USC University of Southern California

Q3 Initiative

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Track #2 - Real-World Optimization Problem - Knapsack

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Superposition Squad

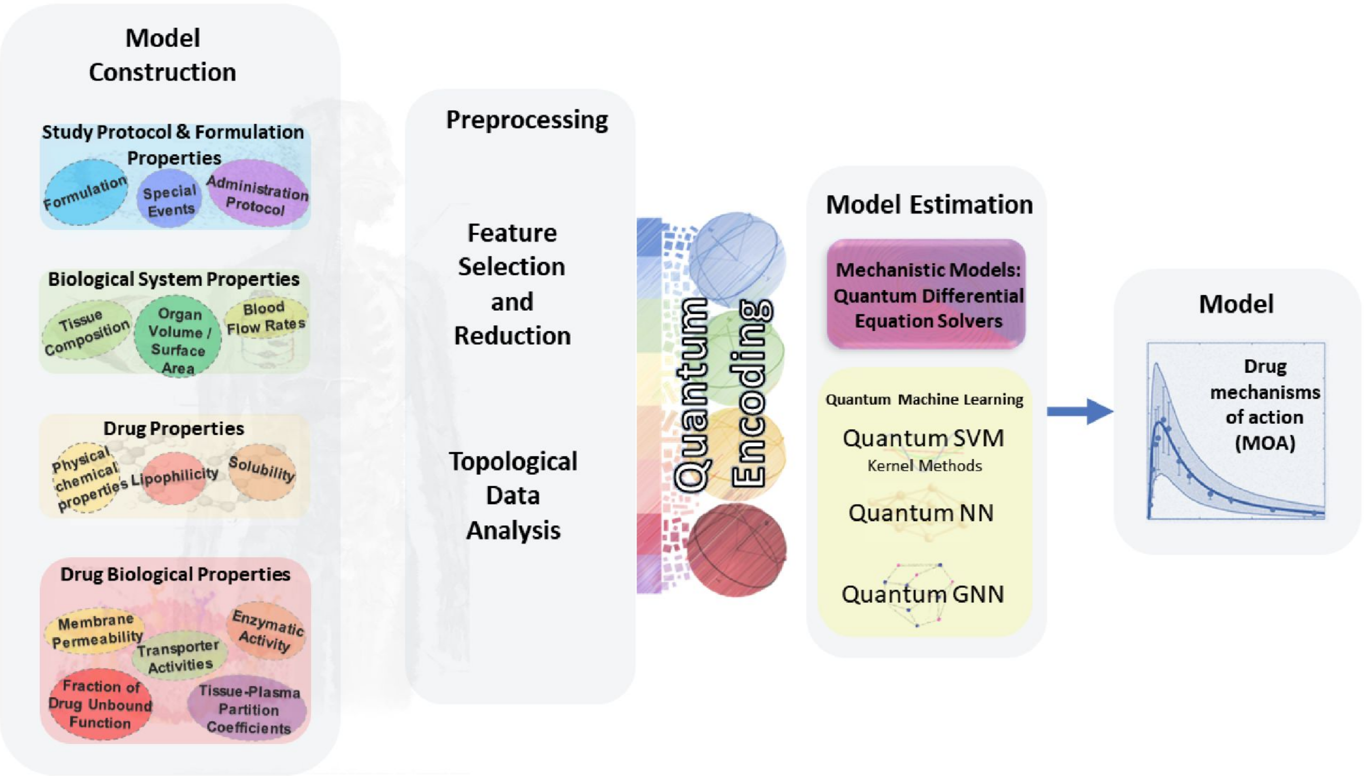
What is the *knapsack* problem?

- A combinatorial optimization problem that states :

Given a set of items, each with a weight and a value, determine which items to include in the collection so that the total weight is less than or equal to a given limit and the total value is as large as possible.

- Often arises in resource allocation where decision-makers have to choose from a set of non-divisible projects or tasks under a fixed budget or time constraint, respectively.
- This decision problem form of the knapsack problem is NP-complete which means that there is no known algorithm that is both correct and fast (polynomial-time) in all cases making it the absolute best problem to solve using quantum computing.

