INTRODUCTION TO QUANTUM ANNEALING

Formulating and solve QUBO Problems

Daniele Ottaviani
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The Quantum Annealing Algorithm

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Quantum Annealing is a quantum algorithm capable of solving optimization problems.
The quantum annealing algorithm was proposed for the first time in 1998 with the paper you see in the figure.

1. 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. Guan and Geen 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 combinatorial optimization, rather than to develop a general algorithm, 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 [3]. 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 [4]. 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 Carlo calculations for the transverse Ising model. It is of interest to study the effects of quantum fluctuations on the spin dynamics of the transverse Ising model.
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In 2018 I had a beer with him!
Annealing Algorithms

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

![Graph of an objective function](image-url)
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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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\text{Initial Hamiltonian} & \quad - \frac{A(s)}{2} \left( \sum_i \hat{\sigma}_x^{(i)} \right) + \frac{B(s)}{2} \left( \sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \right) \\
\text{Final Hamiltonian} & \quad 0
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  - Quadratic Unconstrained Binary Optimization problems (QUBO problems)
  - Graphs and embedding
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When the solver is a QPU, energy is a function of the binary variables that represent its qubits; for classical quantum hybrid solvers, energy might be a more abstract function.
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- When the solver is a QPU, energy is a function of the binary variables that represent its qubits; for classical quantum hybrid solvers, energy might be a more abstract function.
- For most problems, the lower the energy of the objective function, the better the solution. Sometimes any state of local minimum for energy is an acceptable solution to the original problem; for other problems only optimal solutions are acceptable.
Objective Function

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

\[
\begin{align*}
    x + 1 &= 2 \\
    \min_x [2 - (x + 1)]^2
\end{align*}
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\text{Global Minimum} \\
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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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- Mathematically, it is expressed in this form

\[ E_{\text{Ising}}(s) = \sum_{i=1}^{N} h_i s_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} J_{i,j} s_i s_j \]
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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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Game of Switches

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• Suppose we have a certain number of switches, each settable on two possible states represented by the values 1 and -1.

• Furthermore, each switch has a univocally associated weight.
Game of Switches

h = ‘bias’ value associated with each switch
s = the ON/OFF setting of each switch, +1 or -1
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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

$$E(s) = \sum_i h_i s_i$$

- $h = \text{‘bias’ value associated with each switch}$
- $s = \text{the ON/OFF setting of each switch, +1 or -1}$
Game of Switches

\[
\begin{align*}
+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{align*}
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Total: -3.6
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We therefore add to the quantity to be minimized the contribution introduced by the couplers.
Game of Switches

\[ E(s) = \sum_i h_is_i + \sum_{i,j} J_{i,j}s_is_j \]

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

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Game of Switches

\[ s_1 + 0.2s_2 - 0.7s_3^+ \]
\[ 0.4s_4 - 0.8s_5 + 0.5s_6^+ \]
\[ 0.2s_1s_2 - 0.7s_2s_3^+ \]
\[ 0.3s_3s_6 - 0.7s_2s_6^+ \]
\[ - 0.3s_1s_6 - s_1s_5^+ \]
\[ 0.1s_5s_4 + s_6s_4 \]
Game of Switches

2 switches $= 2^2 = 4$ possible answers
Game of Switches

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

10 switches $= 2^{10} = 1024$ possible answers
Game of Switches

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

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

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

- QUBO (Quadratic Unconstrained Binary Optimization) problems are well known problems in the field of combinatorial optimization.
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$$f(x) = \sum_i Q_{i,i} x_i + \sum_{i<j} Q_{i,j} x_i x_j$$
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• Where the diagonal terms of the matrix $Q$ play the role of linear coefficients while the other non-zero elements are the quadratic coefficients.
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- Where the diagonal terms of the matrix $Q$ play the role of linear coefficients while the other non-zero elements are the quadratic coefficients. In matrix form

$$\min_{x \in \{0,1\}^n} x^T Q x.$$
To familiarize yourself with the QUBO formulation, let’s make an example of a realistic problem whose structure can be mapped in this form.
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Suppose we have a certain number of antennas and a certain number of possible sites to place these antennas.
QUBO Problems

