Mathematical formulation

Formulating our optimization problem

Variables:

Nc binaries $x[i]$ where $x[i] = 1$ when we are accelerating at time segment i

Nc binaries $y[i]$ where $y[i] = 1$ when we are braking at time segment i

Nc binaries $z[i]$ used to linearize constraint

Objective function:

We consider that the energy cost from accelerating is worth $(\Delta v)^2$ where Δv is our train's acceleration during a time segment

We consider that the energy we get back from regenerative braking is worth: $\alpha(\Delta v)^2$ where α is the efficiency.

Therefore, our objective function is:

$$Objective(N_c) = \sum_{i \in [0, N_c]} (x[i] - y[i]\alpha)(\Delta v)^2$$

Constraints:

Constraint 1: Simultaneous braking/acceleration

We want to force our train to be either accelerating or braking, to do this we want to impose the constraint:

$$\forall i \in [0, N_c]\ ,\ x[i] \times y[i] = 0$$

However, this constraint formulation is quadratic and non-convex, we will therefore linearize it.

Generally, if we want to deal with constraining $z = xy$ where x is binary and y is bounded ($L \leq y \leq U$), we can create a variable z and add the constraints:

- $z \leq Ux$
- $z \geq Lx$
- $z \leq y - L(1 - x)$
- $z \geq y - U(1 - x)$

And then constraint z.

In our case, $L = 0$ and $U = 1$, therefore we add the constraints:
$\forall i \in [0, Nc]:$

- $z[i] \leq x[i]$
- $z[i] \geq 0$
- $z[i] \leq y[i]$
- $z[i] \geq x[i] + y[i] - 1$

We can remove the second constraint, $z[i]$ being binary.

Constraint 2: Total Distance constraints

We want our train to travel a distance $D \pm tol$.

For each step, we define the velocity at step j as being:

$$v_j = \sum_{i=0}^{j} (x[i] - y[i])(\Delta v)^2$$

And the final distance as being:

$$D_{travelled} = \sum_{i=0}^{N_c} v_i$$

We therefore add the constraints:

- $\sum_{i=0}^{N_c} v_i \leq D + tol$
- $\sum_{i=0}^{N_c} v_i \geq D - tol$

Constraint 3: Net-Zero constraint

We also want our train to be stopped when arriving, therefore, we add the constraint:

- $v_{N_c} = \sum_{i=0}^{N_c} (x[i] - y[i])(\Delta v)^2 = 0$

Constraint 4: Maximum speed constraint

We want our train's maximum speed to be v_{max}, for this we add the constraints:
$\forall i \in [0, N_c]:$

- $v_i \leq v_{max}$

We can simplify this constraint, because we don't have different speed limits on our track. We therefore only add the constraint:

- $\sum_{i=0}^{N_c} x[i]\ \Delta v \leq v_{max}$

Constraint 5: Positive speed constraint

We want to force our speed to remain positive, for this we add the constraint:
$\forall i \in [0, N_c]$:

- $v_i \geq 0$

Converting our problem

Converting inequalities to equalities

In order to convert our inequalities to equalities, we introduce slack variables:

An inequality $x \geq y$ therefore becomes $x + s = y$ by introducing a slack variable $s \geq 0$.

An inequalities $x \geq y$ therefore becomes $x + s = y$ by introducing a slack variable $s \leq 0$.

We therefore apply this to constraints 1,2,4 & 5.

Converting our problem to a Quadratic Unconstrained Binary Optimization (QUBO) problem

In order to run our optimization problem on quantum hardware, we have to input an unconstrained problem. For this, we will convert our constraints (equality) to penalties.

We can write all of our constraints as :

$$h(x,y,z) = \sum_{i=0}^{N_c} (a_i x[i] + b_i y[i] + c_i y[i]) - b = 0$$

By defining a penalty term and adding it to the objective function:

$$Penalty = \lambda (h(x,y,z))^2$$

By default, λ is defined by $\lambda = 10 \times max(\text{absolute coefficient in objective function})$

We therefore apply this to all of our constraints and our problem becomes unconstrained.

Once all of our constraints are transformed to penalties, we are left with a QUBO problem of the form:

$$minimize: \ x^T Q x = \sum_{i,j=1}^{n} Q_{i,j} x_i x_j$$

Converting our QUBO problem to an Ising Hamiltonian

From this QUBO, we will need to extract the Ising Hamiltonian which is done by applying the transformation: $x \rightarrow \frac{\sigma+1}{2}$. Where the $x[i]$ binary variables are turned to spin variables $\in \{-1,+1\}$

The Ising Hamiltonian is defined as:

$$H(\sigma) = \sum_{i,j} J_{i,j}\sigma_i\sigma_j + \sum_i h_i\sigma_i$$

We therefore have:

- $h_i = -\frac{1}{2}\sum_j Q_{i,j} - \frac{Q_{i,i}}{2}$
- $J_{i,j} = \frac{Q_{i,j}}{4}$
- $offset = \frac{1}{4}\sum_{i,j} Q_{i,j}$

We are therefore left with the Ising Hamiltonian and offset.

QAOA

We build a parametrized quantum circuit that we will optimize in order to solve our problem.

