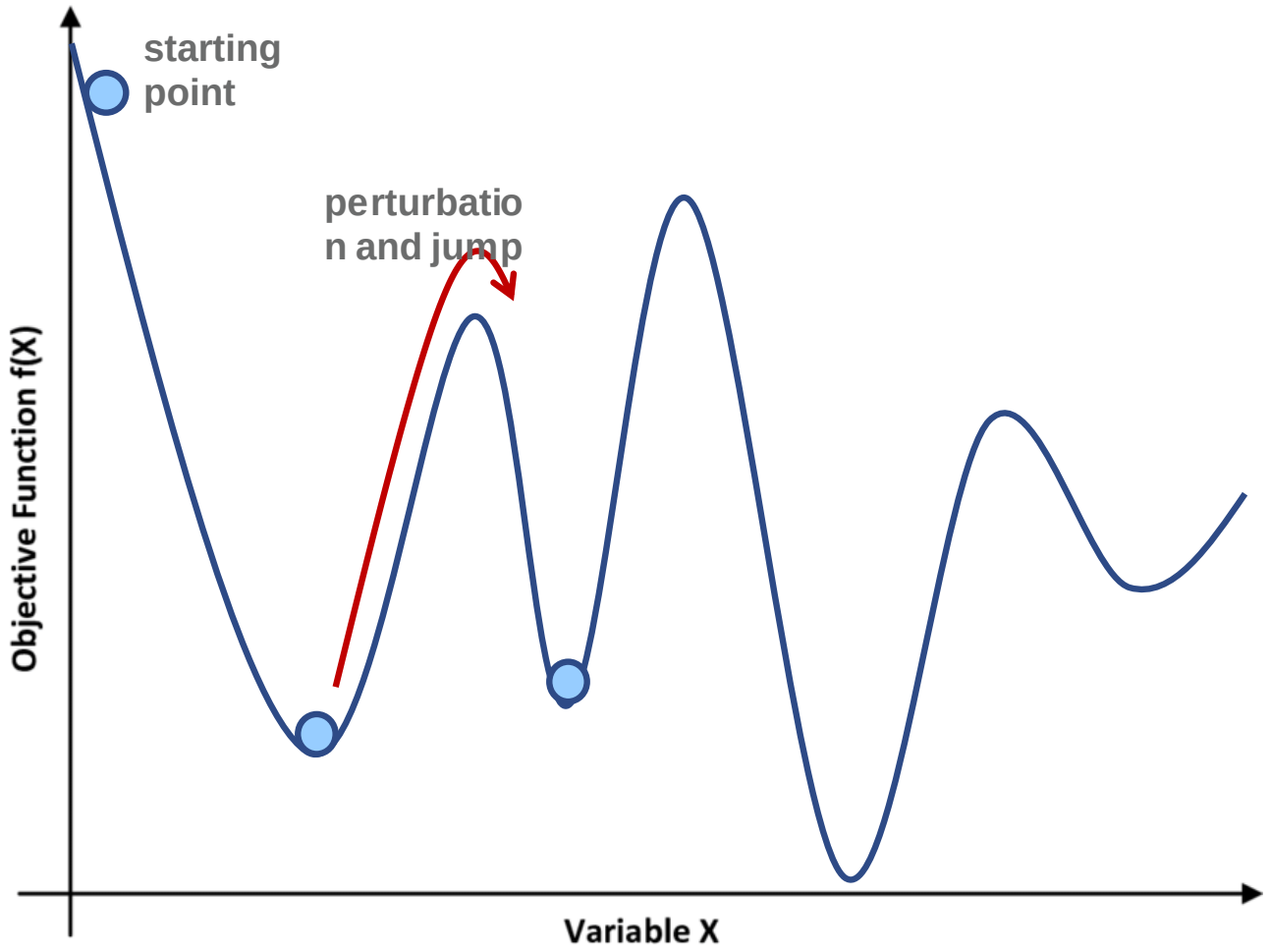

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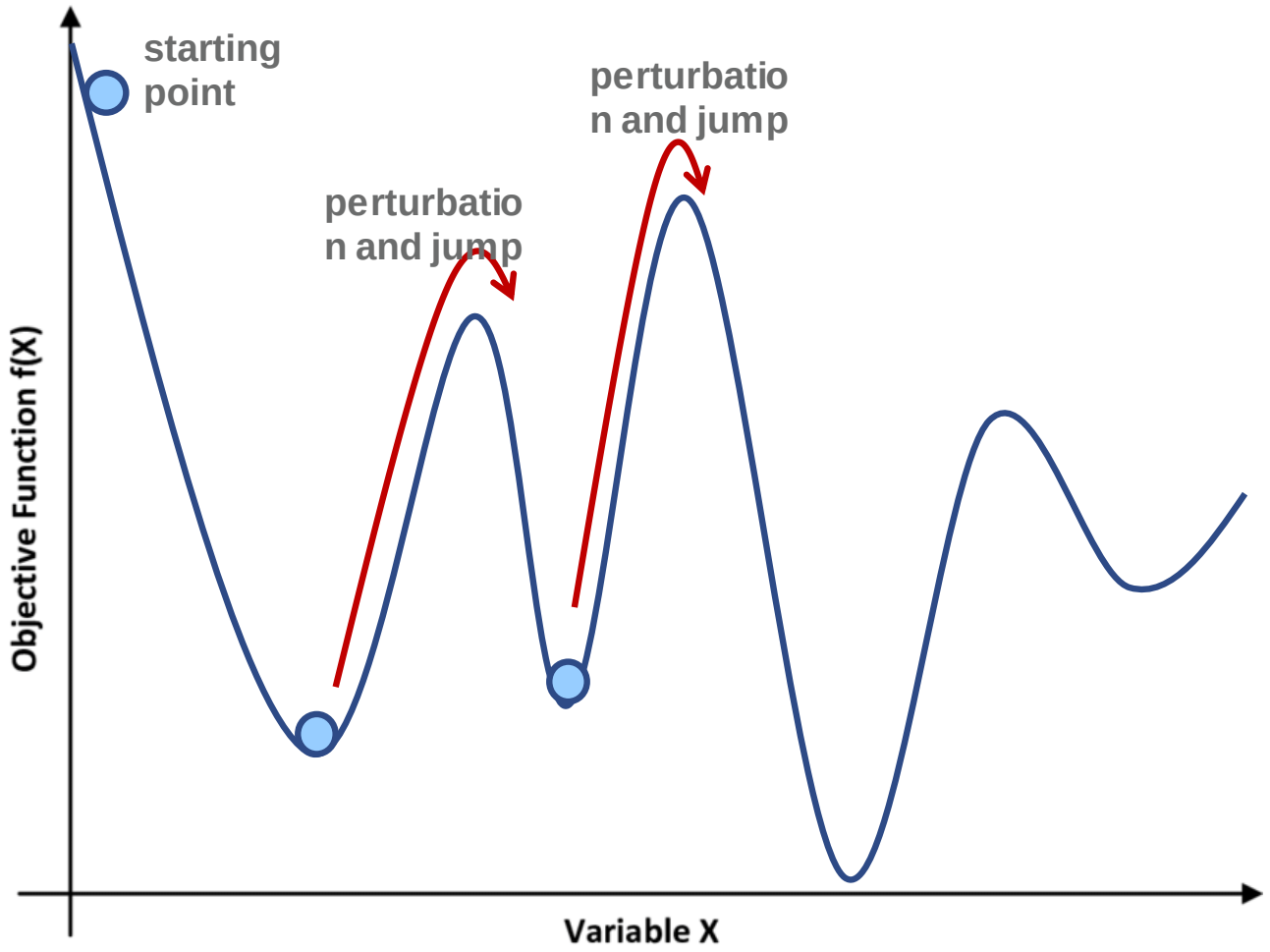

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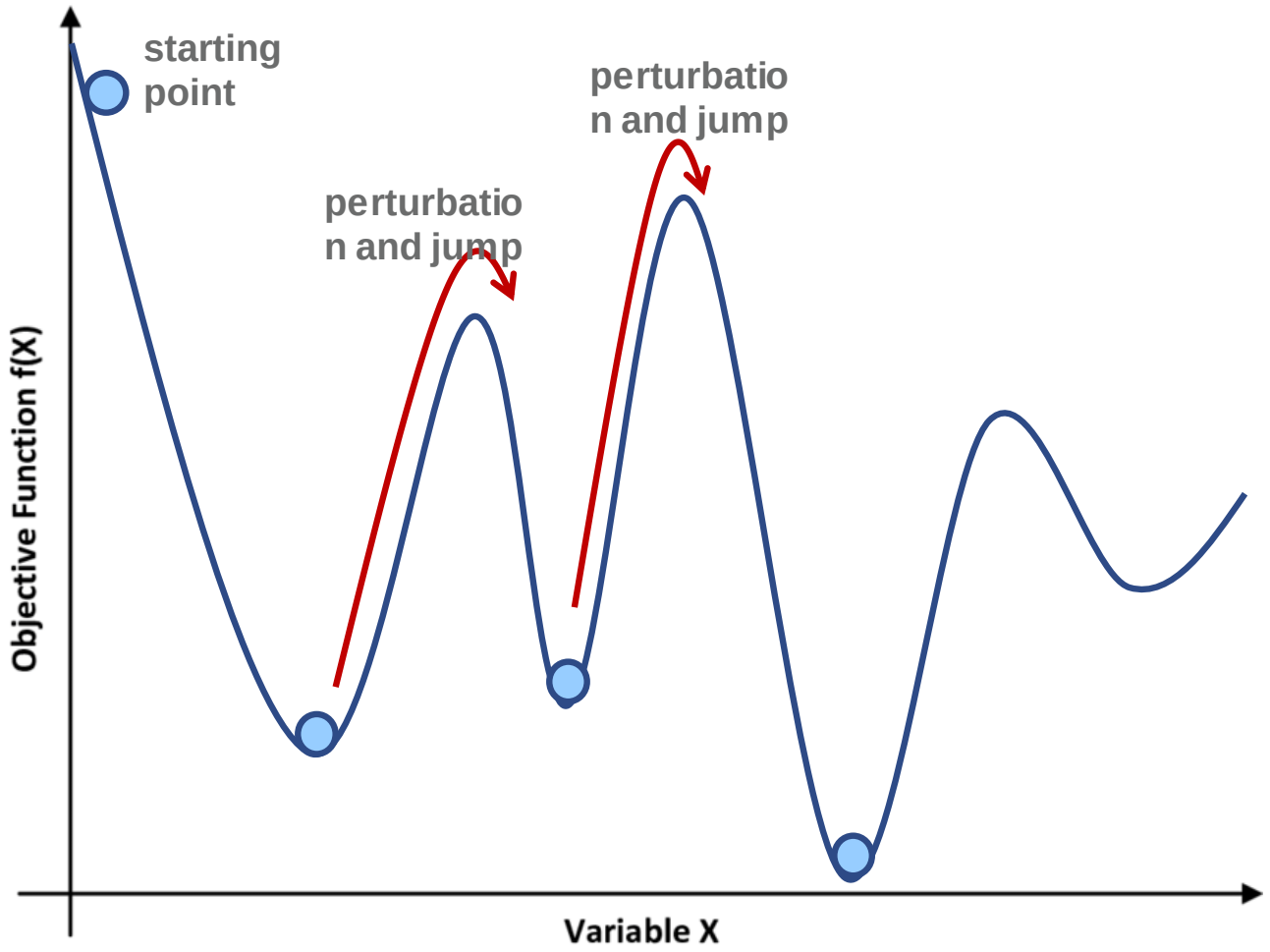

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- There are many algorithms capable of identifying the optimal point of an objective function without having to analyze each of its points
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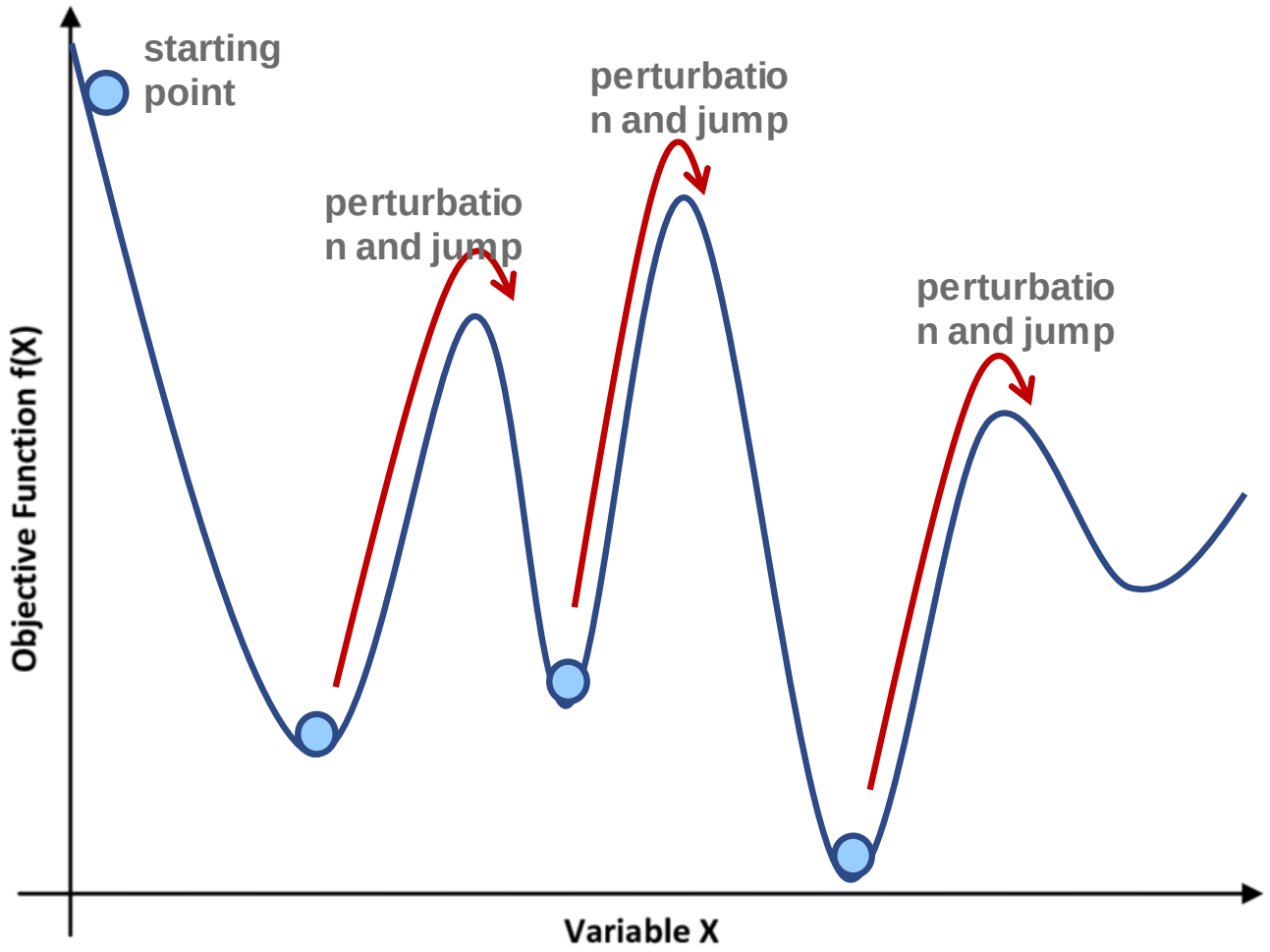

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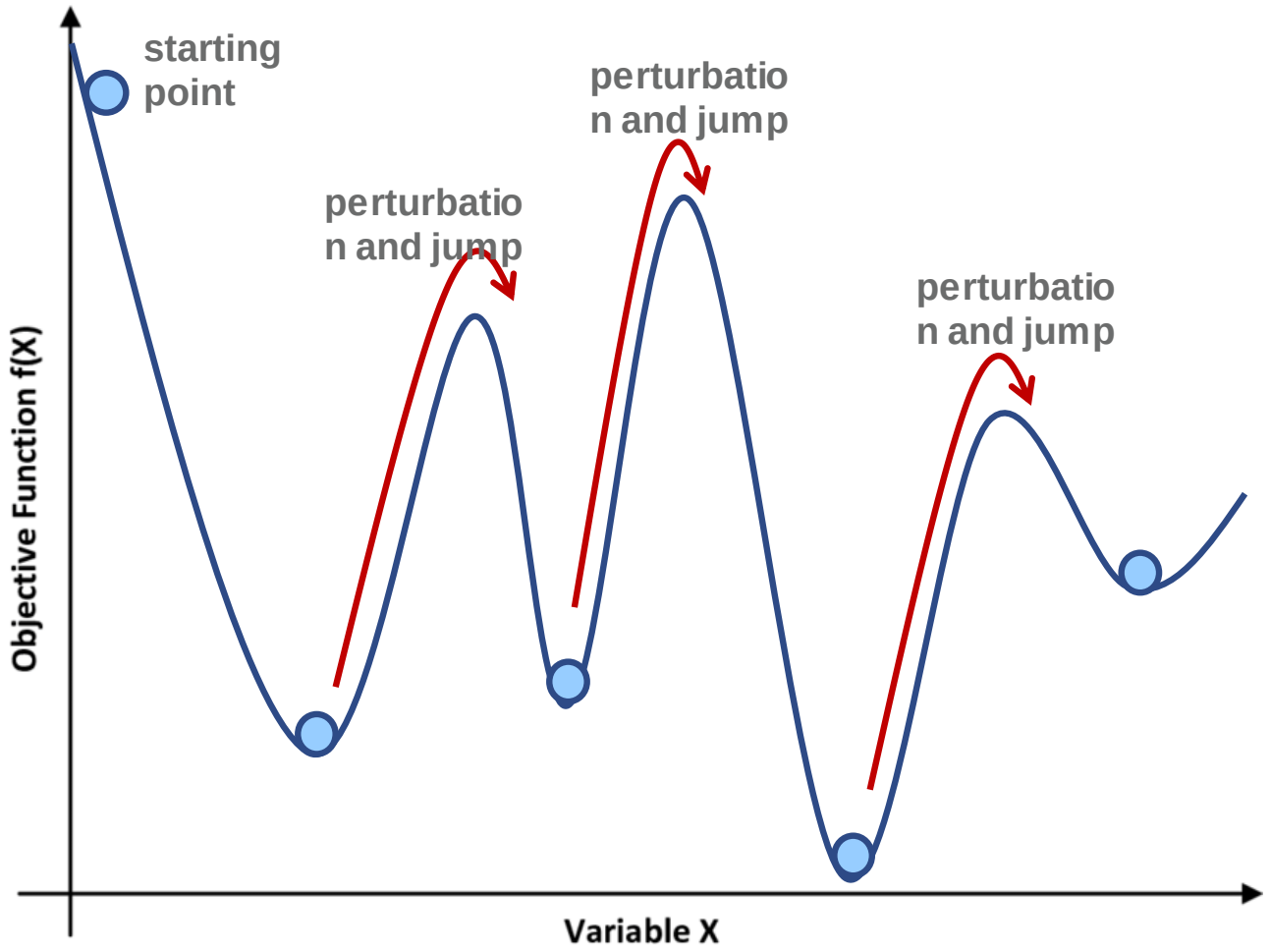

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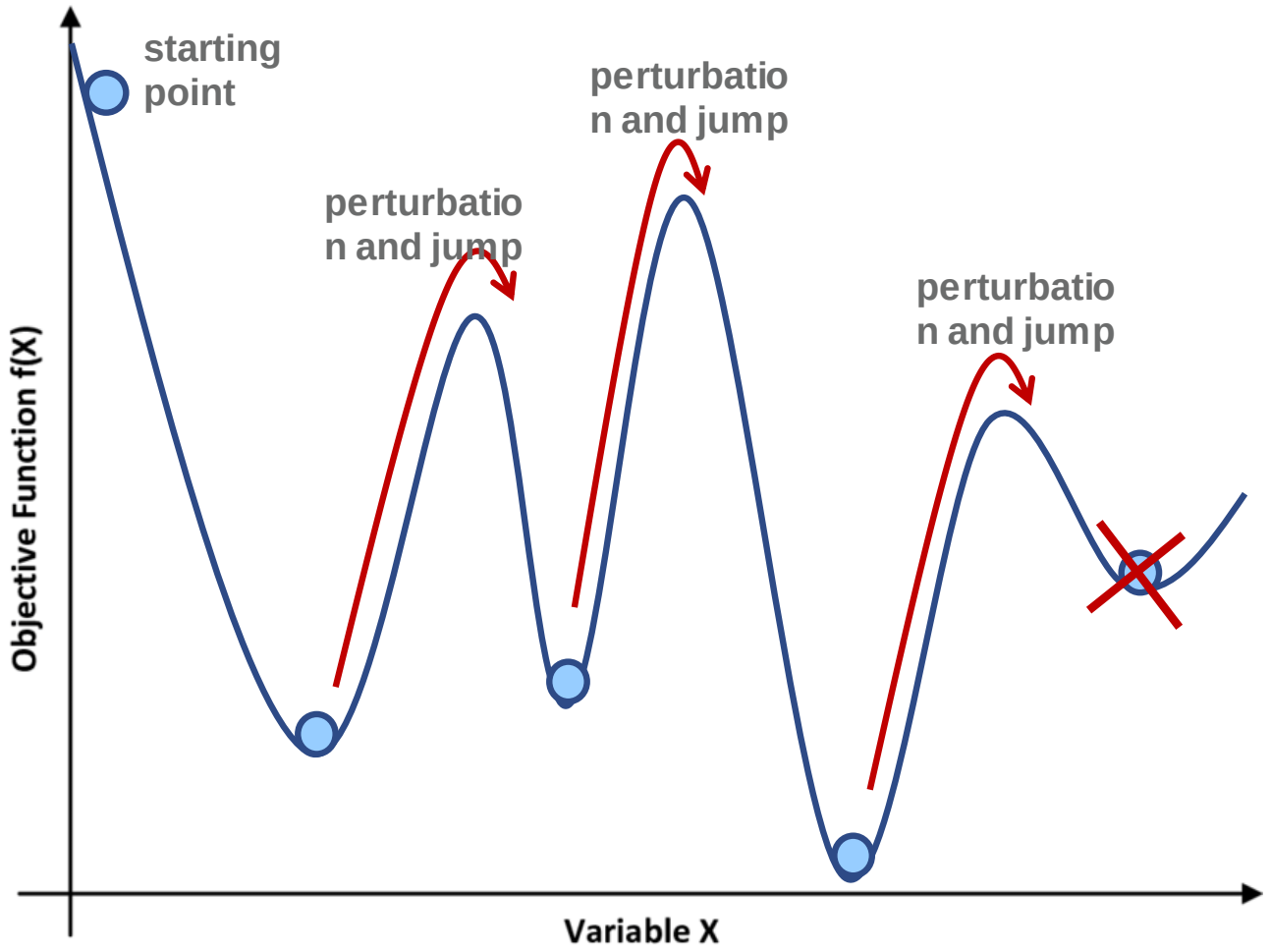

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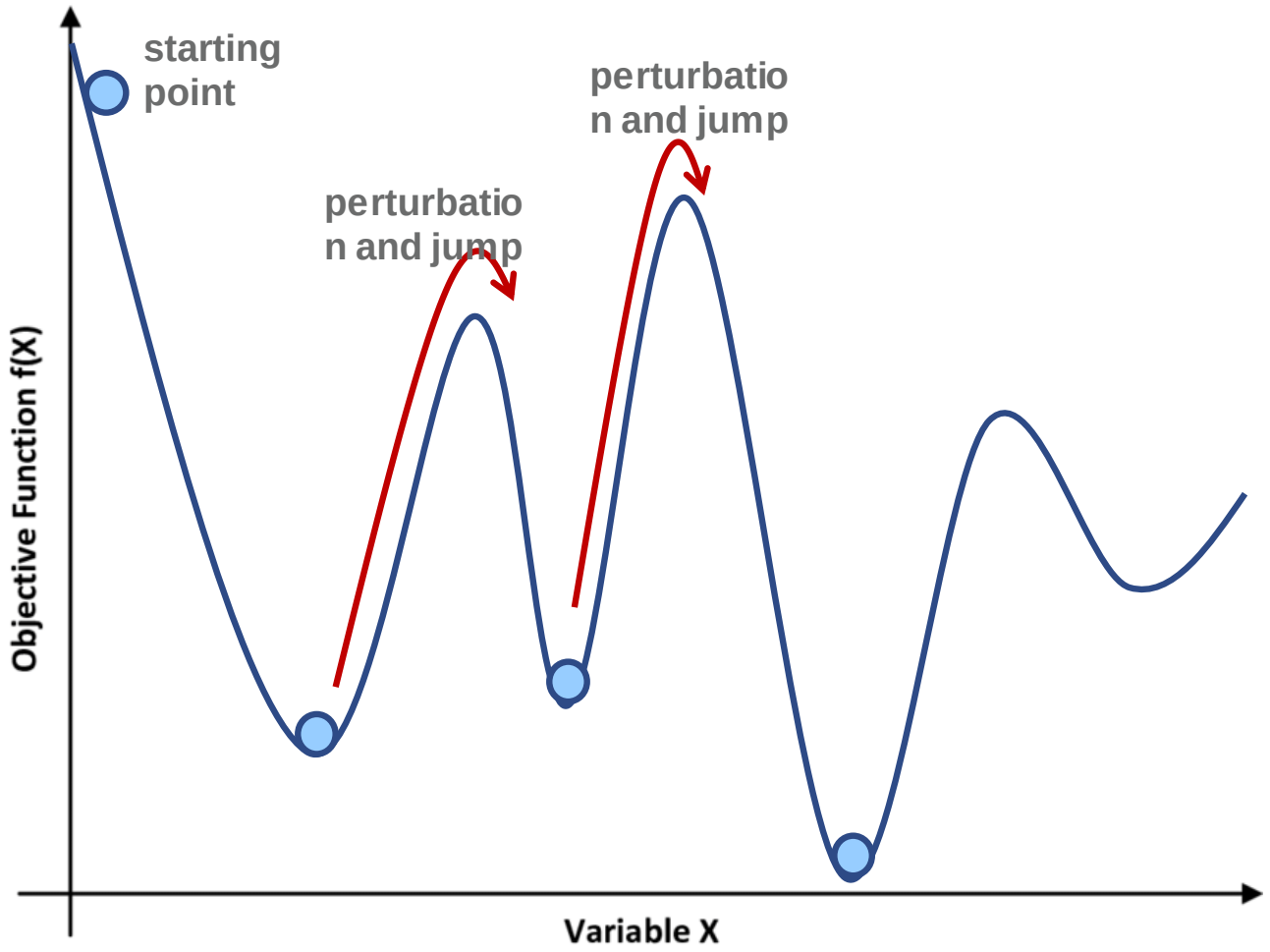

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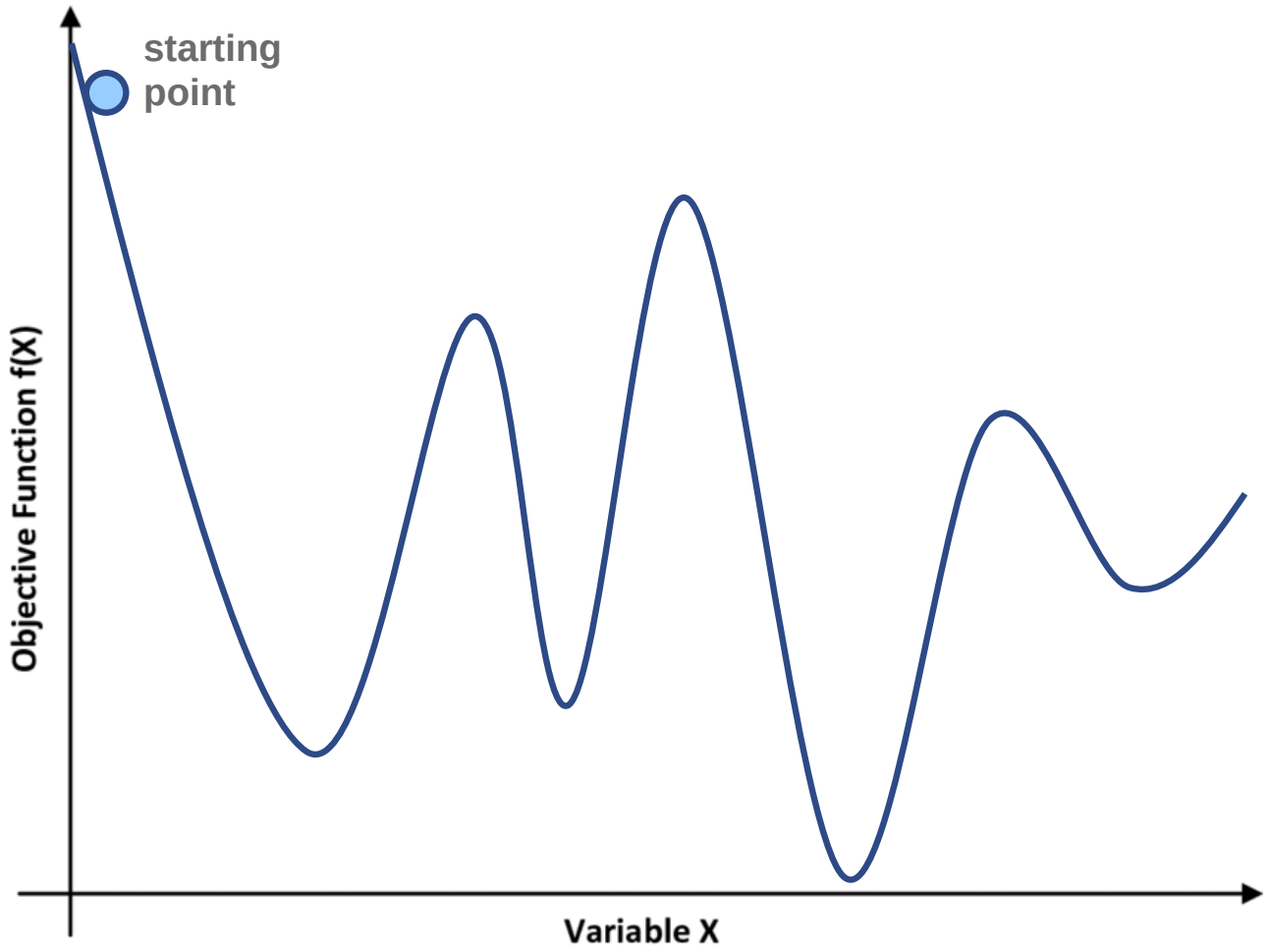

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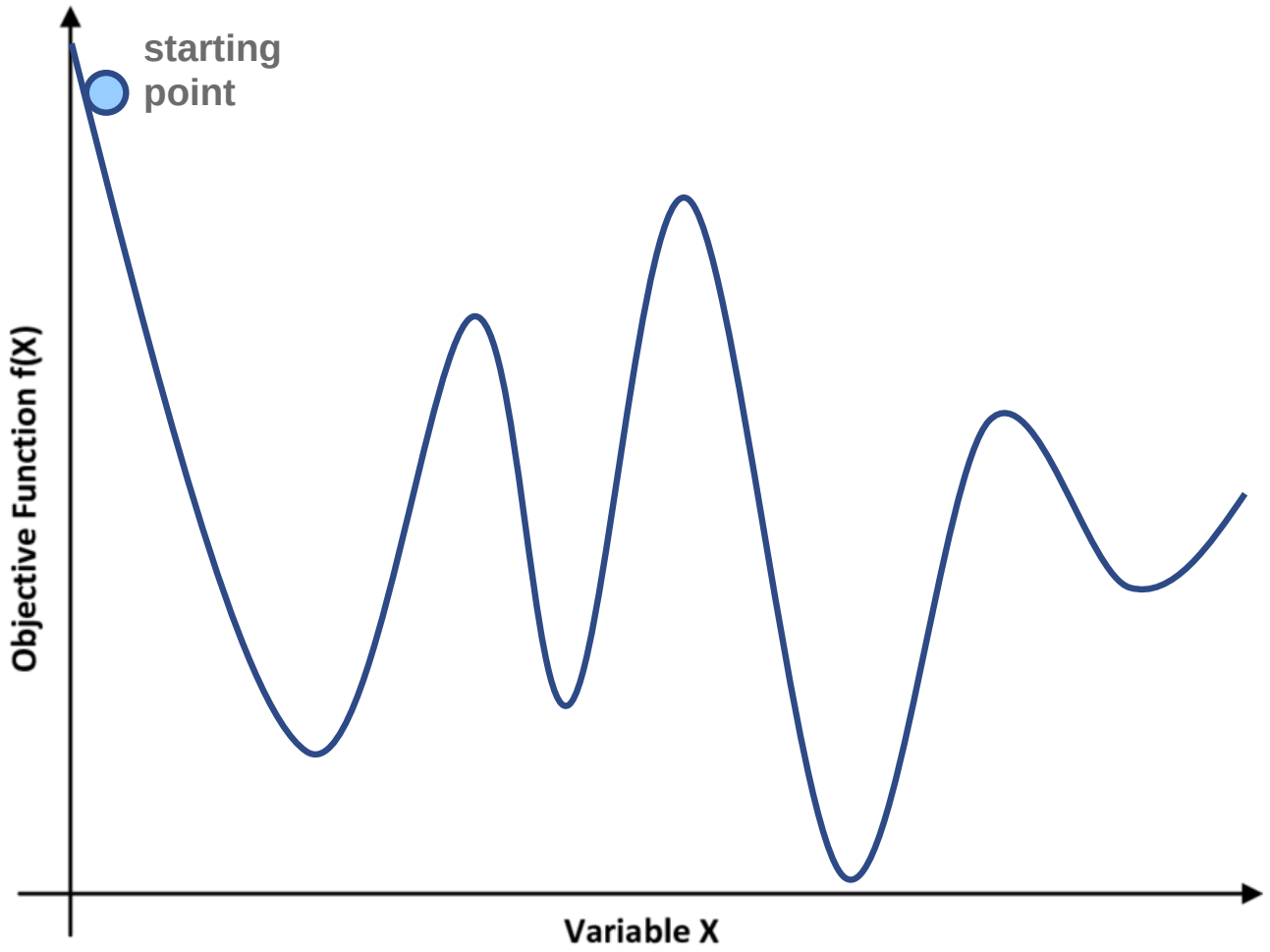

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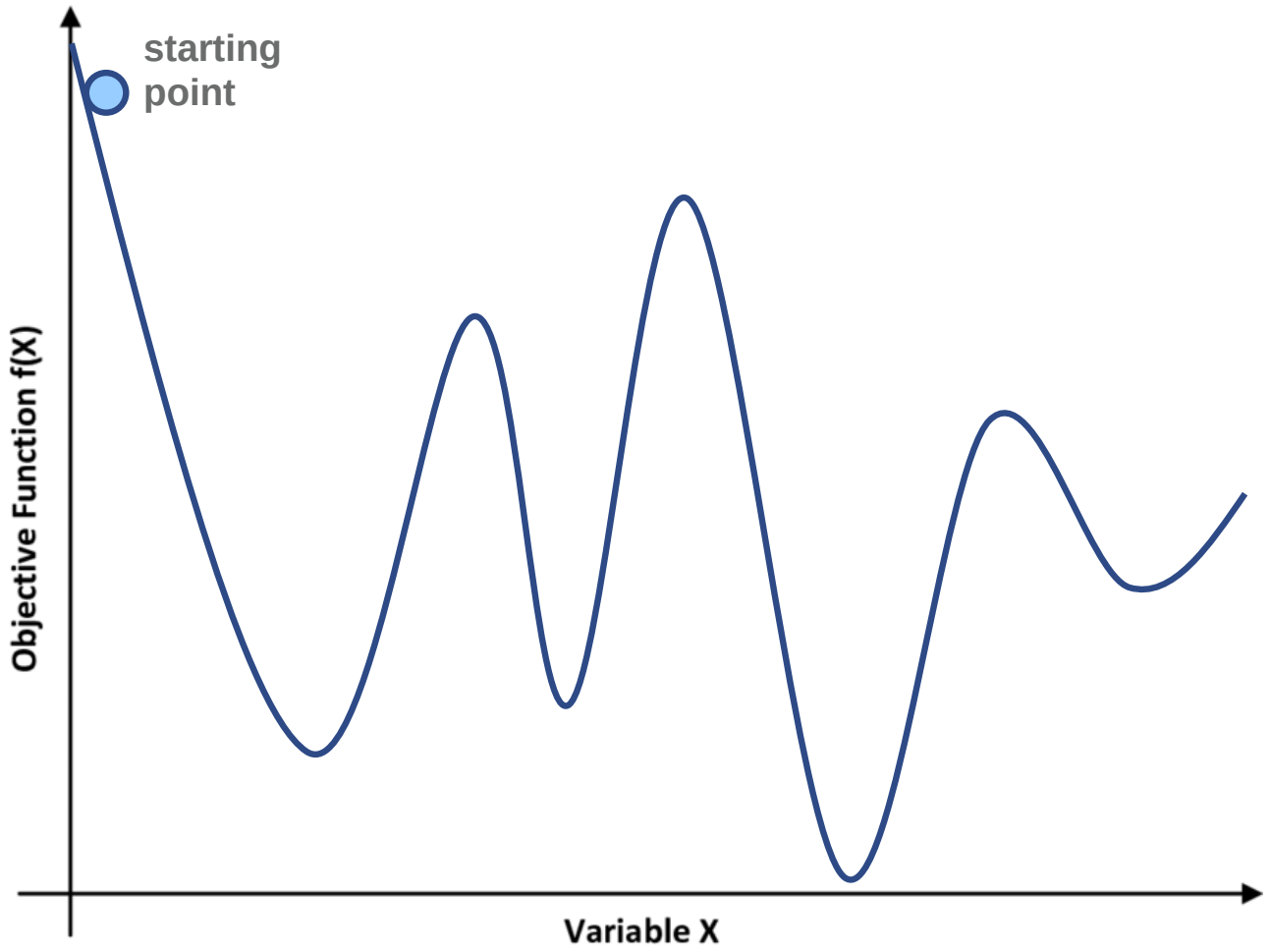

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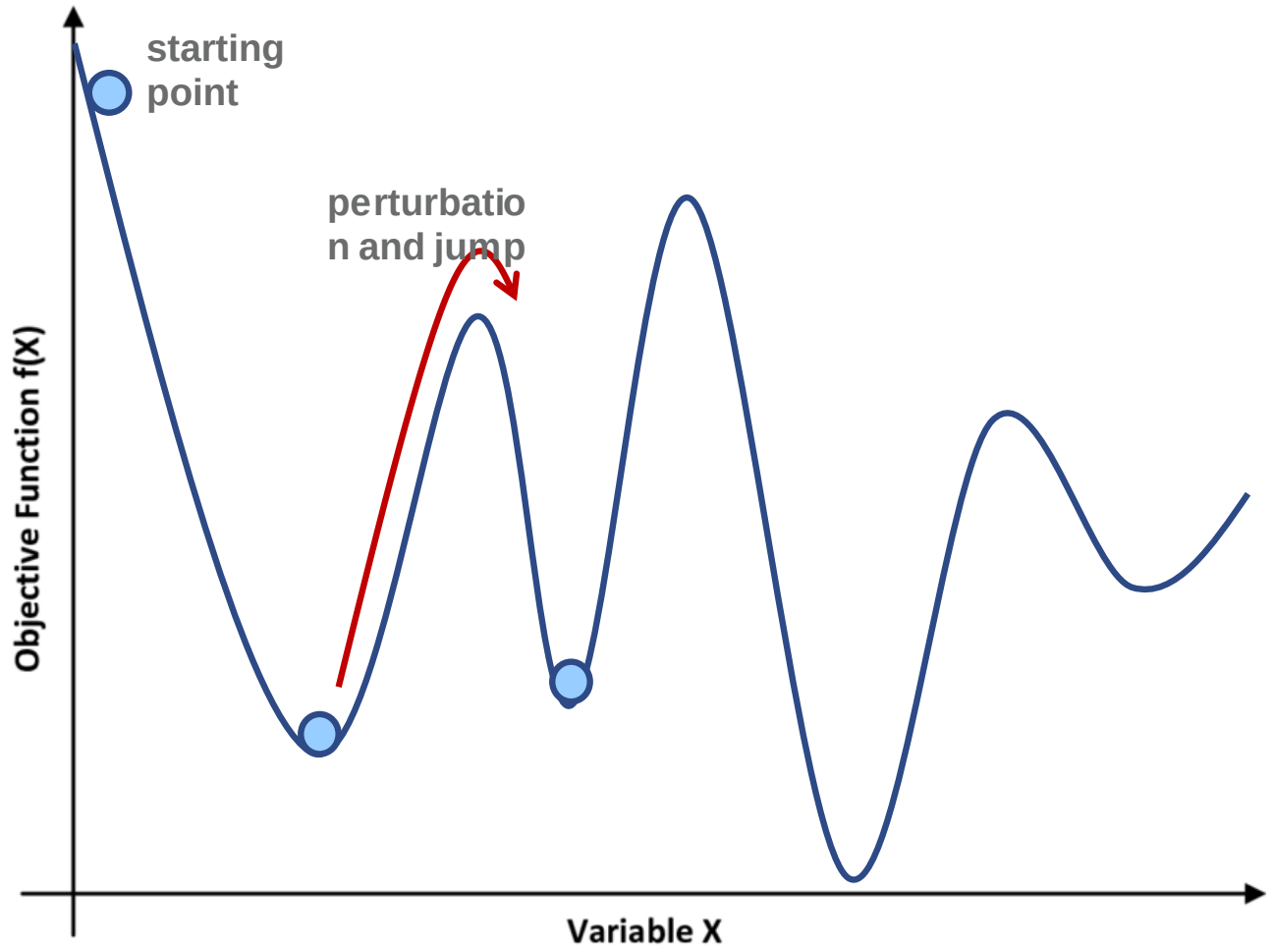

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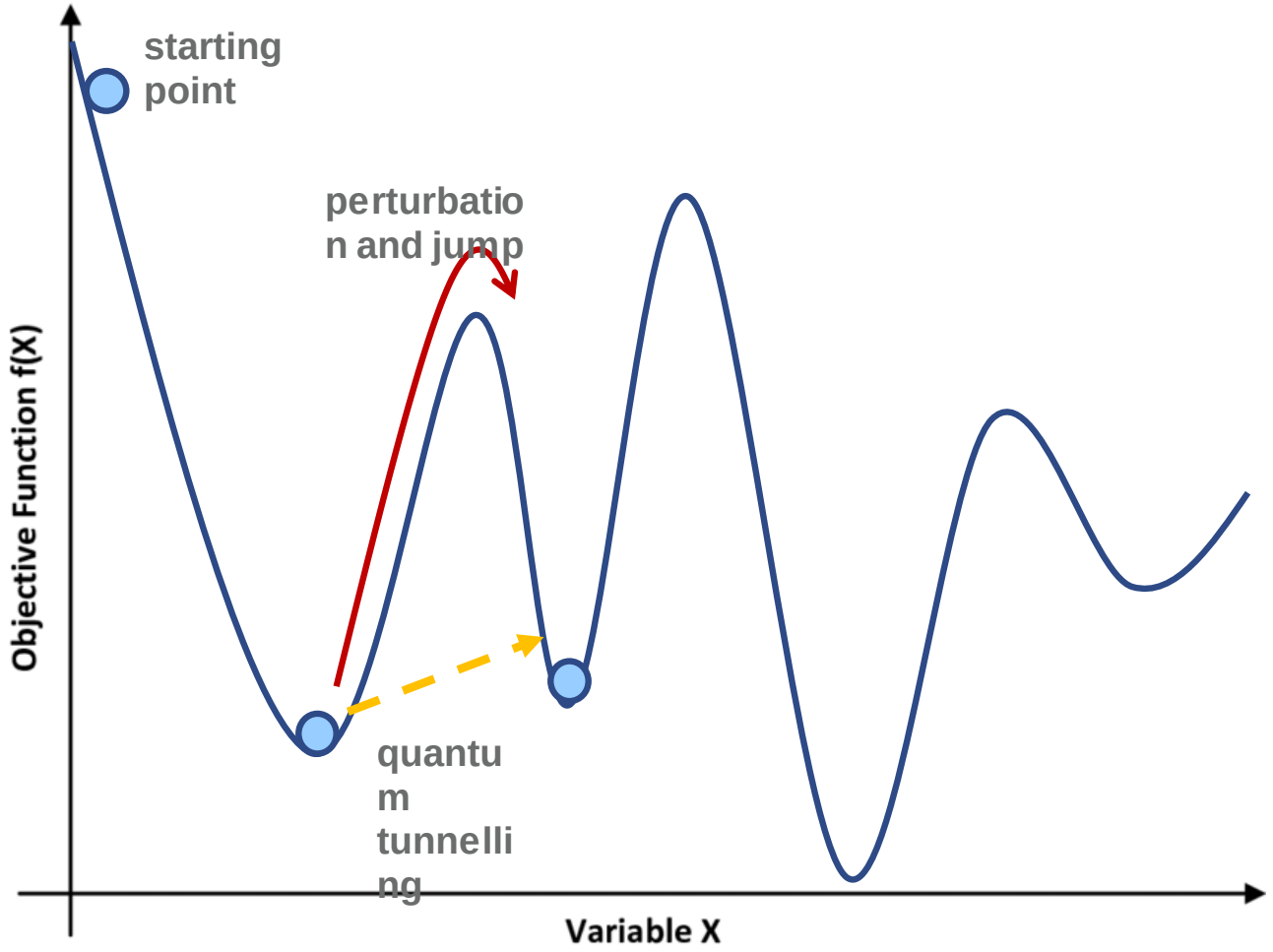