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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.
QUBO Problems

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

We define:

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

\[ A_i = r_i^2 \cdot \pi \]
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\[ \rho_{ij} = \max\left\{ 0, r_i + r_j - \text{dist}\left( c_i, c_j \right) \right\} \]
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\[ \rho_{ij} = \max \left\{ 0, r_i + r_j - \text{dist} \left( c_i, c_j \right) \right\} \]

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

\[ \rho_{ij} = \max \left\{ 0, r_i + r_j - \text{dist} \left( c_i, c_j \right) \right\} \]
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- With the definition of the rho radius, we can define the interference area between the overlap of two antennas $i$ and $j$ as

$$B_{ij} = \rho_{ij}^2 \cdot \pi$$
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$$[q_0, \ldots, q_{19}]$$
QUBO Problems

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

\[ A_i = r_i^2 \cdot \pi \]
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- Minimize interference

\[ \text{QUBO} = \sum_{i < j} B_{ij} q_i q_j \]
Let's formulate our problem. At this stage, we must always think about a minimization problem. To maximize, simply reverse the sign. Keeping in mind that

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

Maximize covering area

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

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

\[ A_i = r_i^2 \cdot \pi \quad B_{ij} = \rho_{ij}^2 \cdot \pi \]

- Maximize covering area

\[ \text{QUBO} = - \sum_{i=0}^{N} A_i q_i + \sum_{i<j} B_{ij} q_i q_j \]
Let’s formulate our problem. At this stage, we must always think about a minimization problem. To maximize, simply reverse the sign. Keeping in mind that

\[ A_i = r_i^2 \cdot \pi \quad B_{i,j} = \rho_{i,j}^2 \cdot \pi \]

- Maximize covering area

\[
\text{QUBO} = -\sum_{i=0}^{N} A_i q_i + \alpha \sum_{i<j} B_{i,j} q_i q_j
\]
QUBO/ISING Equivalency

- Any QUBO problem can be easily mapped into an ISING problem through simple equivalence
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- Any QUBO problem can be easily mapped into an ISING problem through simple equivalence

\[ s_i \mapsto 2x_i - 1 \]
\[ s_i + 1 \]
\[ x_i \mapsto \frac{s_i}{2} \]

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

\[ E_{\text{QUBO}}(x) = \sum_{i} Q_{i,i} x_i + \sum_{i<j} Q_{i,j} x_i x_j \]
QUBO/ISING Equivalency

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- More generally, any mathematical problem can be mapped into a QUBO problem
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\[ E_{\text{ising}}(s) = \sum_{i=1}^{N} h_i s_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} J_{i,j} s_i s_j \]

\[ E_{\text{QUBO}}(x) = \sum_{i=1}^{N} Q_{i,i} x_i + \sum_{i<j} Q_{i,j} x_i x_j \]

- 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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PyQUBO is a Python library, with a C++ backend, written by D-Wave to use its quantum annealer.
Programming a Quantum Annealer

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

- Installation:

  ```
  pip install pyqubo
  ```
Programming a Quantum Annealer

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

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• PyQUBO is a very handy utility for writing problems in QUBO or ISING form. Let's see how to use it.
Programming a Quantum Annealer

• PyQUBO is a python library, with a C ++ backend, written by DWA V E to use its quantum annealer.

• Installation:

```python
pip install pyqubo
```

• PyQUBO is a very handy utility for writing problems in QUBO or ISING form. Let's see how to use it

• Variables: Type Binary (0/1)

```python
>>> 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)
```
Programming a Quantum Annealer

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

- Installation:
  ```
  pip install pyqubo
  ```

- PyQUBO is a very handy utility for writing problems in QUBO or ISING form. Let's see how to use it.