Quantum Knapsack in Real World Drug Discovery



Real World Constraints in Implementation

- Technical Constraints
  - Scalability issues due to hardware limitation.
  - High qubit use from pairwise connections
  - Highly sensitive to penalty terms
- Practical Concerns
  - Upfront costs are high
  - If candidate drugs are selected by underdeveloped quantum–classical hybrid pipelines, explaining decision-making for regulatory approval could be difficult.
- Governance
  - Possibility of misusing tech to create bioweapons and drugs - need robust policies to counter
  - Due to cost & scarcity of hardware only well-funded institutions may benefit, widening gaps in drug-discovery innovation possibly creating monopolies

The Hamiltonian

$$H(x) = -\sum_i v_i x_i + A\left(\sum_i w_i x_i - C\right)^2$$

$$x_i = \frac{1 - Z_i}{2}$$

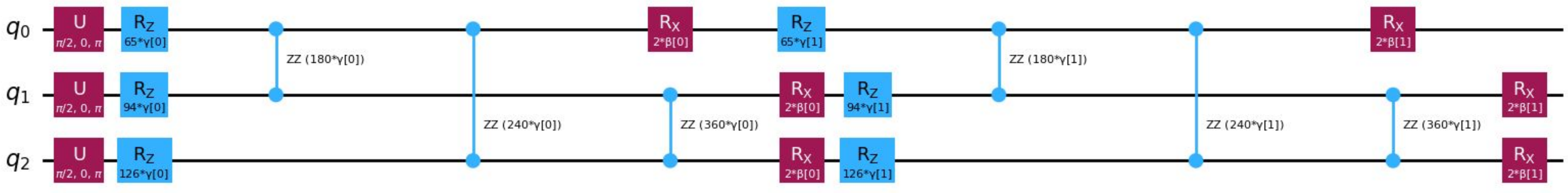
$$v_i x_i = \frac{v_i}{2} I - \frac{v_i}{2} Z_i$$

$$w_{ij} x_i x_j = \frac{w_{ij}}{4} I - \frac{w_{ij}}{4} Z_i - \frac{w_{ij}}{4} Z_j + \frac{w_{ij}}{4} Z_i Z_j$$

- x_i represents a binary select / do not select (1, 0)
    - Map to (1, -1) as orthogonal states are distinguishable
- A is a penalty term, and generally should be >= max(w)
- C is the capacity of the knapsack
- v_i and w_i are value and weight

The QAOA Algorithm

- We are minimizing the expectation value
  - <psi(gamma, beta) | H | psi(gamma, beta)>
  - A classical optimizer tunes gamma and beta to reach this minimum
- Once converged, sampling the tuned circuit should produce the bitstring representing the max items with a higher percentage than other options in the search space