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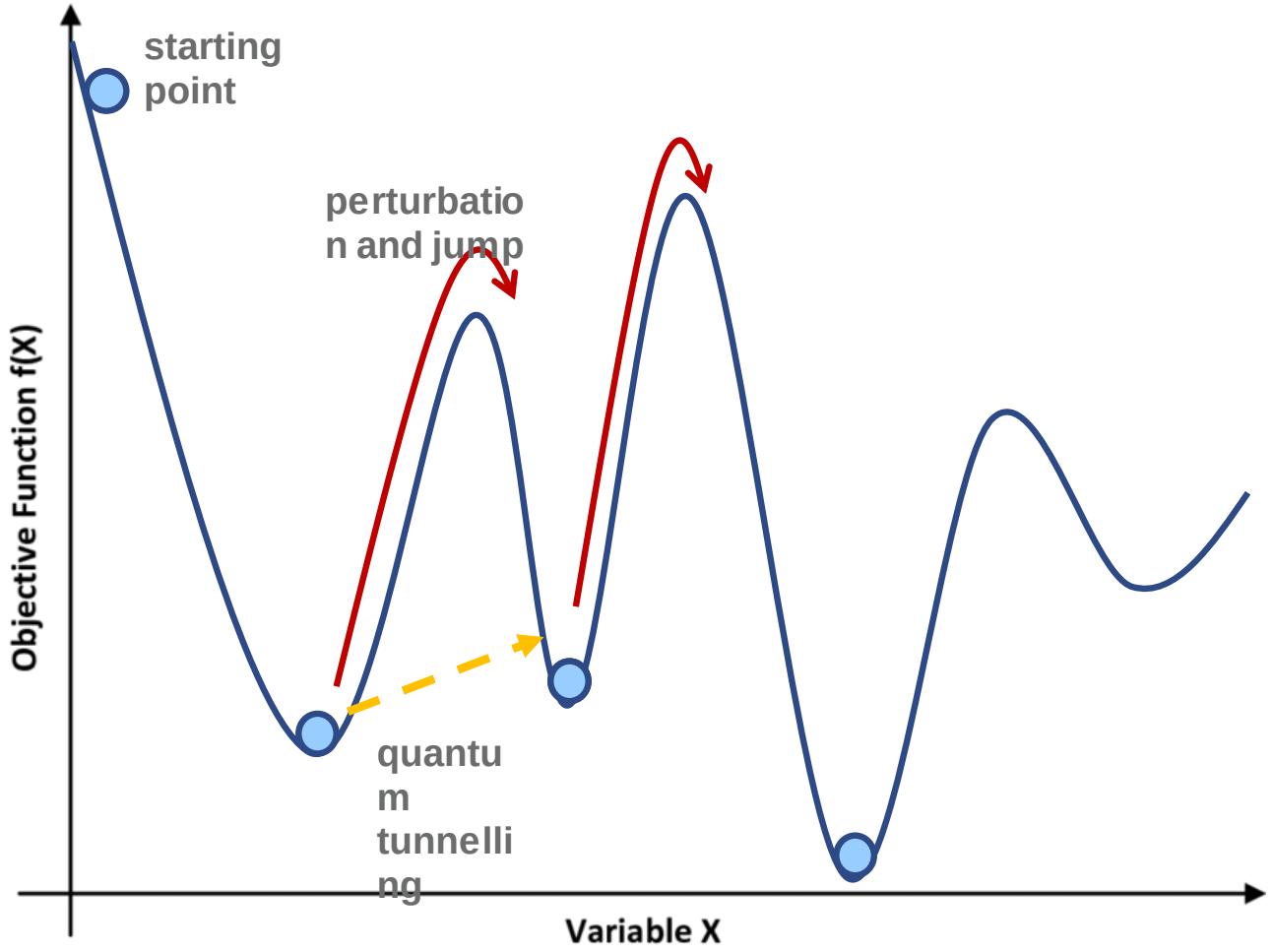

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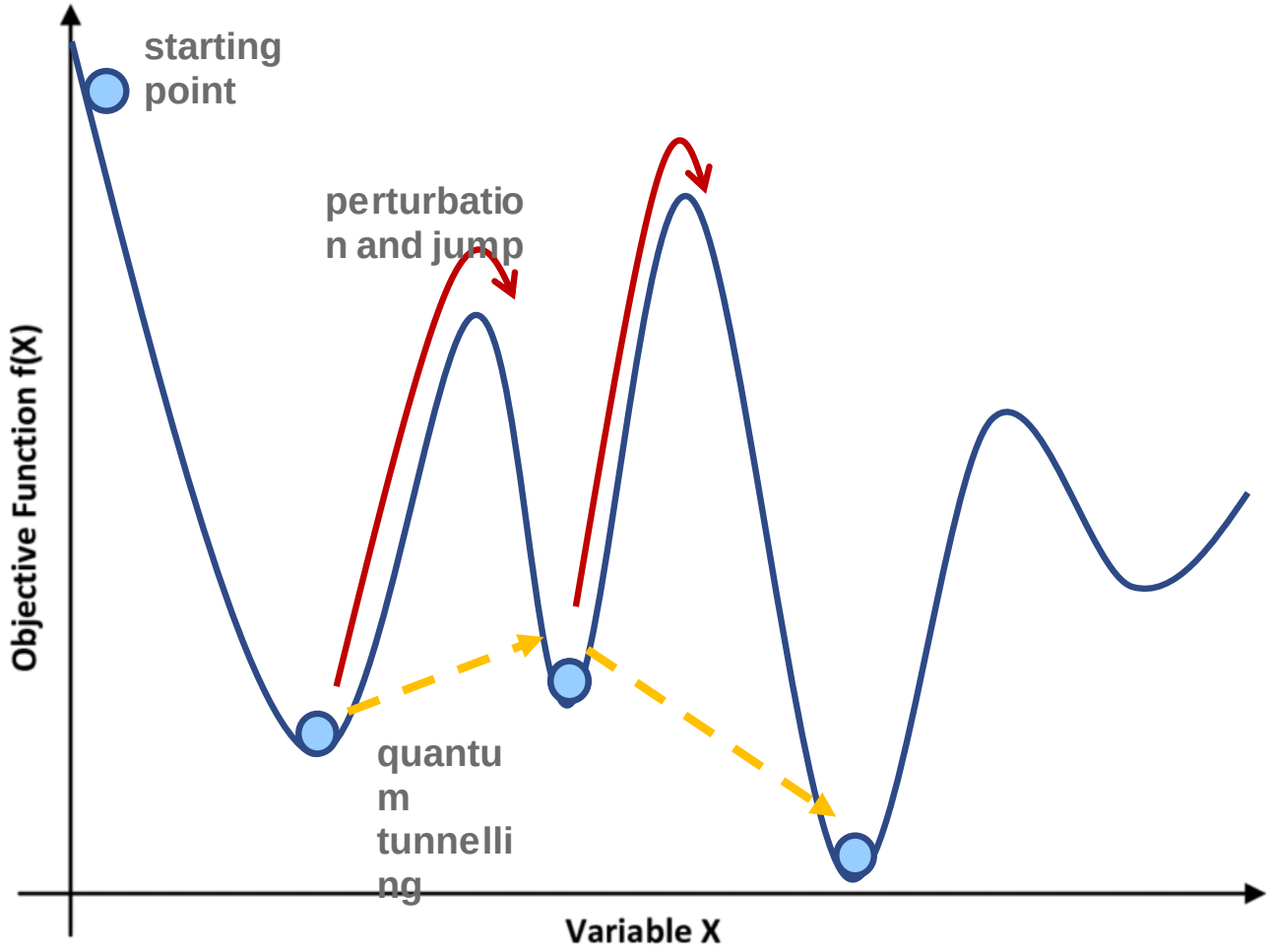

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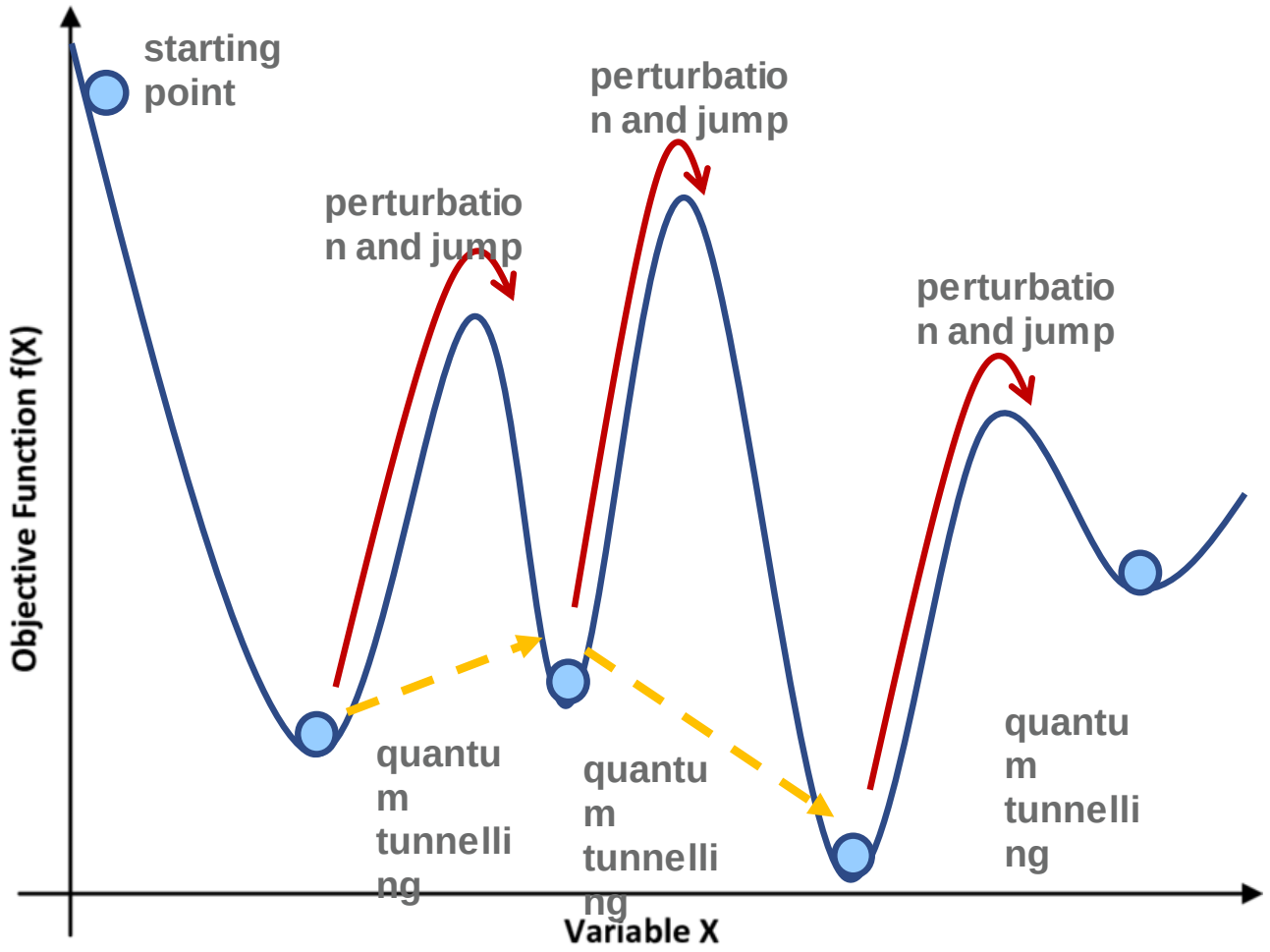

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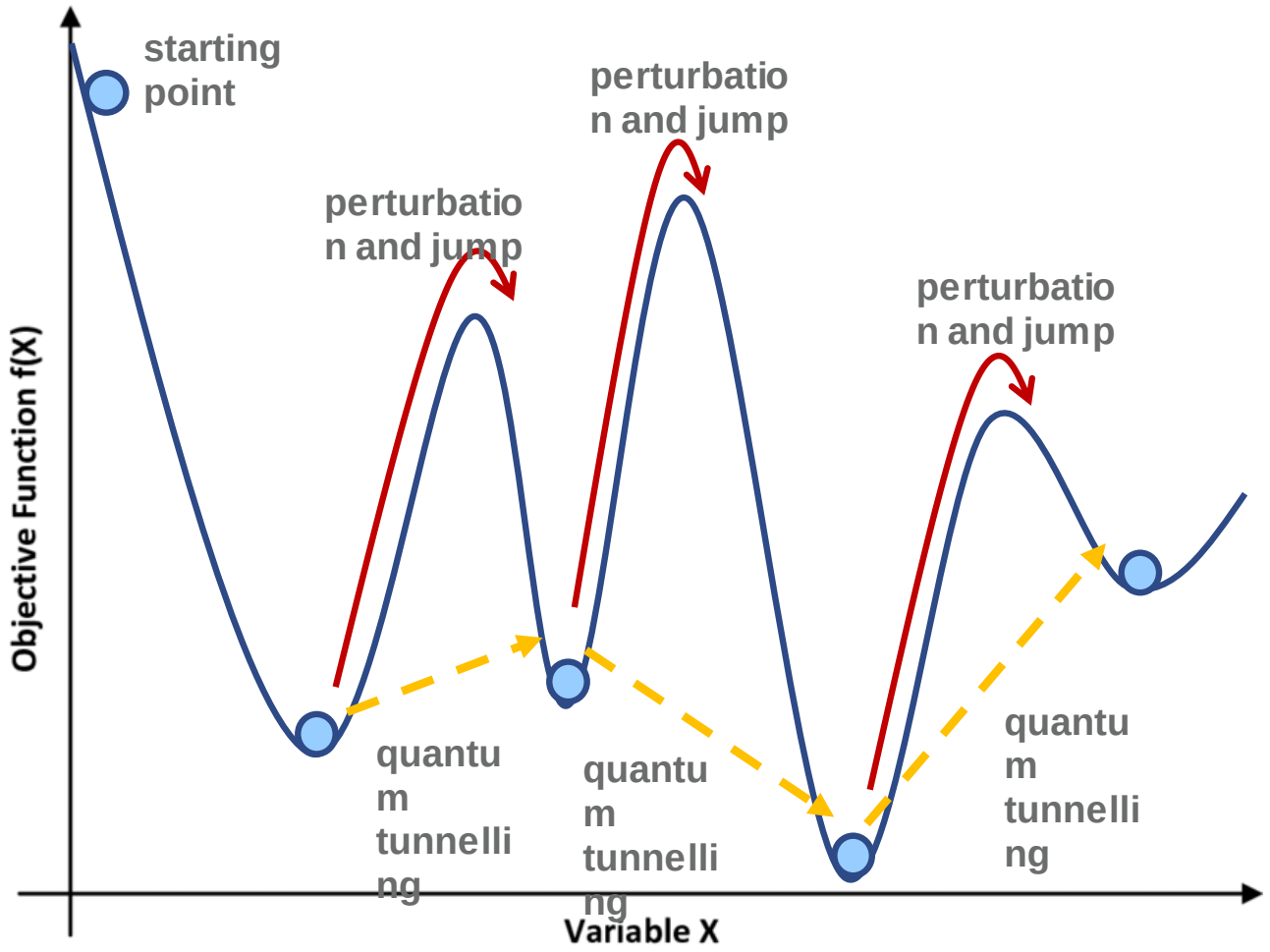

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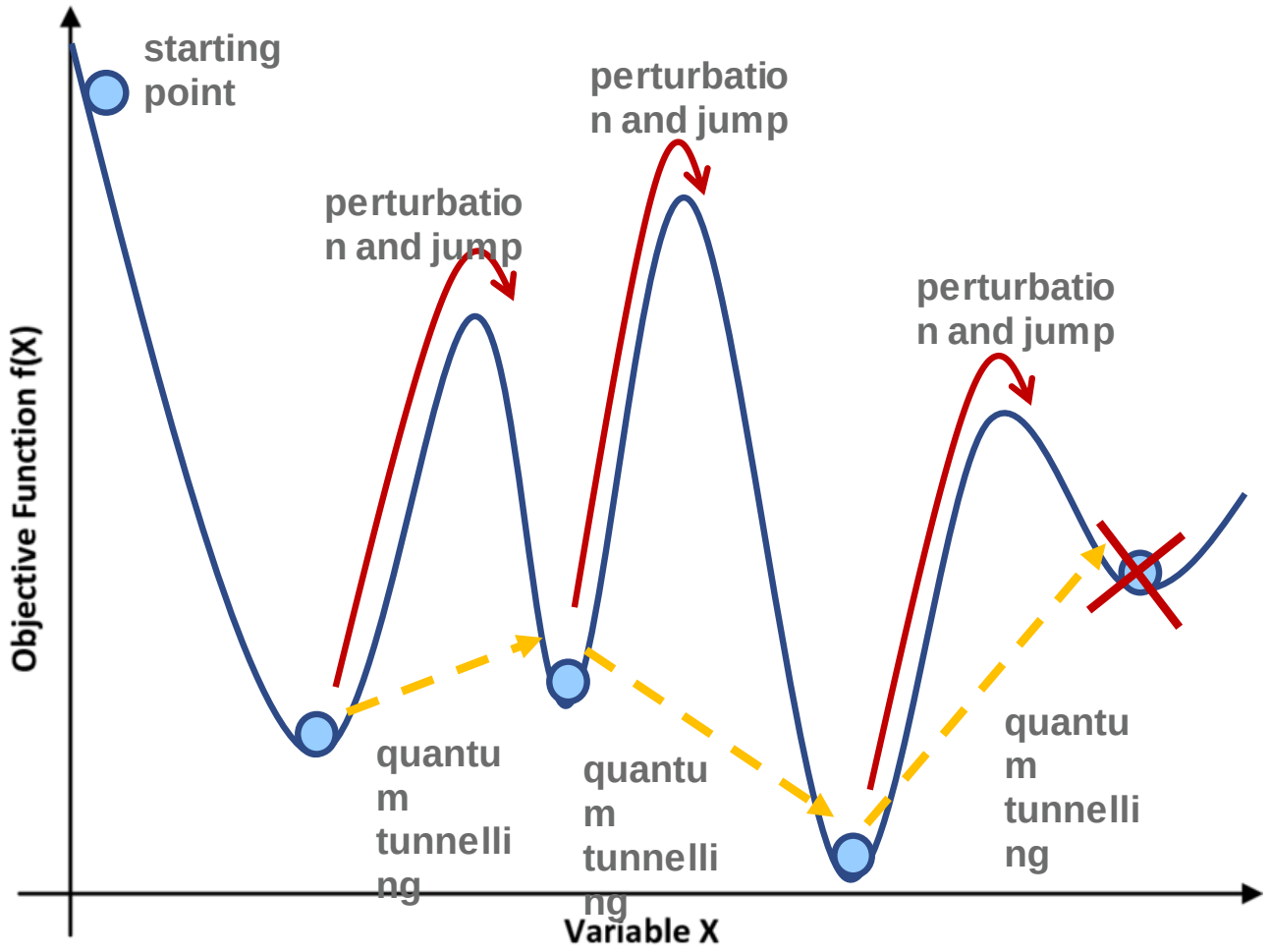
- How does the Quantum Annealing process work? The core of the algorithm is in the **Adiabatic Theorem**:
  A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum



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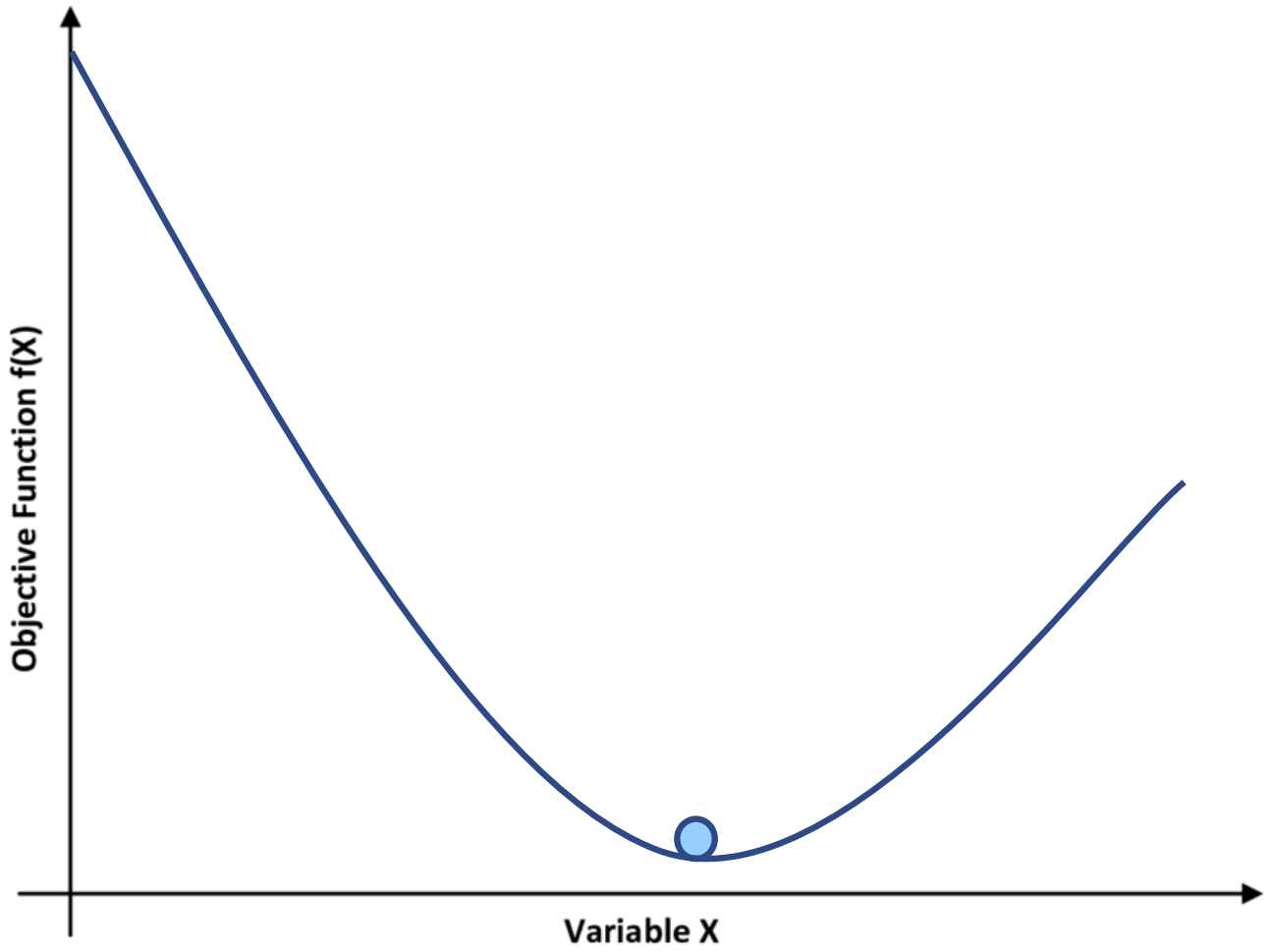

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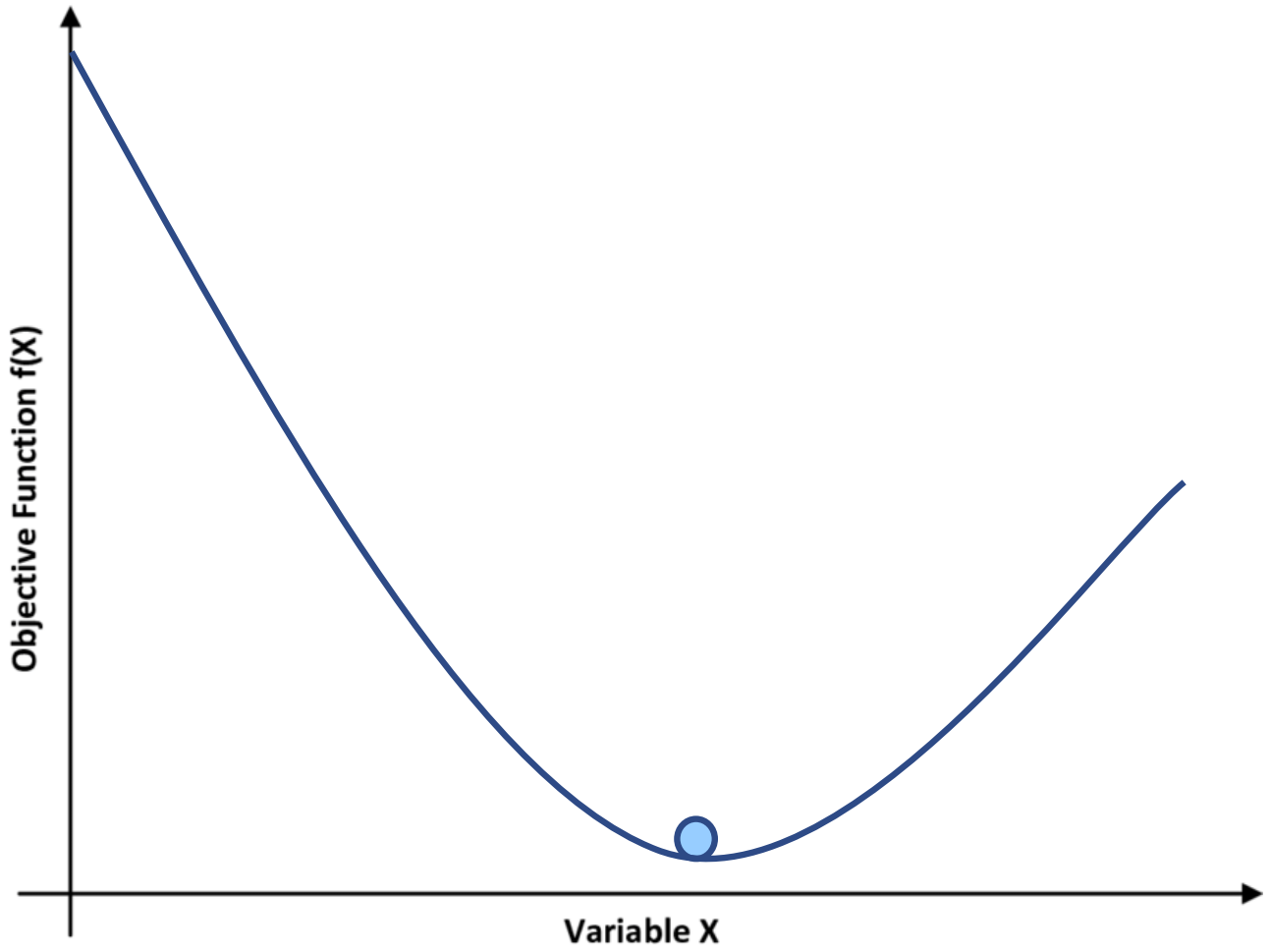

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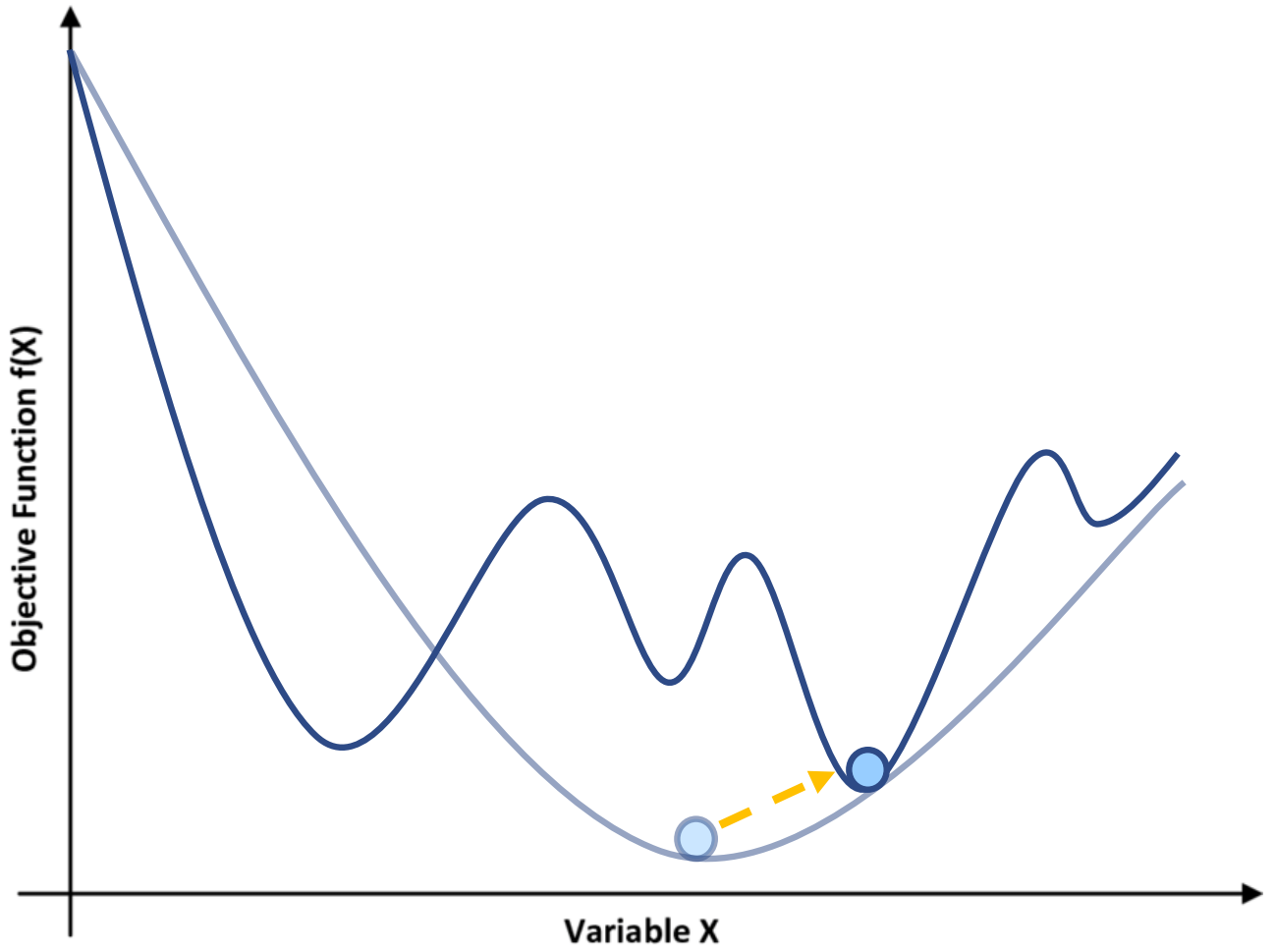

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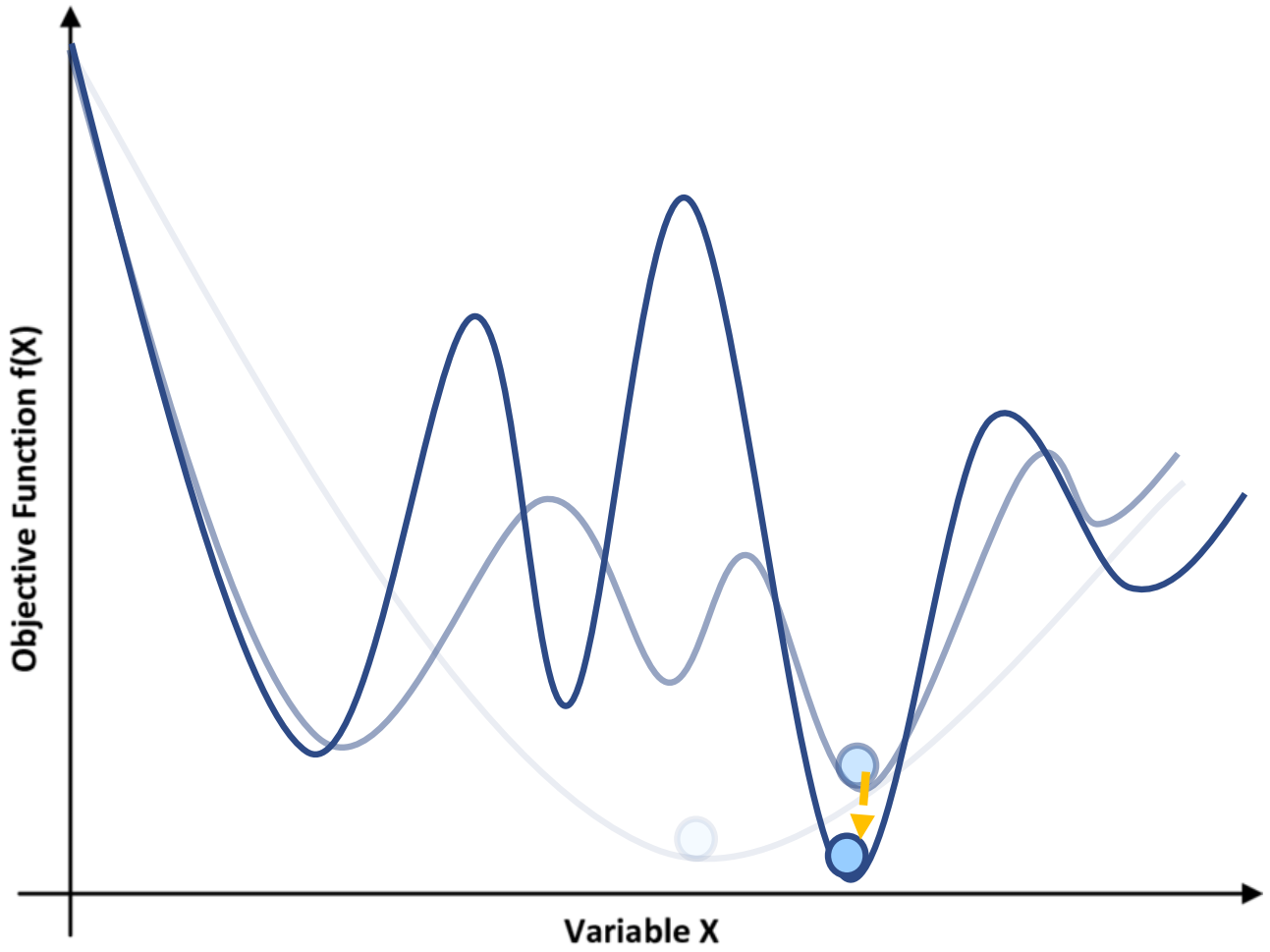

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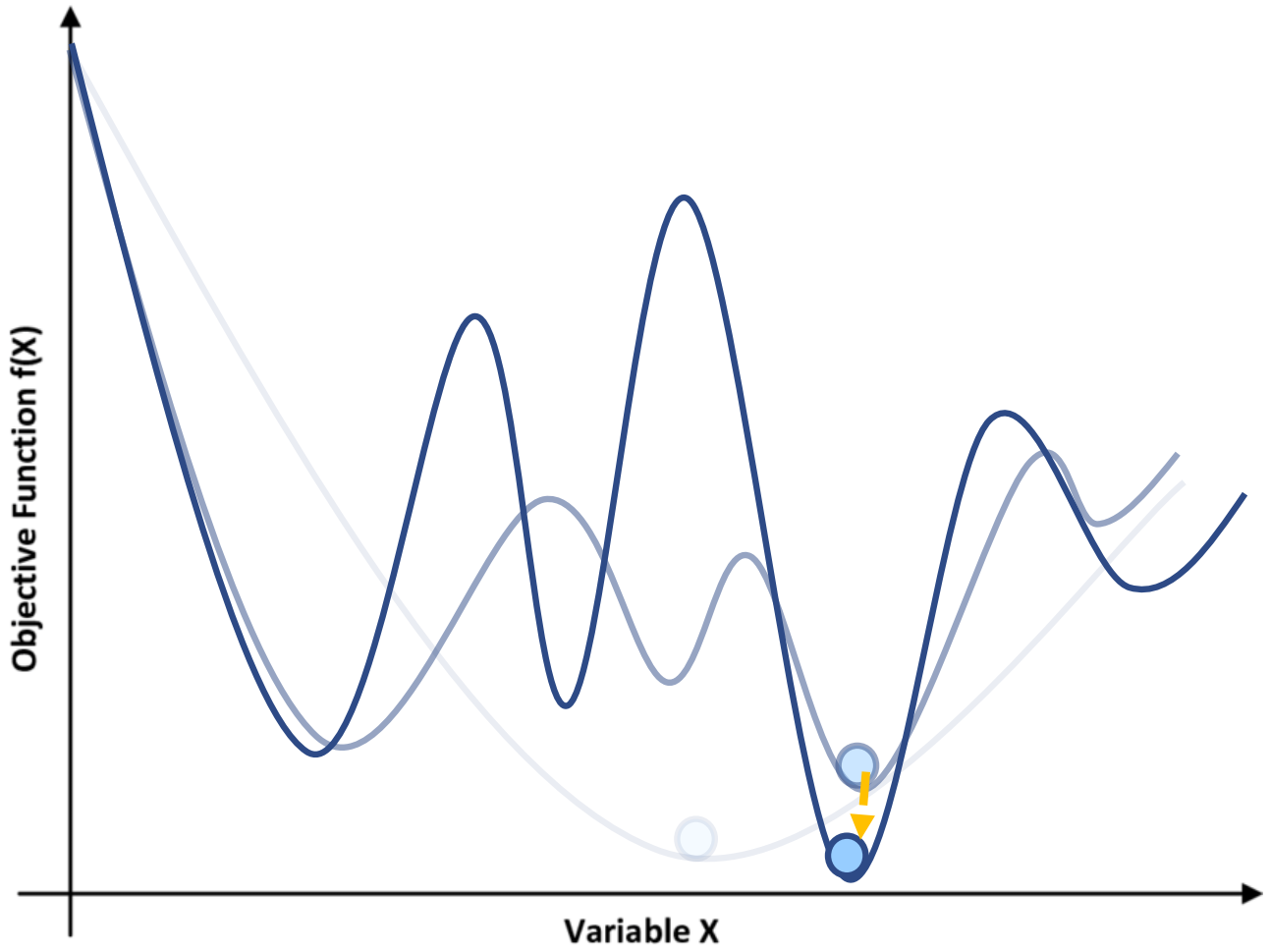

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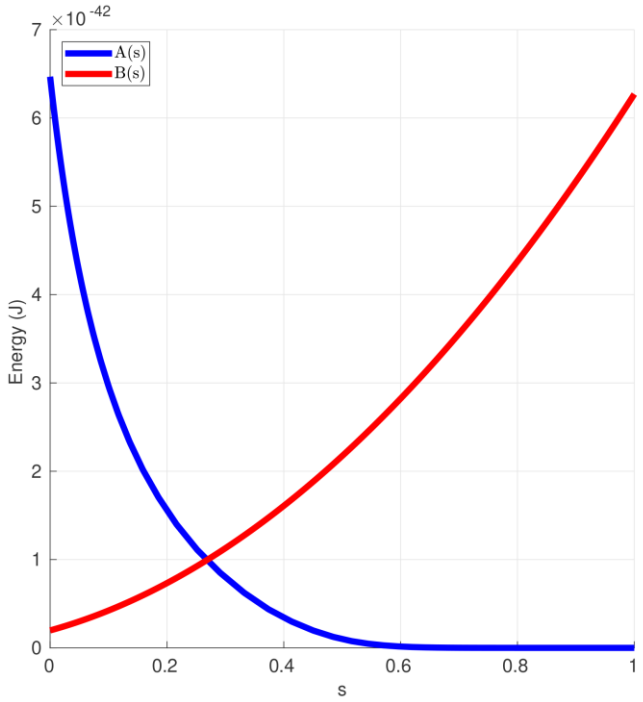

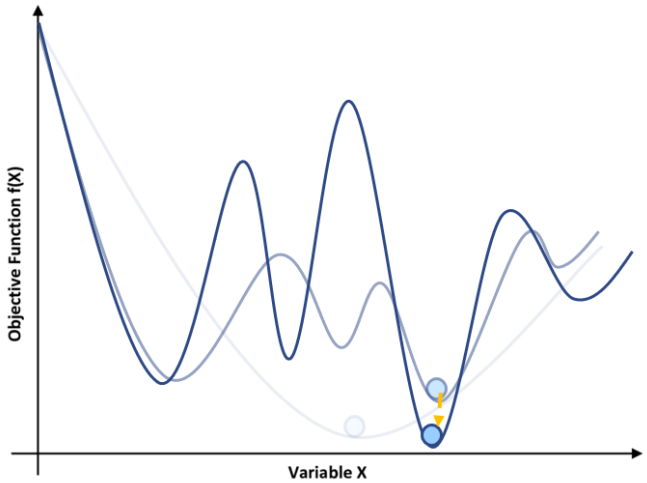

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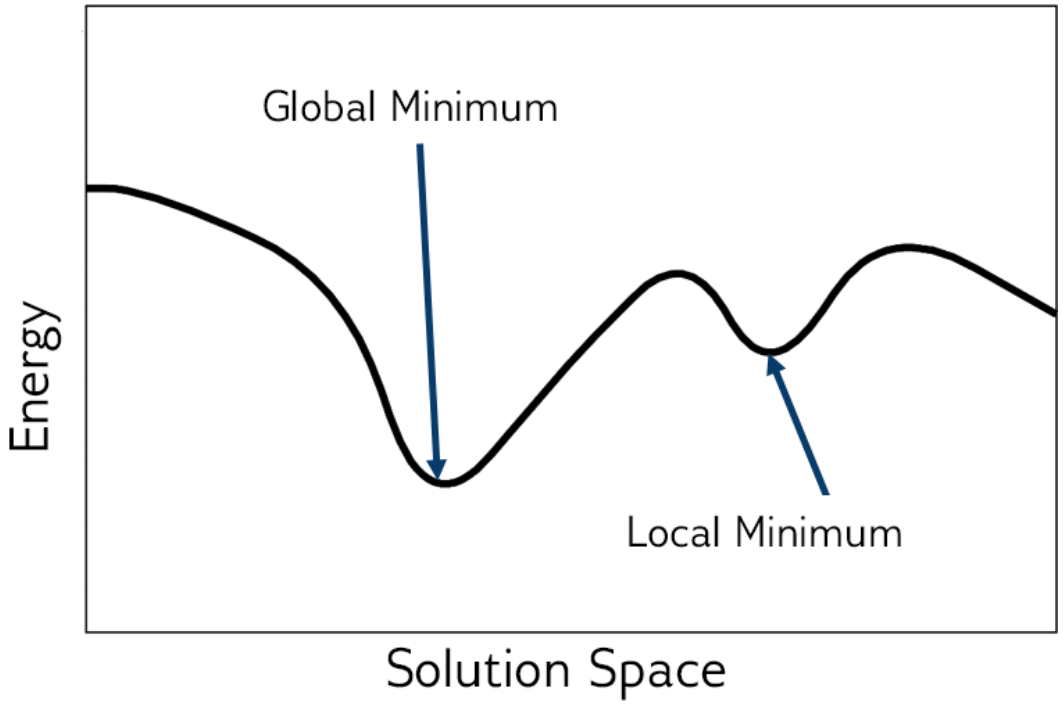

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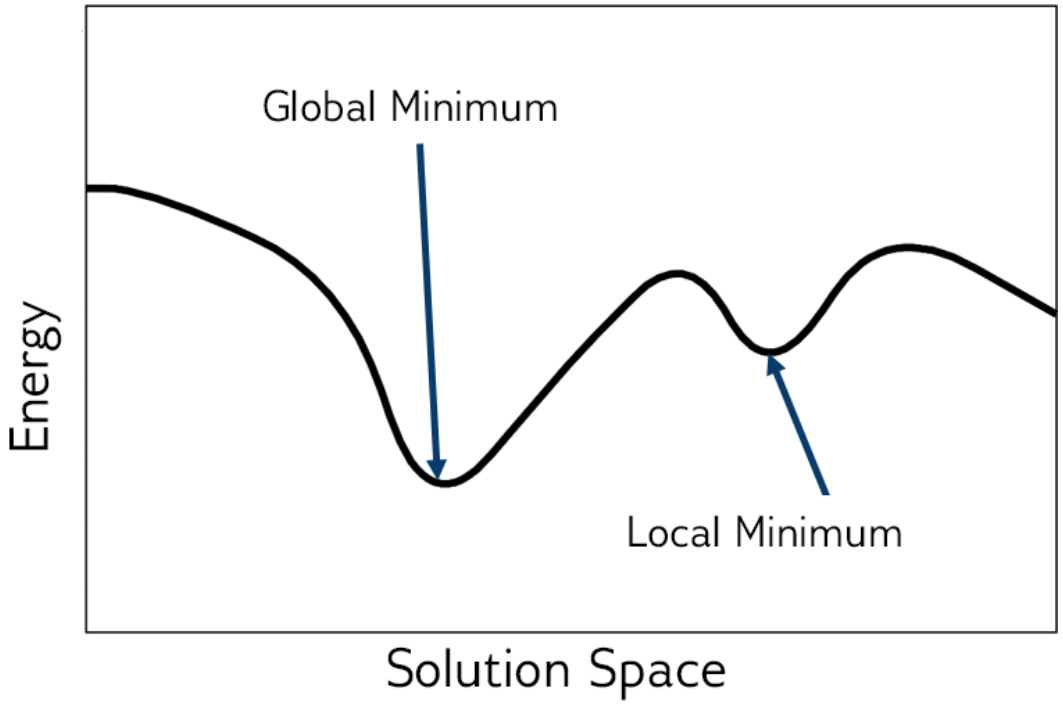

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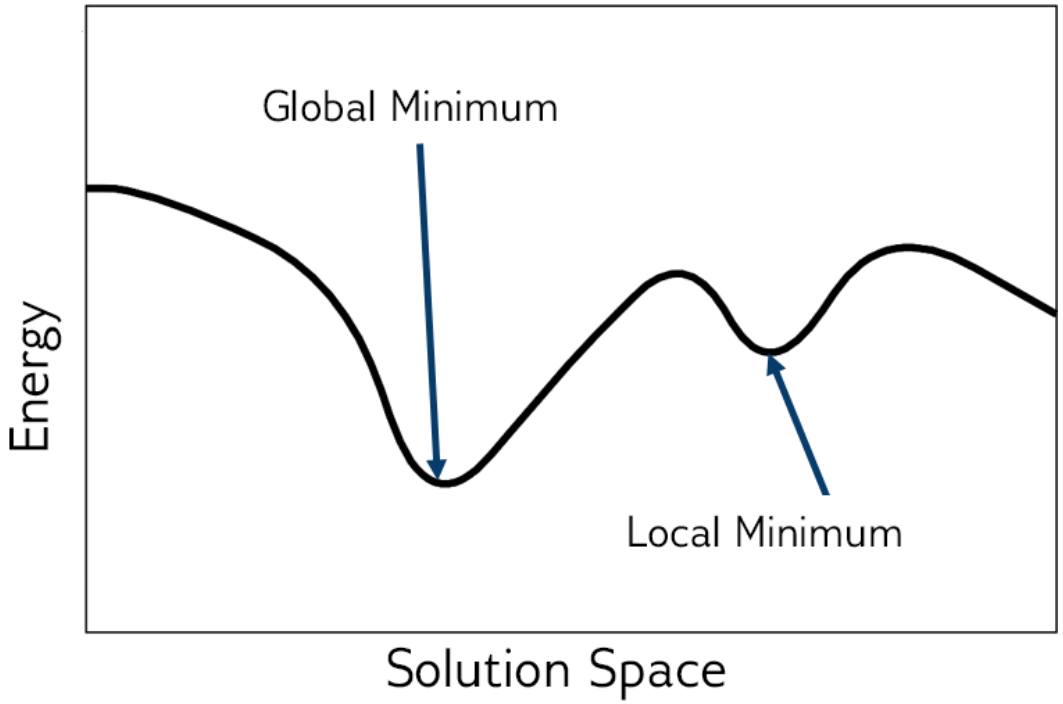

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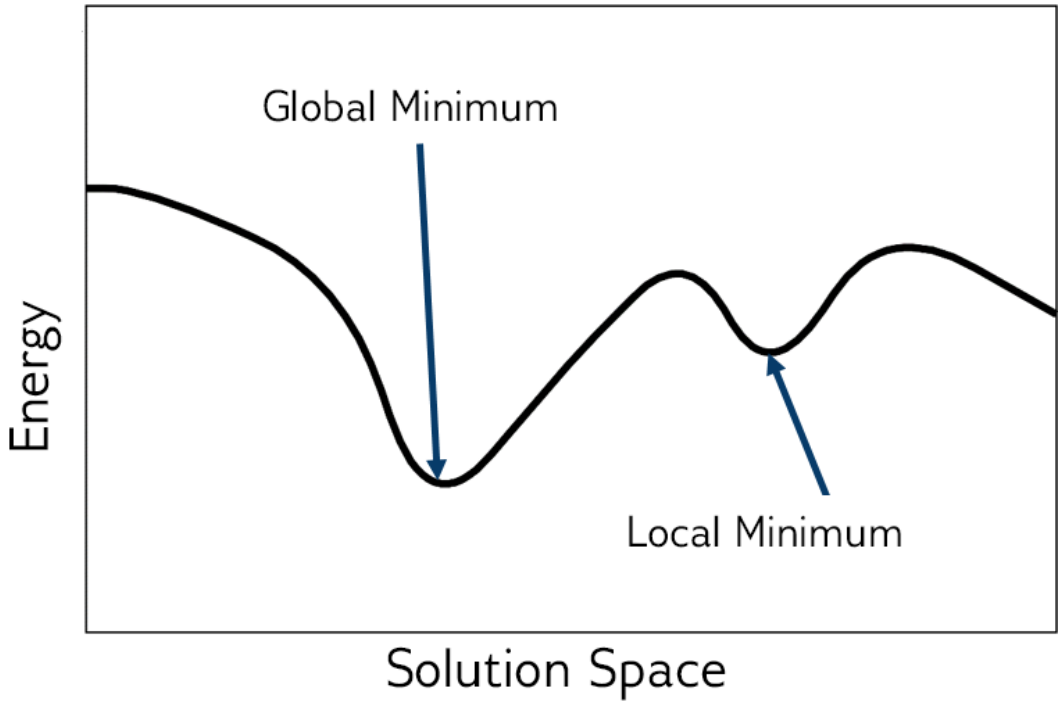
- For most problems, the lower the energy of the objective function, the better the solution. Sometimes any state of local minimum for energy is an acceptable solution to the original problem; for other problems only optimal solutions are acceptable.