- Variables: Type Spin (+1/-1)

  ```
  >>> from pyqubo import Spin
  >>> s1, s2 = Spin('s1'), Spin('s2')
  >>> H = 2*s1*s2 + 3*s1
  >>> 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)

```python
from pyqubo import Array
x = Array.create('x', shape=(2, 3), var_type='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)

```python
>>> 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

```python
>>> 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)

```python
>>> 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

```python
>>> from pyqubo import Binary
>>> x1, x2 = Binary('x1'), Binary('x2')
>>> H = (x1 + x2 - 1)**2
>>> model = H.compile()
>>> bqm = model.to_bqm()
```
- Solve a problem set via pyQUBO
- After setting the Hamiltonian of the problem, it must be compiled and transformed into a `bqm` object

```python
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(pprint(best_sample.sample))
{'x1': 0, 'x2': 1}
```
Exercise 1: Game of Switches

- Try to implement the Game of Switches

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

Adding another weight, J, which multiplies the product of the two switch settings.
Exercise 2: Antenna Placement

- Try to implement the Antenna Placement Problem

\[ A_i = r_i^2 \cdot \pi \quad B_{ij} = \rho_{ij}^2 \cdot \pi \]

\[ QUBO = -\sum_{i=0}^{N} A_i q_i + \alpha \sum_{i<j} B_{ij} q_i q_j \]
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.
Add a Constraint to a QUBO Problem

- Let’s see how to implement a linear constraint in a QUBO problem.
- Everything relies around the concept of *penalty function*
Add a Constraint to a QUBO Problem

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• A penalty function is in fact an **additional quantity** to the original minimization problem, **which must be optimized** in order for the entire problem to be optimized
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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*
Add a Constraint to a QUBO Problem

• Let’s see how to implement a linear constraint in a QUBO problem.
• Everything relies around the concept of penalty function
• A penalty function is in fact an additional quantity to the original minimization problem, which must be optimized in order for the entire problem to be optimized
• Suppose we want to add the following constraint to our antenna optimization problem

• Let $F$ be the exact number of antennas to be placed

• Remembering the mathematical formulation of our problem, requested constraint can be seen as

$$\sum_{i=0}^{N} q_i = F$$
Add a Constraint to a QUBO Problem

- Let’s do some math

\[ \sum_{q_i}^{N} = F \]

\[ i=0 \]
Add a Constraint to a QUBO Problem

- Let's do some math

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

- Let’s do some math

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

- Let’s do some math

\[
\sum_{i=0}^{N} q_i = F \implies \min \left( \sum_{i=0}^{N} q_i - F \right)^2
\]

\[
\left( \sum_{i=0}^{N} q_i - F \right)^2 = \left( \sum_{i=0}^{N} q_i \right)^2 + F^2 - 2F \sum_{i=0}^{N} q_i
\]
Add a Constraint to a QUBO Problem

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\]

\[
= \sum_{i=0}^{N} q_i^2 + 2 \sum_{i<j} q_i q_j - 2F \sum_{i=0}^{N} q_i
\]
Add a Constraint to a QUBO Problem

- Let’s do some math

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

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

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\[ = \sum_{i=0}^{N} (1 - 2F) q_i + \sum_{i<j} q_i q_j \]
Add a Constraint to a QUBO Problem

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

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

\[
\min \left( \beta \cdot \left( \sum_{i=0}^{N} (1 - 2F) q_i + \sum_{i<j} 2q_i q_j \right) \right)
\]
Add a Constraint to a QUBO Problem

\[
\sum_{i=0}^{N} q_i = F \implies \min \left( \sum_{i=0}^{N} q_i - F \right)^2
\]

\[
\min \left( \sum_{i=0}^{N} B (1 - 2F) q_i + \sum_{i<j} 2B q_i q_j \right)
\]
Exercise 2: Antenna Placement

• Implement constraint into the Antenna Placement Problem

\[ A_i = r_i^2 \cdot \pi \]
\[ B_{ij} = \rho_{ij}^2 \cdot \pi \]

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

\[
\min \left( \sum_{i=0}^{N} B (1 - 2F) q_i + \sum_{i<j} 2B q_i q_j \right)
\]
Add a Constraint to a QUBO Problem

- Now suppose we want to add another constraint.