QAOA ansatz with 2 repetitions of the Hamiltonian

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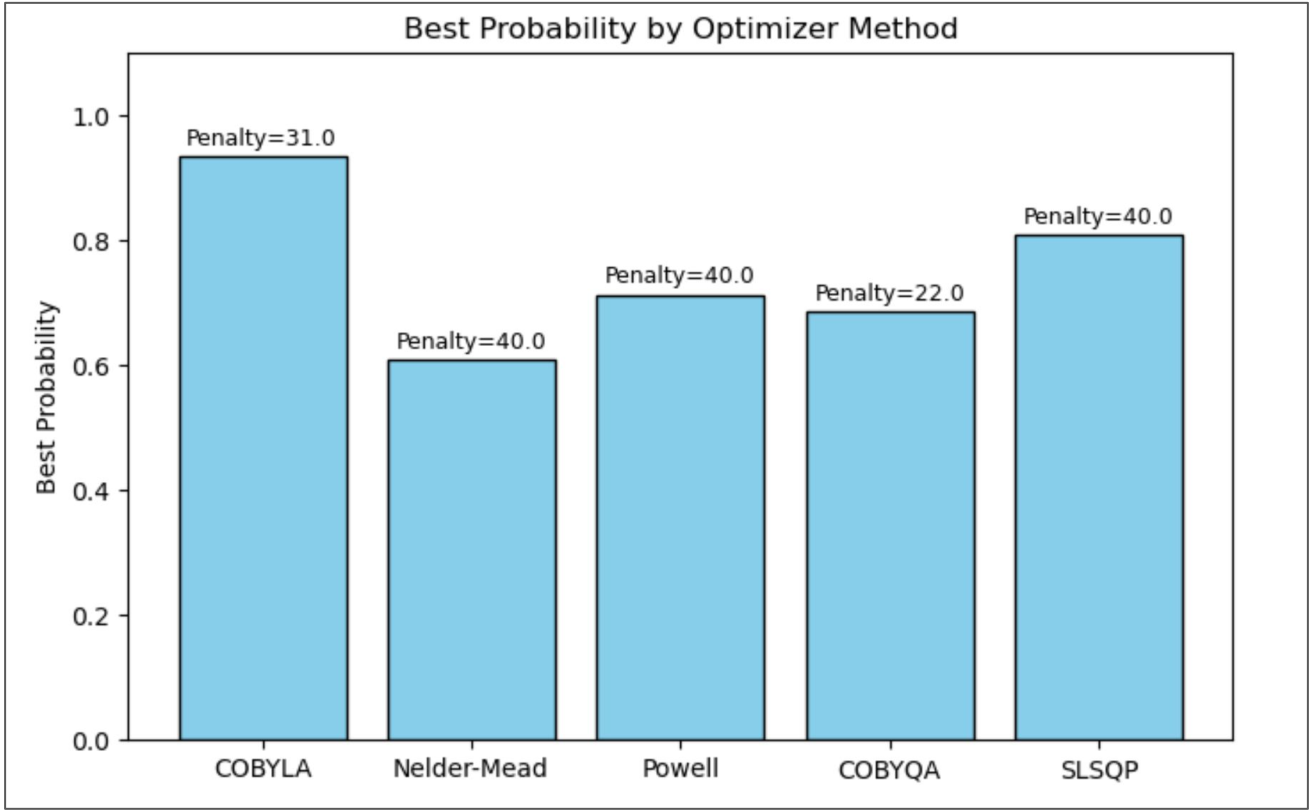
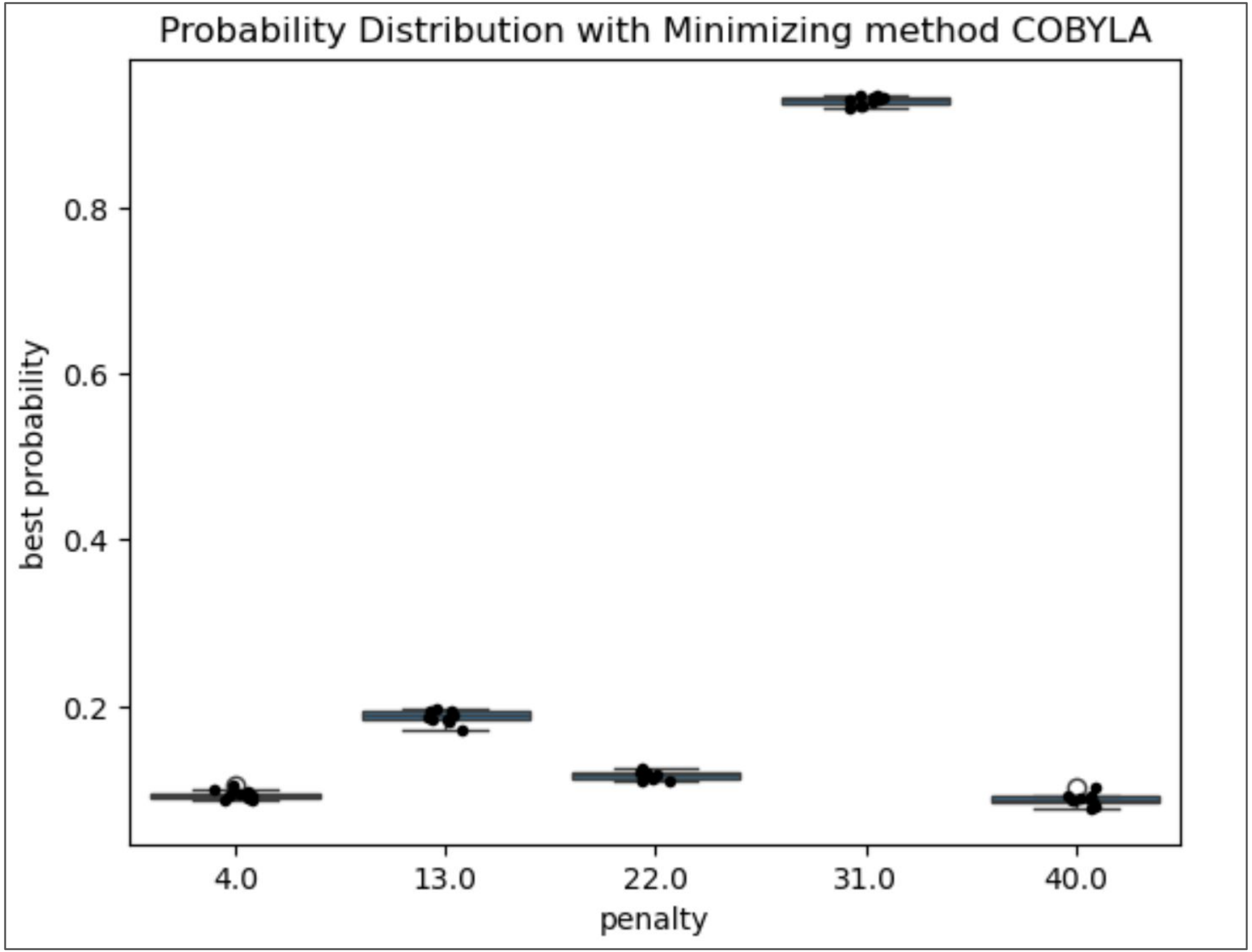
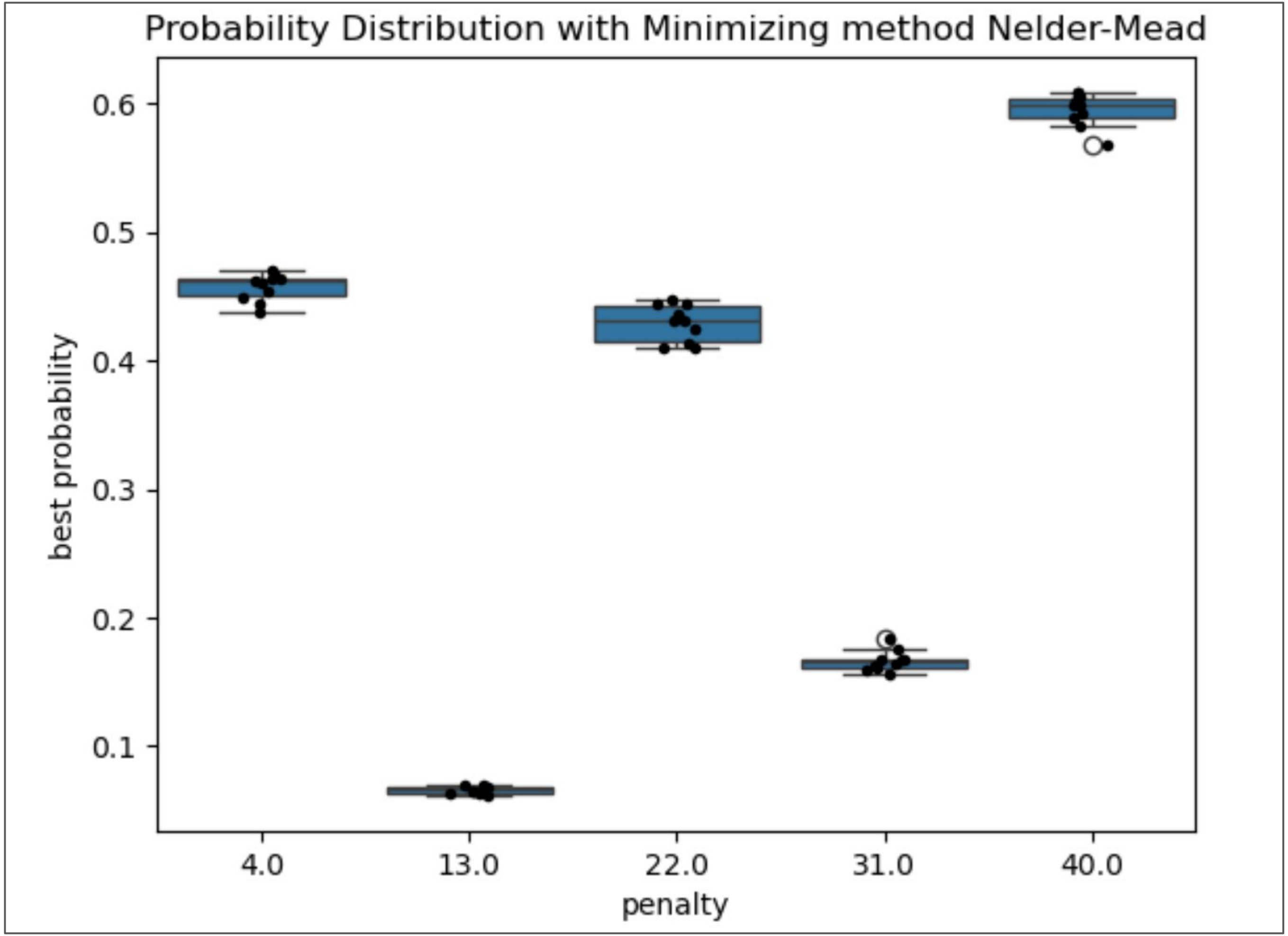