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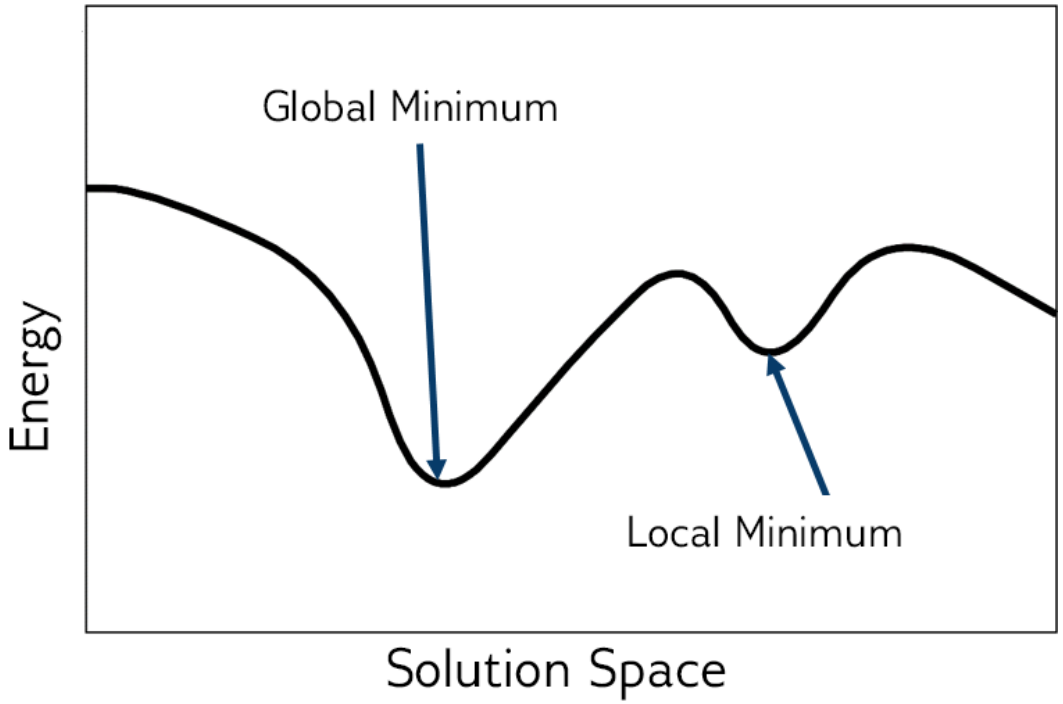

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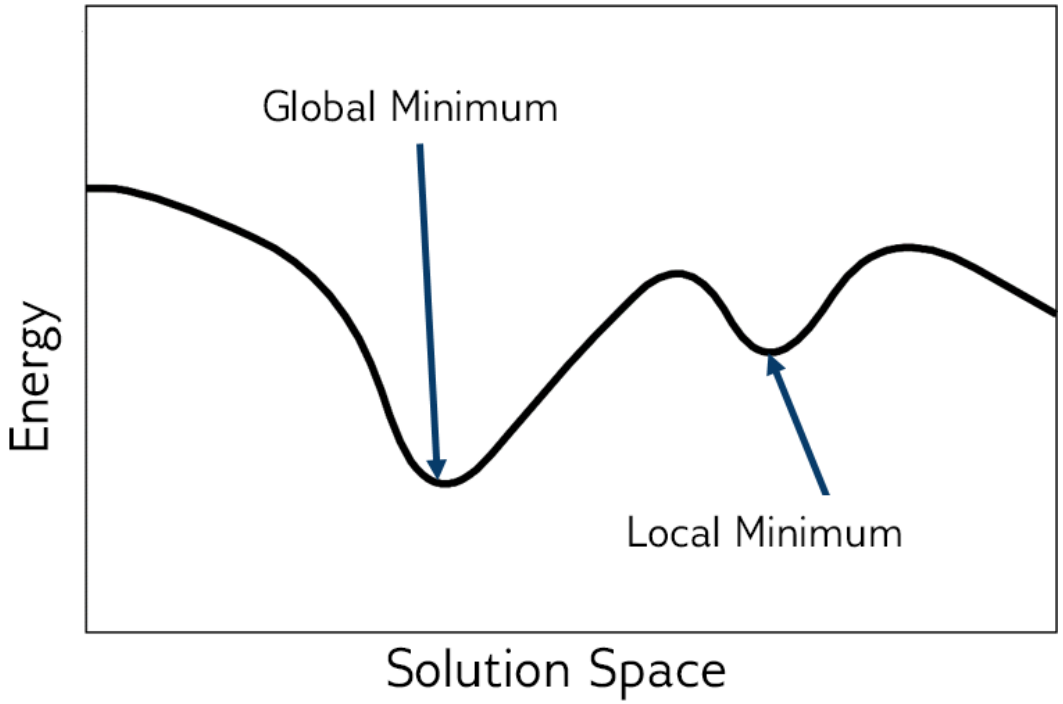

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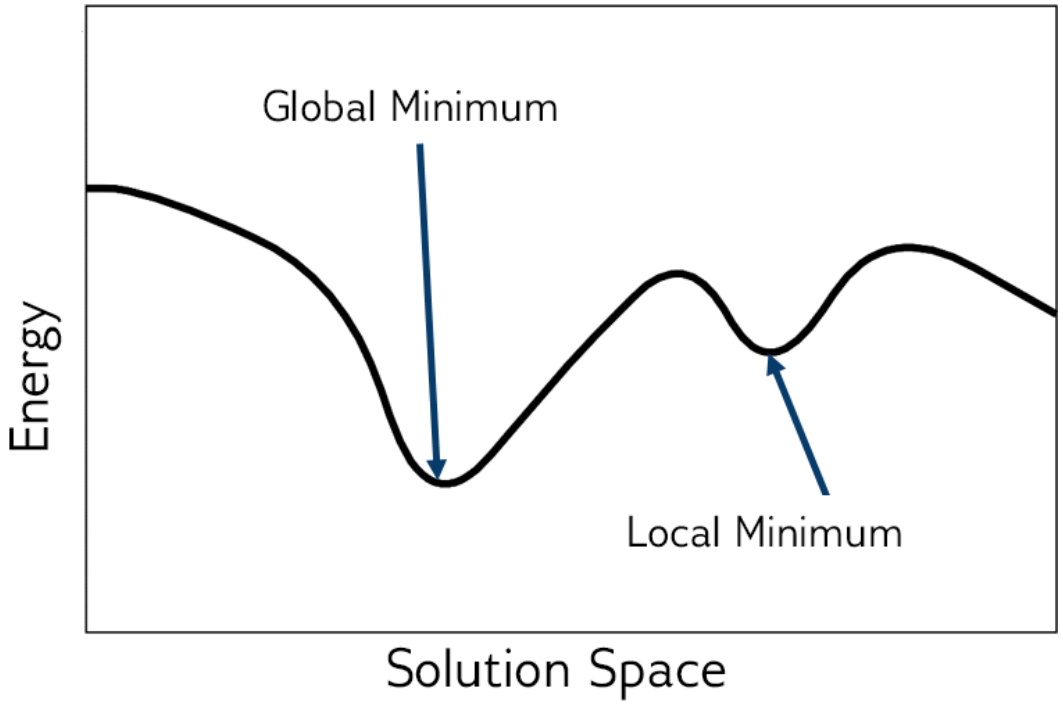

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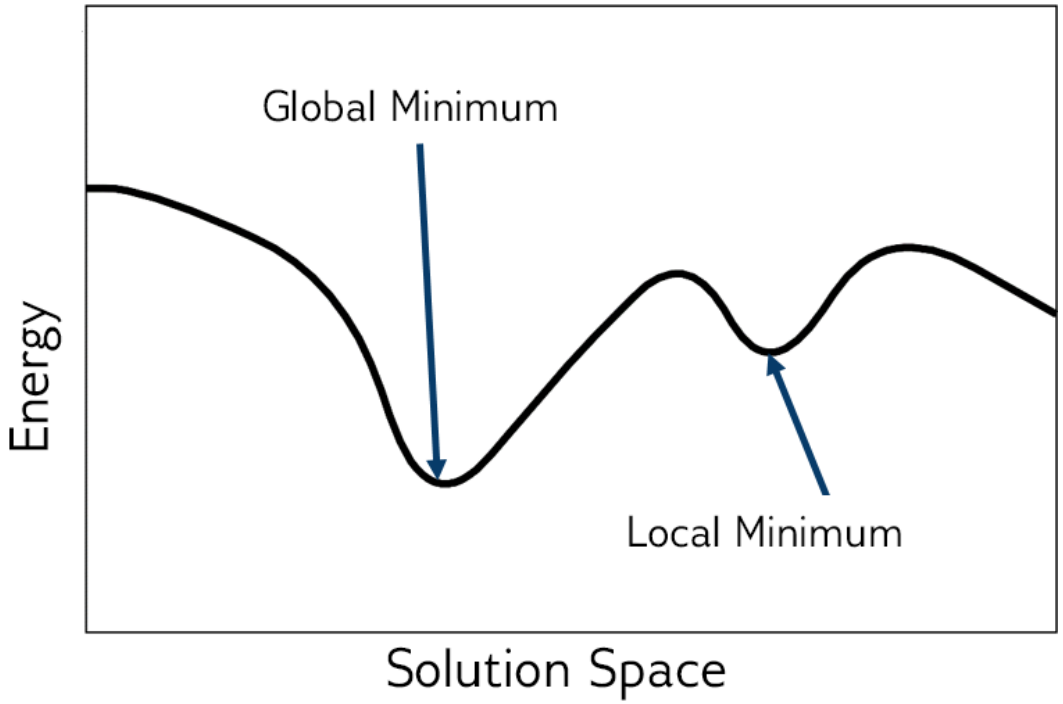
- Although, in some cases it becomes very difficult.
- The objective functions accepted by the quantum annealer of D-Wave are of two types (equivalent to each other): **Ising Hamiltonians and QUBO formulations**



$$x + 1 = 2$$

$$\min_{x} [2 - (x + 1)]^2$$

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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

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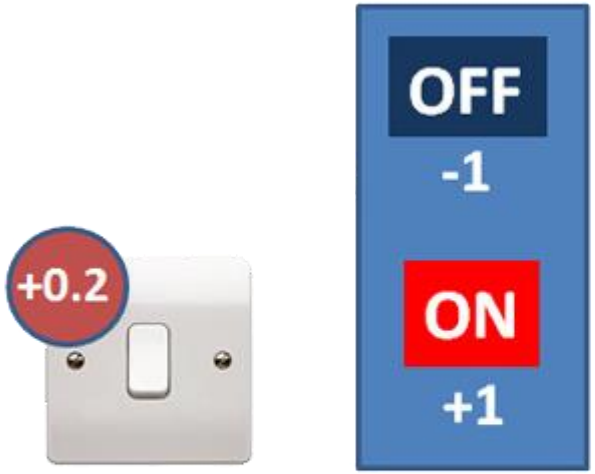

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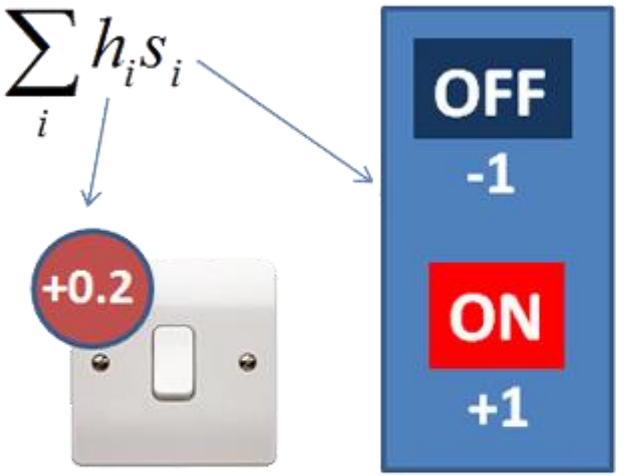

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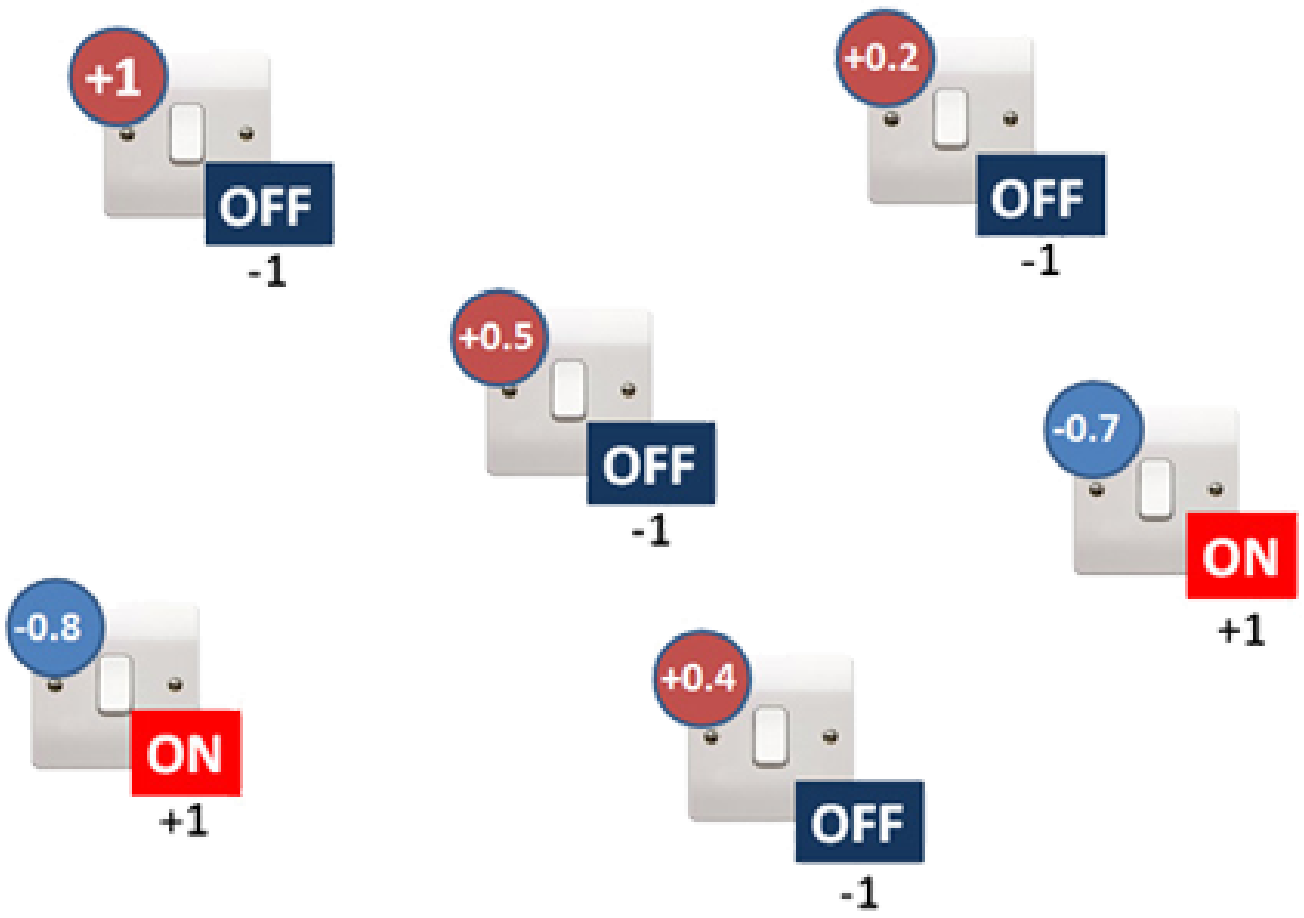
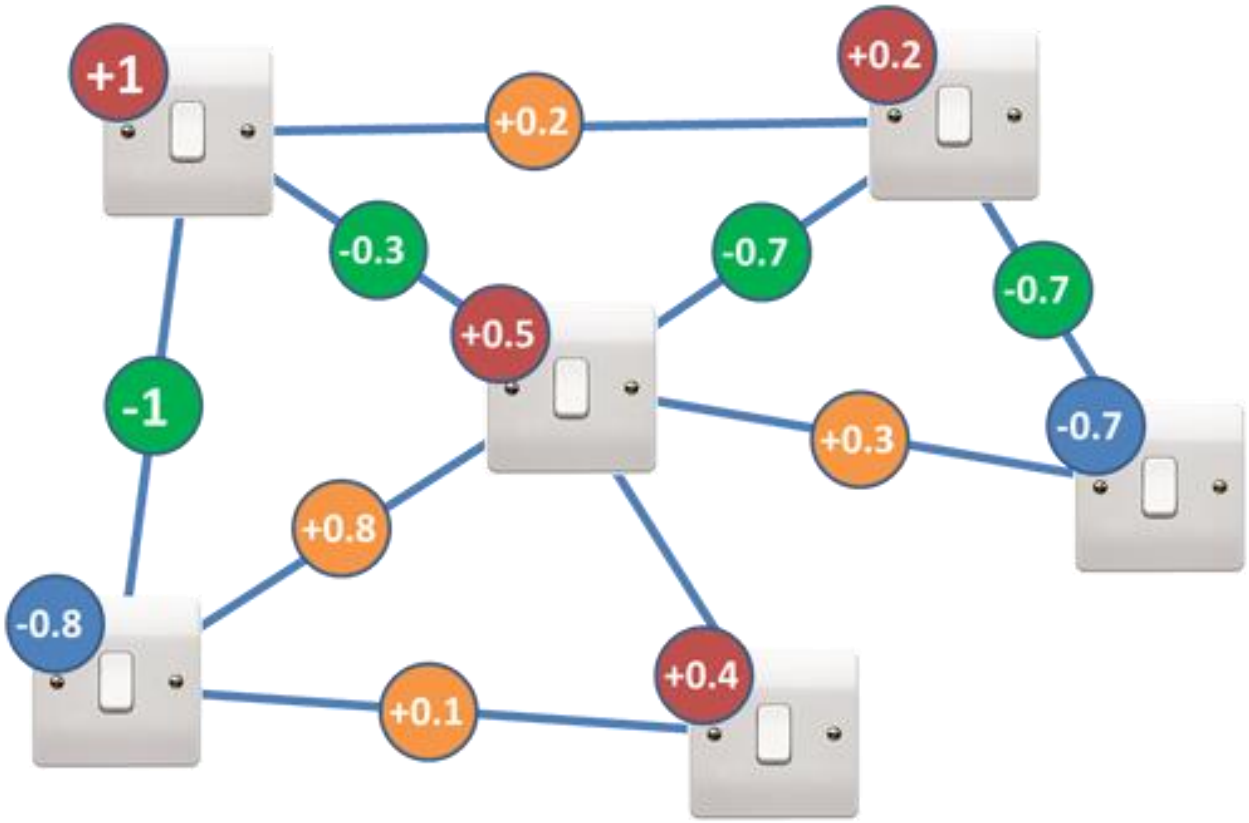


+1	x	-1	=	-1
+0.2	x	-1	=	-0.2
+0.5	x	-1	=	-0.5
-0.8	x	+1	=	-0.8
+0.4	x	-1	=	-0.4
-0.7	x	+1	=	-0.7

Total: -3.6

Game of Switches



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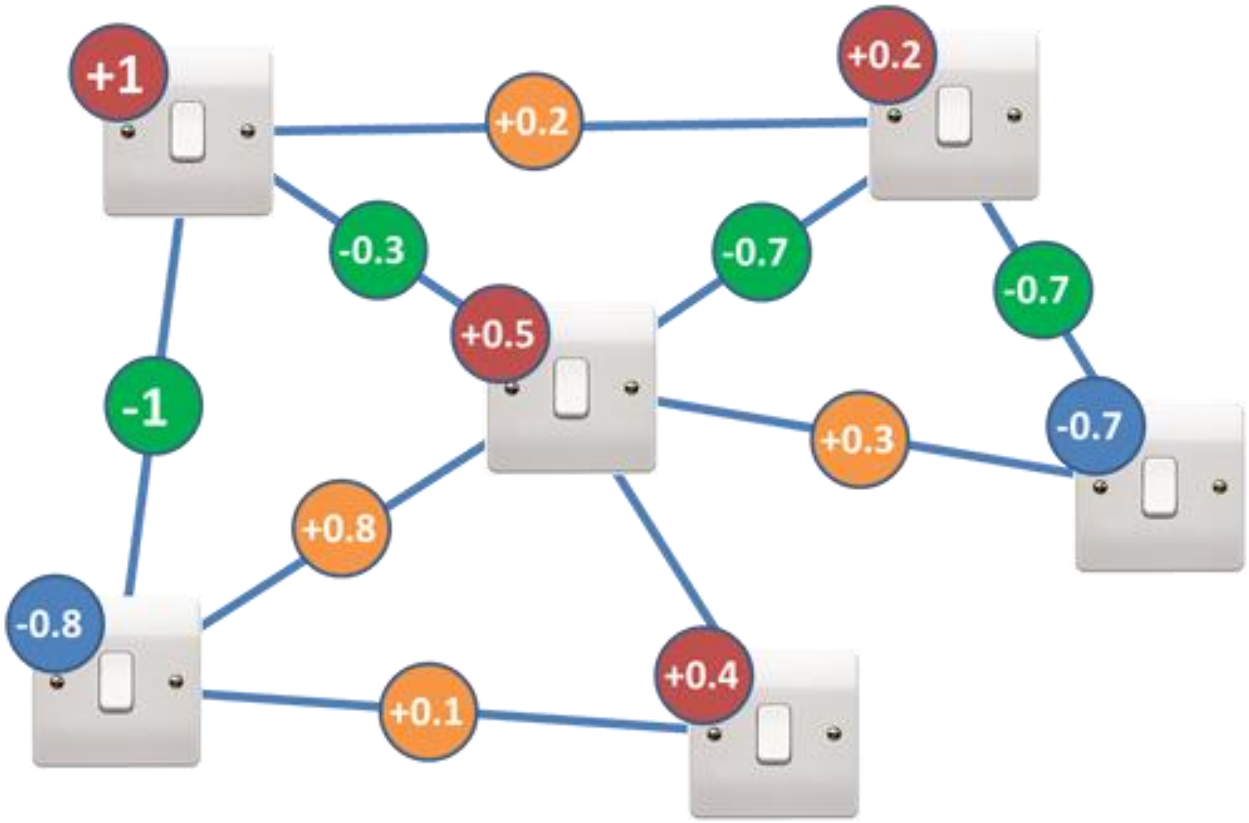

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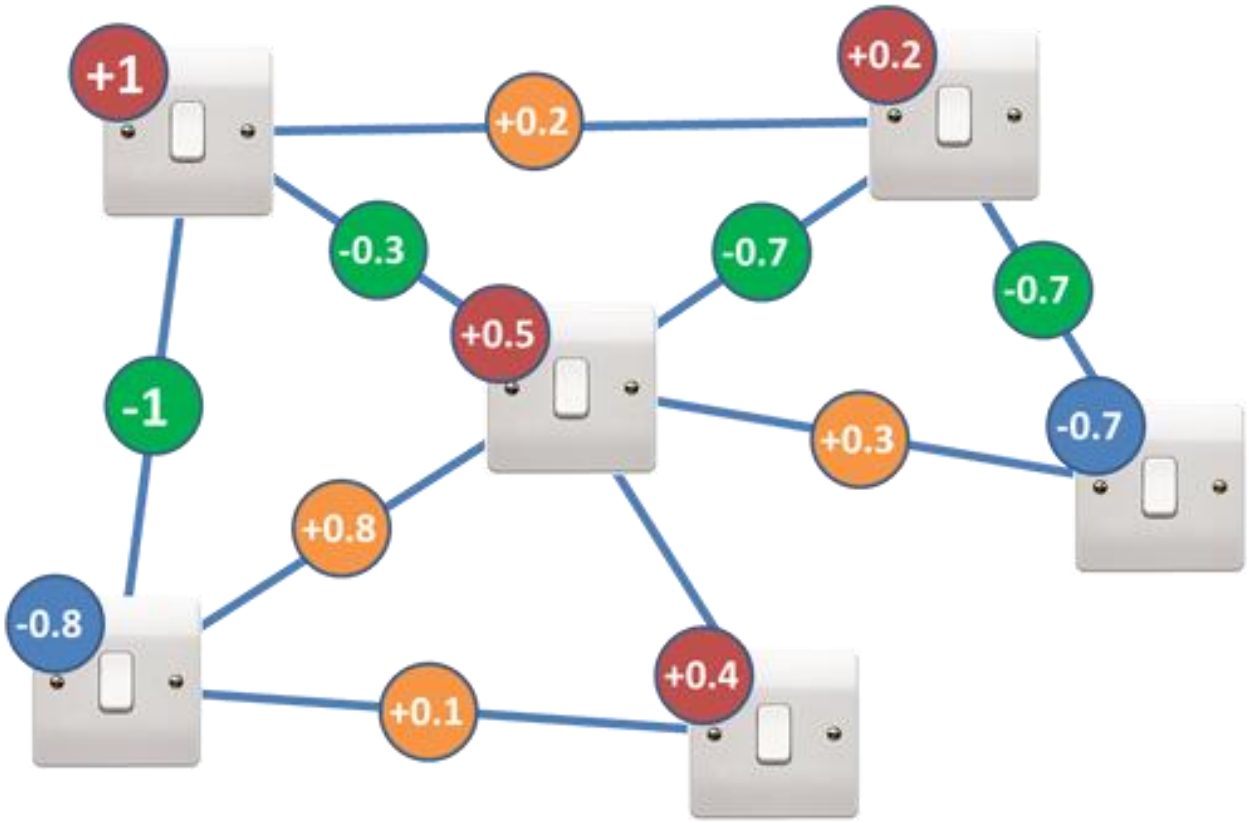

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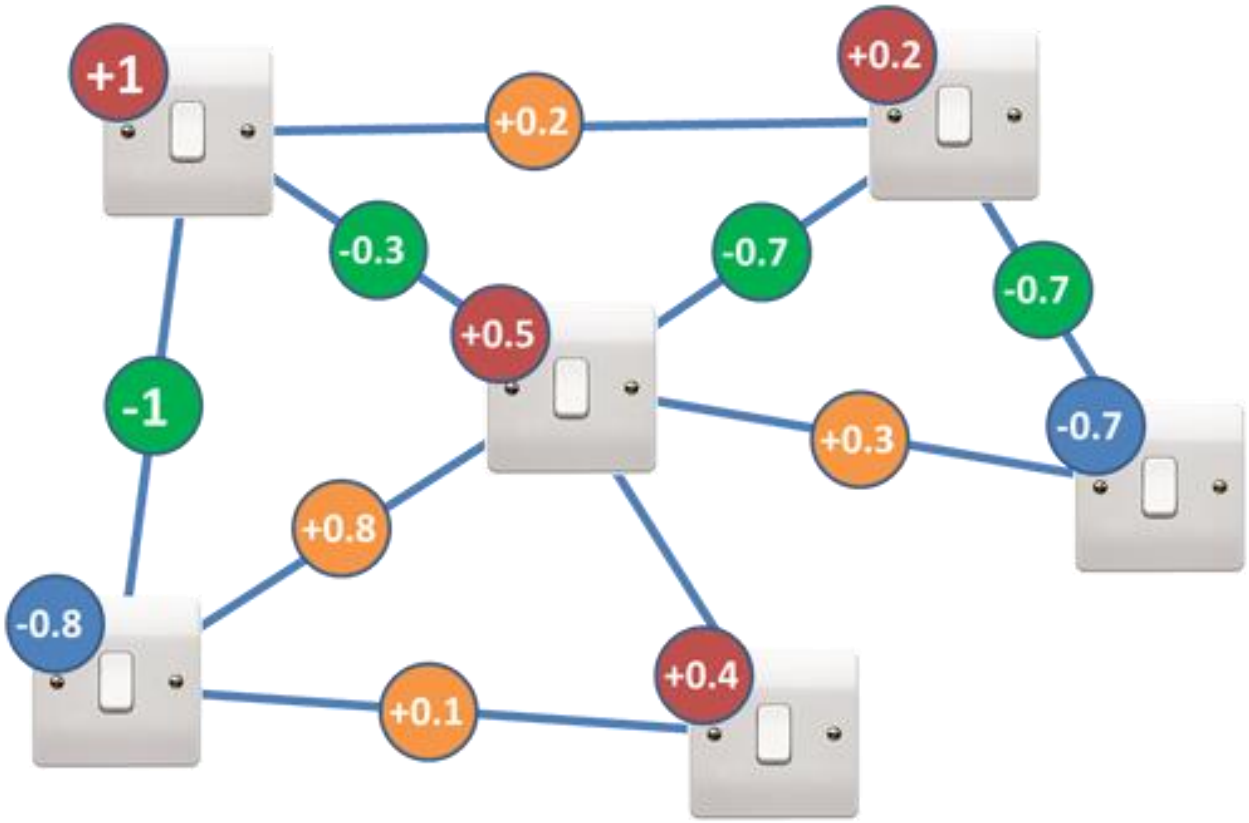

Adding another weight, J, which multiplies the product of the two switch settings.

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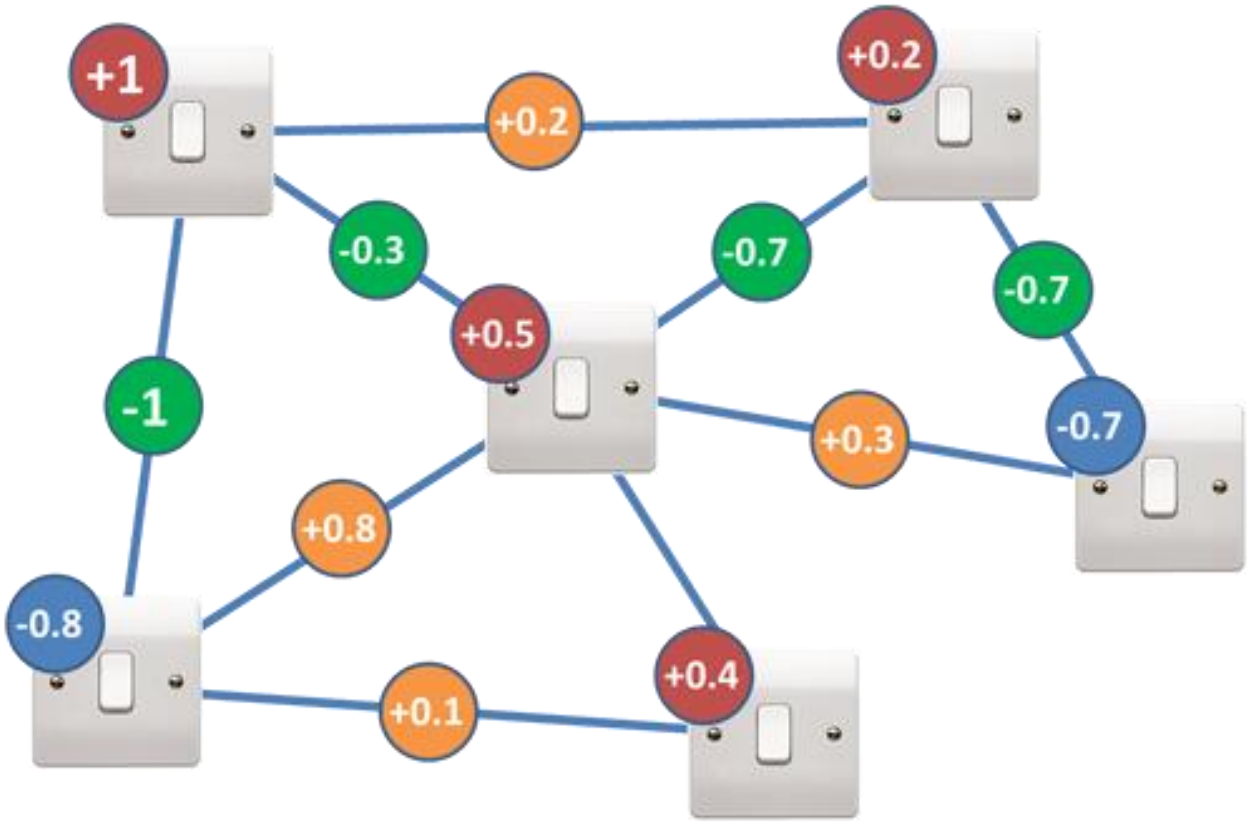

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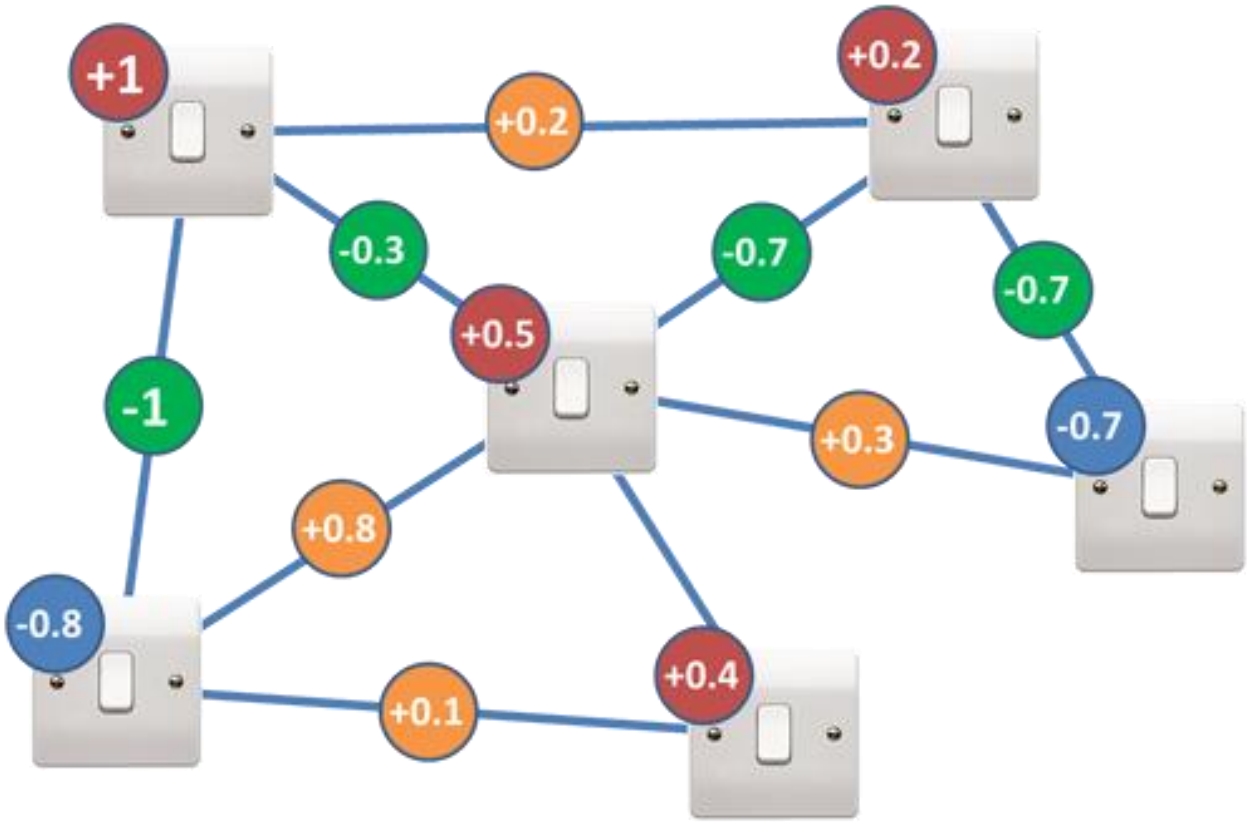

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- We therefore add to the quantity to be minimized the contribution introduced by the couplers

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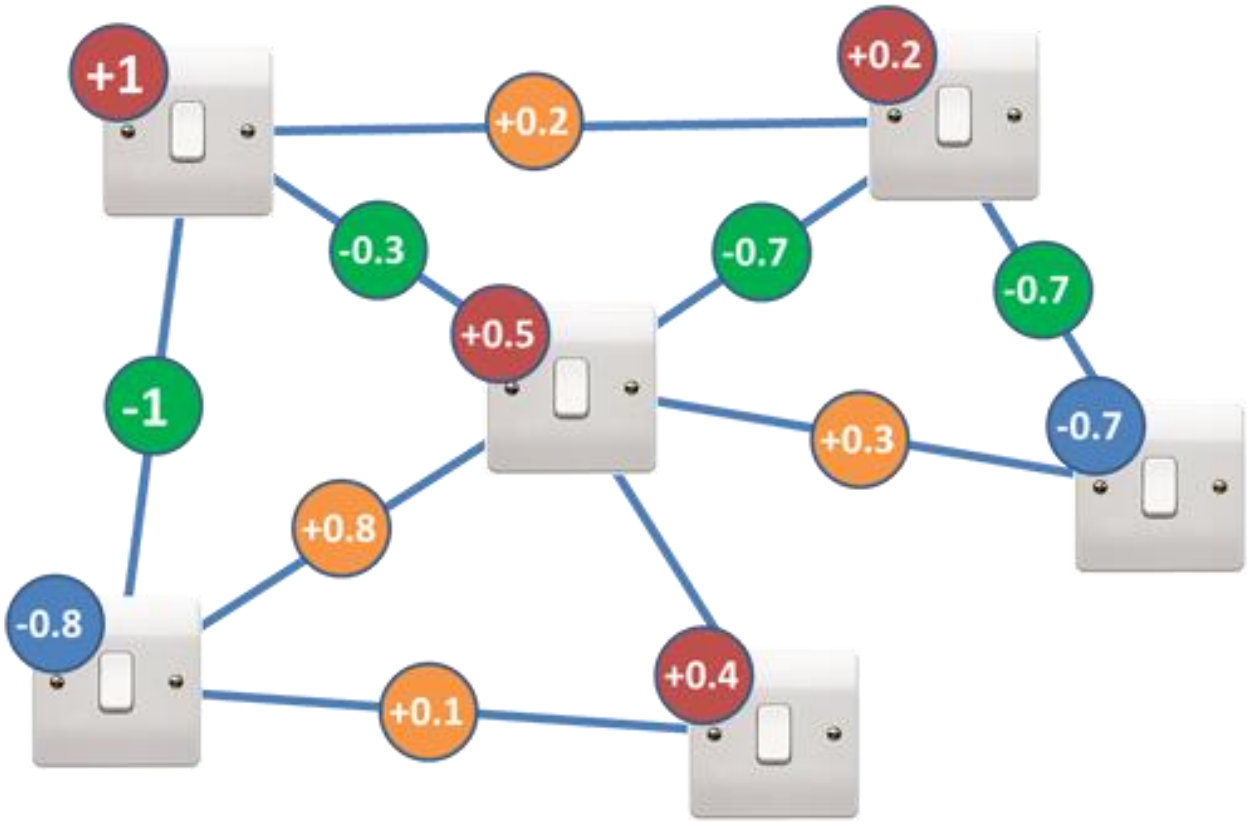