Add a Constraint to a QUBO Problem

- Now suppose we want to add another constraint.
- For some reason, we have received orders from above telling us that certain antennas must be placed, regardless of any other conditions.
Add a Constraint to a QUBO Problem

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- How can we implement this type of request?
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• For some reason, we have received orders from above telling us that certain antennas must be placed, regardless of any other conditions.
• How can we implement this type of request?

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

• Now suppose we want to add another constraint.
• For some reason, we have received orders from above telling us that certain antennas must be placed, regardless of any other conditions.
• How can we implement this type of request?

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

• Consequently, penalty function can be seen as

$$\sum_{i=1}^{N} L_i (q_i - 1)^2$$
Add a Constraint to a QUBO Problem

$$\sum_{i=1}^{N} \lambda_i \left( q_i - 1 \right)^2$$
Add a Constraint to a QUBO Problem

\[ \sum_{i=1}^{N} L_i (q_i - 1)^2 = \sum_{i=1}^{N} L_i q_i + \sum_{i=1}^{N} L_i - \sum_{i=1}^{N} 2L_i q_i = \]
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\[ \sum_{i=1}^{N} L_i (q_i - 1)^2 = \sum_{i=1}^{N} L_i q_i + \sum_{i=1}^{N} L_i - \sum_{i=1}^{N} 2L_i q_i = \]
Add a Constraint to a QUBO Problem

\[
\sum_{i=1}^{N} L_i \left(q_i - 1\right)^2 = \sum_{i=1}^{N} L_i q_i + \sum_{i=1}^{N} L_i - \sum_{i=1}^{N} 2L_i q_i = \\
- \sum_{i=1}^{N} L_i q_i
\]
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
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\[
QUBO = -\sum_{i=0}^{N} A_i q_i + \alpha \sum_{i < j} B_{ij} q_i q_j
\]

\[
\min \left( \sum_{i=0}^{N} B_{ij} (1 - 2q_i) + \sum_{i < j} 2B_{ij} q_i q_j \right)
\]

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

• Now suppose we want to add an inequality constraint to our problem.
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Add a Constraint to a QUBO 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

\[
\sum_{i=0}^{N} q_i \leq F
\]
Add a Constraint to a QUBO Problem

- So far we have seen how to transform constraints involving equalities into penalty functions.
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\[
\begin{align*}
\sum_{i=1}^{N} q_i & \leq F \quad \Rightarrow \quad \sum_{i=1}^{N} q_i = F - \sum_{k=1}^{F} q_k \\
\sum_{i=1}^{N} q_i + \sum_{k=1}^{F} q_i & = F \quad \Rightarrow \quad \sum_{i=1}^{N+F} q_i = F
\end{align*}
\]
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\[ \text{QUBO} = -\sum_{i=0}^{N} A_i q_i + \alpha \sum_{i<j} B_{ij} q_i q_j \]

\[ \min \left( \sum_{i=0}^{N} \left[ (i-j) + \sum_{k=1}^{l} \right] + \sum_{k=1}^{l} q_k \right) - \sum_{i=1}^{N+F} q_i \]

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

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  Let $A_m$ be a measure of area. Turn on the antennas so that the minimum covered area is greater than or equal to $A_m$
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\[
\sum_{i=1}^{N} A_i q_i - \sum_{k=1}^{N} q_k = A_m \quad \Rightarrow \quad \sum_{i=1}^{2N} C_i A_i q_i = A_m
\]
Add a Constraint to a QUBO Problem

\[ \sum_{i=1}^{2N} \zeta_i A_i q_i = A_m \]
Add a Constraint to a QUBO Problem

\[ \sum_{i=1}^{2N} C_i A_i q_i = A_m \Rightarrow \left( \sum_{i=1}^{2N} C_i A_i q_i - A_m \right)^2 \]
Add a Constraint to a QUBO Problem

\[
2N \sum_{i=1}^{2N} c_i A_i q_i = A_m \Rightarrow \left( \sum_{i=1}^{2N} c_i A_i q_i - A_m \right)^2 = \left( \sum_{i=1}^{2N} c_i A_i q_i \right)^2 - 2 \sum_{i=1}^{2N} A_m c_i A_i q_i
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\[\begin{align*}
2N & \sum_{i=1}^{2N} C_i A_i q_i = A_m \Rightarrow \left( \sum_{i=1}^{2N} C_i A_i q_i - A_m \right)^2 = \left( \sum_{i=1}^{2N} C_i A_i q_i \right)^2 - 2N \sum_{i=1}^{2N} A_m C_i A_i q_i \\
2N & \sum_{i=1}^{2N} A_i^2 q_i + 2N \sum_{i<j} C_i C_j A_i A_j q_i - 2N \sum_{i=1}^{2N} A_m C_i A_i q_i
\end{align*}\]
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\[ \sum_{i=1}^{2N} C_i A_i q_i = A_m \Rightarrow \left( \sum_{i=1}^{2N} C_i A_i q_i - A_m \right)^2 = \left( \sum_{i=1}^{2N} C_i A_i q_i \right)^2 - 2 \sum_{i=1}^{2N} A_m C_i A_i q_i \]