Cost Hamiltonian

We apply the Hamiltonian as a phase evolution:

$$U_C(\gamma) = e^{-i\gamma H_C} = \prod_i e^{-i\gamma h_i\sigma_i} \prod_{i<j} e^{-i\gamma J_{i,j}\sigma_i\sigma_j}$$

From the Ising Hamiltonian's definition. This means that each qubit undergoes single-qubit R_Z rotations and two-qubit ZZ interactions.

- $e^{-i\gamma h_i\sigma_i}$ corresponds to rotating qubit i by an angle of γh_i around z.
- $e^{-i\gamma J_{i,j}\sigma_i\sigma_j}$ two-qubit rotation based on the value of $J_{i,j}$

Mix Hamiltonian

We apply a mixing term to encourage the exploration of the solution space, usually:

$$H_m = \sum_i X_i$$

The corresponding unitary:

$$U_M(\beta) = e^{-i\beta H_M} = \prod_i e^{-i\beta X_i}$$

These are single-qubit R_X rotations.

Building the circuit

We start by intializing all qubits to the state: $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$
By applying a Hadamard gate to all qubits, this gives us:

$$|+\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_z |z\rangle$$

We then apply the cost Hamiltonian $U_C(\gamma)$ followed by the mixer Hamiltonian $U_M(\beta)$

We do this p times for p the number of layers which corresponds to the amount of circuit parameters we are going to optimize.
Therefore, we have:

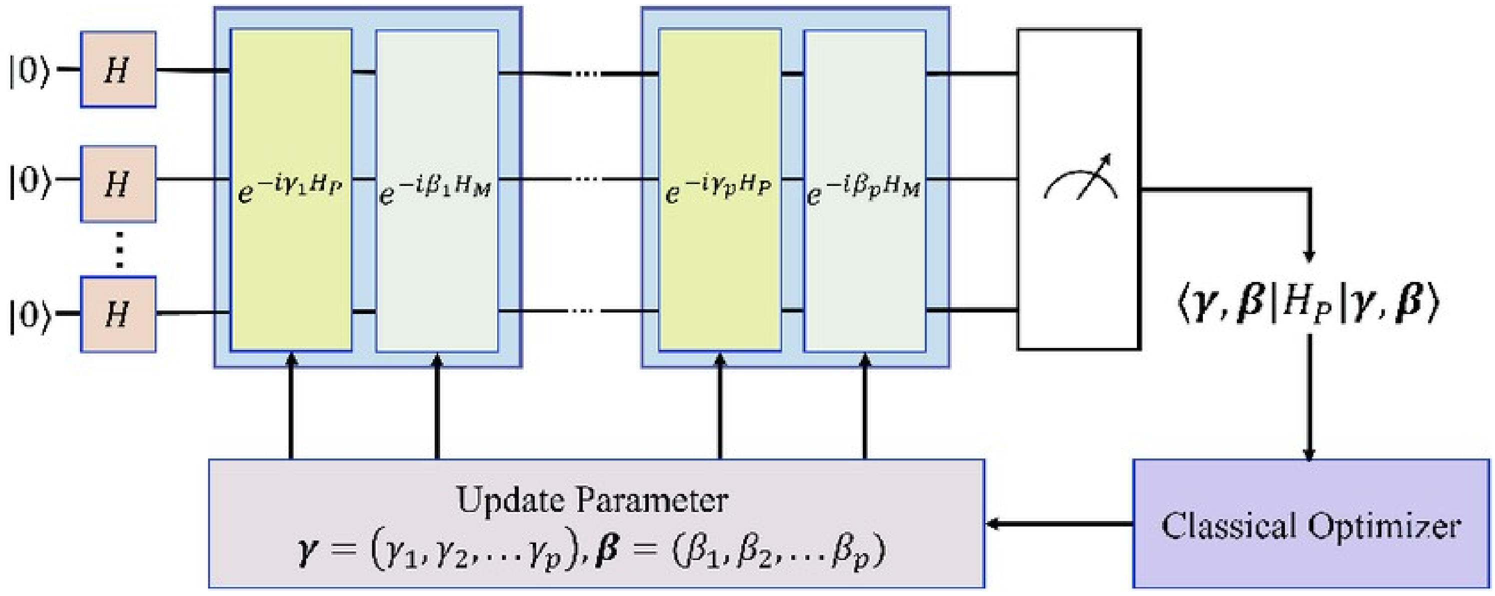
$$|\psi(\gamma, \beta)\rangle = \prod_{j=1}^{p} (U_M(\beta_j)\, U_C(\gamma_j))\ |+\rangle^{\otimes n}$$

At the end, we measure the final quantum state in the computational basis. We do this multiple times to find an average value. This gives us the expected value of the cost Hamiltonian.

We then try to optimize classically $\beta\ and\ \gamma$ in order to minimize:

$$\langle H_C \rangle = |\psi(\gamma, \beta)\rangle\ H_C\ \langle\psi(\gamma, \beta)|$$

This creates a loop represented by the diagram below.


$|0\rangle$
H
$|0\rangle$
H
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H
$e^{-i\gamma_1 H_P}$
$e^{-i\beta_1 H_M}$
$e^{-i\gamma_p H_P}$
$e^{-i\beta_p H_M}$
$\langle \gamma, \beta | H_P | \gamma, \beta \rangle$
Update Parameter
$\gamma = (\gamma_1, \gamma_2, \dots \gamma_p), \beta = (\beta_1, \beta_2, \dots \beta_p)$
Classical Optimizer