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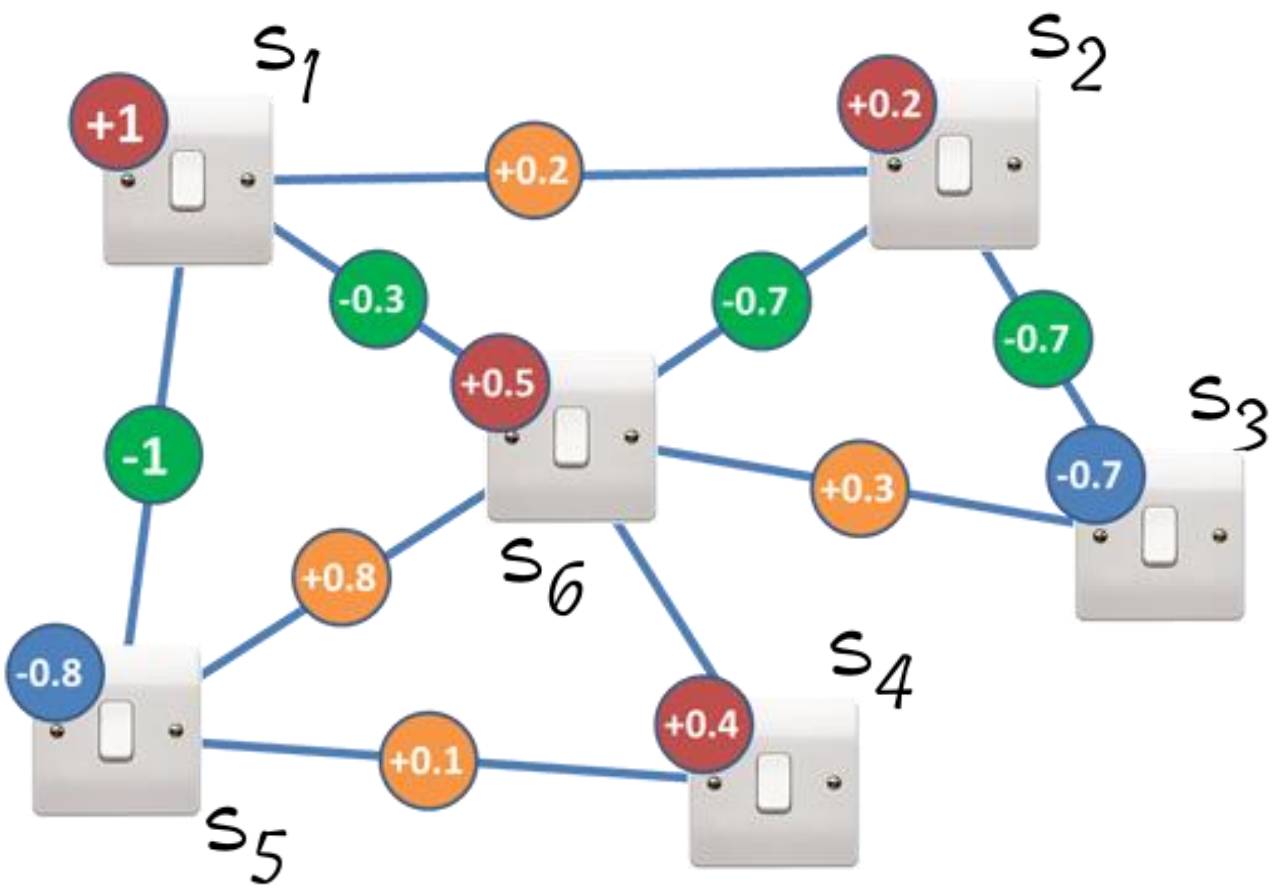

$$s_1 + 0.2s_2 - 0.7s_3 +$$
$$0.4s_4 - 0.8s_5 + 0.5s_6 +$$
$$0.2s_1s_2 - 0.7s_2s_3 +$$
$$0.3s_3s_6 - 0.7s_2s_6 +$$
$$- 0.3s_1s_6 - s_1s_5 +$$
$$0.1s_5s_4 + s_6s_4$$

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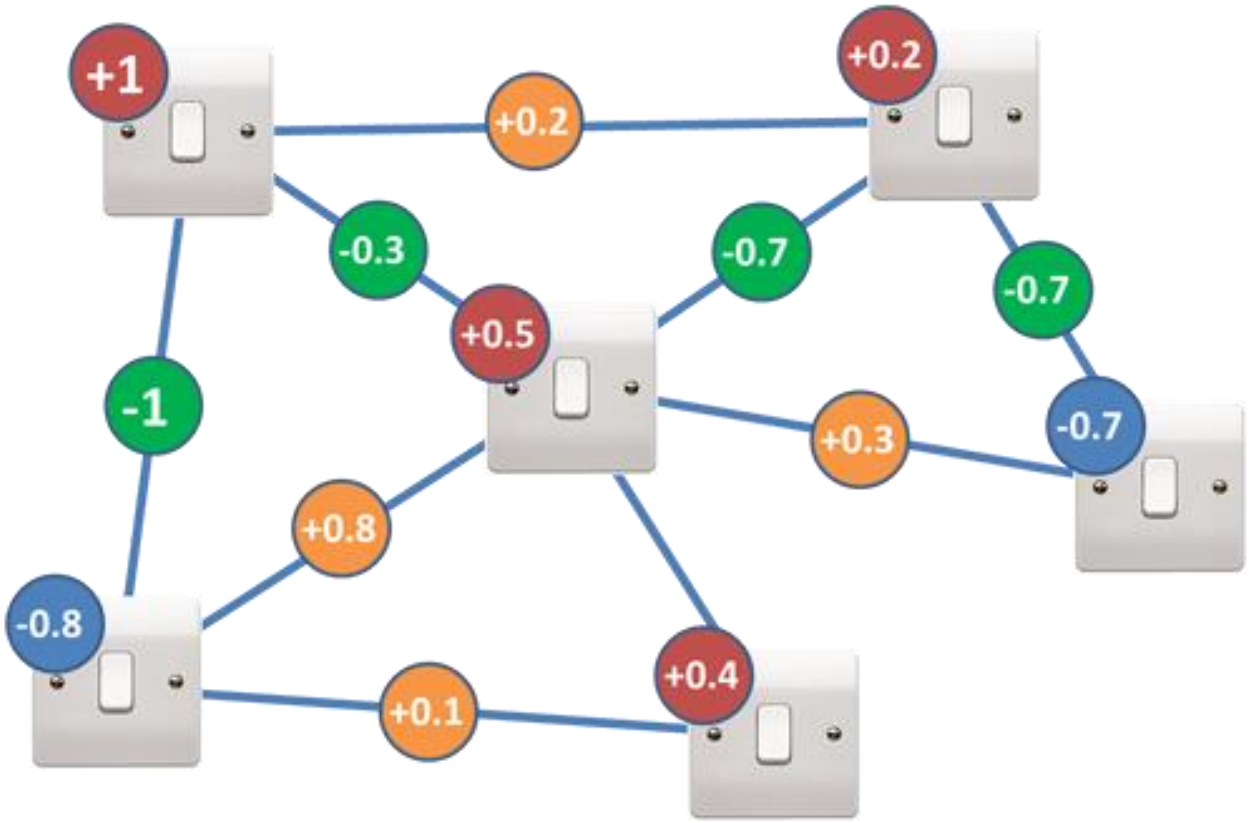

2 switches = 2^2 =
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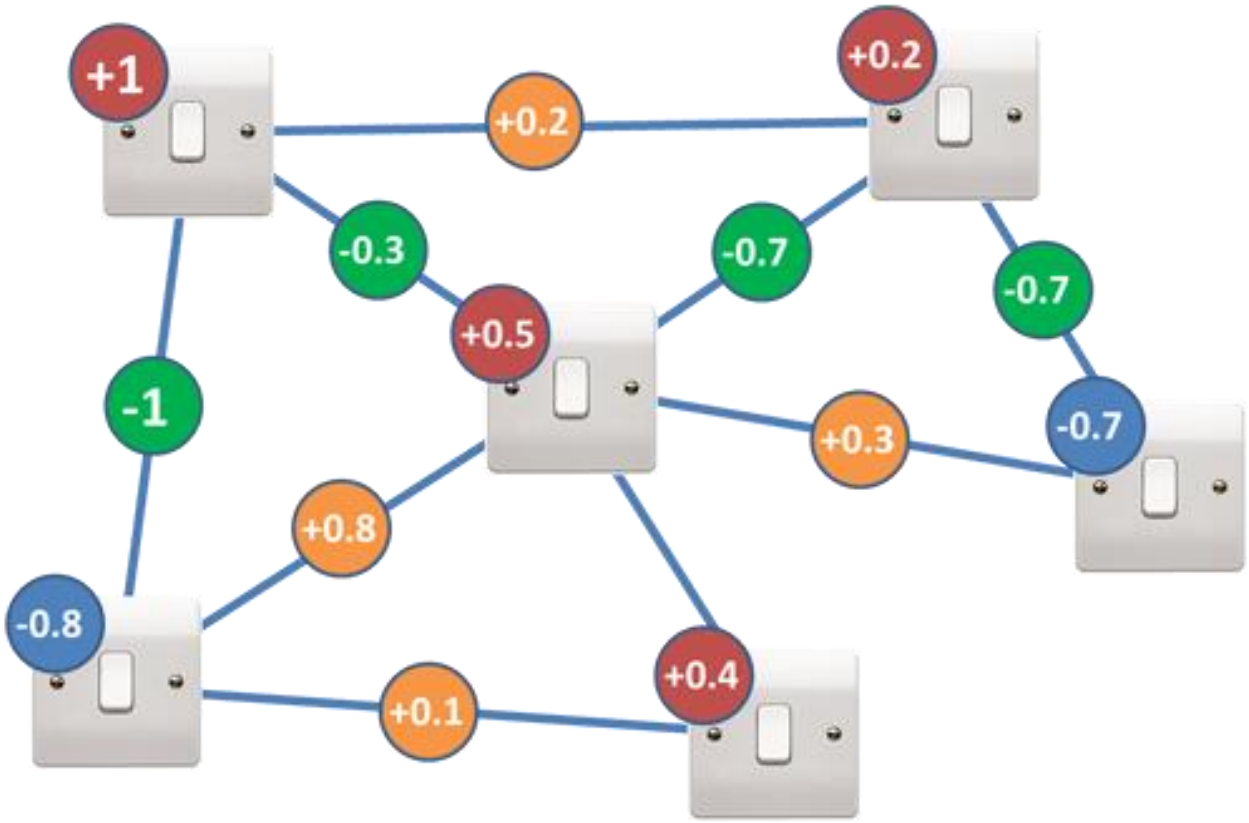

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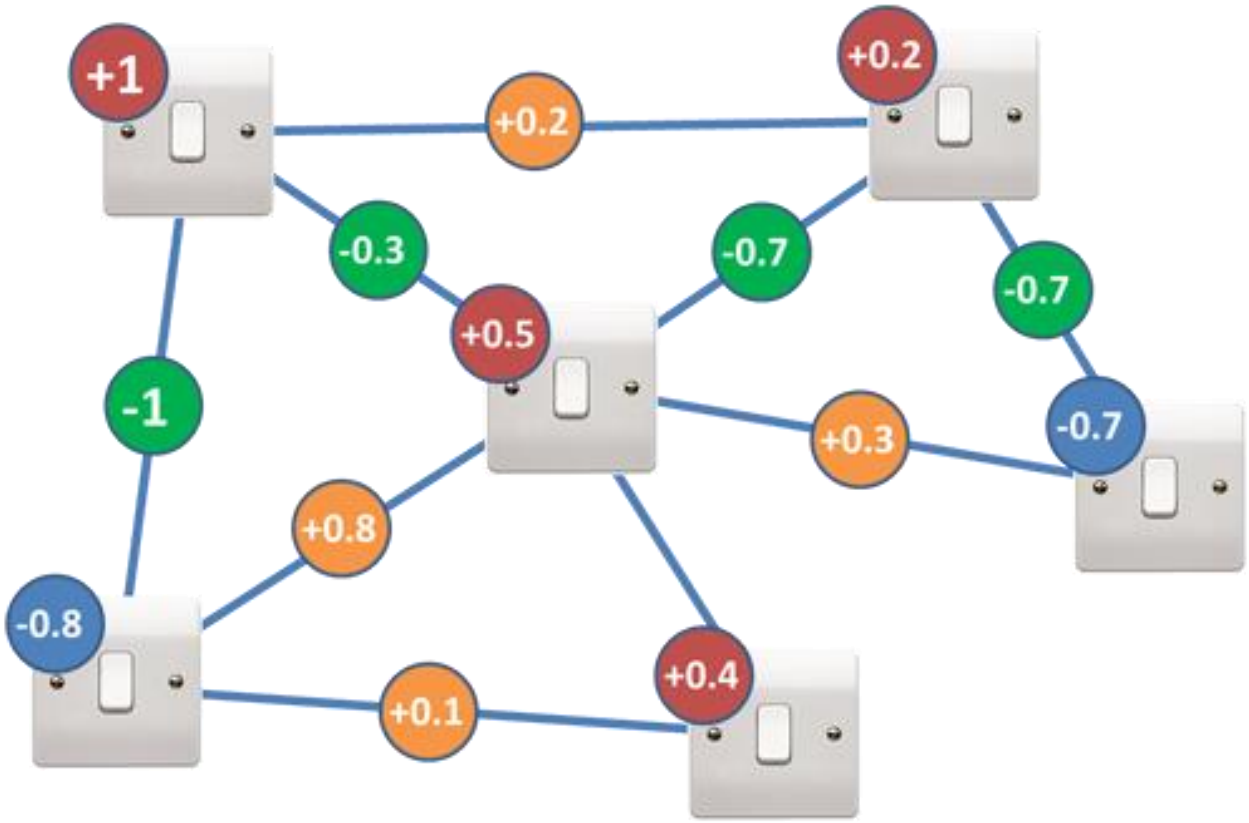

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1,267,650,600,228,229,401,496,703,205,376
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$$\min_{x \in \{0,1\}^n} x^T Q x.$$

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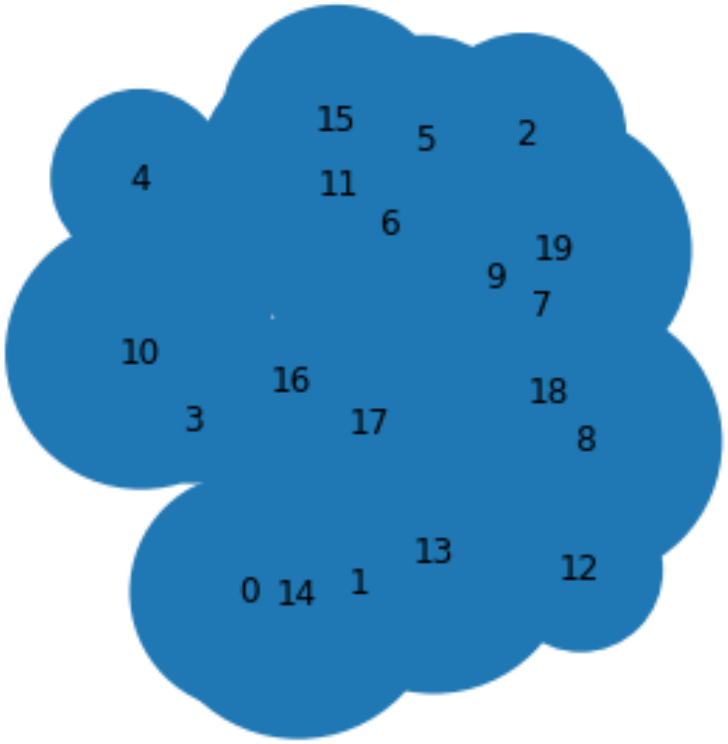

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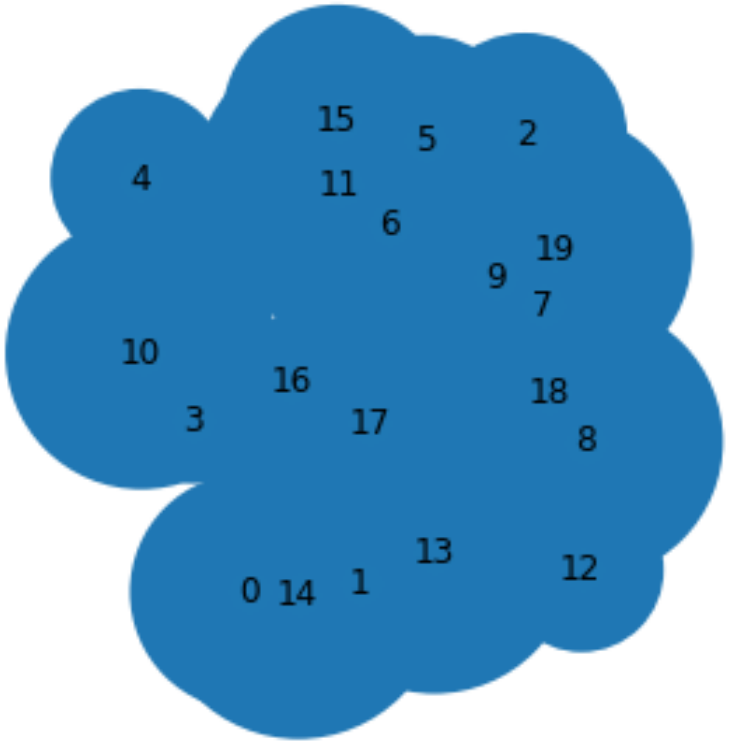

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We define:

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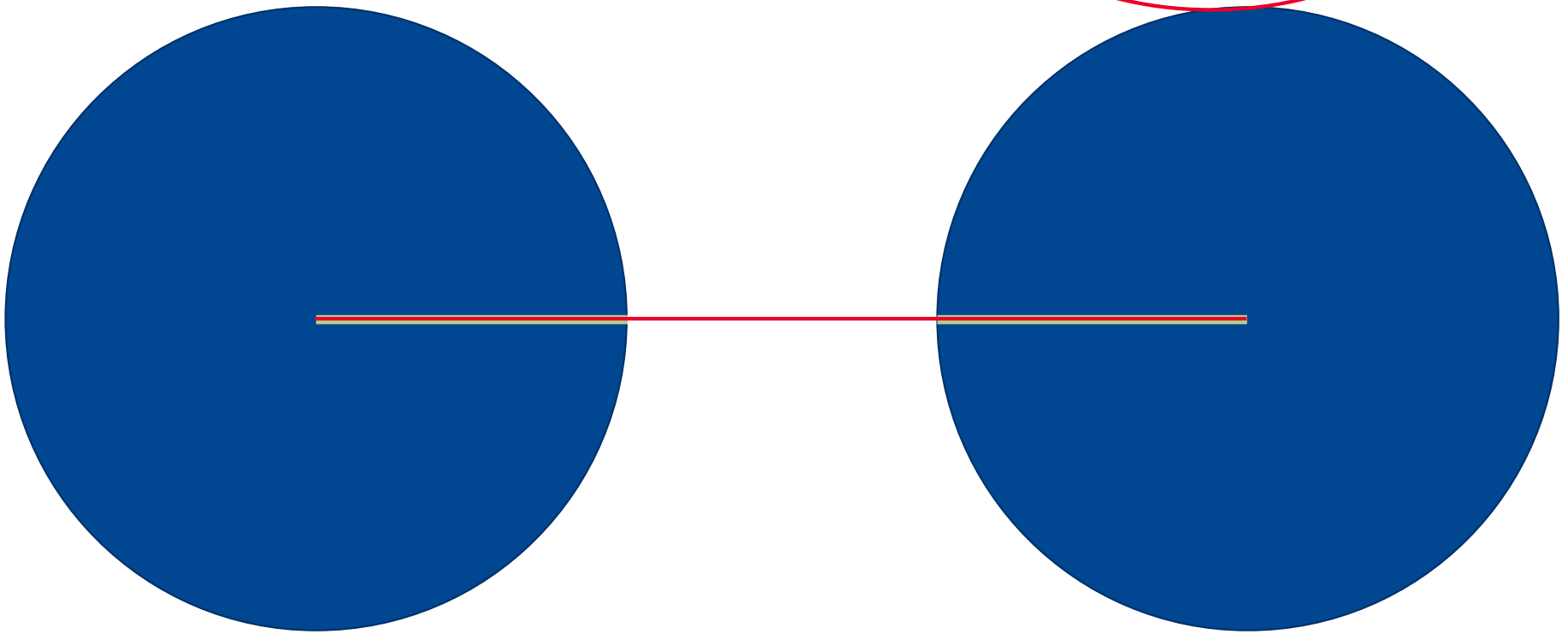

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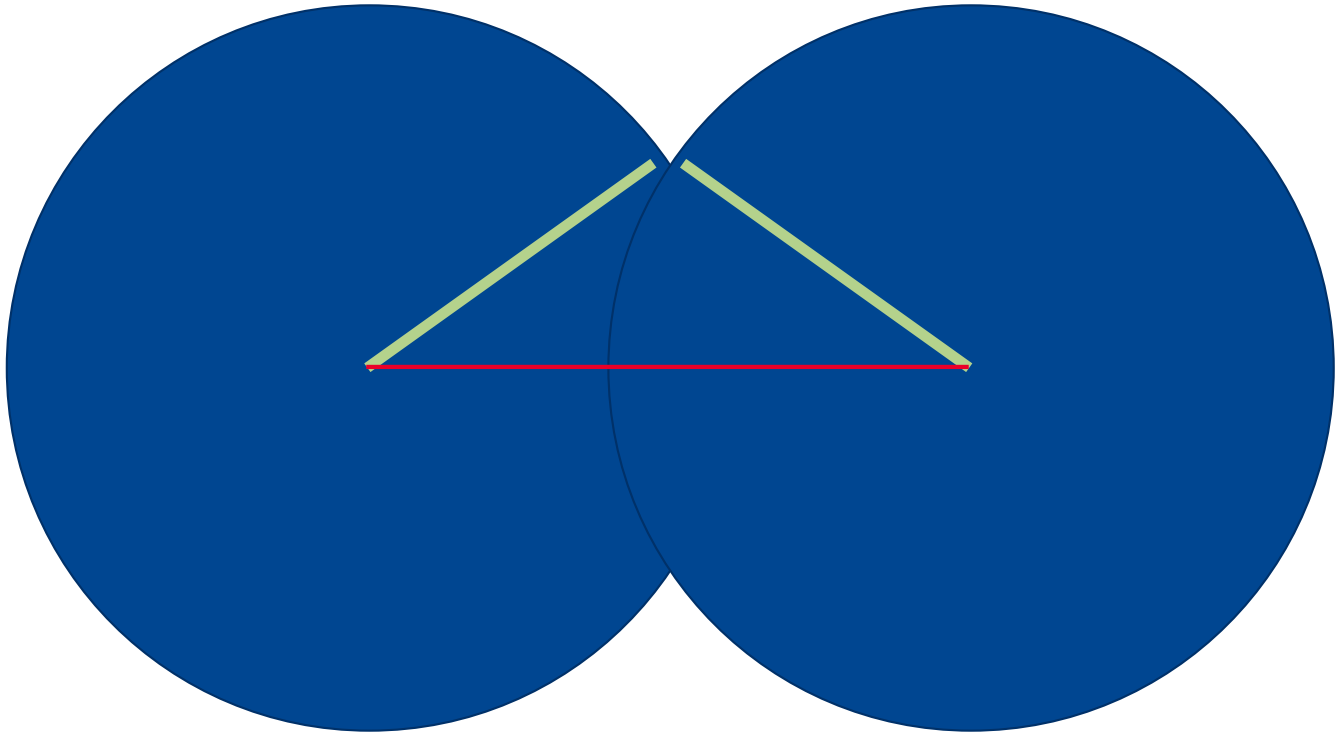

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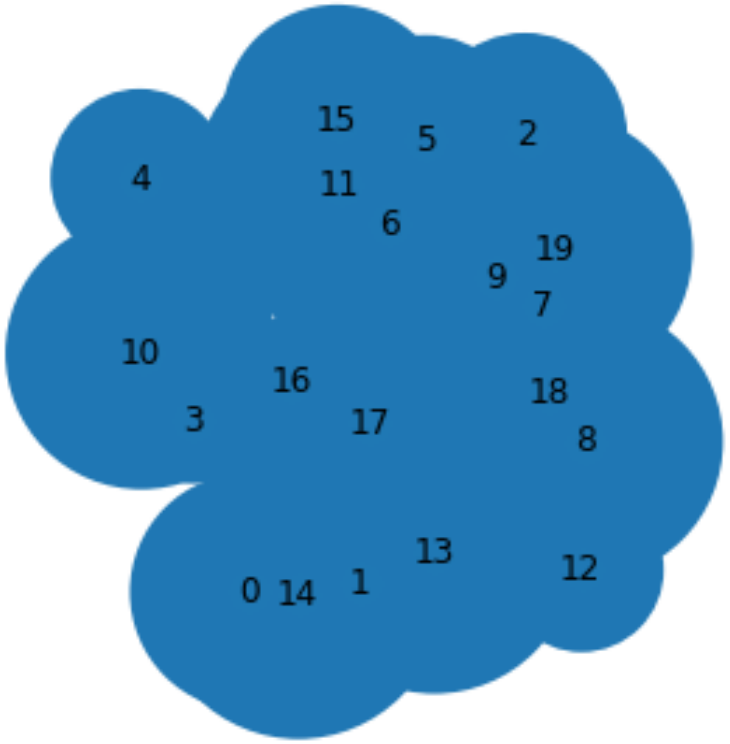

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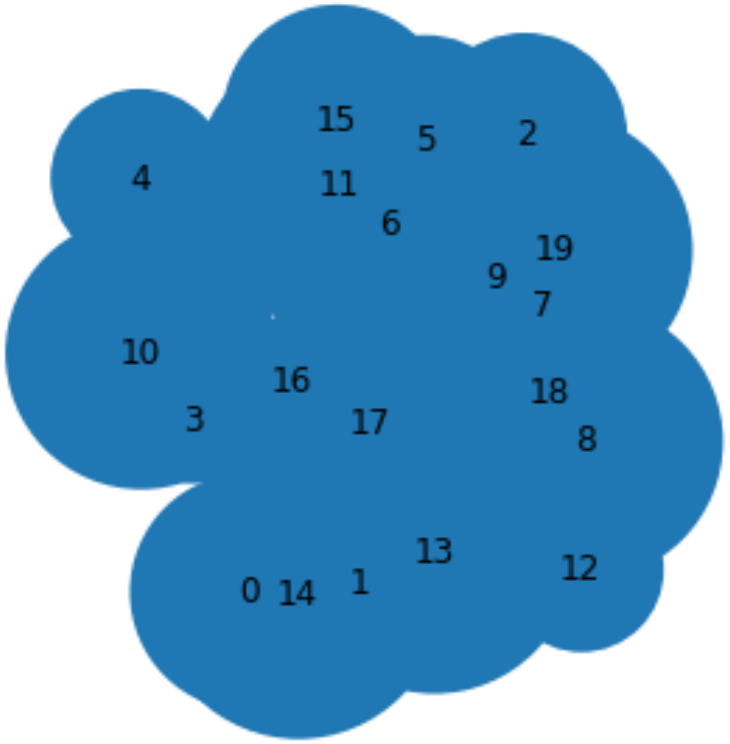
$$[q_0, \dots, q_{19}]$$



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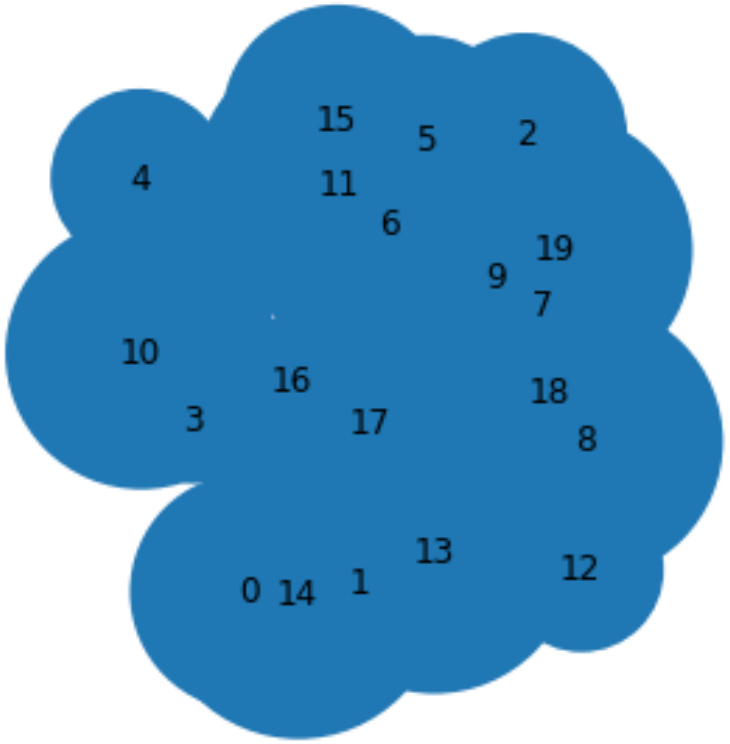

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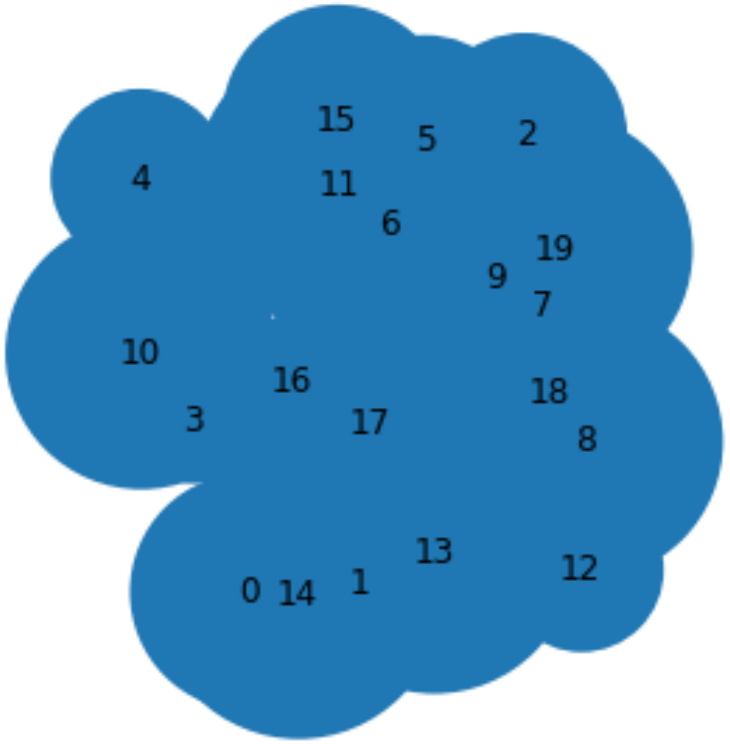

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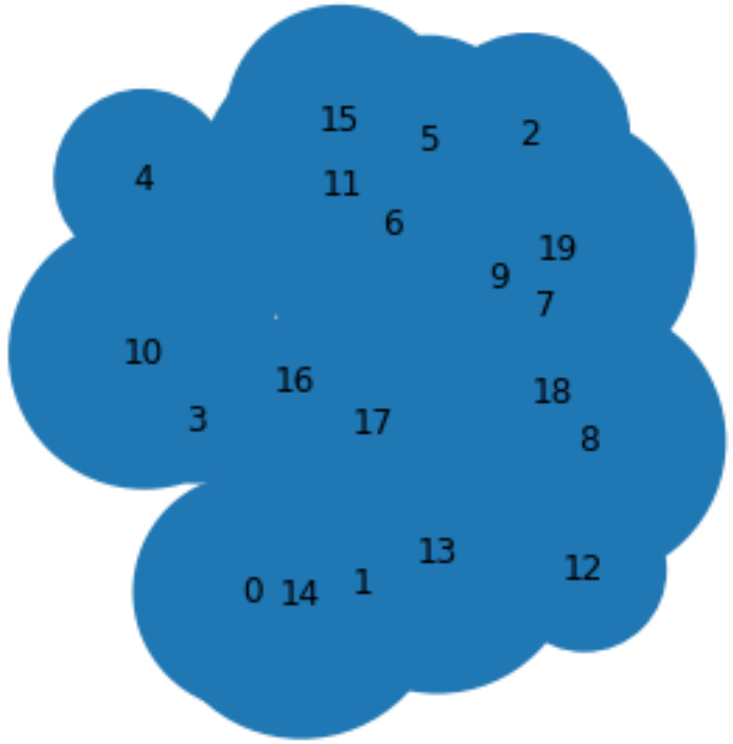

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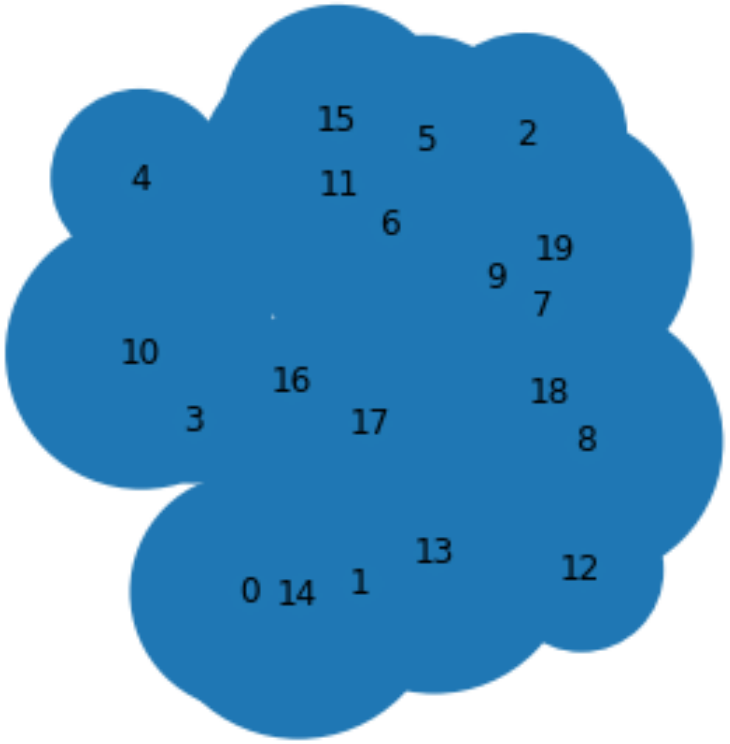

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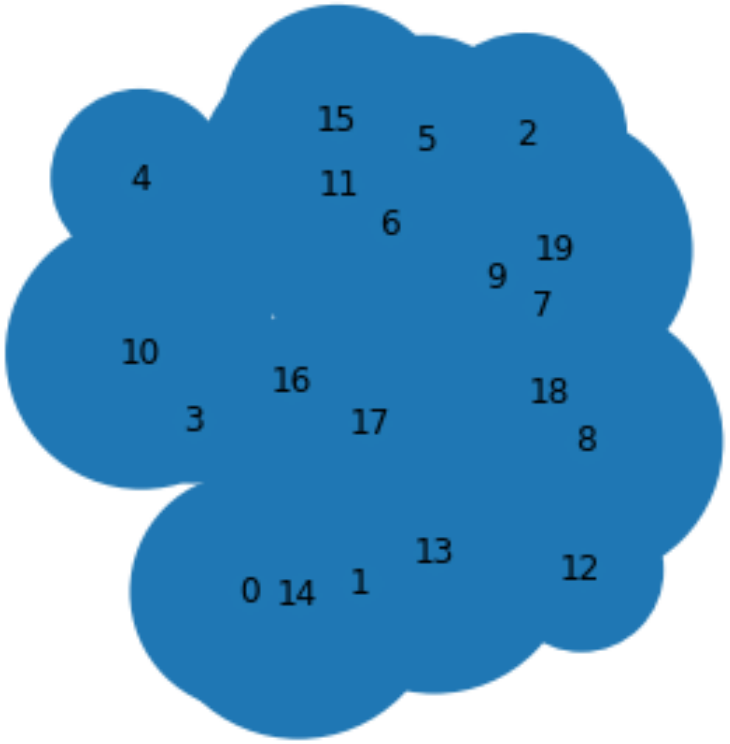

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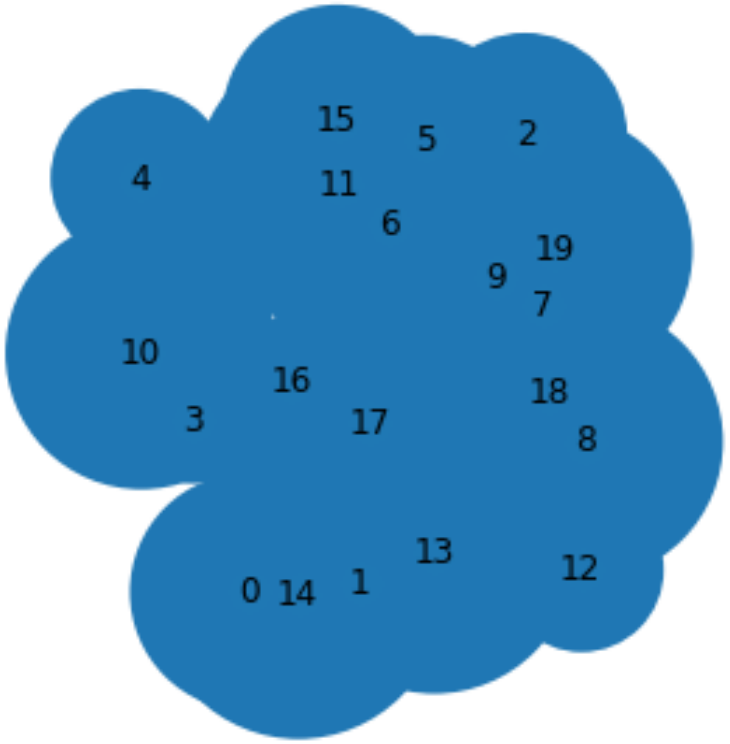

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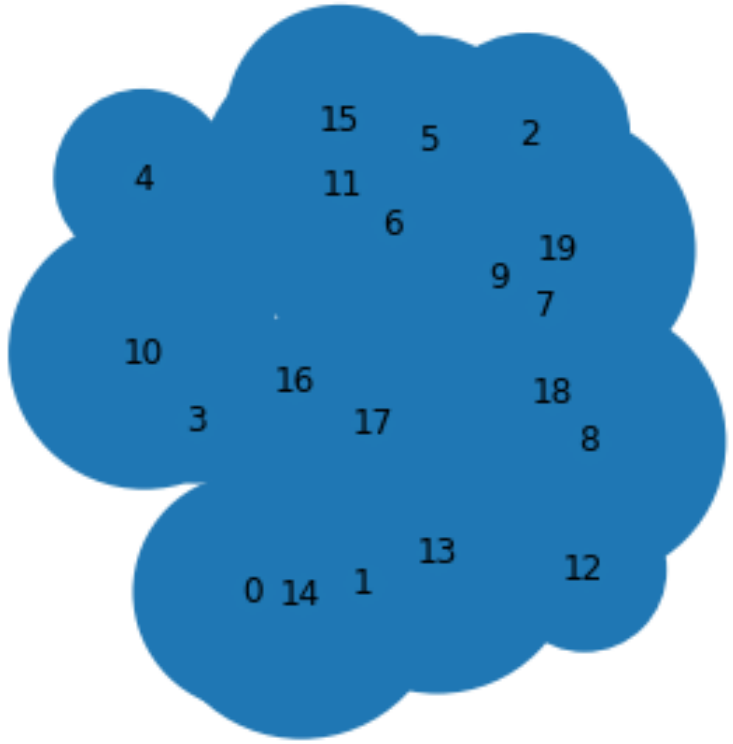

-

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

QUBO/ISING Equivalency

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$$x_i \mapsto \frac{s_i + 1}{2}$$

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

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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 :)

Programming a Quantum Annealer

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```
>>> 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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```
>>> 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

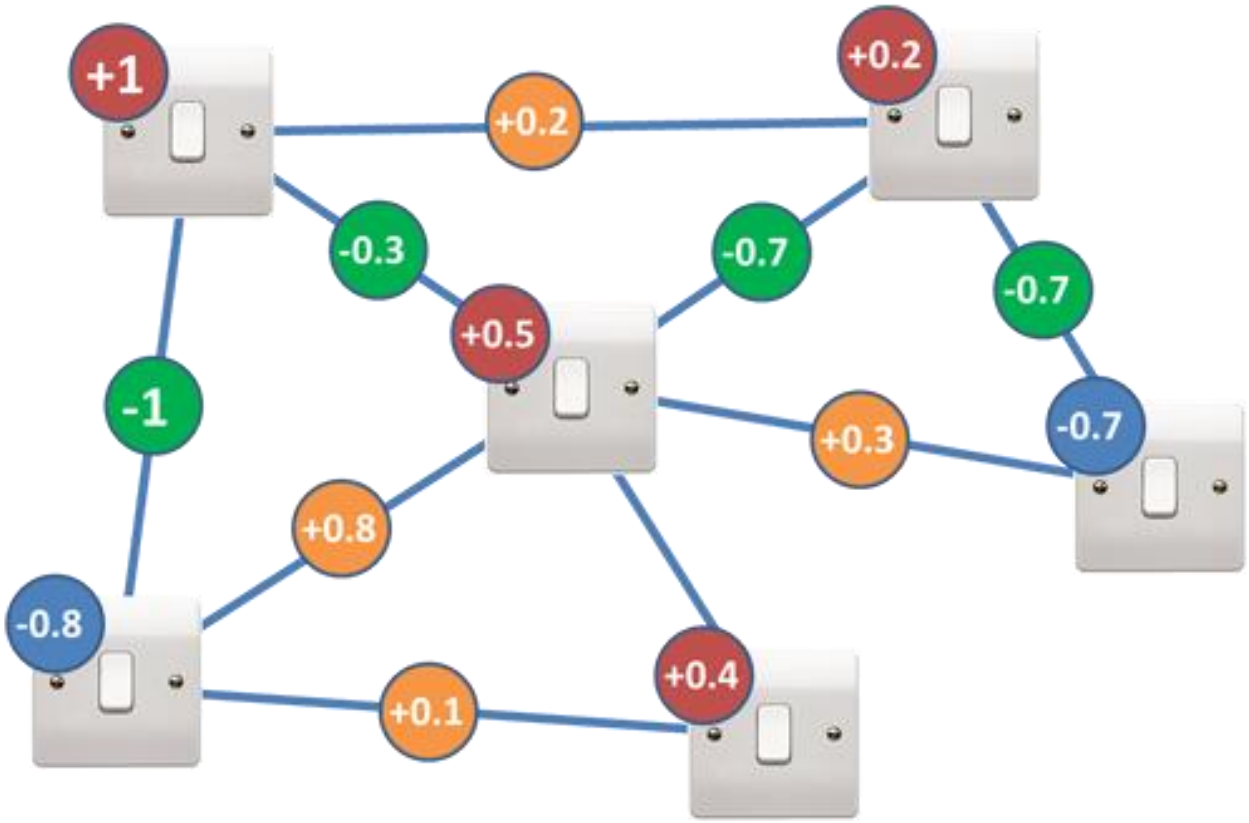
- Solve a problem set via pyQUBO
- After setting the Hamiltonian of the problem, it must be compiled and transformed into a bqm object