\[ \sum_{i=1}^{2N} A_i^2 q_i + 2 \sum_{i<j} C_i C_j A_i A_j q_i - 2 \sum_{i=1}^{2N} A_m C_i A_i q_i = \sum_{i=1}^{2N} \left( A_i^2 - 2 A_m C_i A_i \right) q_i + \sum_{i<j} C_i C_j A_i A_j q_i \]
Exercise 2: Antenna Placement

- Implement constraint into the Antenna Placement Problem

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\min \left( \sum_{i=0}^{N} (B_{ij} (i - x_i) + \sum_{i < j} B_{ij} q_i q_j) \right) - \sum_{i=1}^{N} C_i A_i 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!
Add High Order terms to our problem

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

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

<table>
<thead>
<tr>
<th>$x, y, z$</th>
<th>$xyz$</th>
<th>$x + y + z - 2$</th>
<th>$\max_w {w(x + y + z - 2)}$</th>
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<td>-2</td>
<td>$0_{w=0}$</td>
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<td>0</td>
<td>-1</td>
<td>$0_{w=0}$</td>
</tr>
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<td>0, 1, 0</td>
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\[ A_i = r_i^2 \cdot \pi \quad \text{and} \quad B_{ij} = \rho_{ij}^2 \cdot \pi \]

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

\[ \min \left( \sum_{l=0}^{N} \left( \sum_{i=0}^{l} B_{ij} q_i q_j + \sum_{i>j} B_{ij} q_i q_j \right) \right) = \sum_{l=0}^{N} \sum_{i=0}^{l} q_i q_j = F \]

\[ \sum_{l=0}^{N} \sum_{i=0}^{l} C_l A_i q_i = A_m \]

- Add High Order Terms to QUBO problem with pyqubo
Mathematically speaking, an undirected graph is defined as a set of vertices $V = \{v_1, \ldots, v_N\}$.
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$$H(a, b) = 5a + 7ab - 3b$$
Graphs

- Mathematically speaking, an undirected graph is defined as a set of vertices $V = \{v_1, \ldots, v_N\}$
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$$H(a, b) = 5a + 7ab - 3b$$
Embedding a problem on a graph

- But what if the graph with which we want to represent the QUBO function does not have enough vertices or edges to do so?
Embedding a problem on a graph

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• This procedure is called embedding
Embedding a problem on a graph

• Suppose we have a QUBO problem that can be translated with the following graph
Embedding a problem on a graph

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

\[ A_i = r_i^2 \cdot \pi \]

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\[
\text{QUBO} = -\sum_{i=0}^{N} A_i q_i + \alpha \sum_{i<j} B_{ij} q_i q_j \quad \text{min} \left( \left( \sum_{i=0}^{N} B_{ij} (1 - 2q_j) + \sum_{i<j} B_{ij} q_i q_j \right) \right) -\sum_{i=1}^{N} \chi_i q_i - \sum_{i=1}^{N+F} q_i = F
- 2N \sum_{i=1}^{N} C_i A_i q_i = A_m
- \]

- 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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• 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

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Exercise 3: N-Queens Puzzle

- Let's think about how to turn the problem into a QUBO problem.
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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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Exercise 3: N-Queens Puzzle

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= \sum_{i=1}^{N} (1 - 2N) q_i + \sum_{i<j} 2q_i q_j
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• If we go through the previous slides, we can easily realize that every constraint can be implemented with what we already know
• The only problem is the large amount of math!
Exercise 3: N-Queens Puzzle

- Let us then consider the problem from another point of view.
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- 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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- 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.
- This matrix has as elements all the possible pairs of squares on the chessboard (NxNxNxN).
Exercise 3: N-Queens Puzzle

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- 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.
- This matrix has as elements all the possible pairs of squares on the chessboard (NxNxNxN).
- 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.
Exercise 3: N-Queens Puzzle

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

