DATA SCIENCE SUMMIT

Logistics Optimization

SURROGATE OPTIMIZATION FOR QUBO SOLVERS USING QROSS METHOD

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Agenda

QROSS: QUBO RELAXATION PARAMETER OPTIMISATION VIA LEARNING SOLVER SURROGATES

Most of Logistics and resource allocation problems are really just combinatorial optimization problems. An increasingly popular method for solving such problems is to first convert it into a Quadratic Unconstrained Binary Optimization(QUBO) problem and solve it using a QUBO solver.

However, this method introduces hyper-parameters that balances the objective and penalty terms for the constraints, and the chosen value significantly impacts the results from the solver. Therefore, tuning these parameter is an important task. Existing hyper-parameter tuning methods require making multiple expensive calls to a QUBO Solver. This makes it impractical for scenarios where solutions to similar combinatorial problems are required. In our project, we build surrogate models of QUBO solvers which learn from solved data from these solvers and predict the feasibility and fitness of relaxation parameter for a given instance.

QROSS: QUBO RELAXATION PARAMETER OPTIMISATION VIA LEARNING SOLVER SURROGATES

A PREPRINT

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Optimizing Logistics: The Travelling Salesman Problem

Problem Statement: Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?

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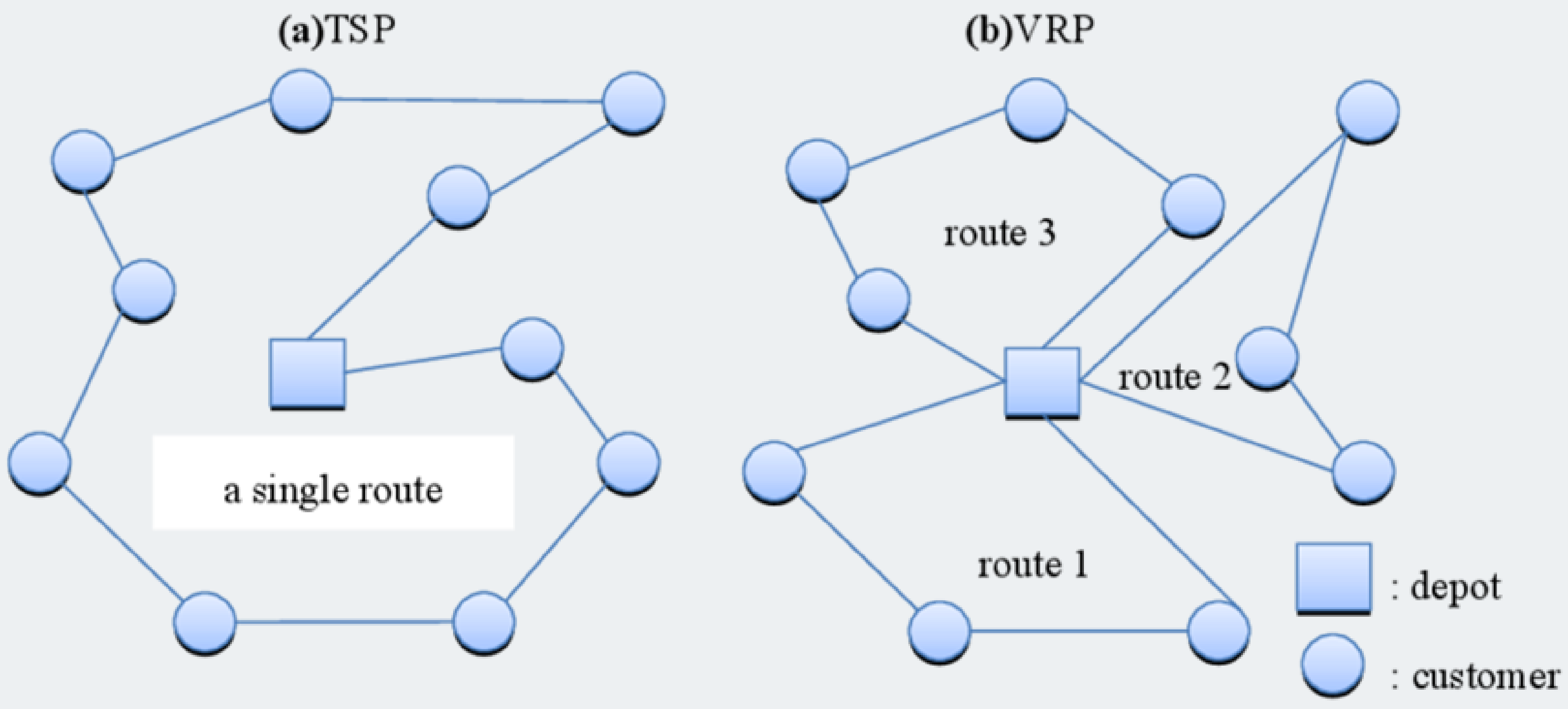
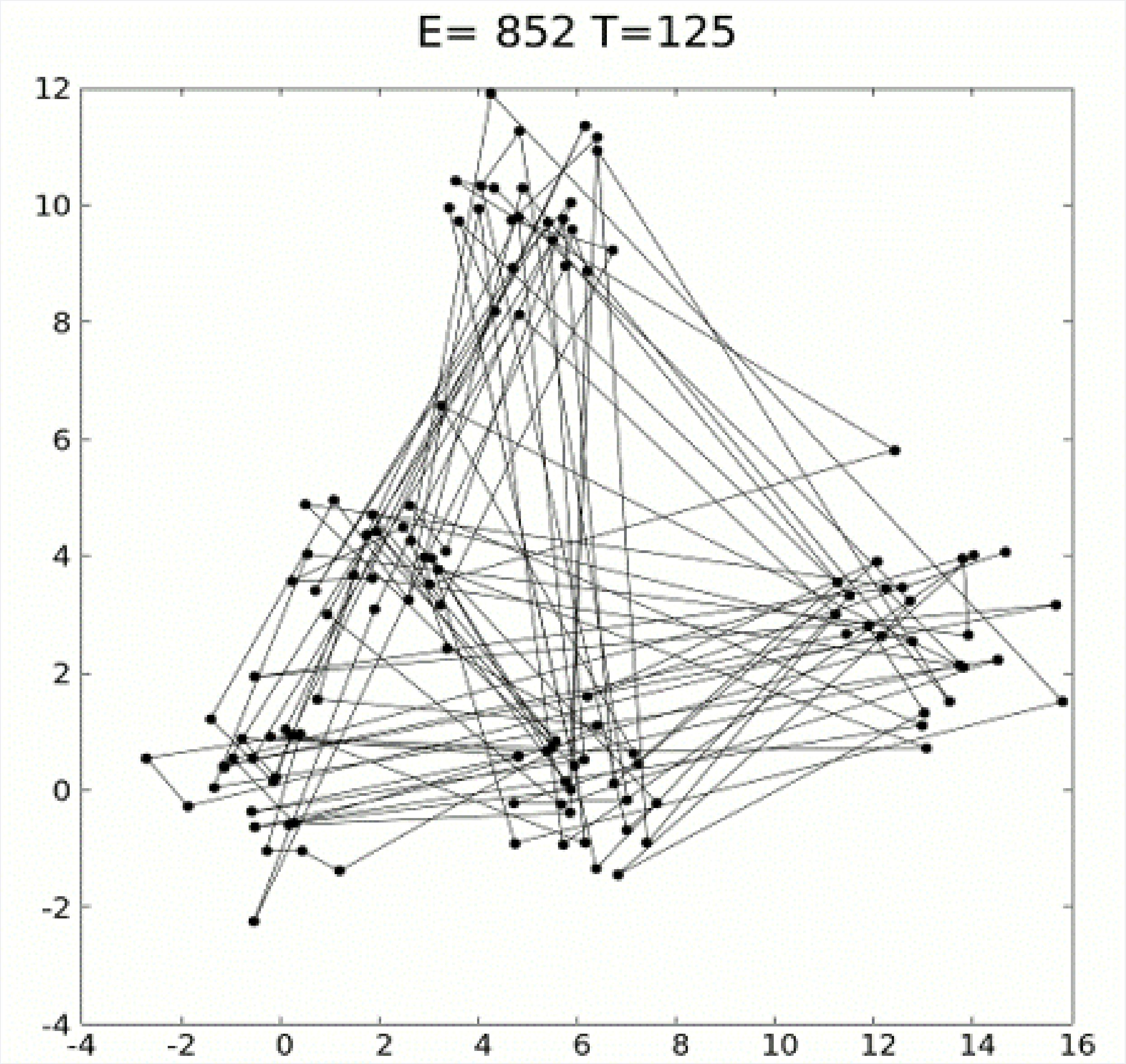