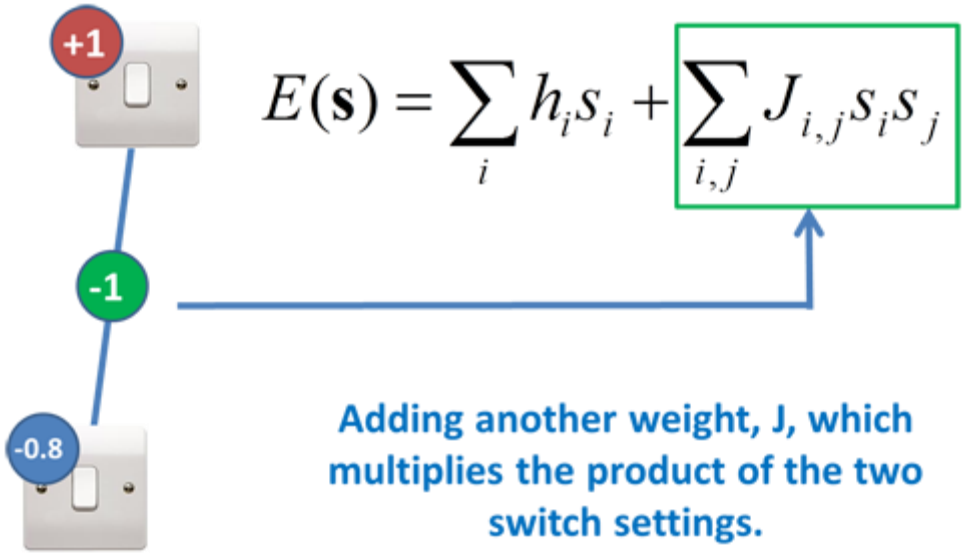
```
>>> from pyqubo import Binary
>>> x1, x2 = Binary('x1'), Binary('x2')
>>> H = (x1 + x2 - 1)**2
>>> model = H.compile()
>>> bqm = model.to_bqm()
```

```
>>> 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



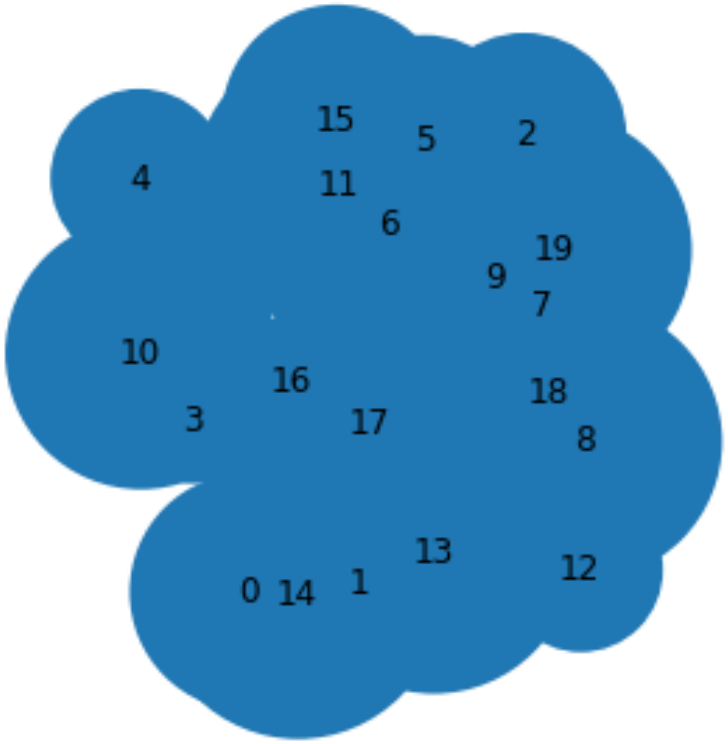


Exercise 2: Antenna Placement

- Try to implement the Antenna Placement Problem

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

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



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.

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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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$$= \sum_{i=0}^{N} q_i^2 + 2 \sum_{i<j} q_i q_j - 2F \sum_{i=0}^{N} q_i$$

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

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Add a Constraint to a QUBO Problem

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

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

Exercise 2: Antenna Placement

- Implement constraint into the Antenna Placement Problem

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

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

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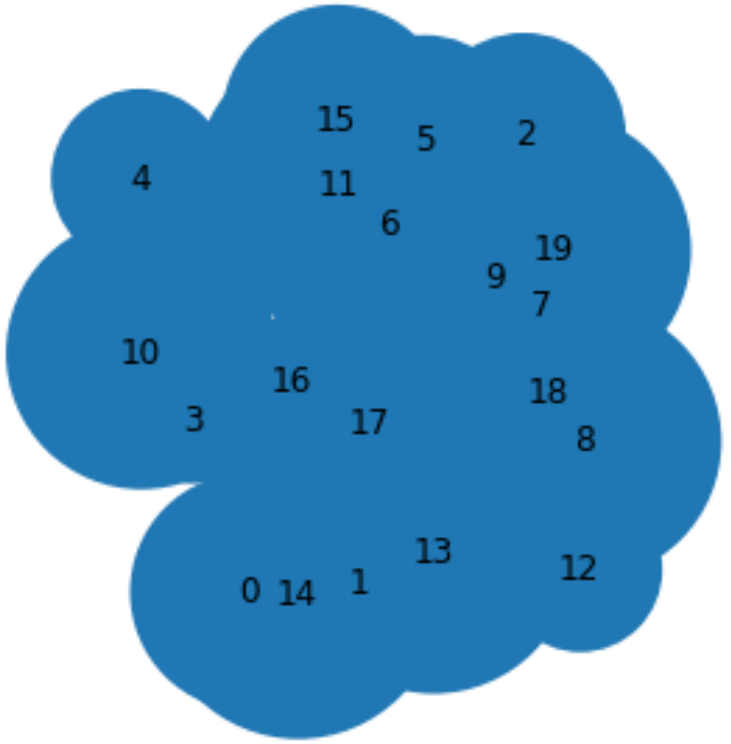

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- First of all we consider a vector L, of length equal to the number of antennas available. We mark with 0 the free antennas and with 1 the antennas that must necessarily be activated.

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- Consequently, penalty funct

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

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

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

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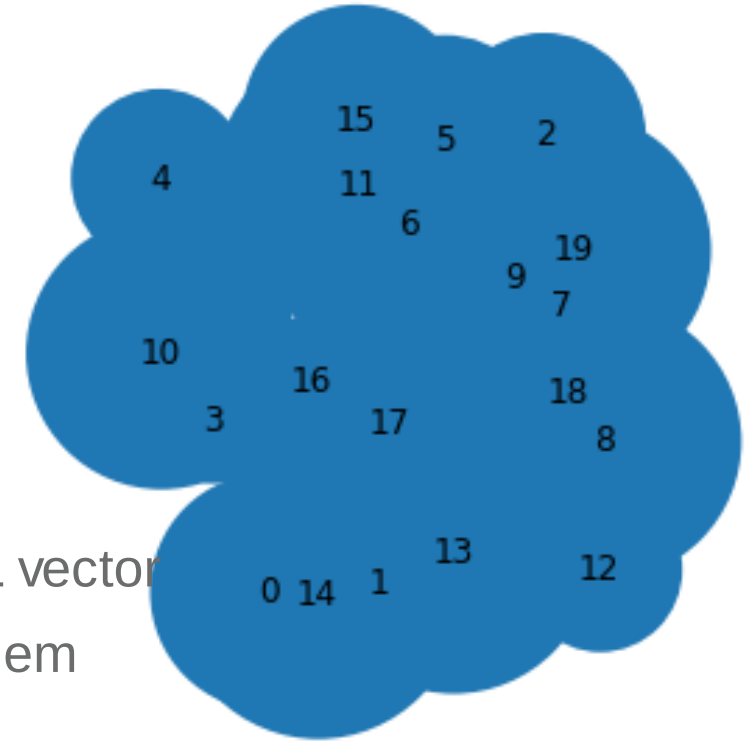

$$-\sum_{i=1}^{N} \gamma L_i q_i$$

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

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- Now suppose we want to add an **inequality** constraint to our problem.

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- An example could be

- *Let F be the maximum number of antennas that can be placed*

- Mathematically, the constraint appears in the form

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

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- So far we have seen how to transform constraints involving equalities into penalty functions

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- 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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$$\sum_{i=1}^{N} q_i + \sum_{k=1}^{F} q_k = F$$

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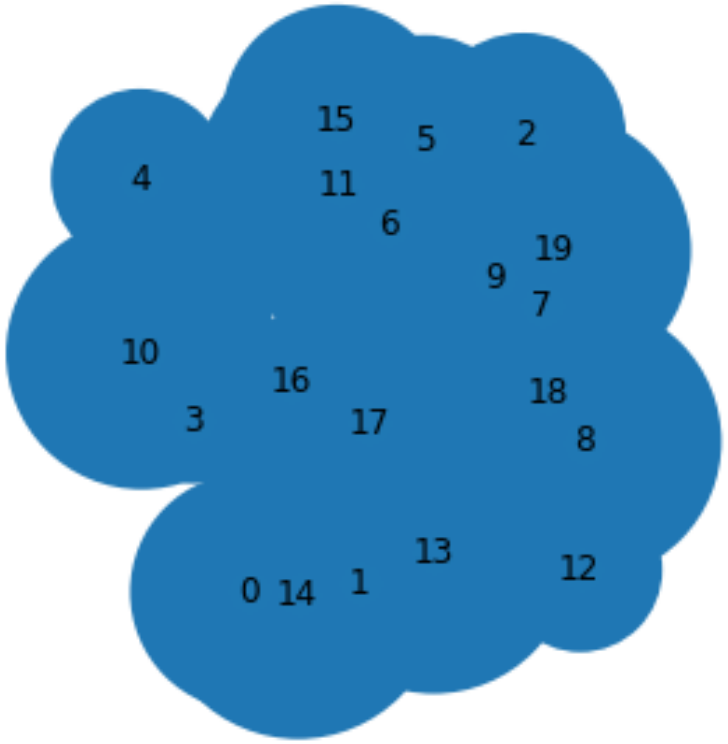
$$\min\left(\left(\sum_{i=0}^{N} \beta(1-2F)q_i + \sum_{i<j} 2\beta q_i q_j\right)\right) - \sum_{i=1}^{N} \gamma L_i q_i$$

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

- 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



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

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

$$\sum_{i=1}^{N} A_i q_i \geq A_m \quad \Rightarrow \quad \sum_{i=1}^{N} A_i q_i = A_m + \sum_{k=1}^{N} A_k q_k$$

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

Add a Constraint to a QUBO Problem

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Exercise 2: Antenna Placement

- Implement constraint into the Antenna Placement Problem

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

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

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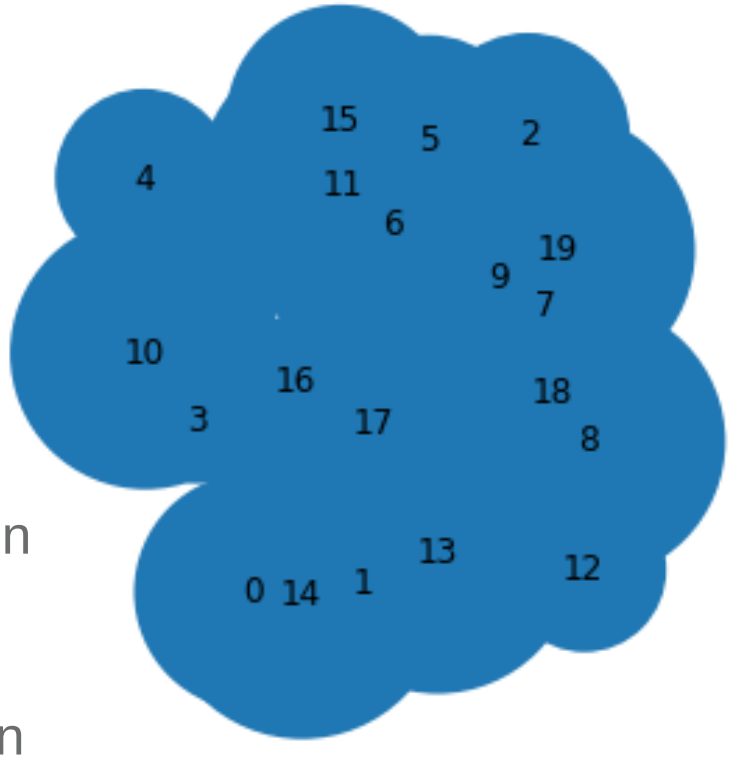

- Add N more qubits to the formulation
- These qubits are a sort of ghost qubits: they don't interact with the other part of the problem formulation
- Do the math!

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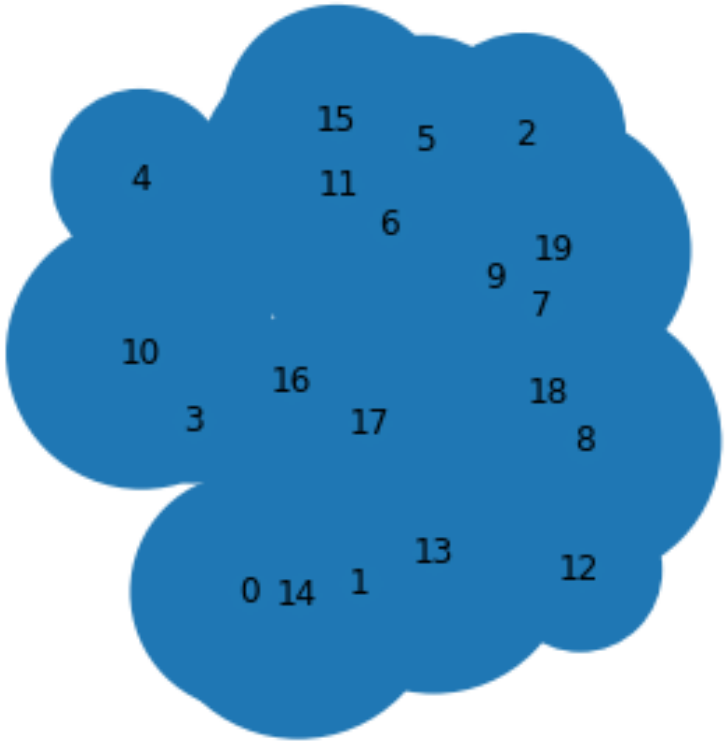
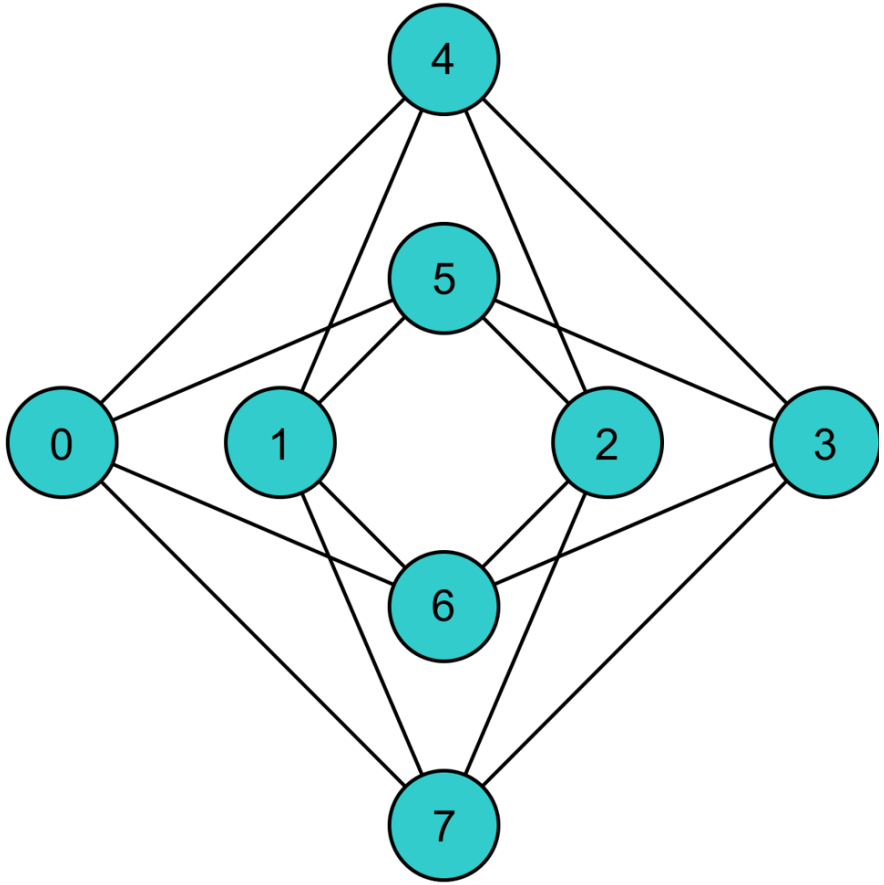


- Add High Order Terms to QUBO problem with pyqubo

Graphs



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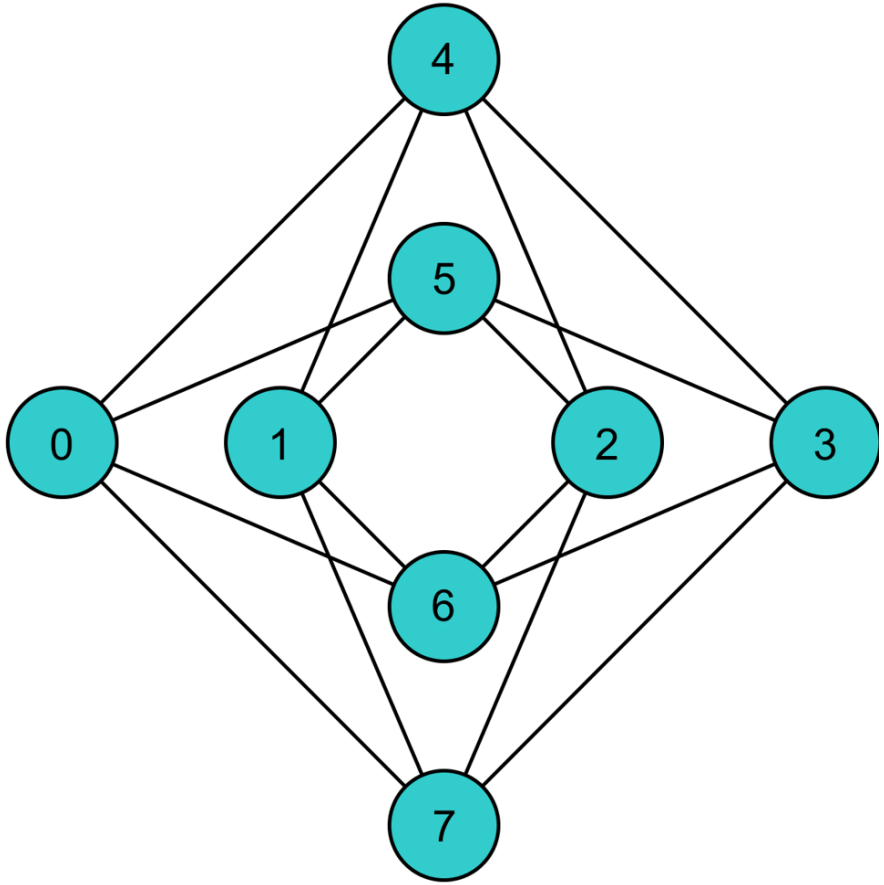

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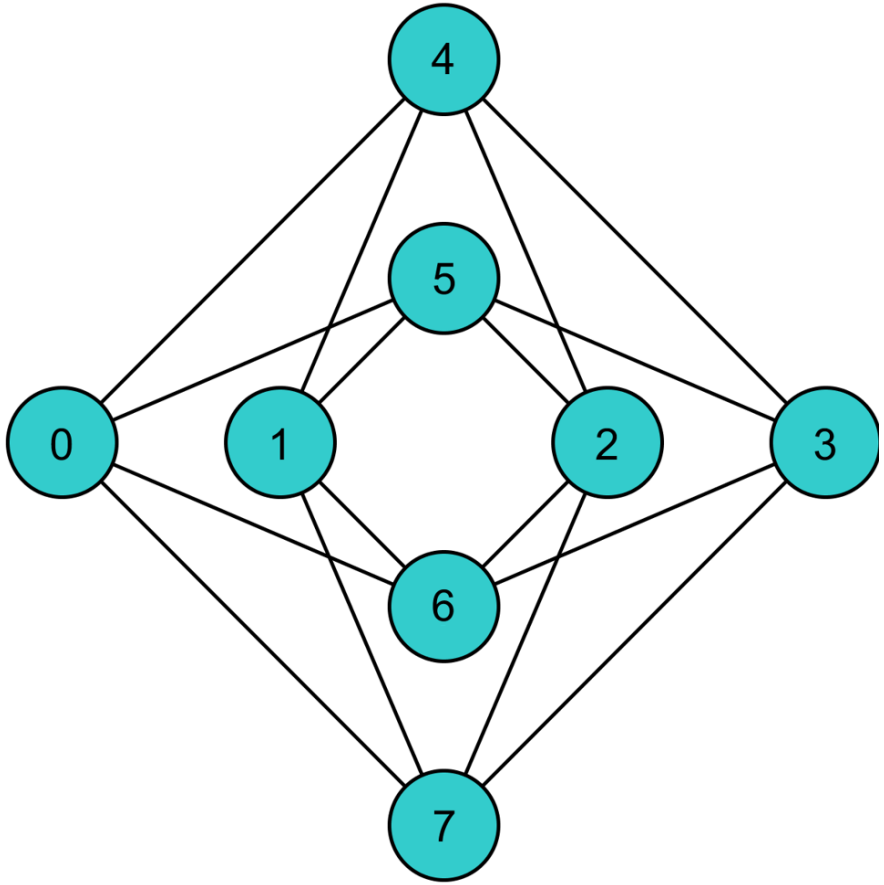

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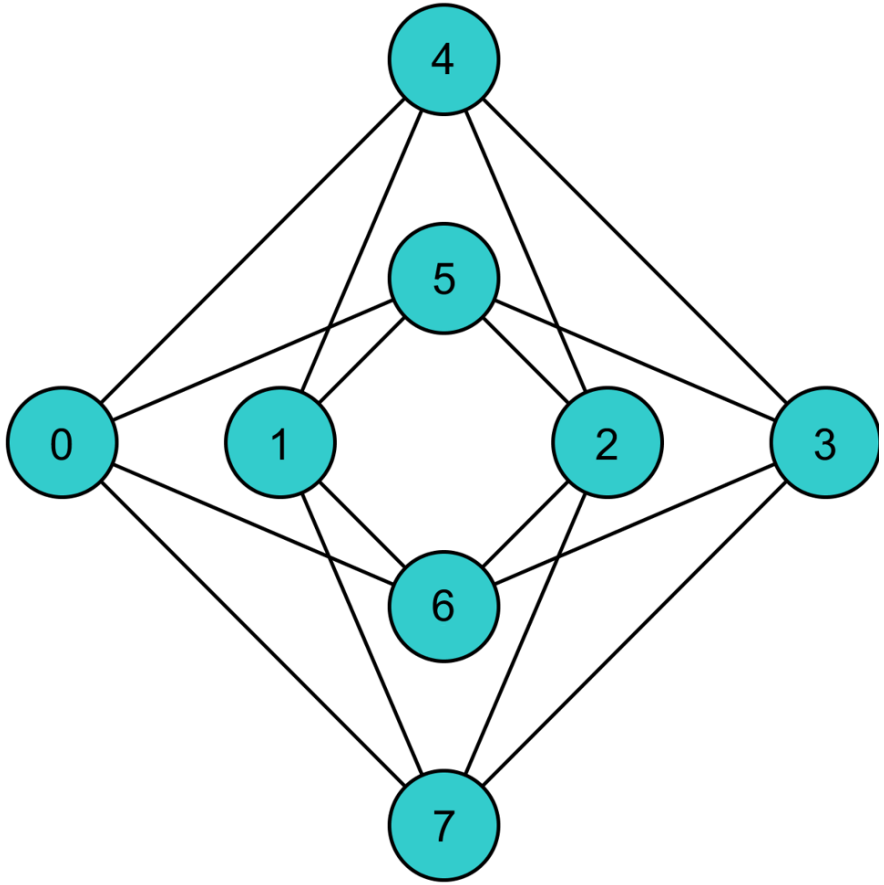

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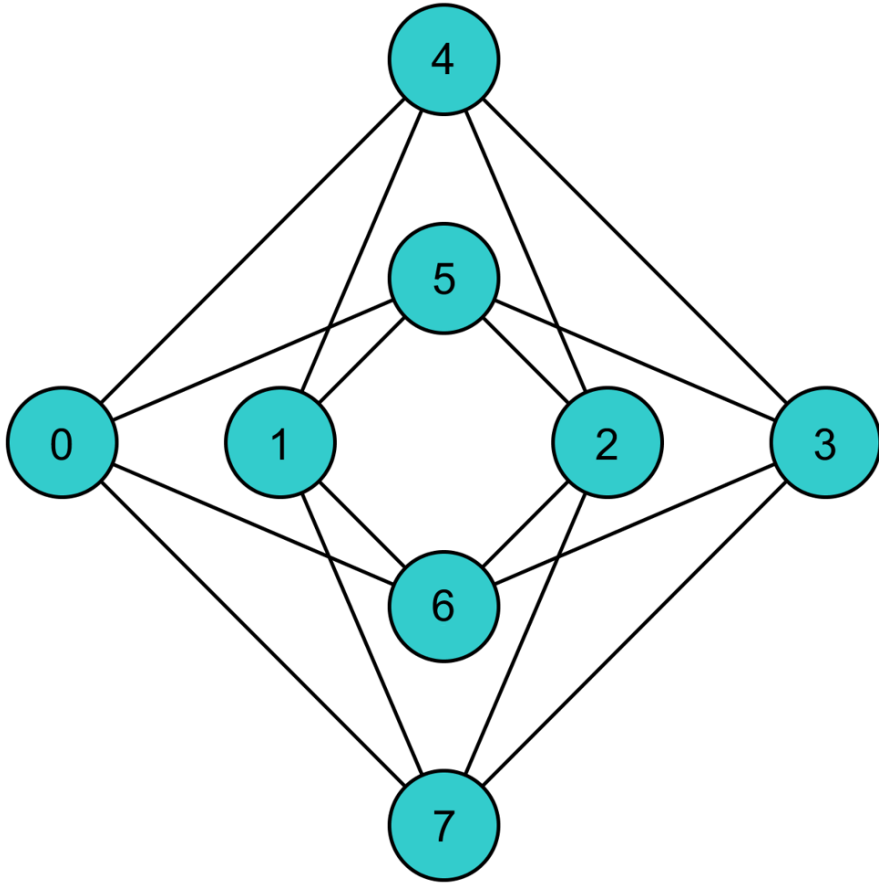

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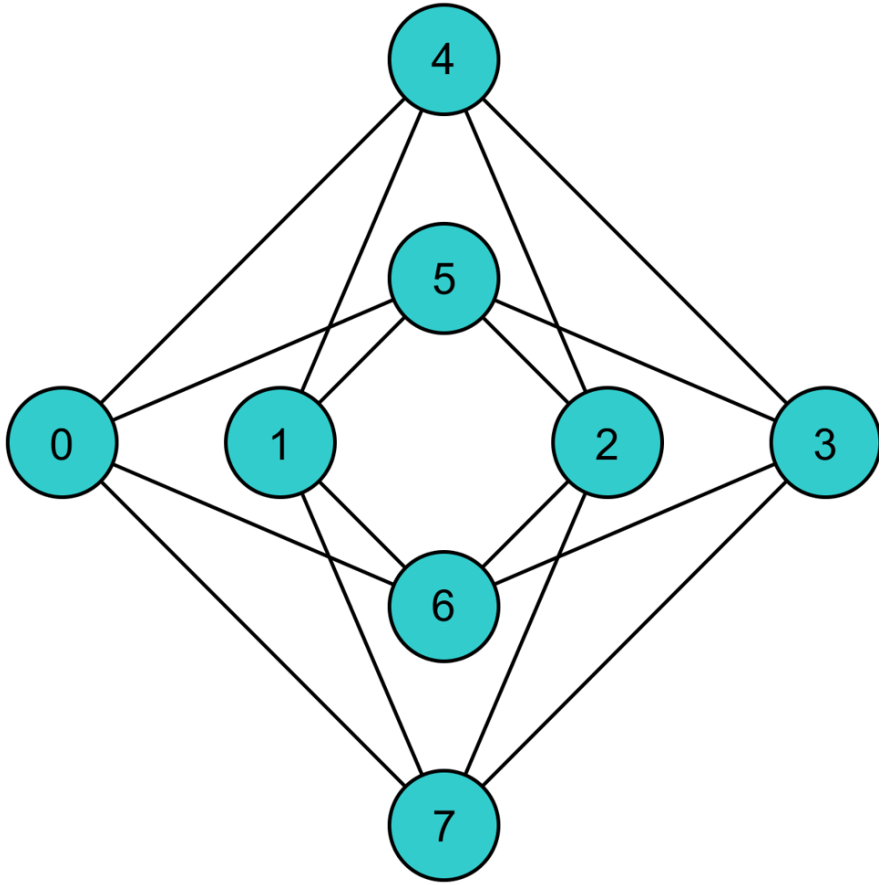

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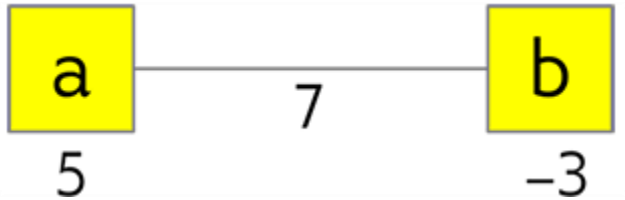
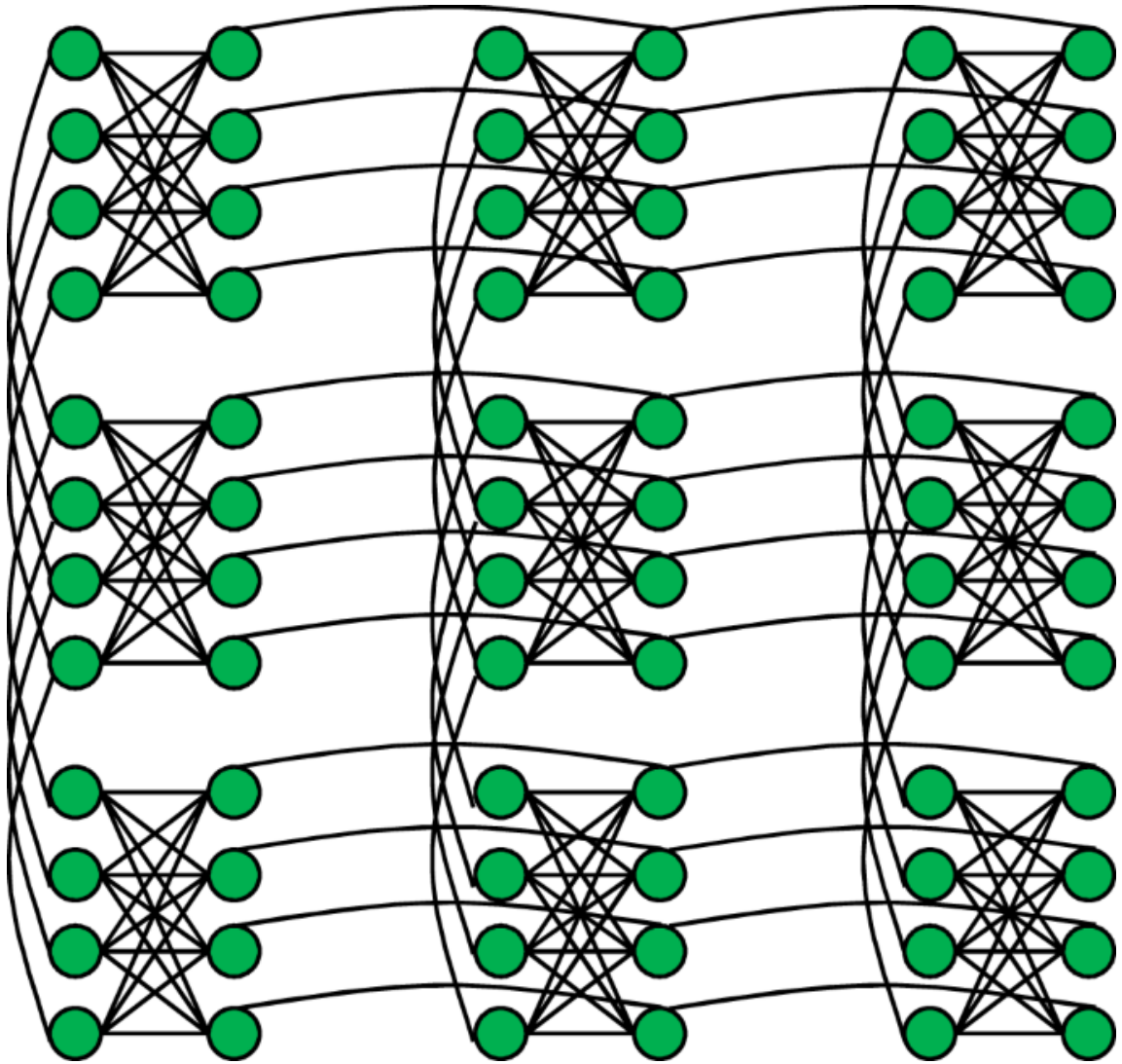


Embedding a problem on a graph



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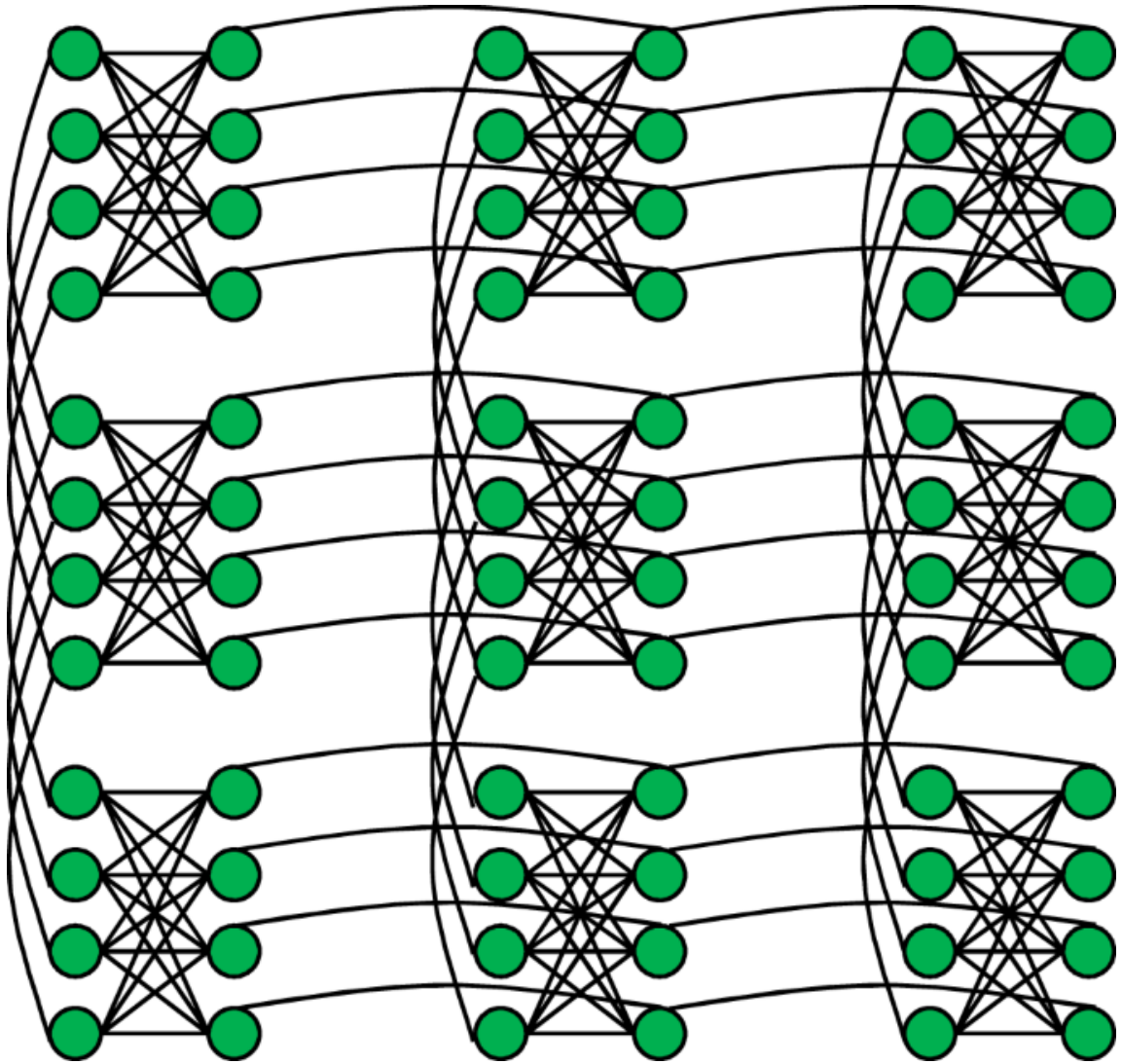

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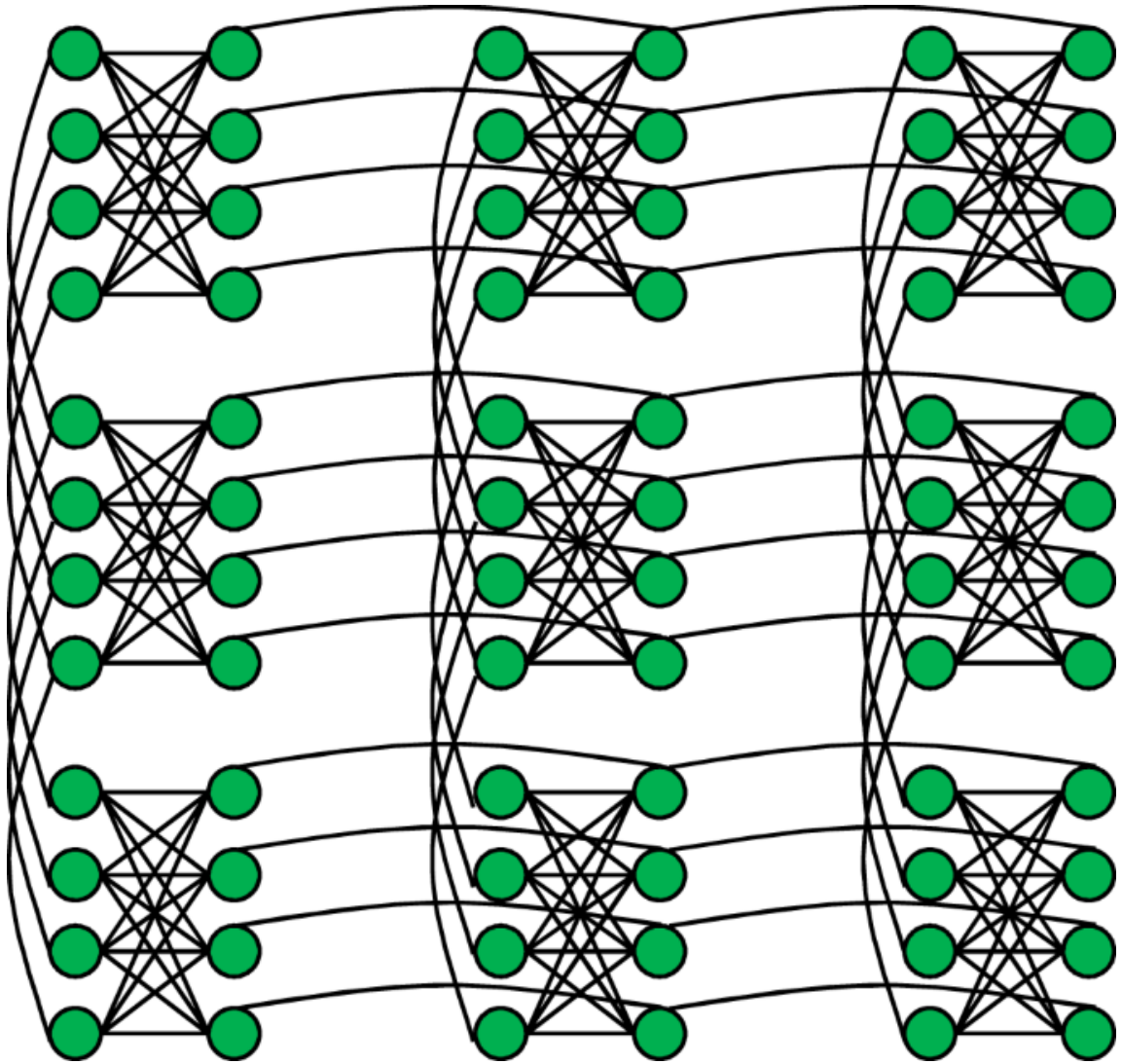

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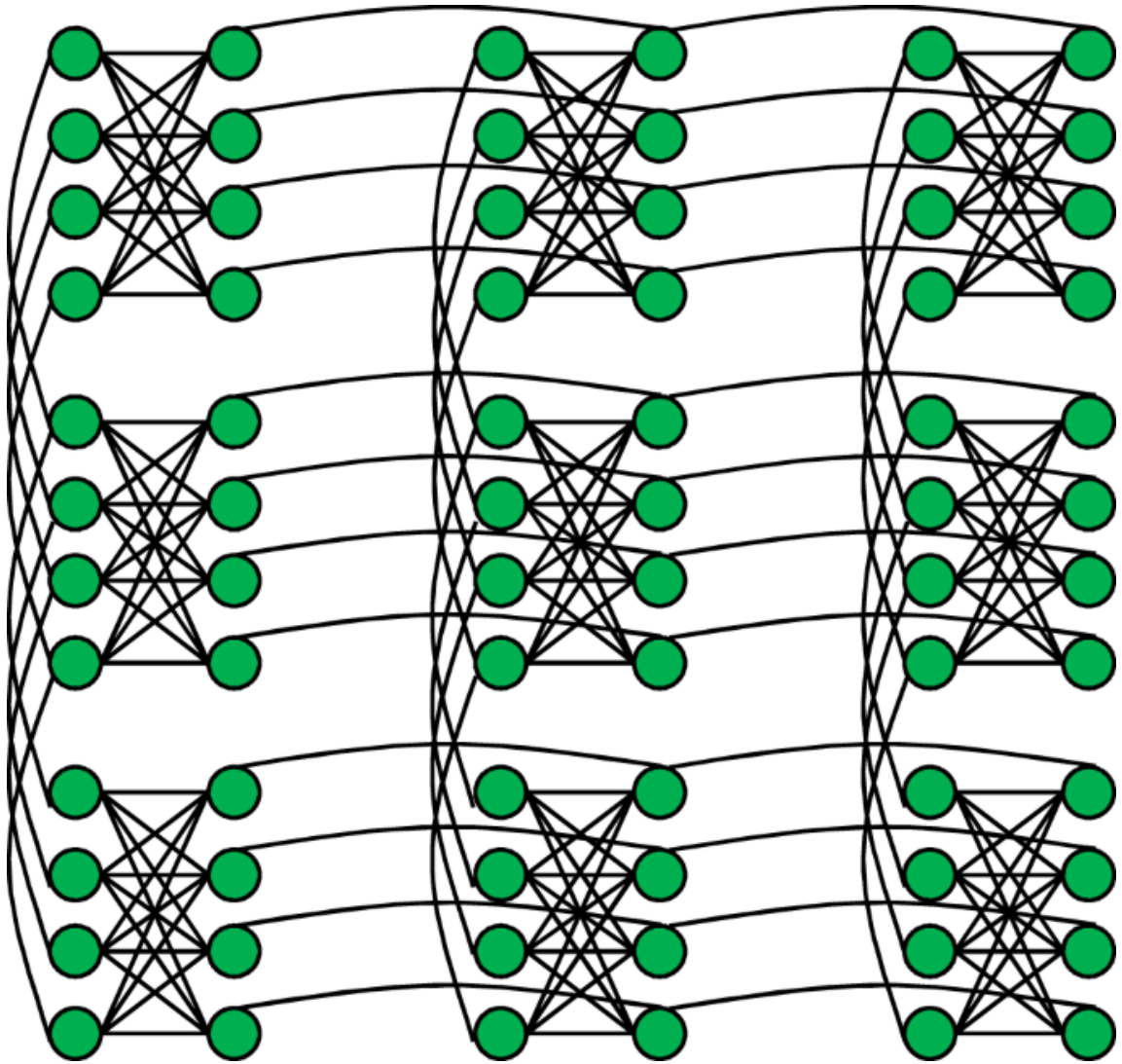

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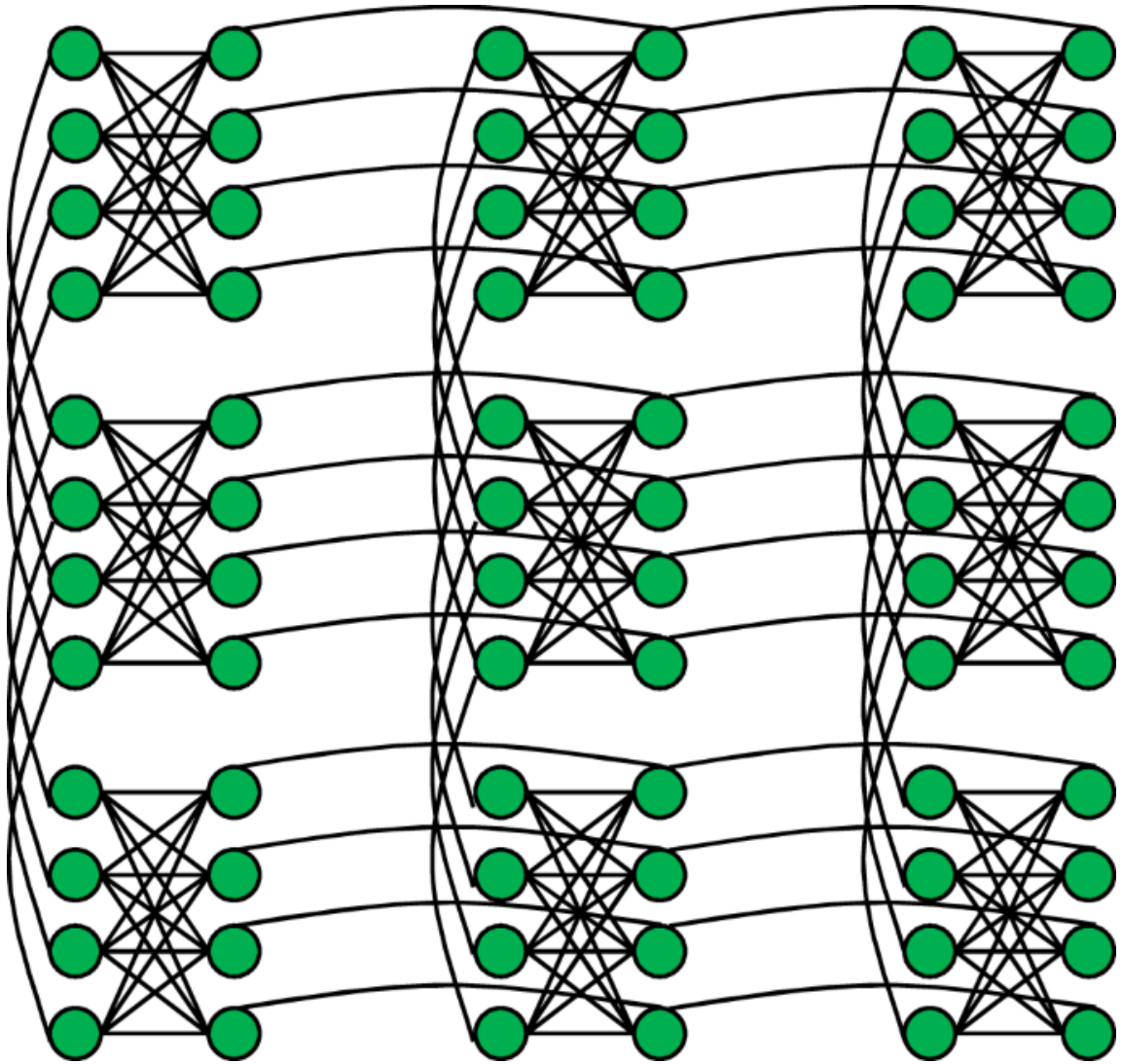