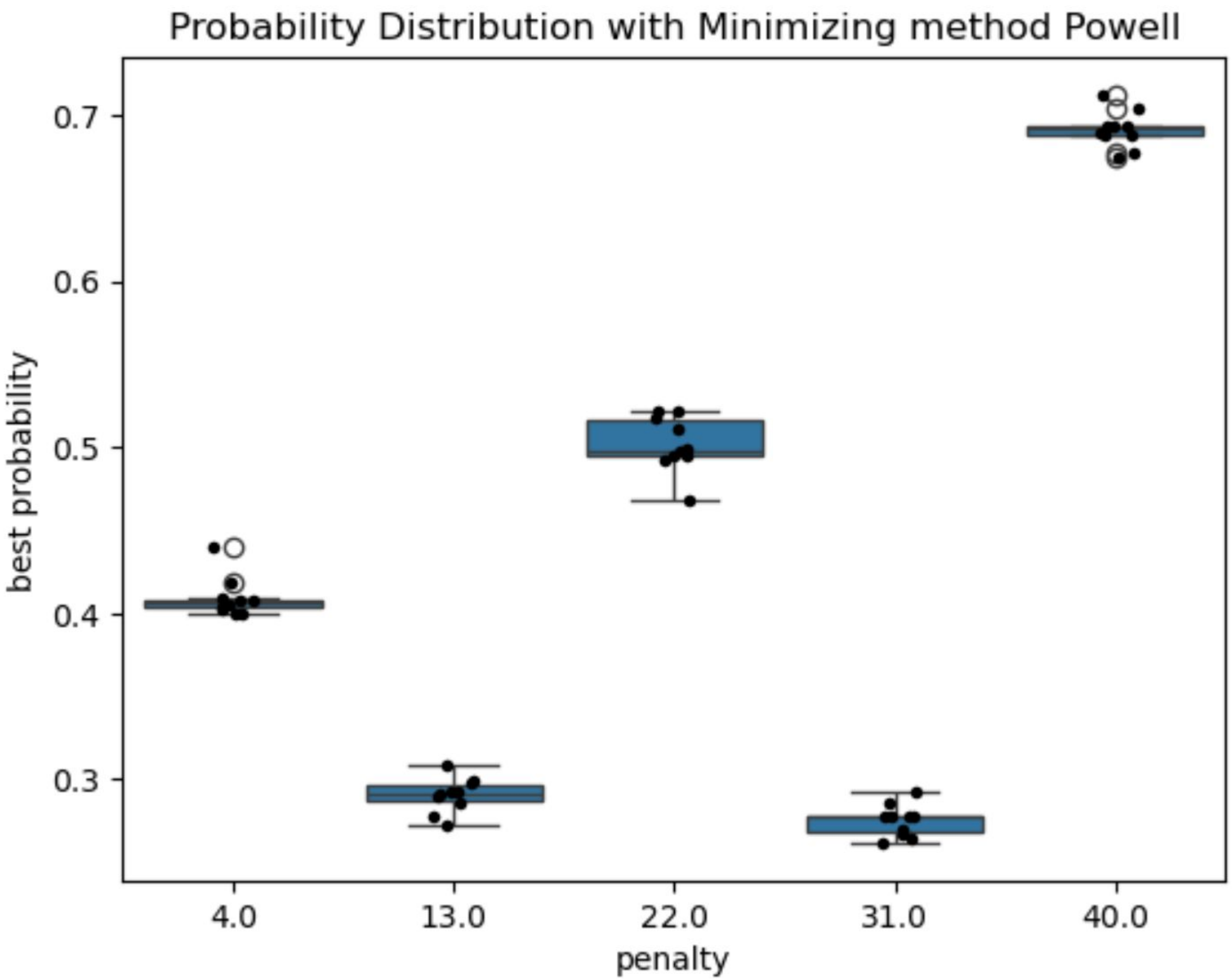
Fine Tuning the Minimization Algorithm