```python
def ROW(row, dim):
    C = np.zeros((dim, dim), dtype=int)
    C[row, :] = 1
    return C.flatten()
```
Exercise 3: N-Queens Puzzle

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

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

- This function calculates a linearized vector containing all the possible pairs of squares on the board.
Exercise 3: N-Queens Puzzle

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

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

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

• 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
Exercise 3: N-Queens Puzzle

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

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

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

- 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. 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. 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. 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. 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. 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. 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. 1. 1. 1. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 0.1]]
```
Exercise 3: N-Queens Puzzle

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

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

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

- 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.

- Basically I’m saying: if two squares are part of the same row, it increases their weight by a factor $w$
Exercise 3: N-Queens Puzzle

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

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

```python
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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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. 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:

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

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

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

```python
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)
```

```
R = ROW(1, 4)

[[0 0 0 0]
 [1 1 1 1]
 [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 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 0 0 0 0 0 0 0 0]]
```
Exercise 3: N-Queens Puzzle

- Same thing for columns

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

```python
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
```

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]
```

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

CINECA Quantum Computing Lab
Exercise 3: N-Queens Puzzle

- Same thing for columns

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

```python
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
```

```python
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]
```

```python
[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. 0. 1. 1. 1. 1. 0. 0. 0. 1. 0. 0. 1. 0.
[0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 0. 1. 0. 0. 1. 0.
[0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1. 0.
[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. 0. 0. 0. 1. 1. 1. 1. 0.
[0. 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. 0. 0. 0. 1.
[0. 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. 0. 0. 1. 0.
```
Exercise 3: N-Queens Puzzle

- Same thing for diagonals

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

[0 1 0 0 0 1 0 0 0 1 0 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. 0. 0. 1. 0. 1. 0. 0. 0. 0. 1.]
 [0. 0. 1. 0. 1. 0. 1. 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. 1. 0. 0. 0. 1. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 0. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 0. 0. 1. 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. 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. 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. 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. 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.]]
```
Exercise 3: N-Queens Puzzle

- Same thing for diagonals

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

```python
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]
```
Exercise 3: N-Queens Puzzle

- Same thing for diagonals

```python
def DIAG2(k, dim):
    d = np.ones(dim-abs(k), dtype=int)
    C = np.flipud(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]]
```