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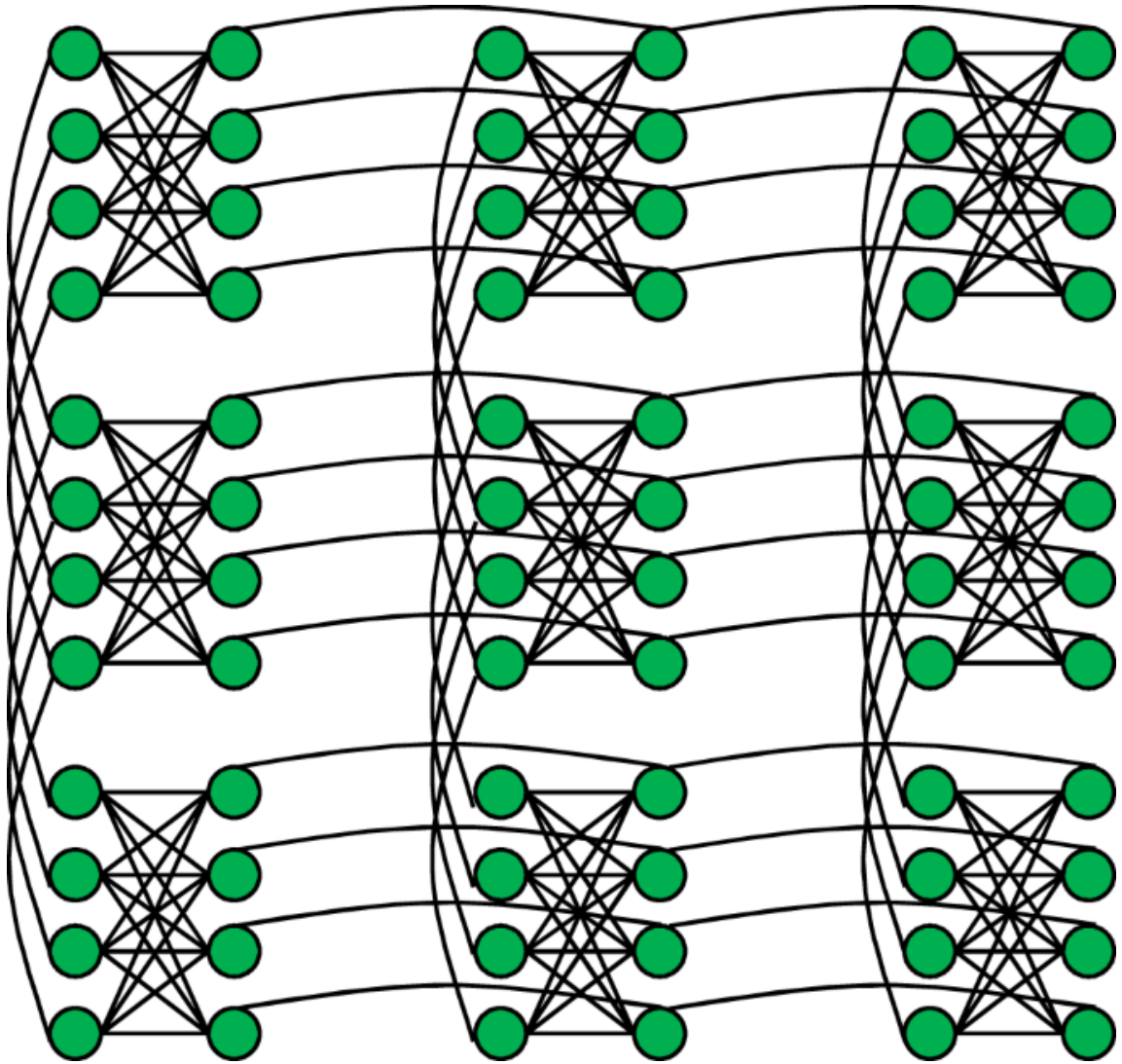

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Embedding a problem on a graph

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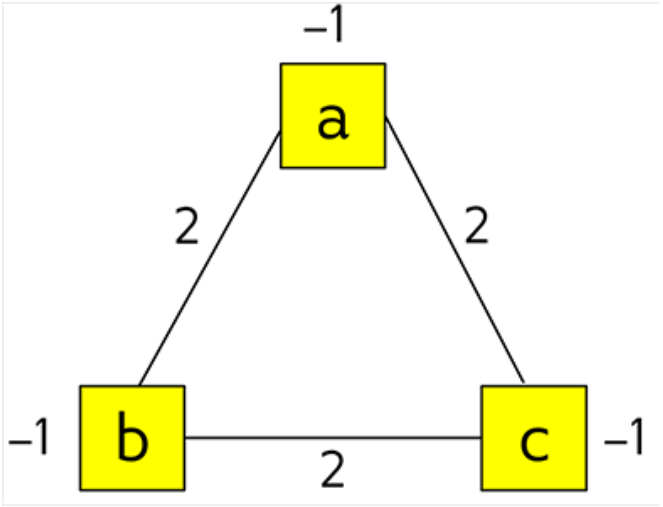
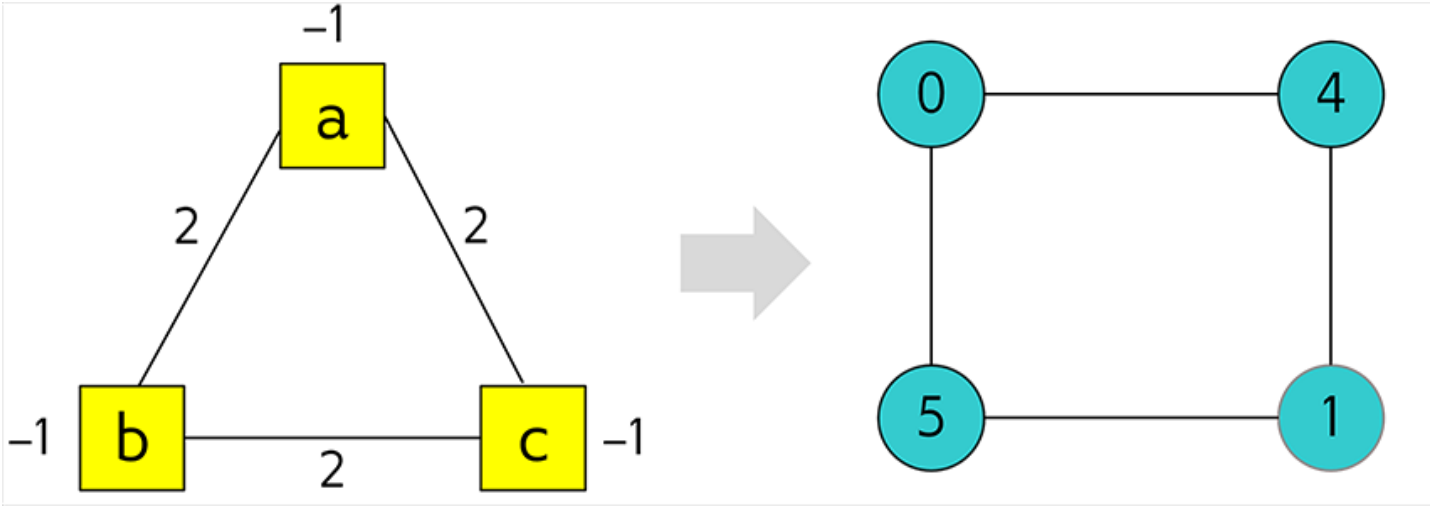


Embedding a problem on a graph

- 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



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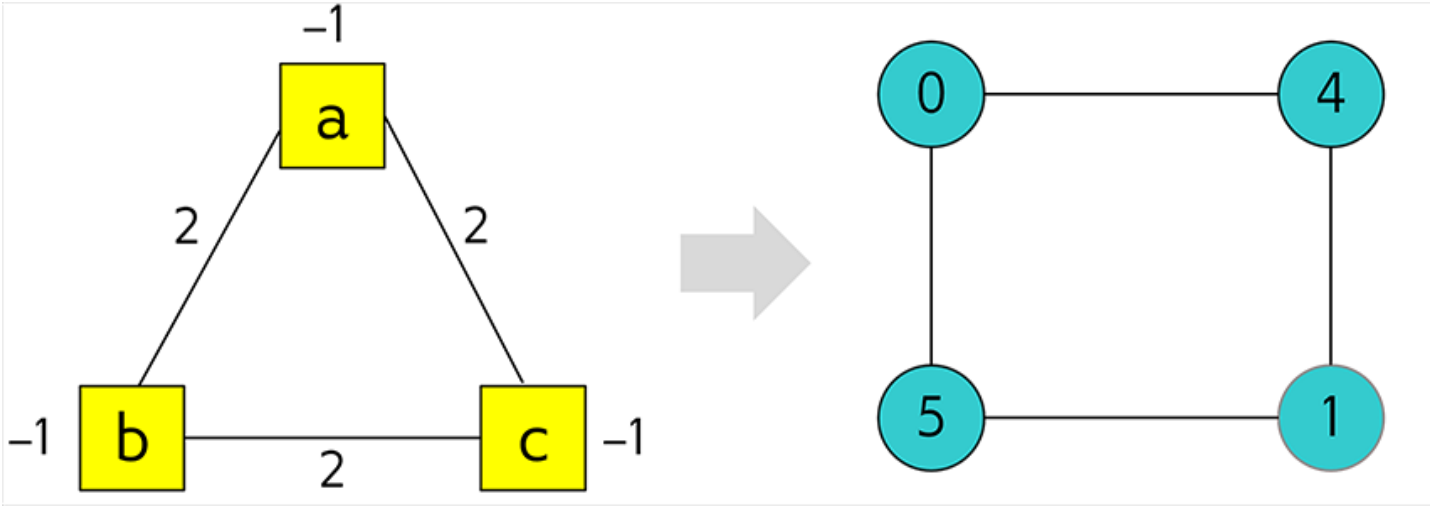

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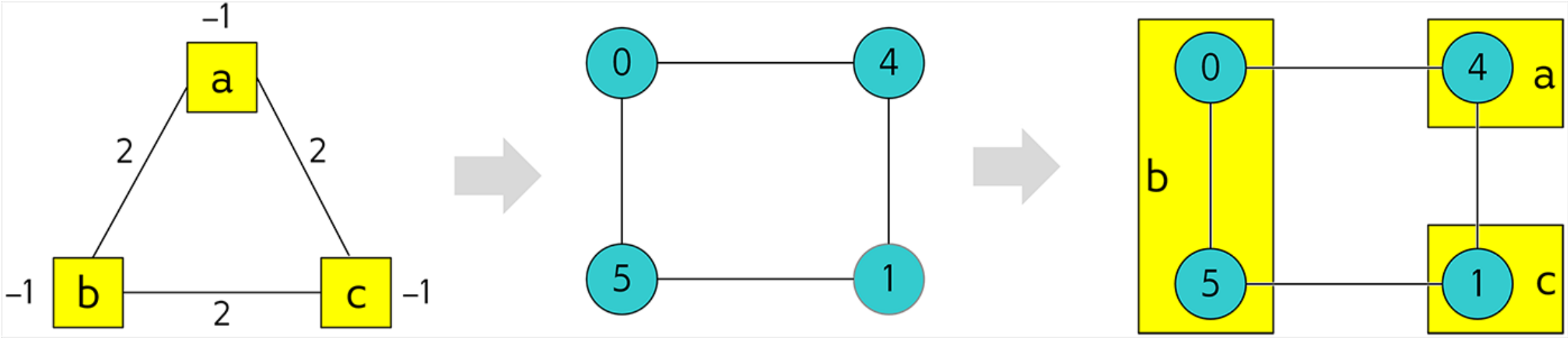

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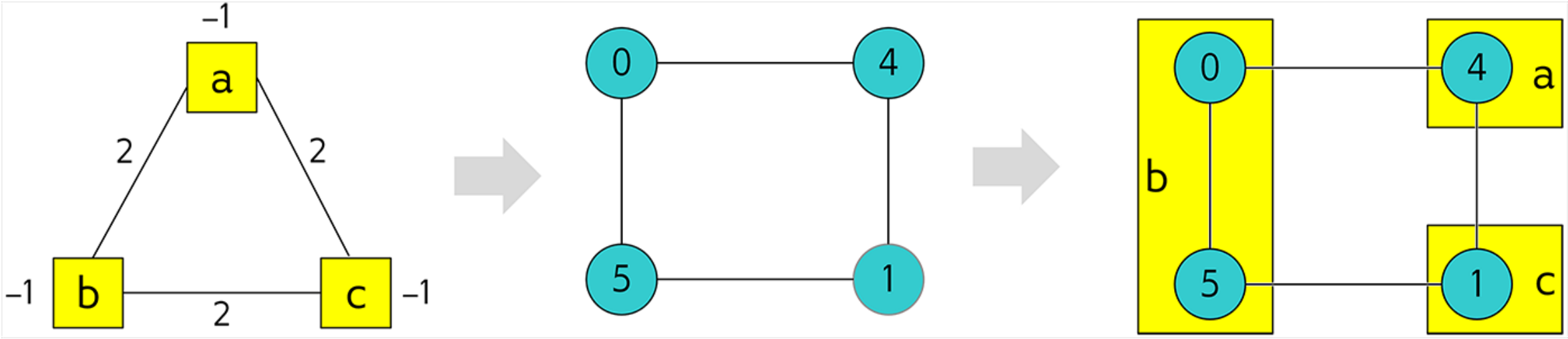
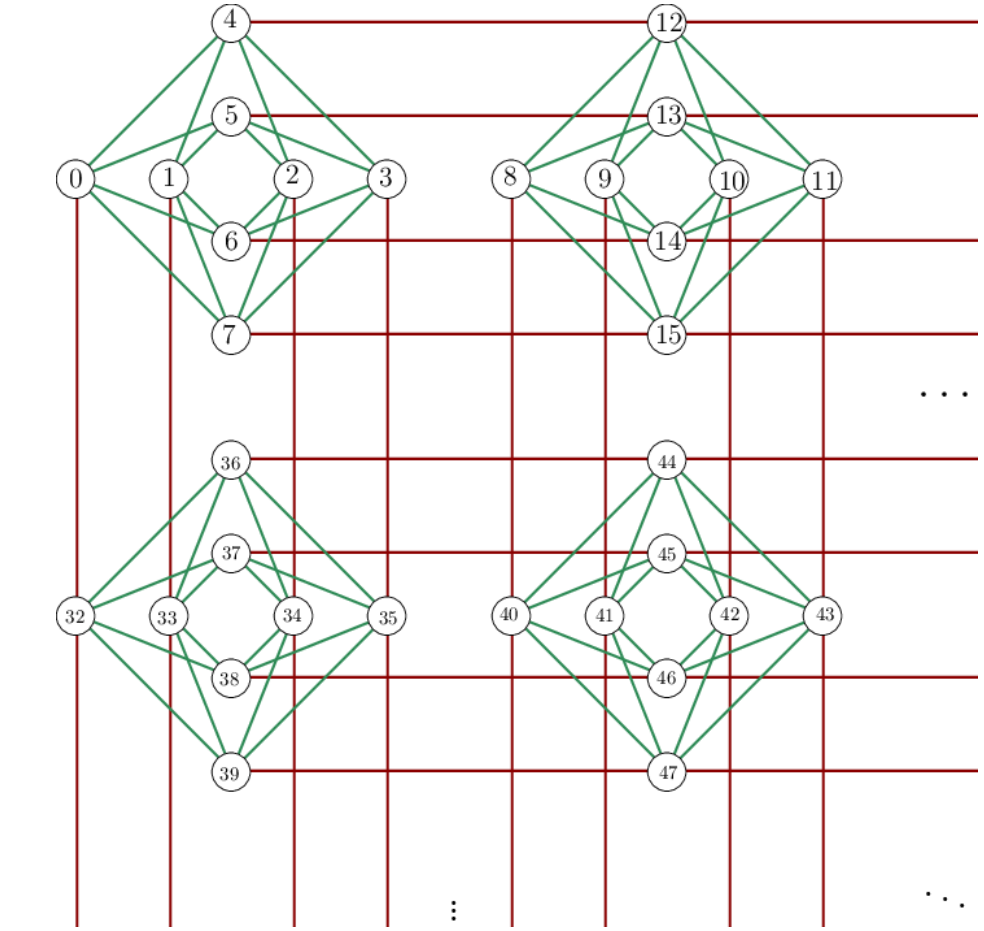
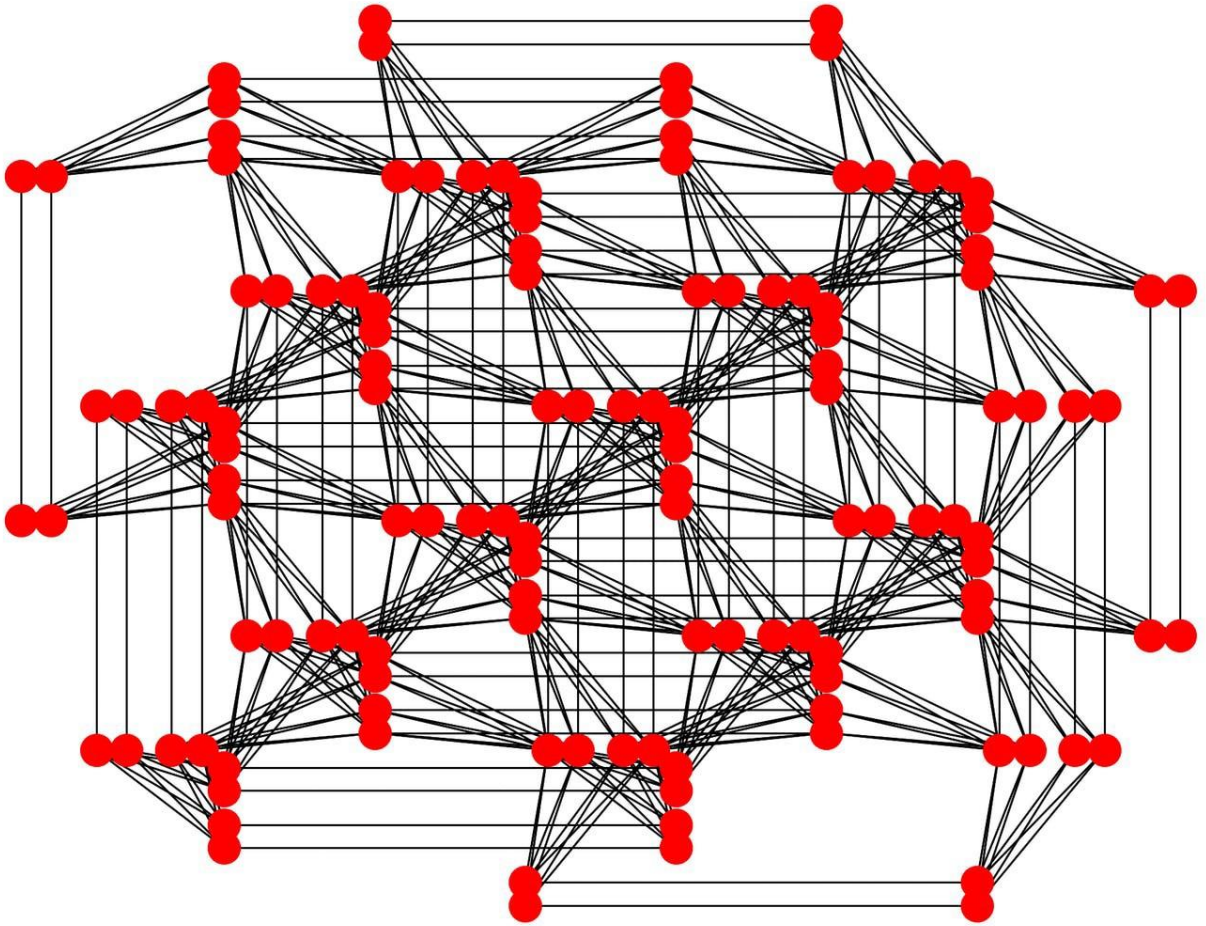
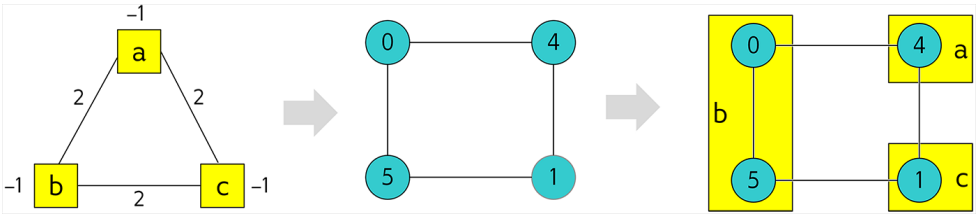
- In a certain sense, we can say that the qubits engaged in embedding are placed in entanglement relationship: they are forced to collapse in the same classical state



Embedding on Chimera and Pegasus







CINECA QUANTUM COMPUTING LAB

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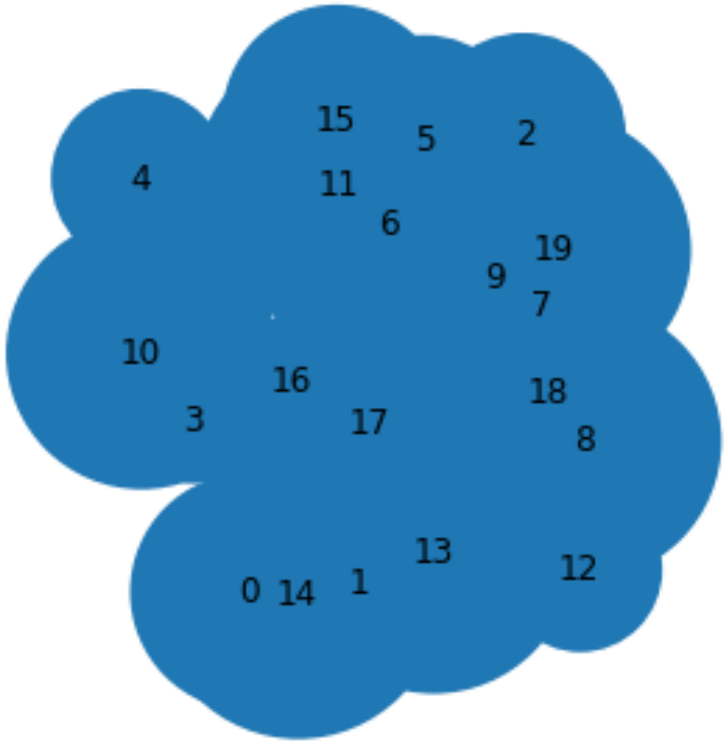

- Try the embedding on Pegasus and Chimera

Exercise 3: N-Queens Puzzle

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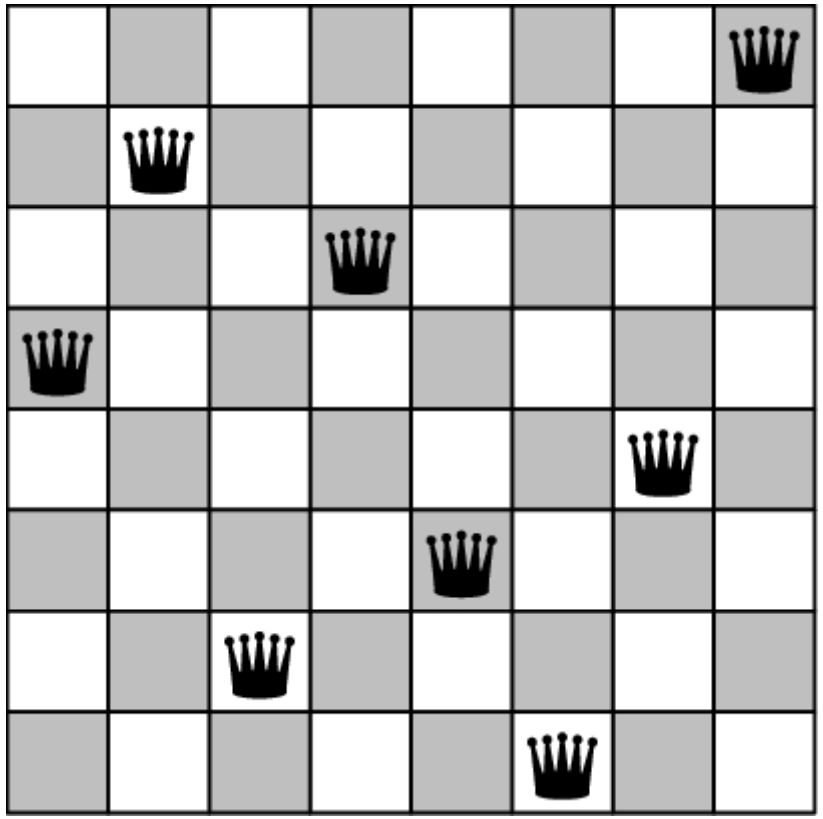

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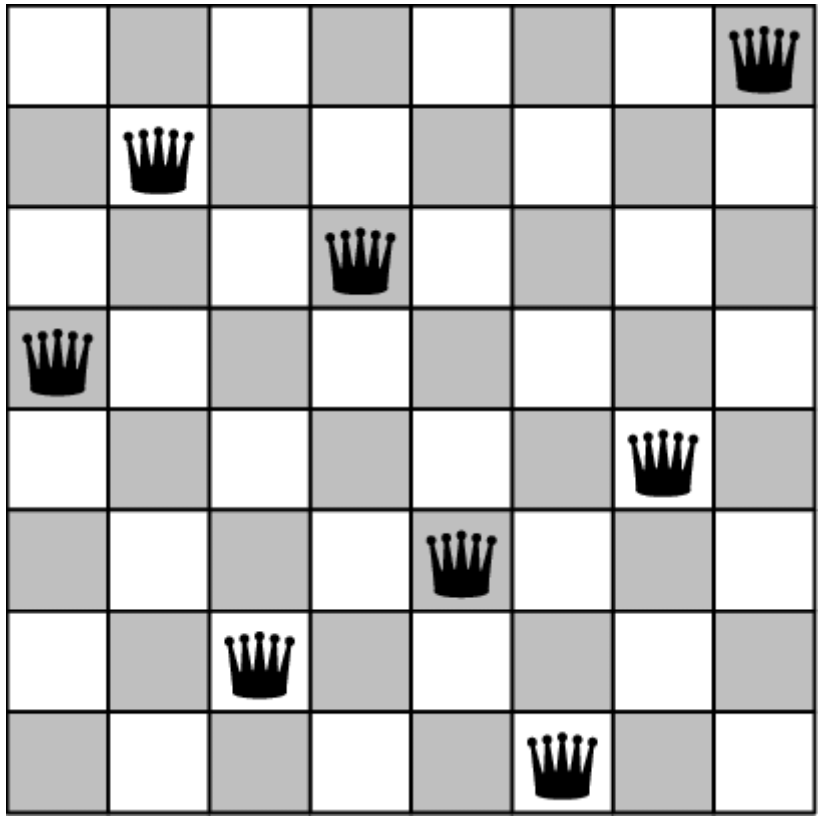

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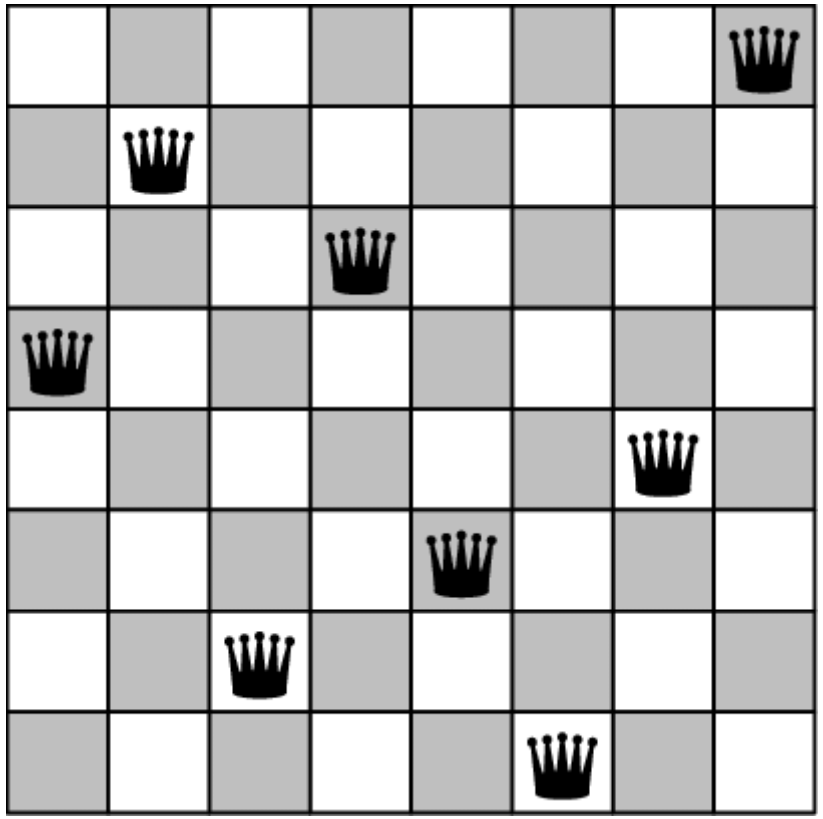

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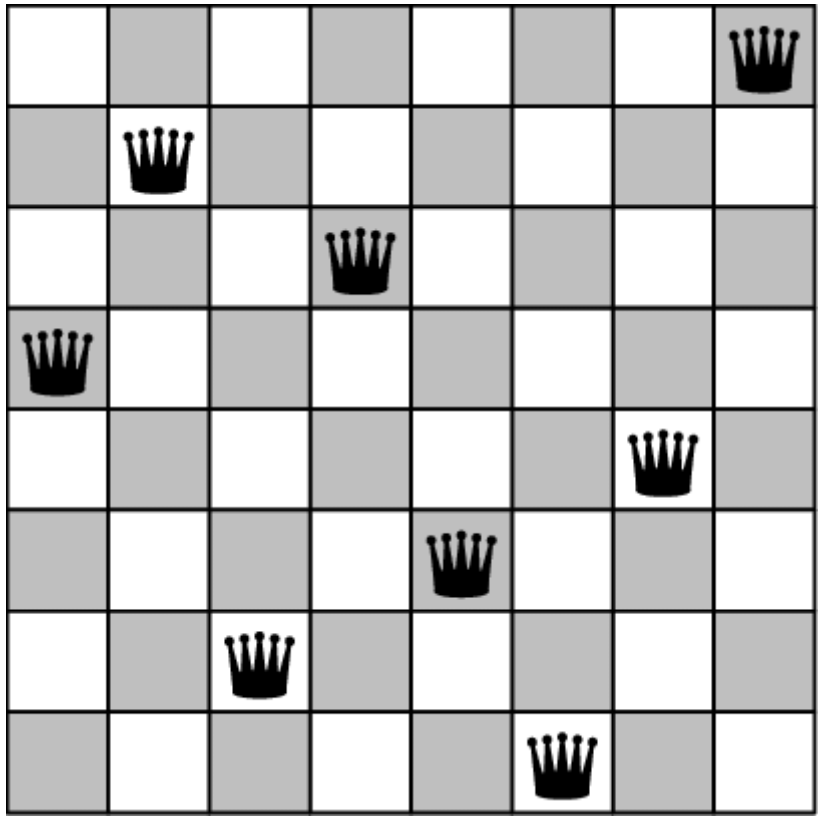
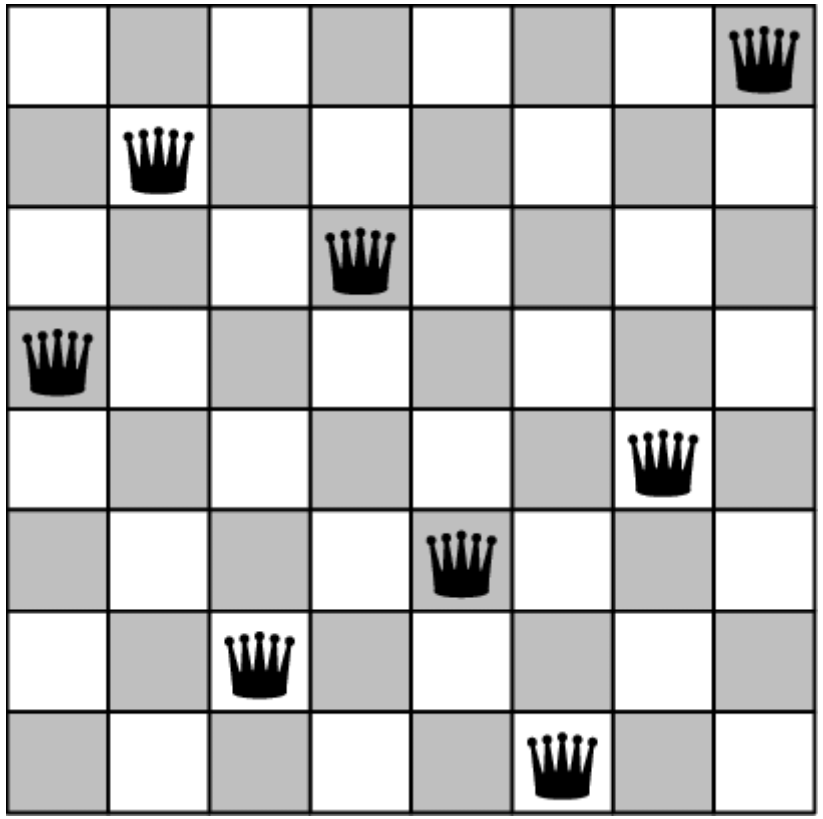
- The game is generalized as follows: let's consider a chessboard **of dimension NxN**. Find a way **to arrange N queens** on the chessboard so that none of them are in check by any of the other queens



Exercise 3: N-Queens Puzzle

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



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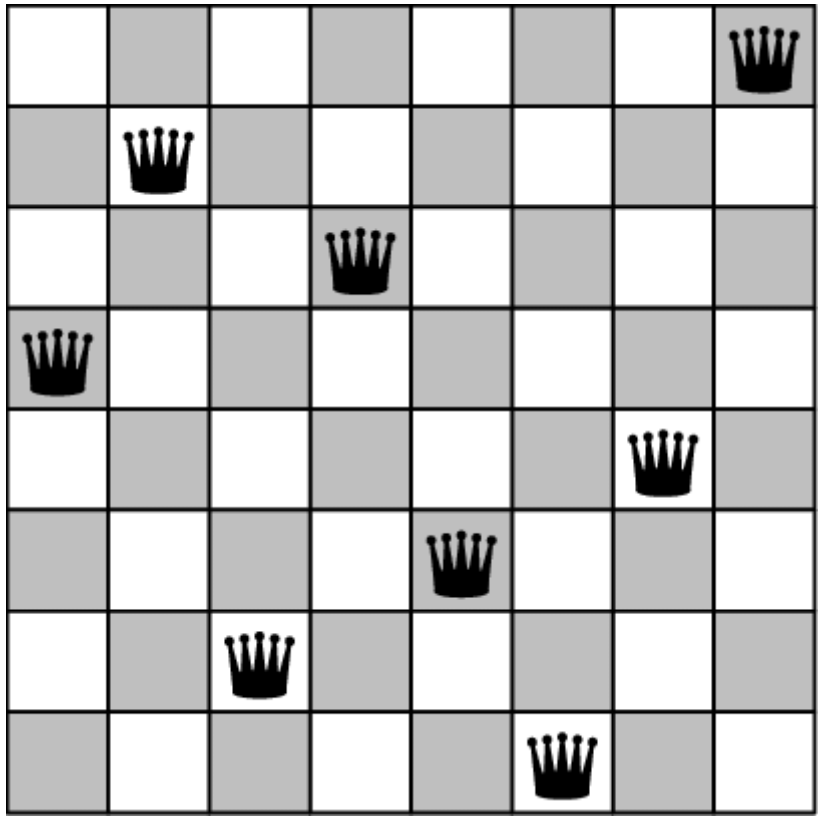

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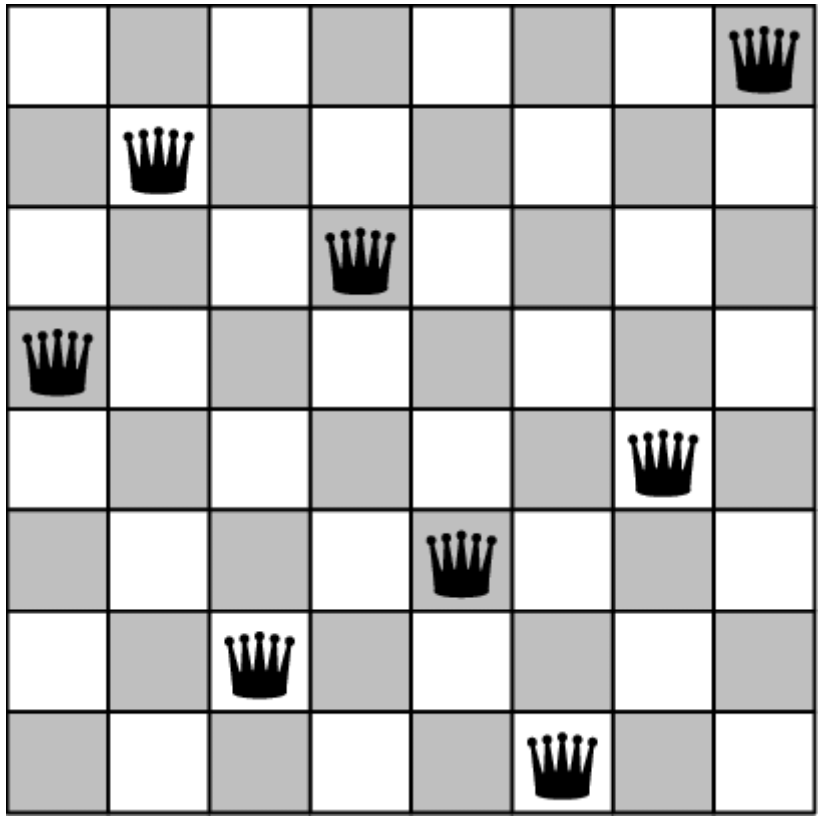

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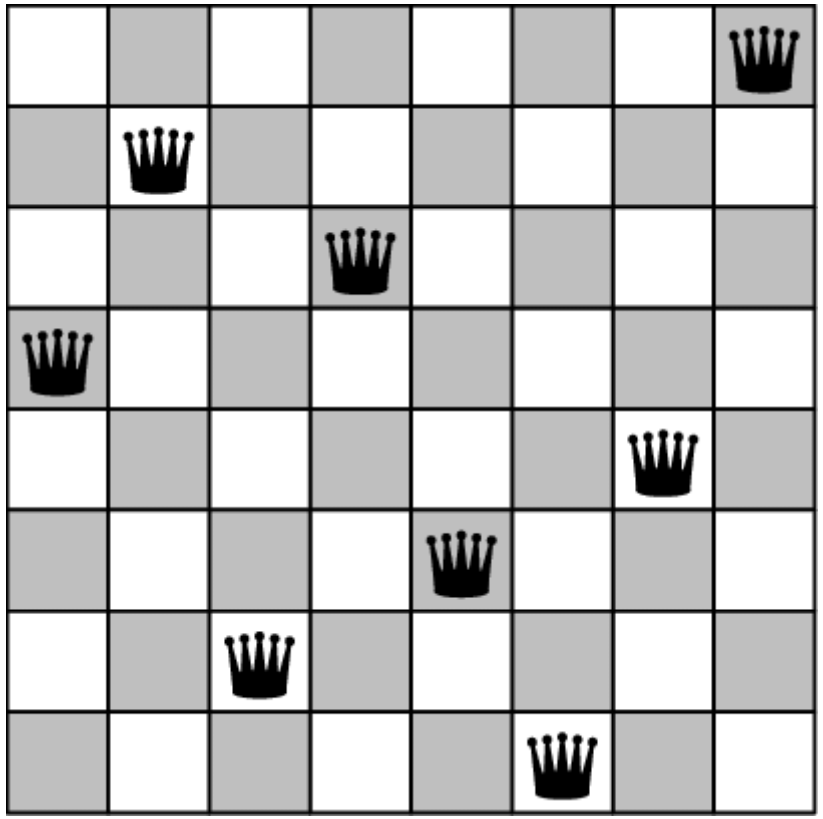

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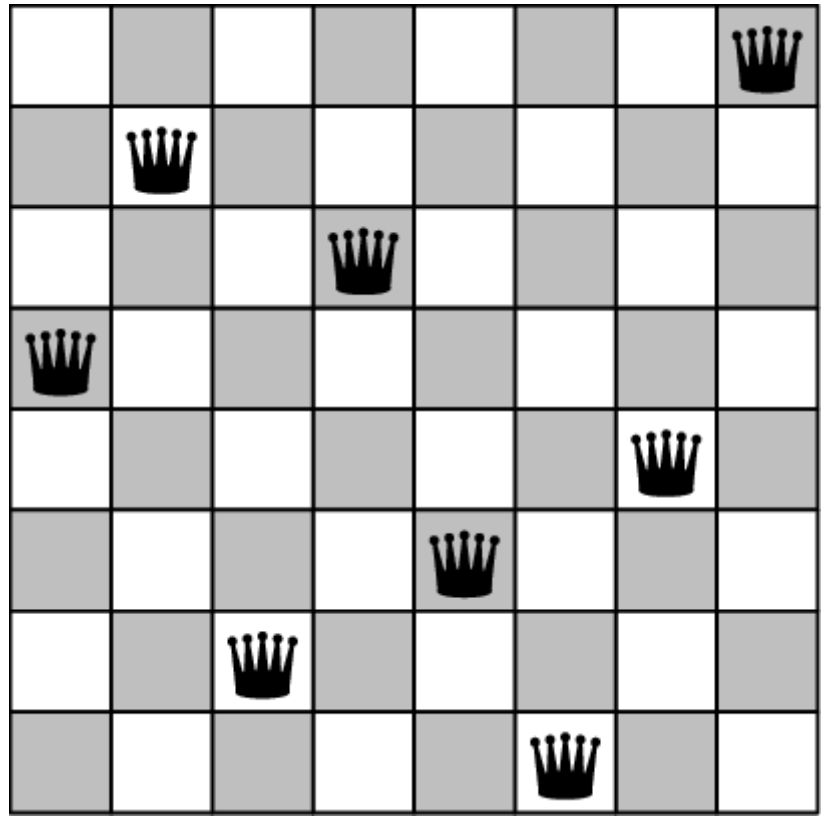

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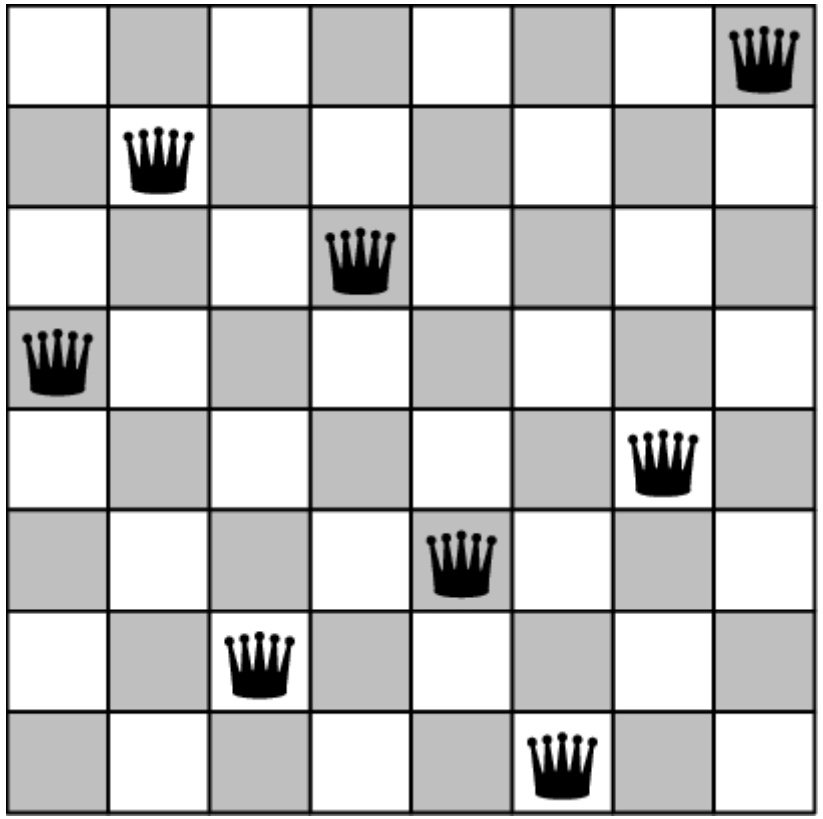
$$\sum_{i=1}^{N} q_i = N$$



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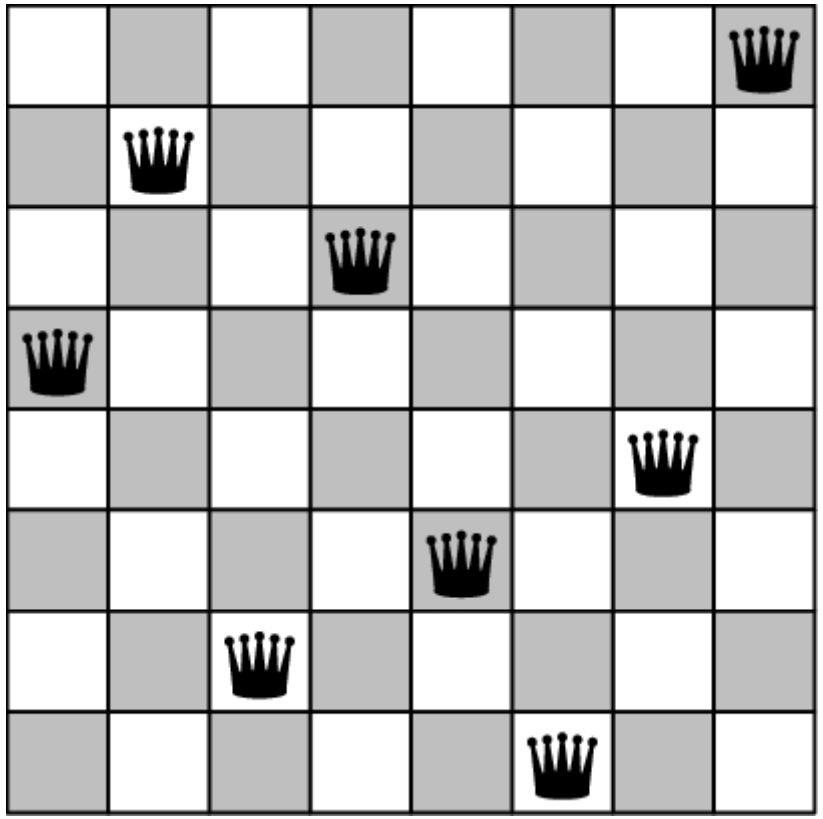
$$\sum_{i=1}^{N} q_i = N \Rightarrow \min \left(\sum_{i=1}^{N} q_i - N \right)^2$$



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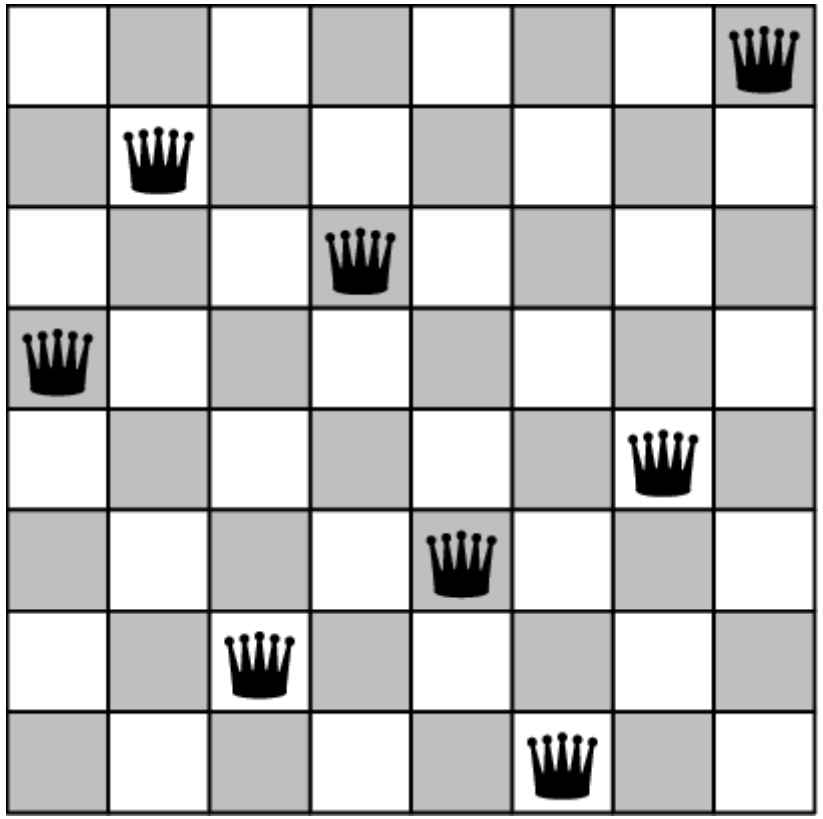
$$\left(\sum_{i=1}^{N} q_i - N \right)^2$$



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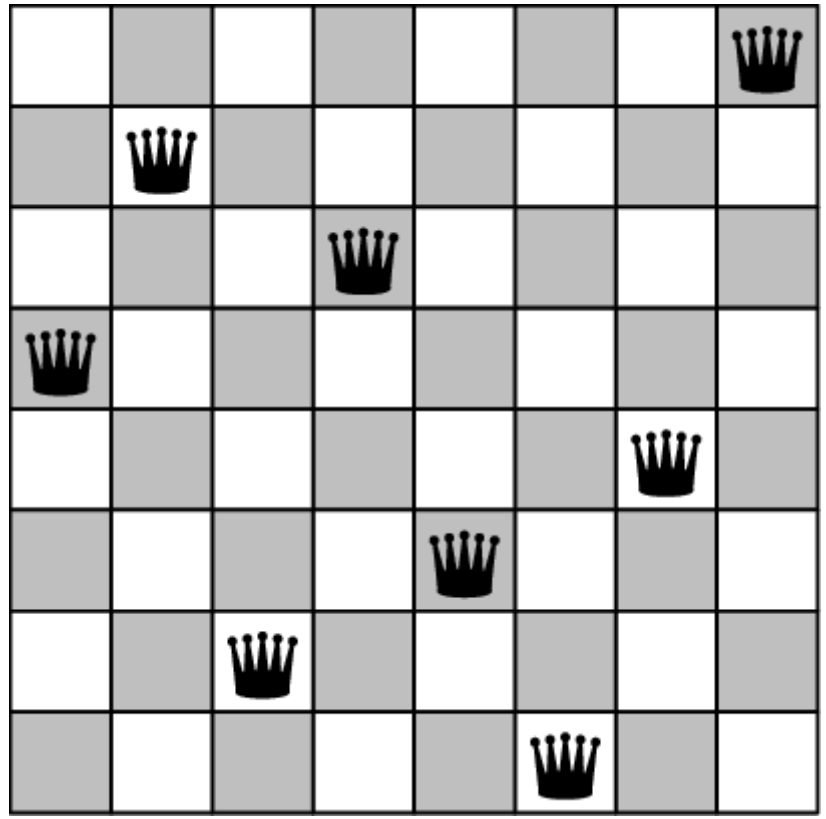
$$\left(\sum_{i=1}^{N} q_i - N\right)^2 = \left(\sum_{i=1}^{N} q_i\right)^2 - 2\sum_{i=1}^{N} q_i$$



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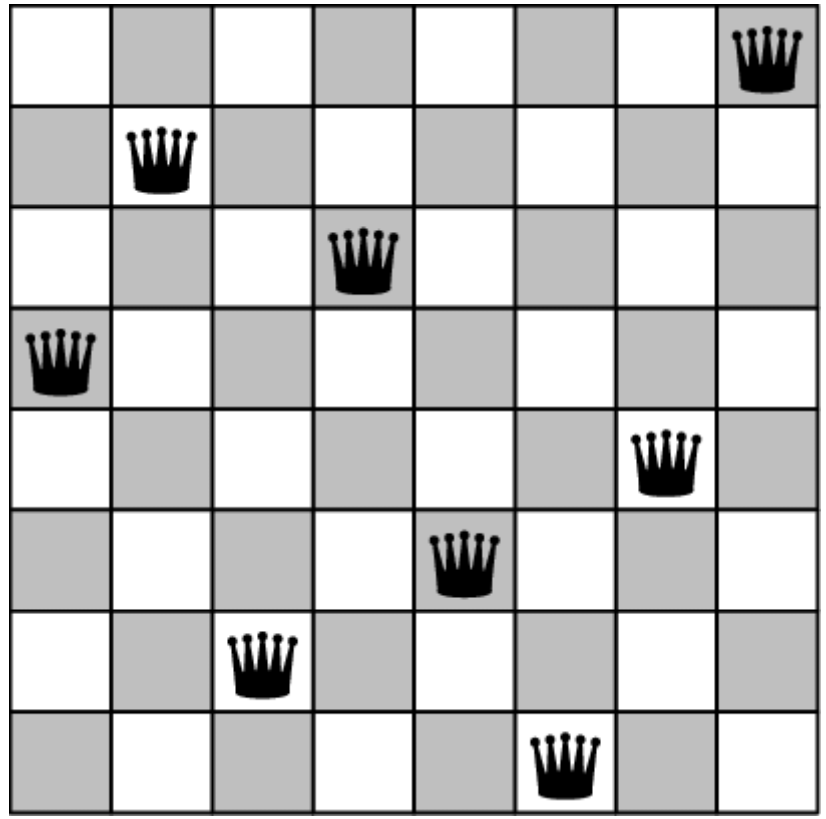

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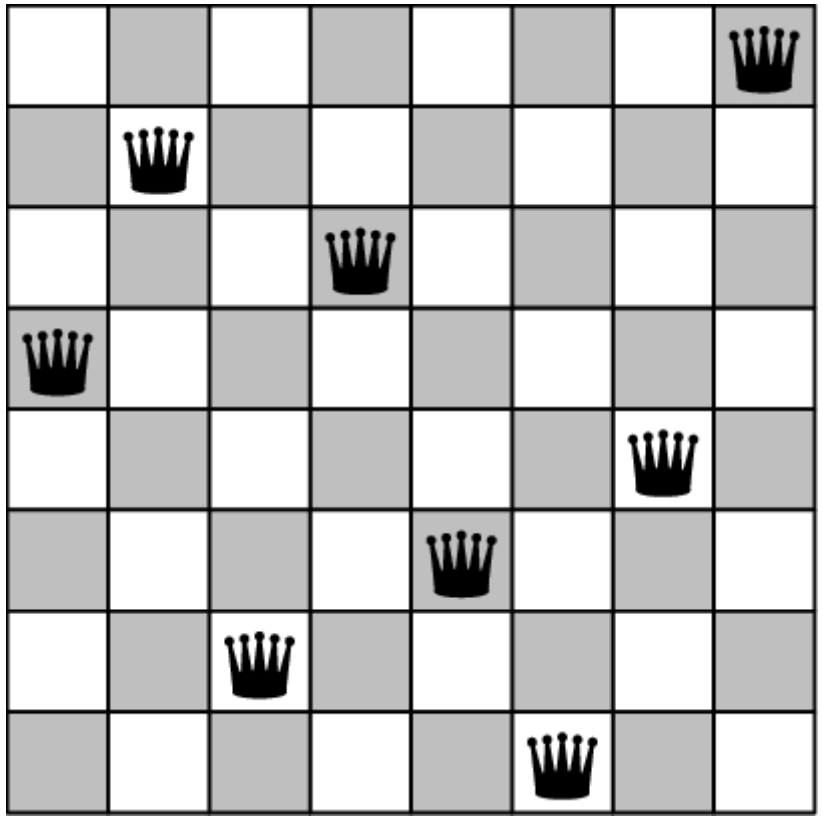

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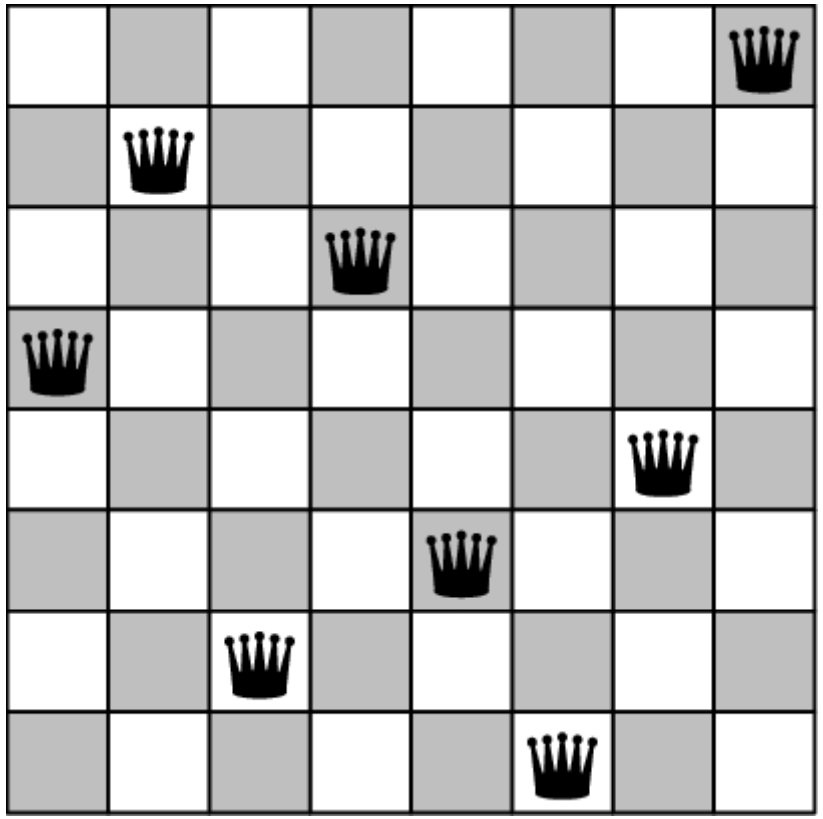

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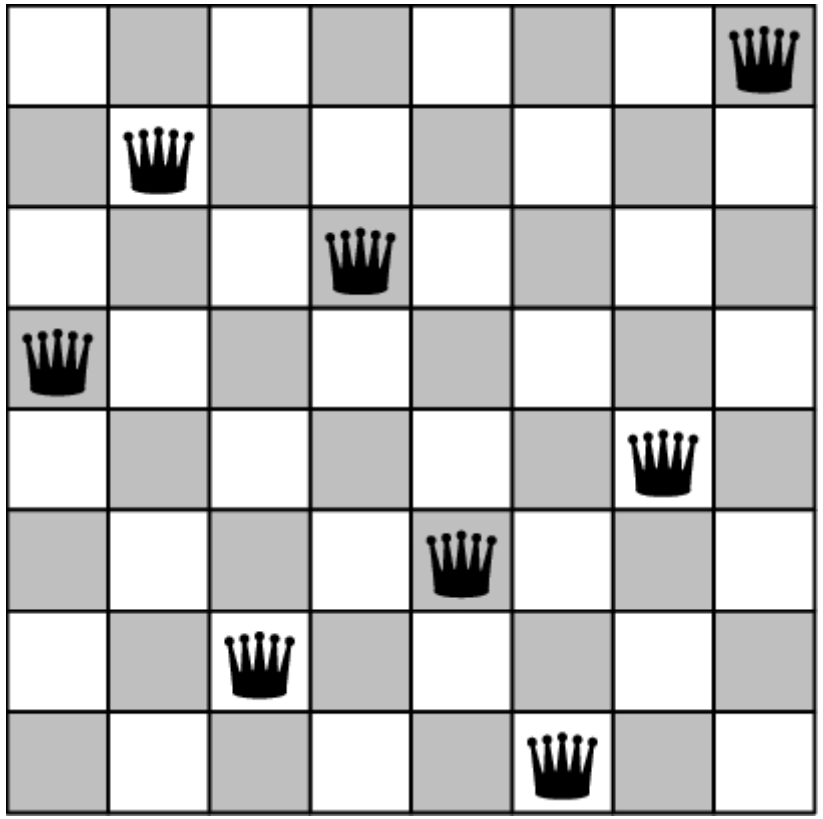

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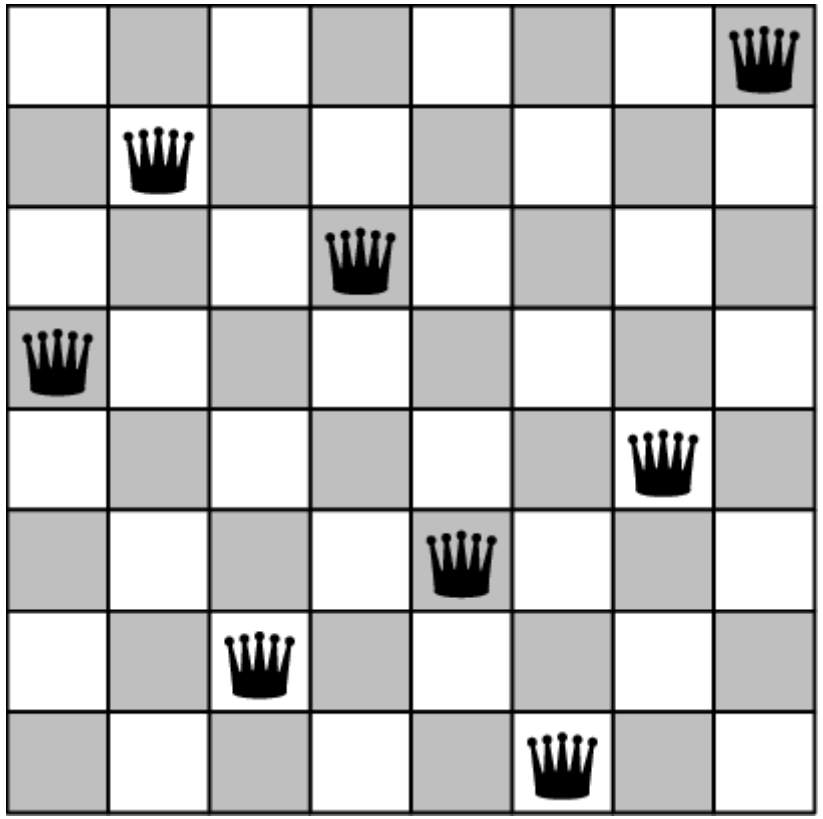

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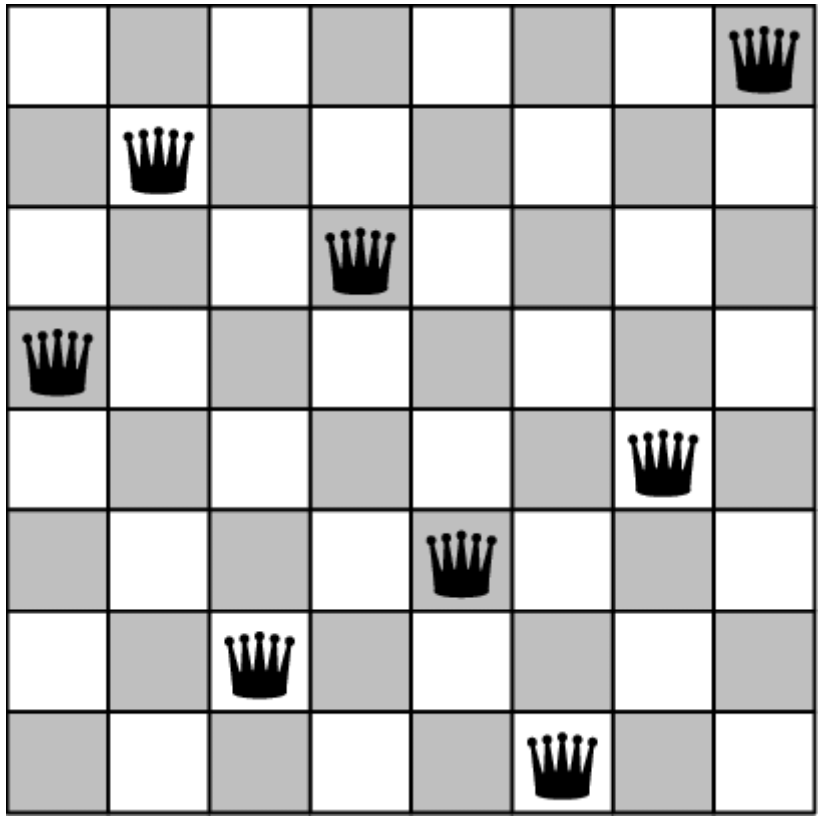

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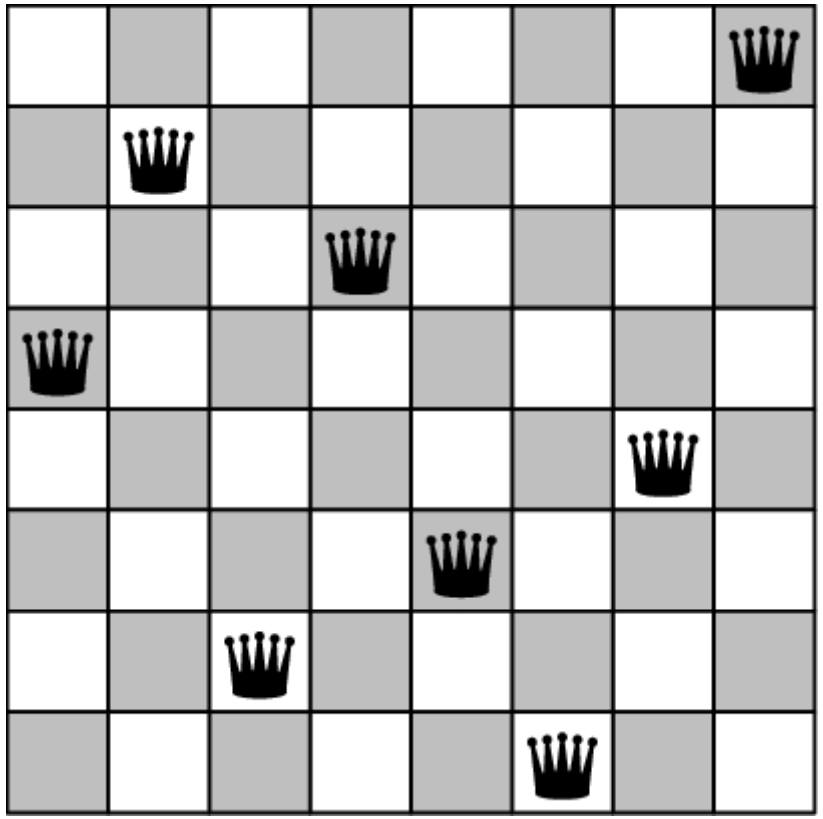

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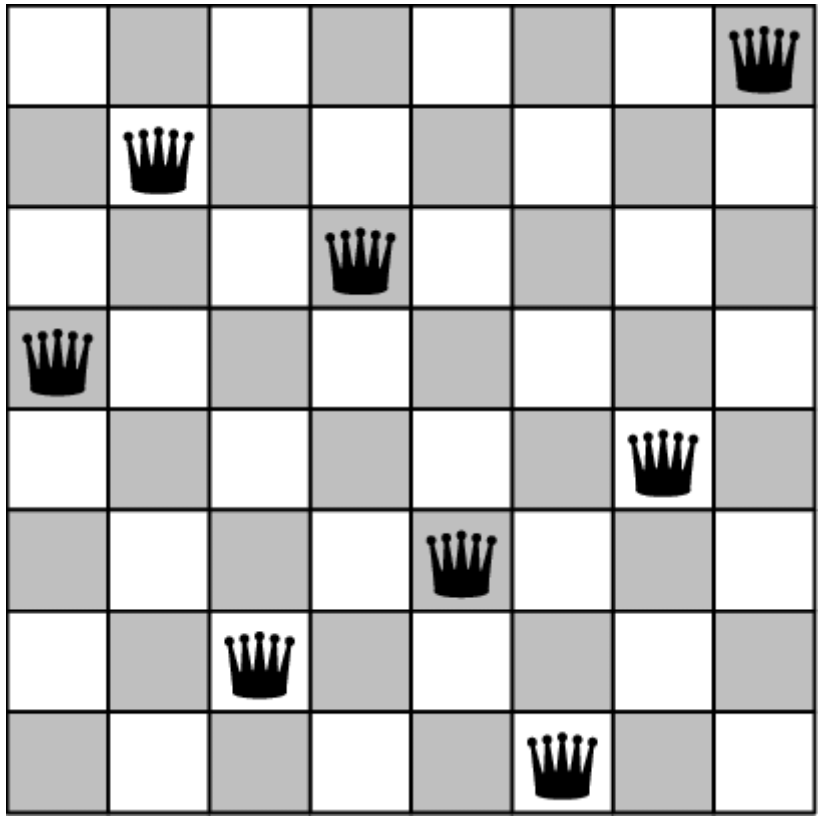

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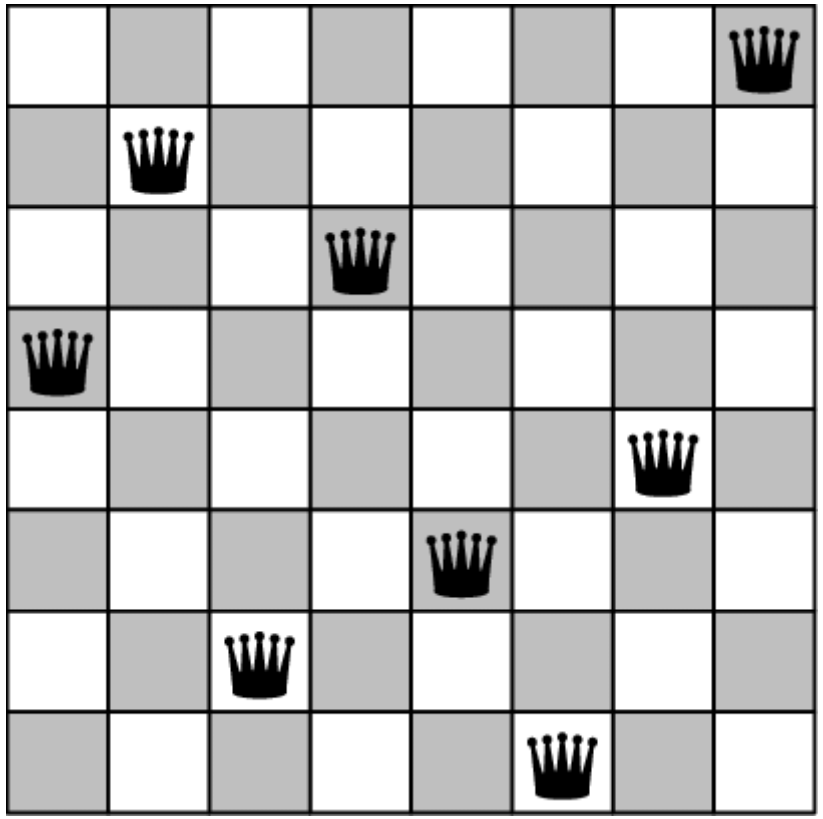

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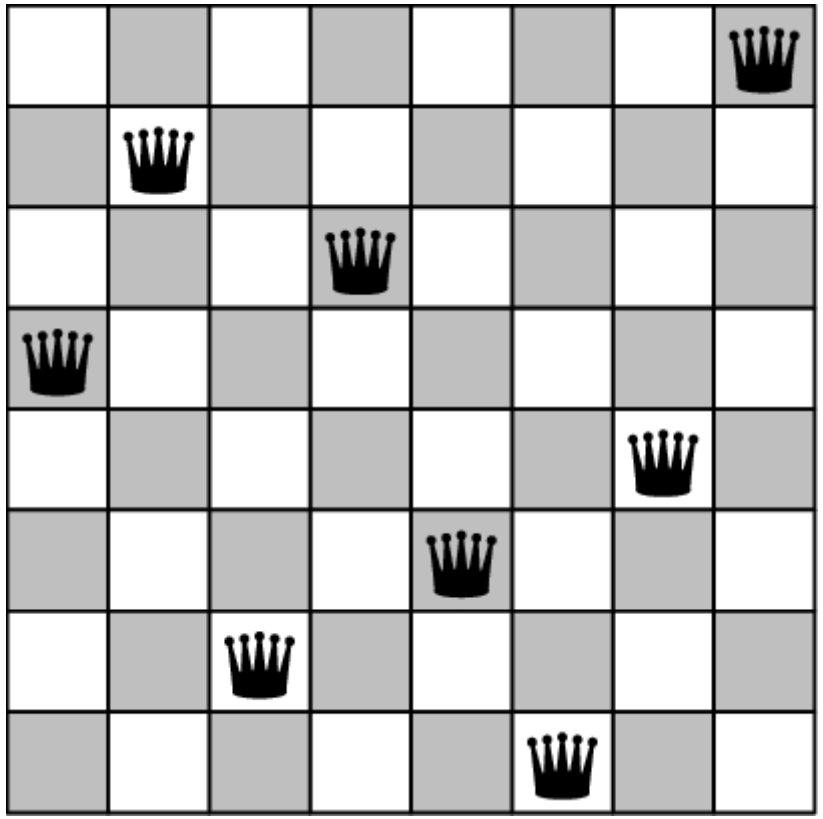

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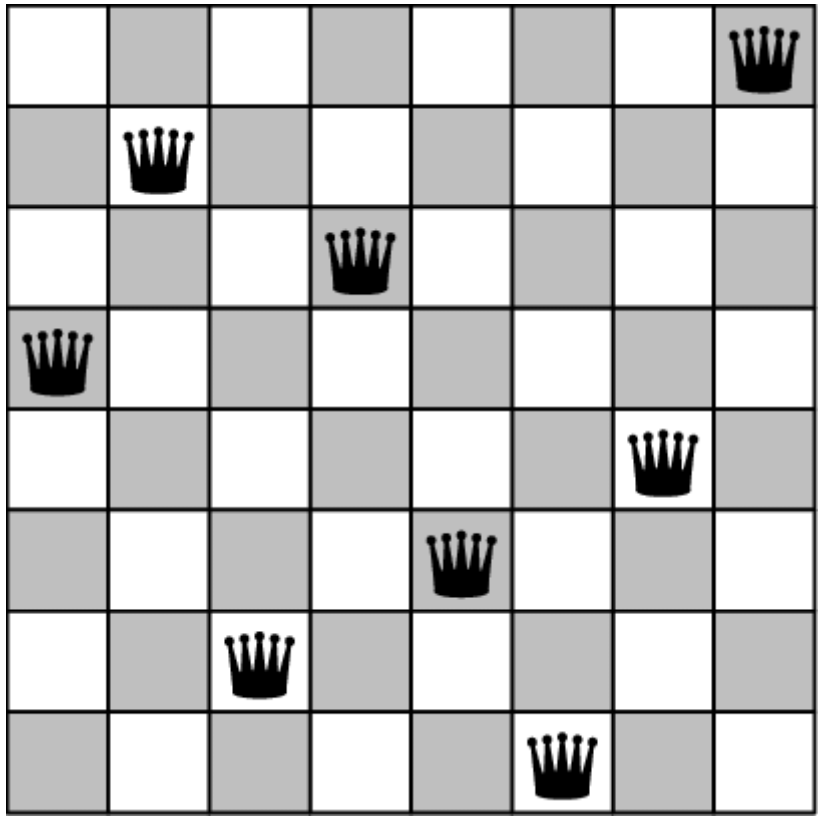

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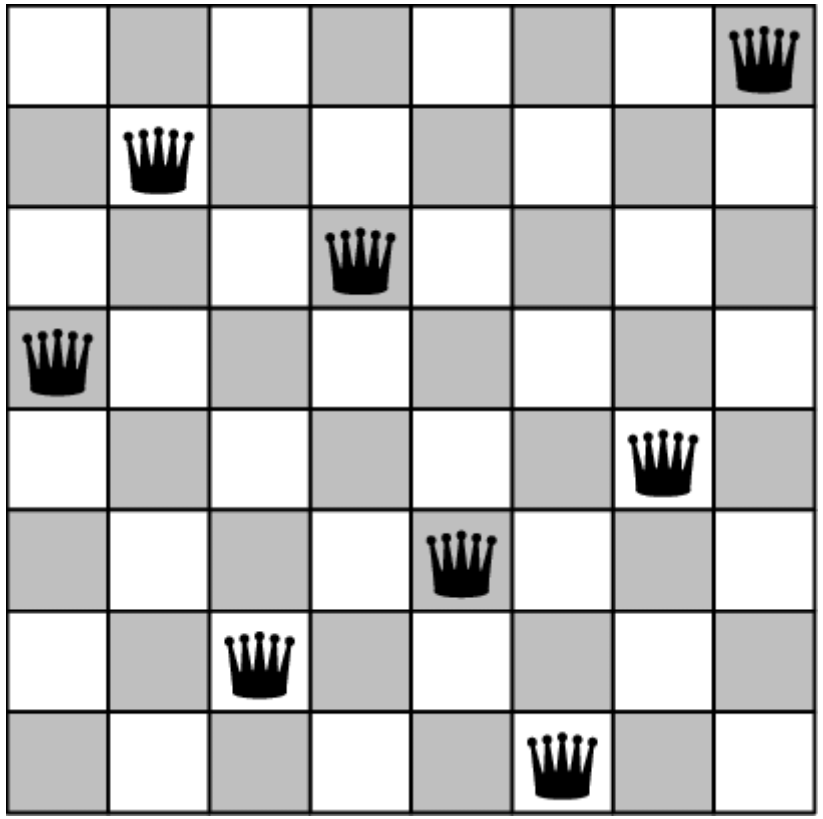

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- Let us then consider the problem from another point of view.
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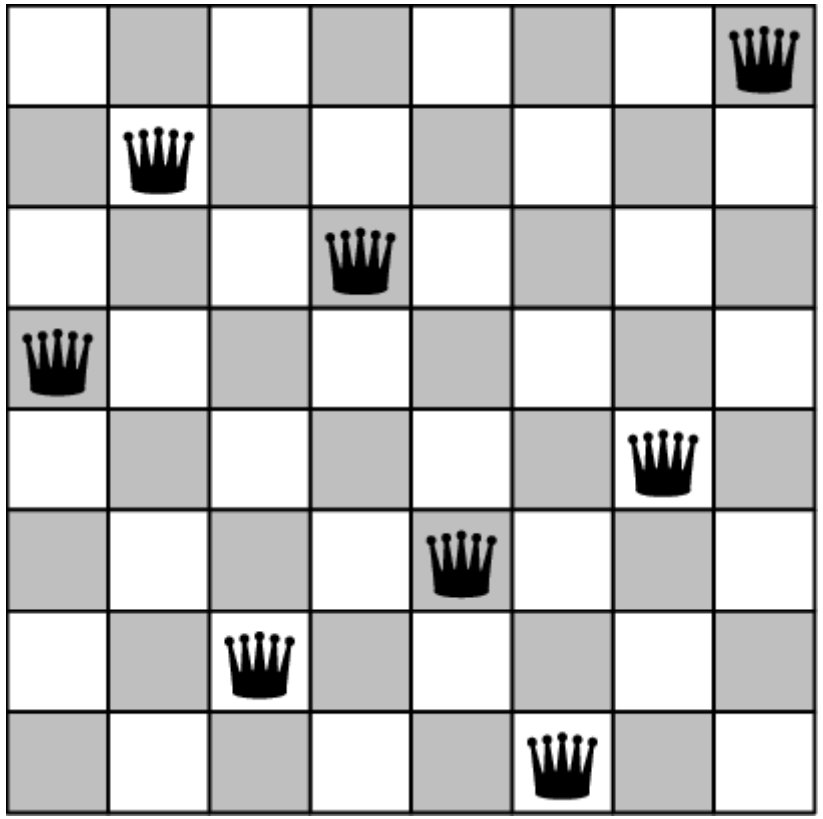

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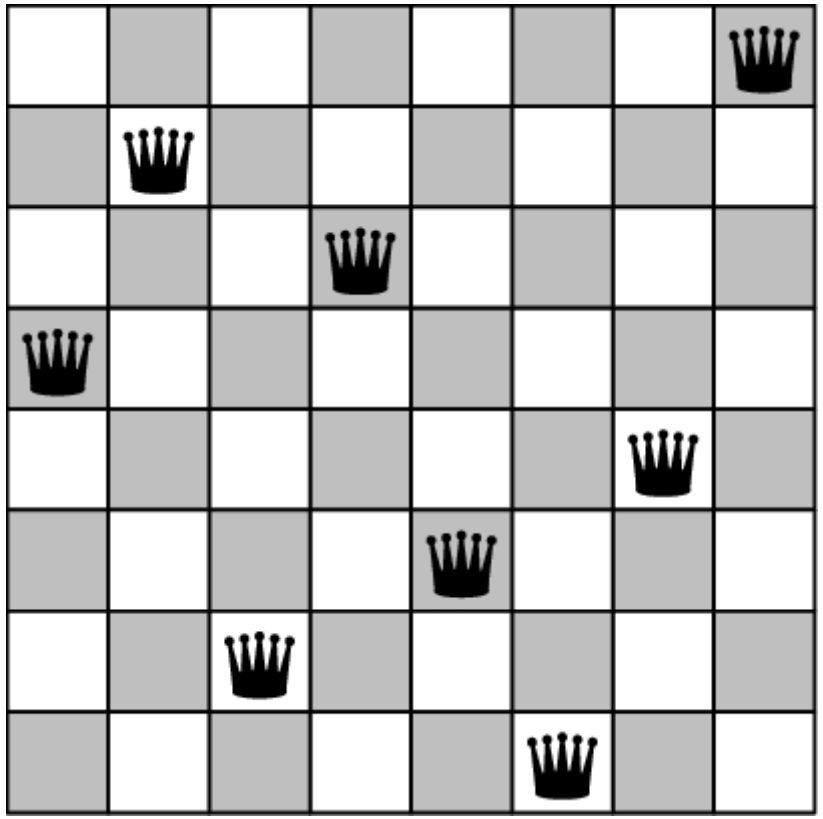
- This matrix has as elements all the possible pairs of squares on the chessboard (NxNxNxN)



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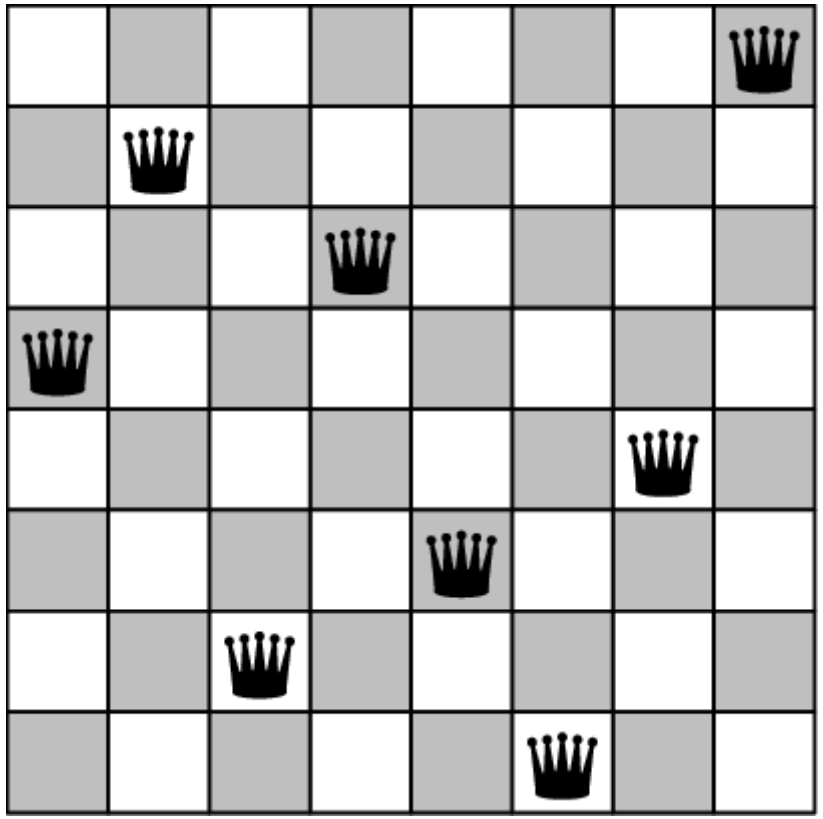

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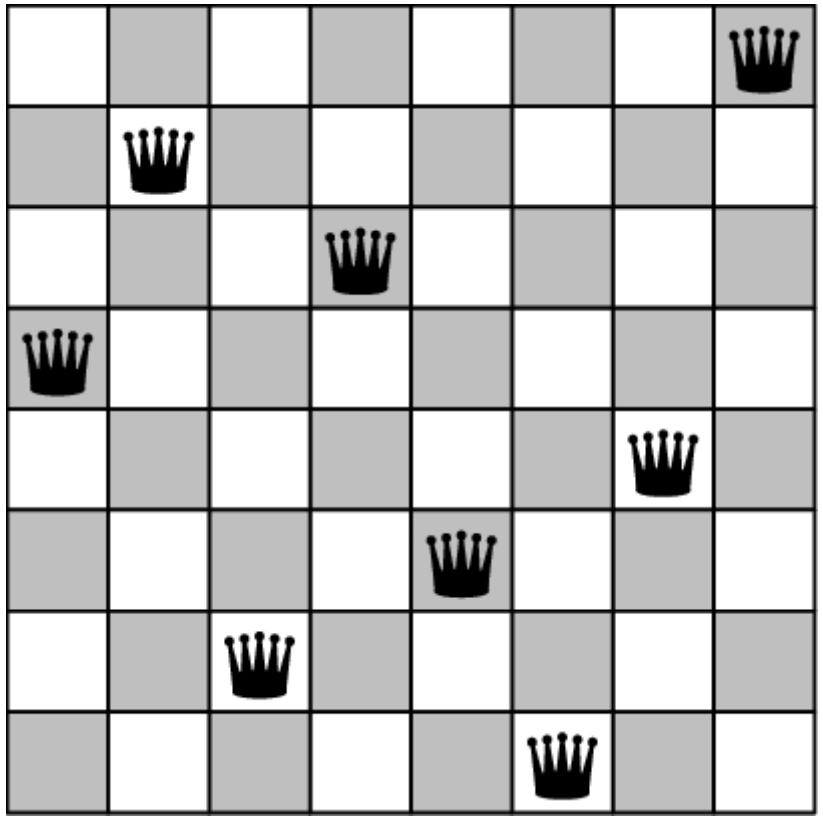

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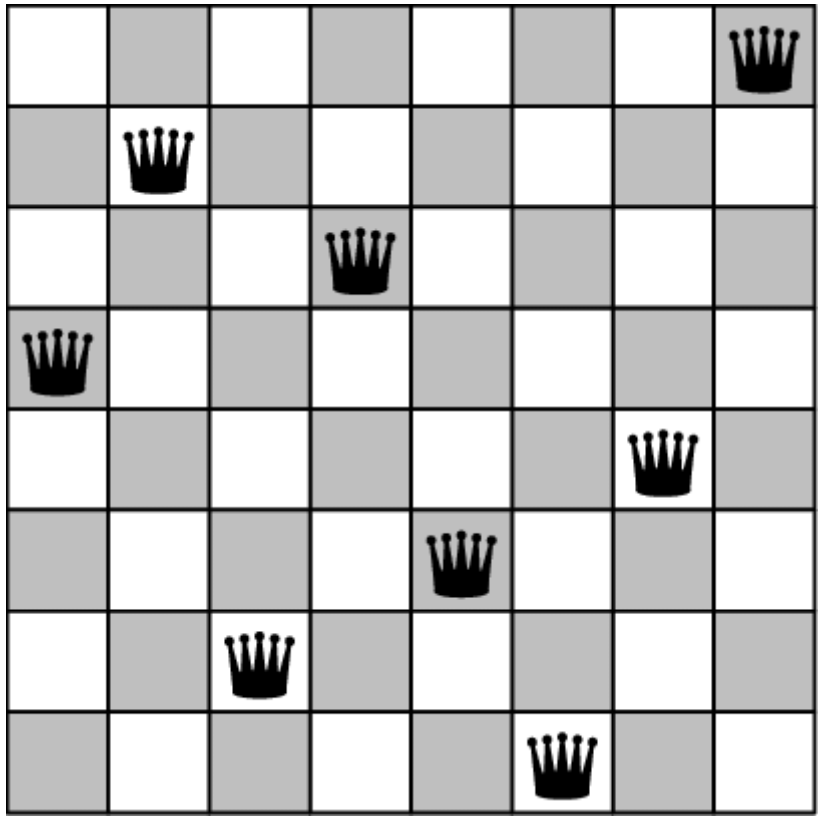

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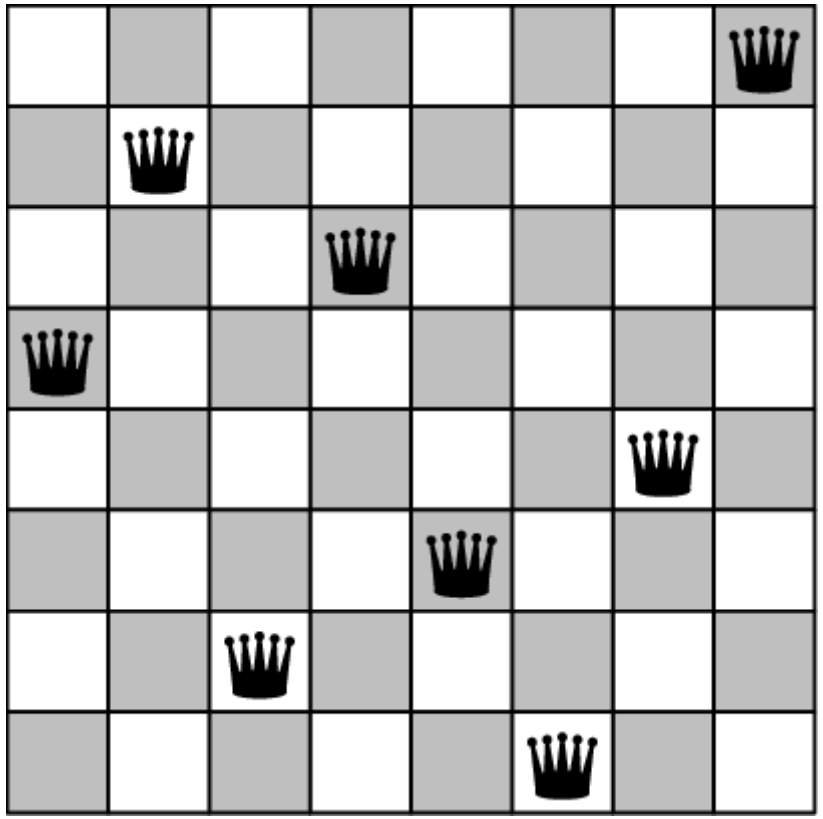

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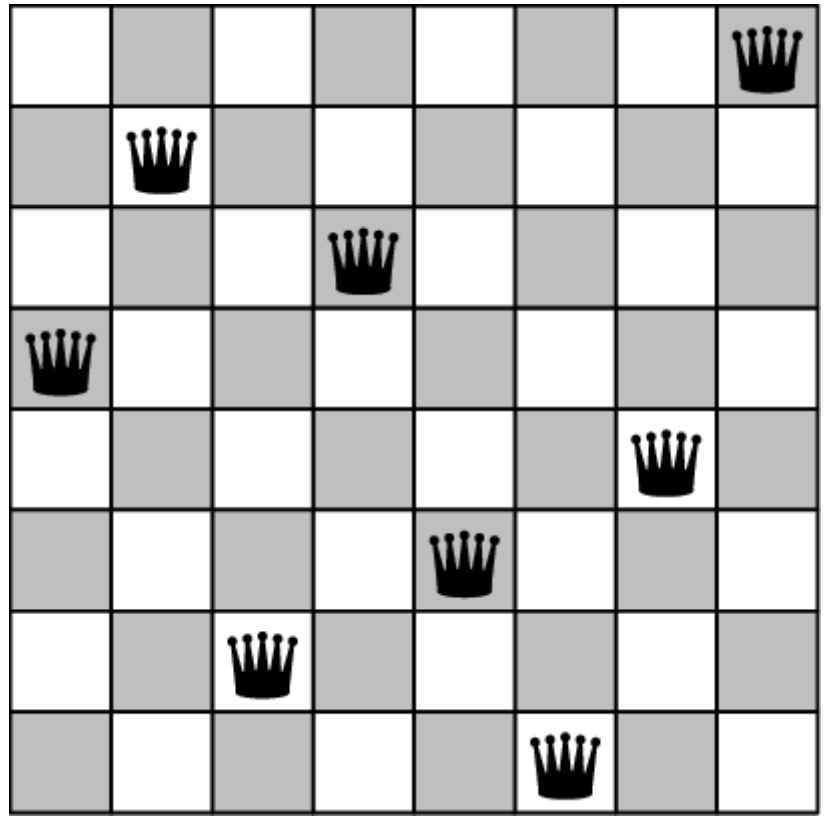

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- With this definition, I can start building the penalty matrix like this