Probability Distribution with Minimizing method COBYLA
best probability
0.2
0.4
0.6
0.8
4.0
13.0
22.0
31.0
40.0
penalty


Probability Distribution with Minimizing method Nelder-Mead
best probability
0.1
0.2
0.3
0.4
0.5
0.6
4.0
13.0
22.0
31.0
40.0
penalty



Probability Distribution with Minimizing method Powell
best probability
0.7
0.6
0.5
0.4
0.3
4.0
13.0
22.0
31.0
40.0
penalty

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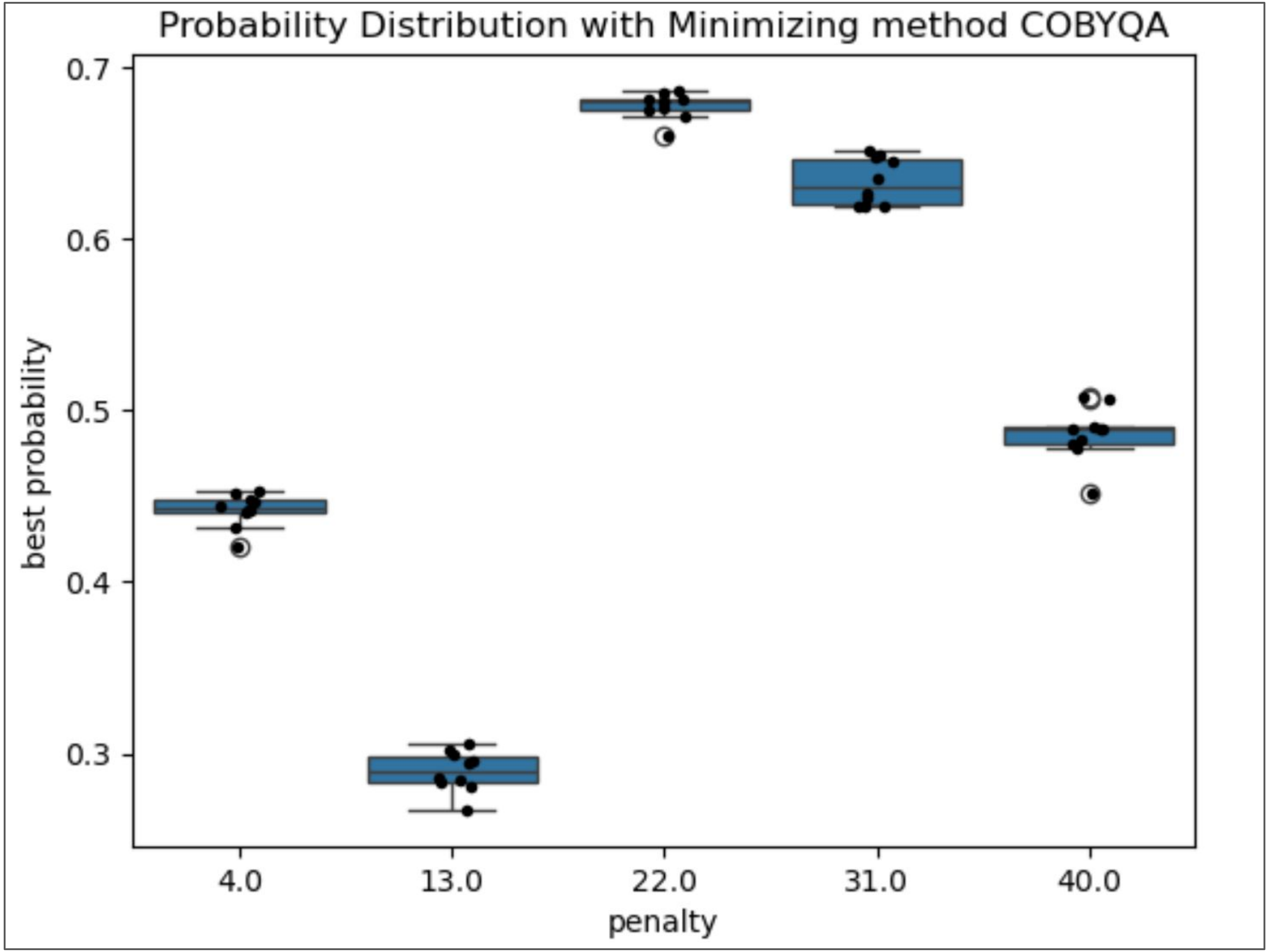
Probability Distribution with Minimizing method COBYQA
best probability
0.7
0.6
0.5
0.4
0.3
4.0
13.0
22.0
31.0
40.0
penalty