```
for k in range(-N,N):
    B[] = B[] + D[k]
```

```
[[0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1.]
 [0. 0. 1. 1. 1. 1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1.]
 [0. 0. 1. 1. 0. 1. 1. 1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 1. 1. 1. 1. 0. 0. 1. 0. 1. 0. 1. 0. 1. 0.]]
```
Quantum Annealing with continuous variables:
Low-Rank Matrix Factorization

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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:

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

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 $Ax = b$, where

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

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

We will find $x$ solving

$$\min_{x \in [0,1]^3} ||Ax - b||_2^2$$

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

Attempt number 1: Forward Annealing

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

\[
\begin{bmatrix}
0.179 \\
0.338 \\
0.483 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
0.178 \\
0.333 \\
0.489 \\
\end{bmatrix}
\]
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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

Reverse Quantum Annealing for Local Refinement of Solutions

WHITEPAPER

![Graphs showing probability and mean Hamming distance against reversal distance.](image-url)
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**Attempt number 2:**
Forward Annealing + Reverse Annealing

- **Forward Annealing**
  - $x_0$
  - $x_{\text{start}} = x_0$

- **Starting point:** $x_{\text{start}}$

- **Reverse Annealing**
  - $x_{\text{new}}$

- **Is $x_{\text{new}}$ better than $x_{\text{start}}$?**
  - **No**
  - **Yes**

- **$x_{\text{start}} = x_{\text{new}}$**
Advanced Annealing Techniques

Attempt number 2:
Forward Annealing + Reverse Annealing

- Forward Annealing: $x_0$, $x_{\text{start}} = x_0$
- Reverse Annealing: $x_{\text{new}}$

Flowchart:
- $x_{\text{start}} = x_{\text{new}}$
- Is $x_{\text{new}}$ better than $x_{\text{start}}$?
  - No
  - Yes

Pie chart:
- 82% Solved
- 18% Not Solved
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.
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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.
Advanced Annealing Techniques

Attempt number 3:
Forward Annealing + Reverse Annealing with pause

- Forward Annealing
  \[ \rightarrow x_0 \quad x_{\text{start}} = x_0 \]
  \[ \text{pause} = 0 \]

- Starting point: \( x_{\text{start}} \)
  Reverse Annealing with pause
  \[ \rightarrow x_{\text{new}} \]
  \[ \text{pause} = \text{pause} + dt \]

- \( x_{\text{start}} = x_{\text{new}} \)
  \[ \text{pause} = 0 \]

- Is \( x_{\text{new}} \) better than \( x_{\text{start}} \)?
  \[ \text{No} \quad \text{Yes} \]
Attempt number 3: Forward Annealing + Reverse Annealing with pause

Forward Annealing
\[ x_0 \quad x_{\text{start}} = x_0 \quad \text{pause} = 0 \]

Starting point: \( x_{\text{start}} \)
Reverse Annealing with pause
\[ x_{\text{new}} \]

\[ \text{pause} = \text{pause} + dt \]

\[ x_{\text{start}} = x_{\text{new}} \quad \text{pause} = 0 \]

Is \( x_{\text{new}} \) better than \( x_{\text{start}} \)?

No

Yes
Advanced Annealing Techniques

Attempt number 3:
Forward Annealing + Reverse Annealing with pause

- Not Solved
- Solved

24%
76%

Flowchart:

Forward Annealing
\[ x_0 \quad x_{\text{start}} = x_0 \quad \text{pause} = 0 \]

Starting point: \( x_{\text{start}} \)
Reverse Annealing with pause
\[ \rightarrow x_{\text{new}} \]

\[ \text{pause} = \text{pause} + dt \]
\[ x_{\text{start}} = x_{\text{new}} \quad \text{pause} = 0 \]

Is \( x_{\text{new}} \) better than \( x_{\text{start}} \)?

No

Yes