```
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.]
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- 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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 [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. 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.]]
```

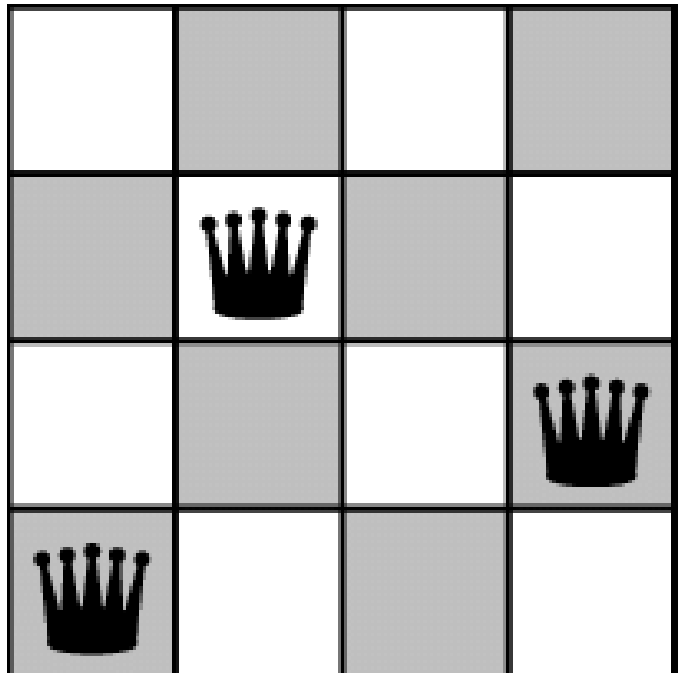
Exercise 3: N-Queens Puzzle

- 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)
```