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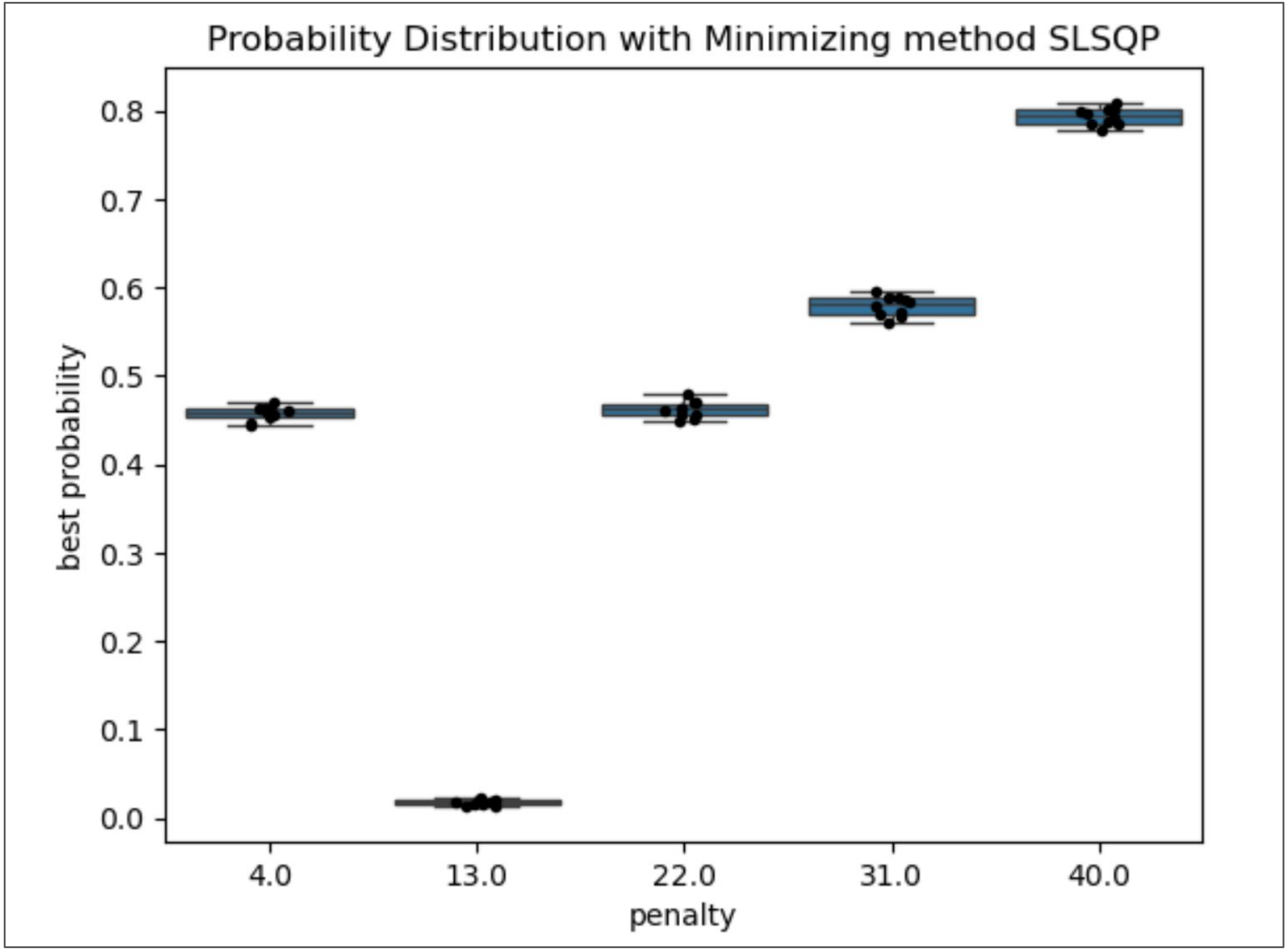

Probability Distribution with Minimizing method SLSQP
best probability
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
4.0
13.0
22.0
31.0
40.0
penalty

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Thank You!

Citations

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