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

Exercise 3: N-Queens Puzzle

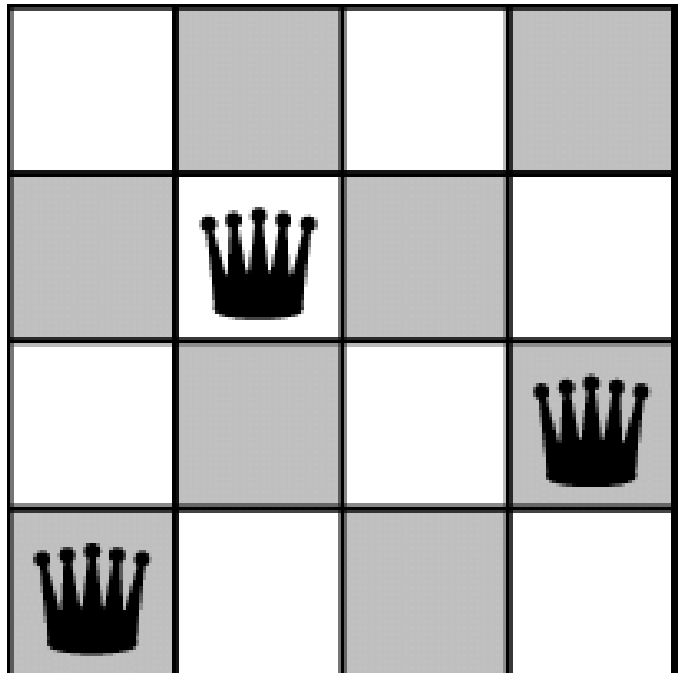
- One way to do this, is to define a function in this way

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

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

```
[[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 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. 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.]]
```

Exercise 3: N-Queens Puzzle

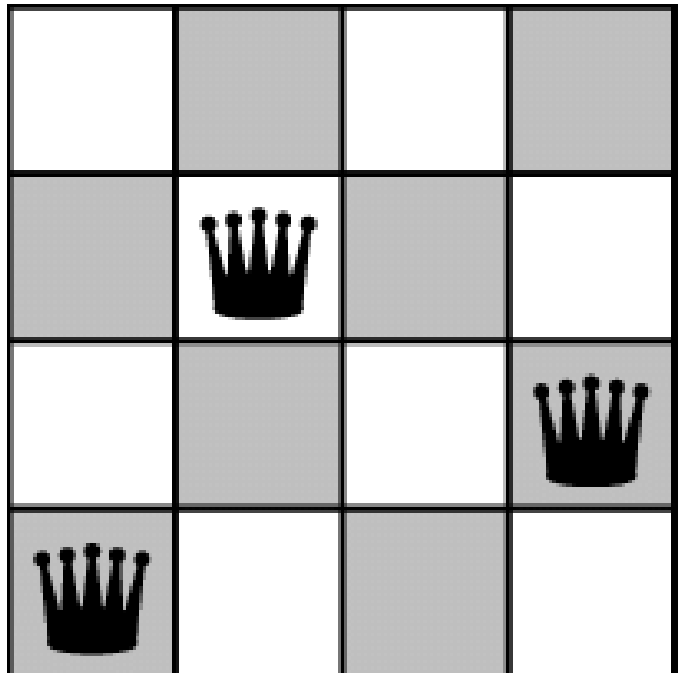
- One way to do this, is to define a function in this way

```
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. 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. 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

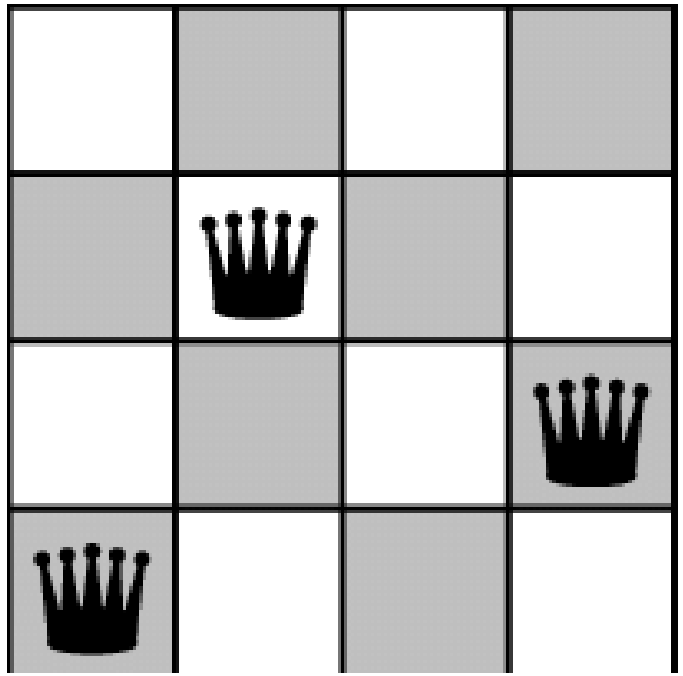
- Same thing for columns

```
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. 1. 0. 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. 1. 1. 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. 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

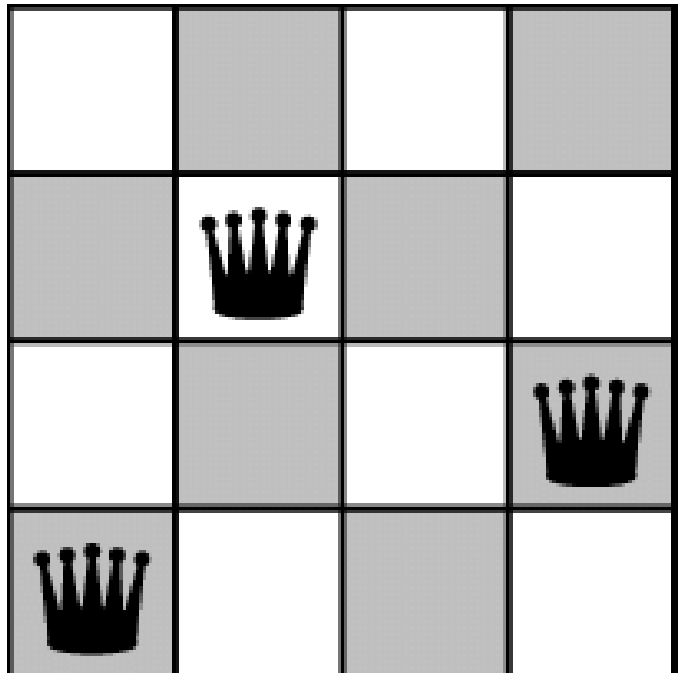
- Same thing for columns

```
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. 1. 0. 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. 1. 1. 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. 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

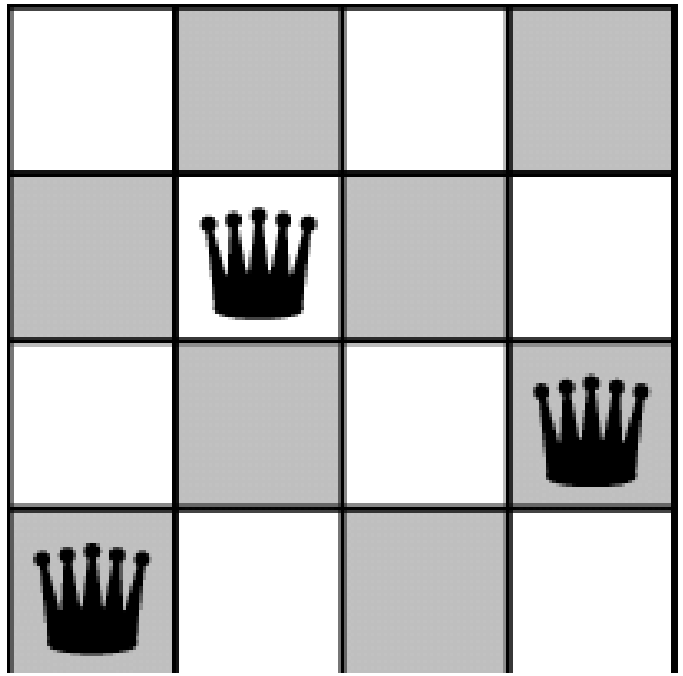
- Same thing for diagonals

```
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. 1. 0. 0. 0. 1. 0. 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

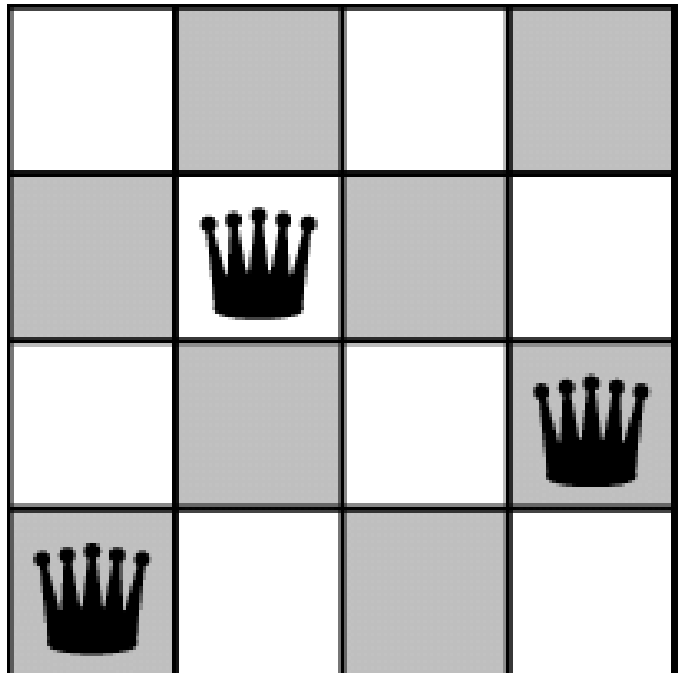
- Same thing for diagonals

```
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 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. 1. 0. 0. 0. 1. 0. 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

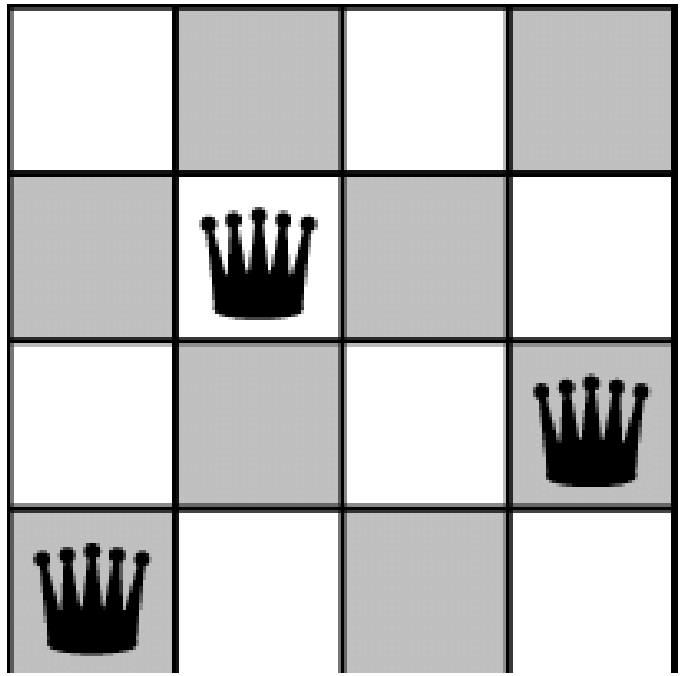
- Same thing for diagonals

```
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. 1. 0. 0. 0. 1. 0. 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. 1. 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

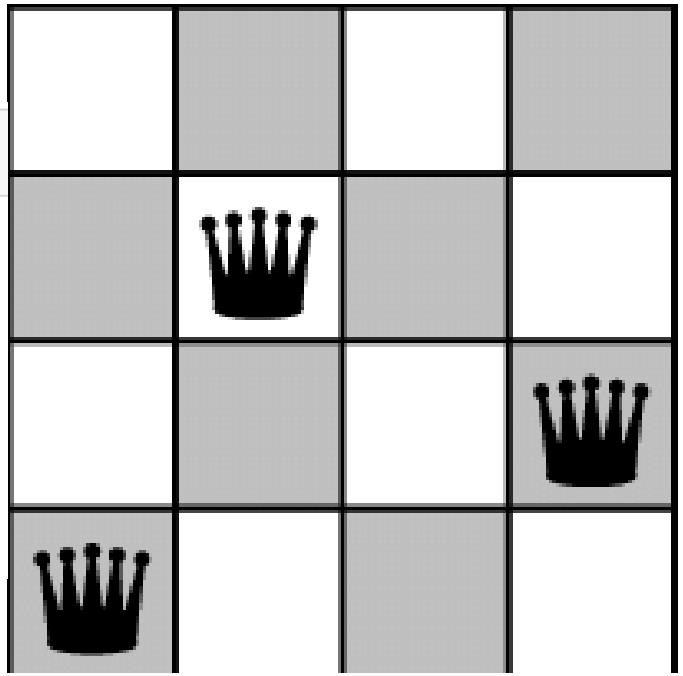
- Same thing for diagonals

```
def 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. 0. 1. 1. 0. 1. 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. 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. 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.]]
```

Calendar Optimization

- The problem is: given a certain number of teams and a certain number of groups, find the best arrangement.
- A travel cost is available for each pair of teams (which includes all the costs that the team has to face in order to go to face the other team)
- The best arrangement will be the one that minimizes travel costs for all groups
- **How can we implement such a problem into the D-Wave Quantum Annealer?**
- **First of all, we have to find a suitable QUBO form**

- Idea: for each team, we allocate (#number_of_groups) qubits with the constraint ”only one can be 1, the others have to be 0”
- **In this way we can imagine the qubits as “group indicators”**
- **We will need N_teams * N_groups Qubits**

	AlbinoLeffe	Alessandria	Arezzo	...
G1	0	1	0	...
G2	1	0	0	...
G3	0	0	1	...

The Problem

- B: matrix of travel costs. Problem: minimize the total cost --> **Example with 3 groups**

$$\min\left(\sum_{i<j} B_{ij}q_iq_j + \sum_{i<j} B_{ij}q_iq_j + \sum_{i<j} B_{ij}q_iq_j\right)$$

- Or

$$\min\left(\sum_{i<j} \mathbf{B}_{ij}q_iq_j\right) \qquad \mathbf{B} = \begin{pmatrix} B & 0 & 0 \\ 0 & B & 0 \\ 0 & 0 & B \end{pmatrix}$$

The Problem

- To solve the problem realistically we need to insert the constraints as boundary conditions of the problem. Without them, in fact, the solution would be trivial: all the values of the qubits would be 0.
- Sum of the teams belonging to a single group equal to (#number_of_teams_per_group → P

$$N_{groups} = 3; \qquad P = \frac{N_{teams}}{N_{groups}}$$

$$\sum_k \left(\sum_i C_i^k q_i - P \right)^2$$

$$C^0 = [\overbrace{1,1,\ldots,1}^{N_{teams}}, \underbrace{0,0,\ldots,0}_{N_{teams}}, \overbrace{0,0,\ldots,0}^{N_{teams}}]$$

$$C^1 = [\overbrace{0,0,\ldots,0}^{N_{teams}}, \underbrace{1,1,\ldots,1}_{N_{teams}}, \overbrace{0,0,\ldots,0}^{N_{teams}}]$$

$$C^2 = [\overbrace{0,0,\ldots,0}^{N_{teams}}, \underbrace{0,0,\ldots,0}_{N_{teams}}, \overbrace{1,1,\ldots,1}^{N_{teams}}]$$

The Problem

- To solve the problem realistically we need to insert the constraints as boundary conditions of the problem. Without them, in fact, the solution would be trivial: all the values of the qubits would be 0.
- Sum of the teams belonging to a single group equal to (#number_of_teams_per_group → P)

$$\sum_k \left(\sum_i C_i^k q_i - P \right)^2$$

$$\sum_i (1 - 2P)\, q_i + \sum_{i<j} 2 C_{ij} q_i q_j$$

$$C_{ij} = \sum_k C_i^k C_j^k$$

The Problem

- To solve the problem realistically we need to insert the constraints as boundary conditions of the problem. Without them, in fact, the solution would be trivial: all the values of the qubits would be 0.
- Sum of the teams belonging to a single group equal to (#number_of_teams_per_group).
- Sum of the qubits representing a single team equal to 1

$$-\sum_i q_i + 2\sum_{i<j} V_{ij} q_i q_j$$

$$V_{ij} = \sum_s V_i^s V_j^s$$

$$V^0 = \left[\overbrace{1,0,0,\ldots,0,0}^{N_{teams}}, \underbrace{1,0,0,\ldots,0,0}_{N_{teams}}, \overbrace{1,0,0,\ldots,0,0}^{N_{teams}}\right]$$

$$V^1 = \left[\overbrace{0,1,0,\ldots,0,0}^{N_{teams}}, \underbrace{0,1,0,\ldots,0,0}_{N_{teams}}, \overbrace{0,1,0,\ldots,0,0}^{N_{teams}}\right]$$

$$\ldots$$

$$V^{N_{teams}-1} = \left[\overbrace{0,0,0,\ldots,1,0}^{N_{teams}}, \underbrace{0,0,0,\ldots,1,0}_{N_{teams}}, \overbrace{0,0,0,\ldots,1,0}^{N_{teams}}\right]$$

$$V^{N_{teams}} = \left[\overbrace{0,0,0,\ldots,0,1}^{N_{teams}}, \underbrace{0,0,0,\ldots,0,1}_{N_{teams}}, \overbrace{0,0,0,\ldots,0,1}^{N_{teams}}\right]$$

The Problem

- To solve the problem realistically we need to insert the constraints as boundary conditions of the problem. Without them, in fact, the solution would be trivial: all the values of the qubits would be 0.
- Sum of the teams belonging to a single group equal to (#number_of_teams_per_group).
- Sum of the qubits representing a single team equal to 1
- Fixed teams (array L used to “block” the selected teams into a group)

$$-\sum_i L_i q_i$$

The Problem

- To solve the problem realistically we need to insert the constraints as boundary conditions of the problem. Without them, in fact, the solution would be trivial: all the values of the qubits would be 0.
- Sum of the teams belonging to a single group equal to (#number_of_teams_per_group).
- Sum of the qubits representing a single team equal to 1
- Fixed teams (array L used to “block” the selected teams into a group)

$$\min \left(\sum_i \left(\alpha(1-2P) - \beta - \gamma L_i \right) q_i + \sum_{i<j} \left(\mathbf{B}_{ij} + 2\alpha C_{ij} + 2\beta V_{ij} \right) q_{ij} \right)$$

Quantum Annealing with continuous variables: Low-Rank Matrix Factorization

Daniele Ottaviani
CINECA

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

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:

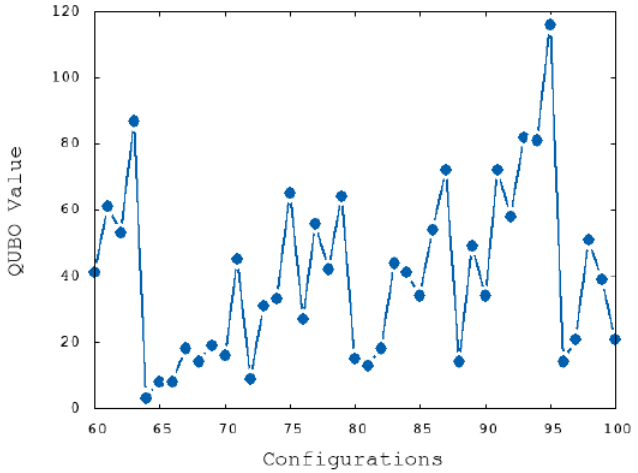
$$\min_{\mathbf{q}=(q_0,\ \ldots,\ q_{N-1})} \left(\sum_{e=0}^{N-1} \left(c^2 2^{2e} - bc2^{e+1} \right) q_e + \sum_{e<f} \left(c^2 2^{e+f+1} \right) q_e q_f \right)$$

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

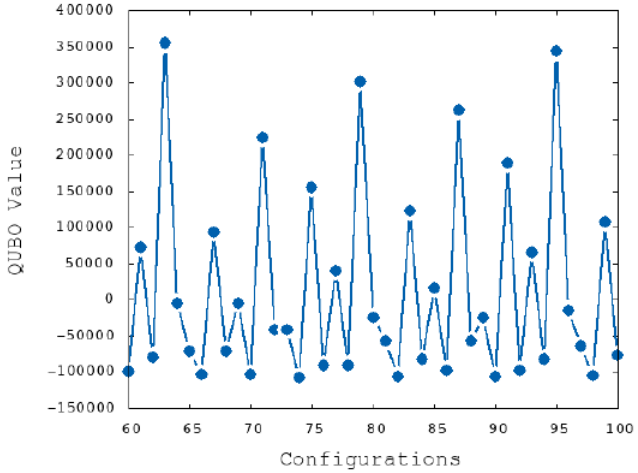
Graphical representation

**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

Solving a linear system

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

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

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

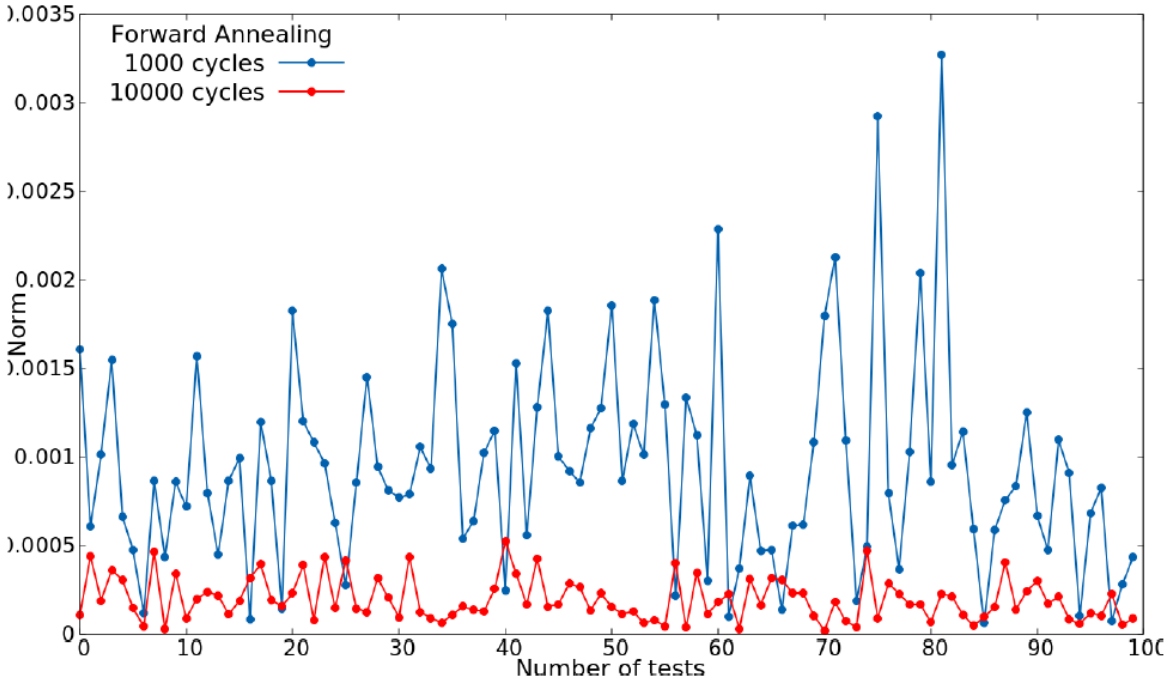
We will find $\mathbf{x}$ solving $\min_{\mathbf{x}\in[0,1]^3} ||A\mathbf{x} - b||_2^2$

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

Advanced Annealing Techiques

Attempt number 1: Forward Annealing

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



$$\begin{bmatrix} 0.179 \\ 0.338 \\ 0.483 \end{bmatrix}$$

$$\left(\begin{bmatrix} 0.178 \\ 0.333 \\ 0.489 \end{bmatrix} \right)$$

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

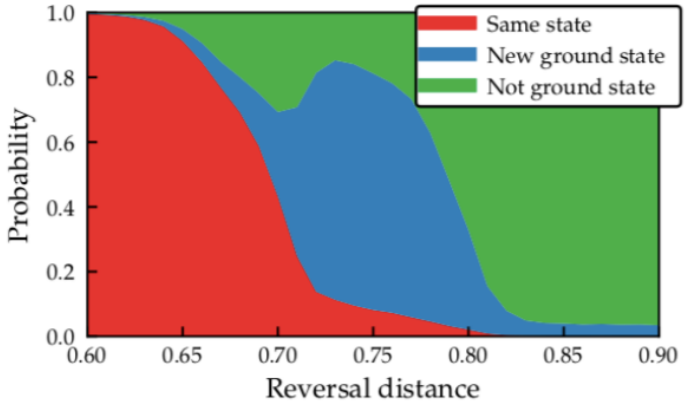
Advanced Annealing Techiques

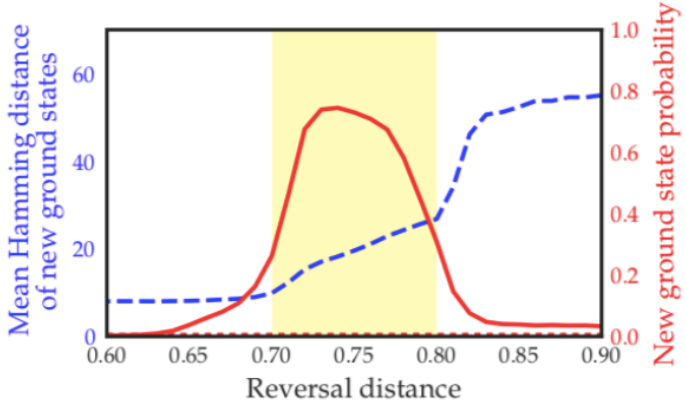
Tuning the reversal distance

D-Wave
The Quantum Computing Company™

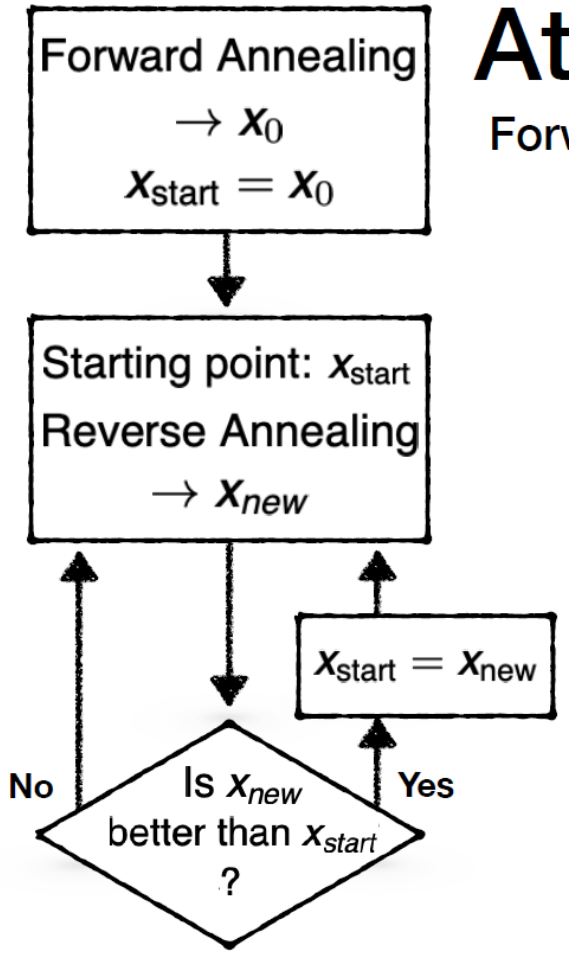
Reverse Quantum Annealing for Local Refinement of Solutions

WHITEPAPER





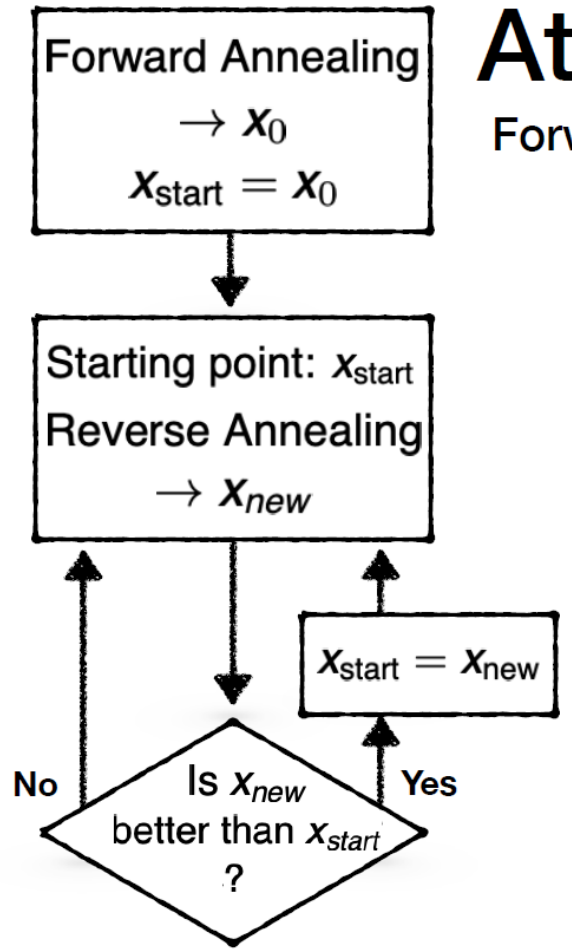
Advanced Annealing Techiques



Attempt number 2:

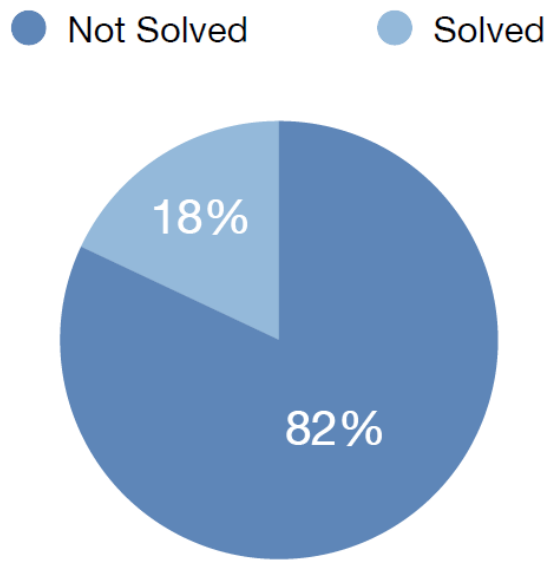
Forward Annealing + Reverse Annealing

Advanced Annealing Techiques



Attempt number 2:

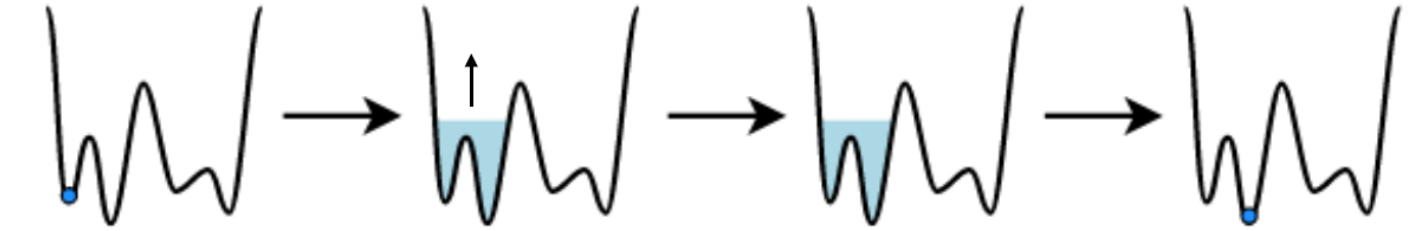
Forward Annealing + Reverse Annealing



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:



Starting point chosen by the user | Backward Annealing | Pause | Forward Annealing

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.

Correlation between pause and search radius

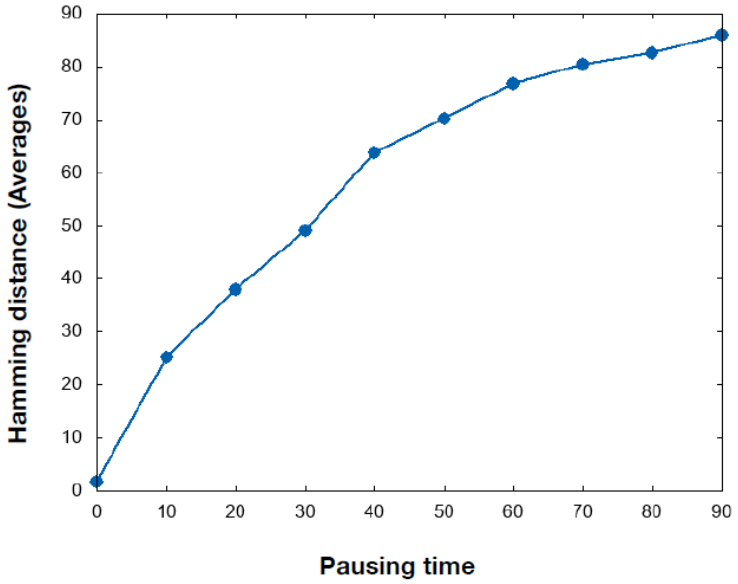
We can realize a posteriori the search radius of a reverse annealing search by analyzing the average distance between the solutions found by each cycle.

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:

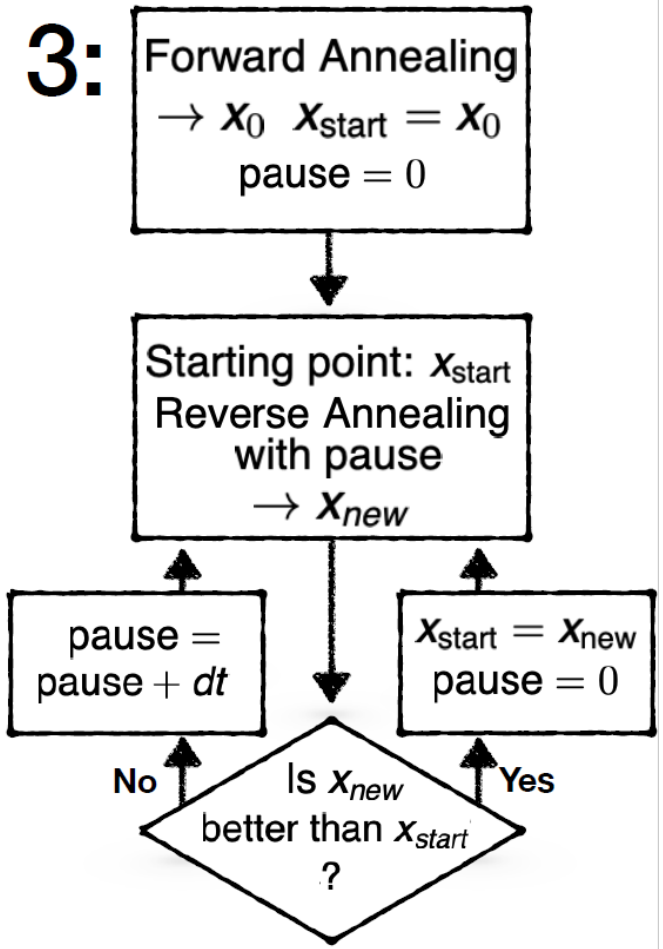
too little is not enough,
too much can lead to wrong results



Advanced Annealing Techiques

Attempt number 3:

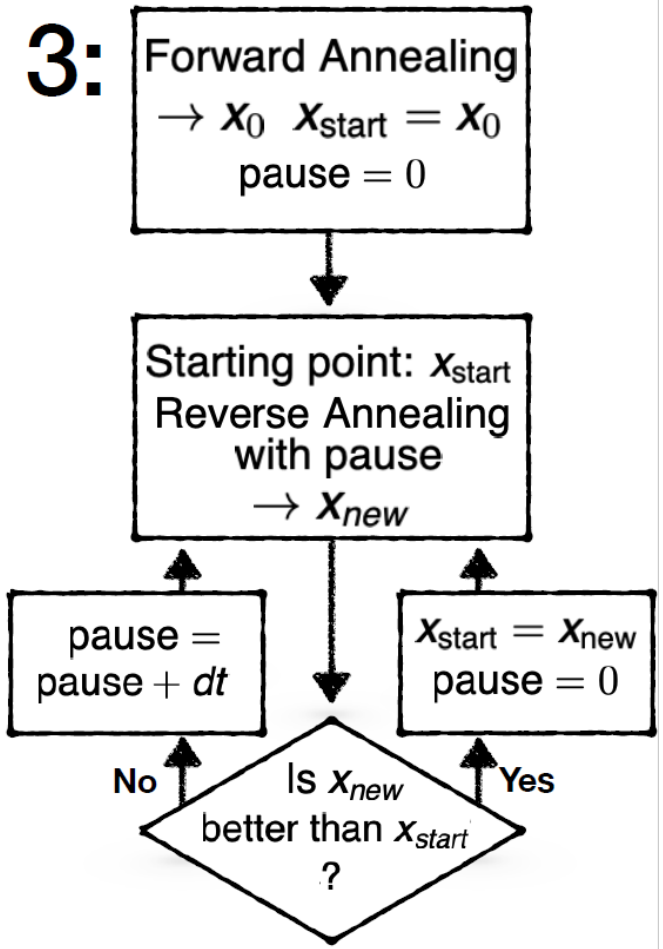
Forward Annealing +
Reverse Annealing with pause



Advanced Annealing Techiques

Attempt number 3:

Forward Annealing +
Reverse Annealing with pause



Advanced Annealing Techiques

Attempt number 3:

Forward Annealing +
Reverse Annealing with pause