We are given a list of vertices and their pairwise distances, and we want to visit every vertex exactly once and return to the starting point. The goal is to minimize the distance of the tour, i.e., we want to find the shortest Hamiltonian cycle.





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Quadratic Unconstrained Binary Optimization(QUBO)

The objective form of QUBO being closely related to the Hamiltonian of the Ising Model, makes it suitable to be solved through processes such as quantum annealing and simulated annealing.

QUBO formulation for TSP & Relaxation Parameter

The formulation is as follows:

$$\min_x H_B(x) + AH_A(x)$$

Where:

$$H_B(x) = \sum_{(u,v)\in E} d_{uv} \sum_{j=1}^{n} x_{u,j} x_{v,j+1}$$

describes the total distance travelled, and

$$H_A = \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{n} x_{v,j}\right)^2 + \sum_{j=0}^{n} \left(1 - \sum_{v=1}^{n} x_{v,j}\right)^2$$

describes the constraints to be a feasible cycle

Here d_uv is the distance between cities u and v. The first subscript of x represents the city and the second represents the order in which the city is to be visited. 'A' is the relaxation parameter, as one increases the parameter value, the constraints dominates the QUBO objective, that is, a solver is now more likely to find a feasible solution. However the part of the function corresponding to original objective becomes less prominent, and there is a chance that the solutions returned by the solver won't be optimal.

A promising relaxation parameter therefore balances the weight of objective and feasibility.

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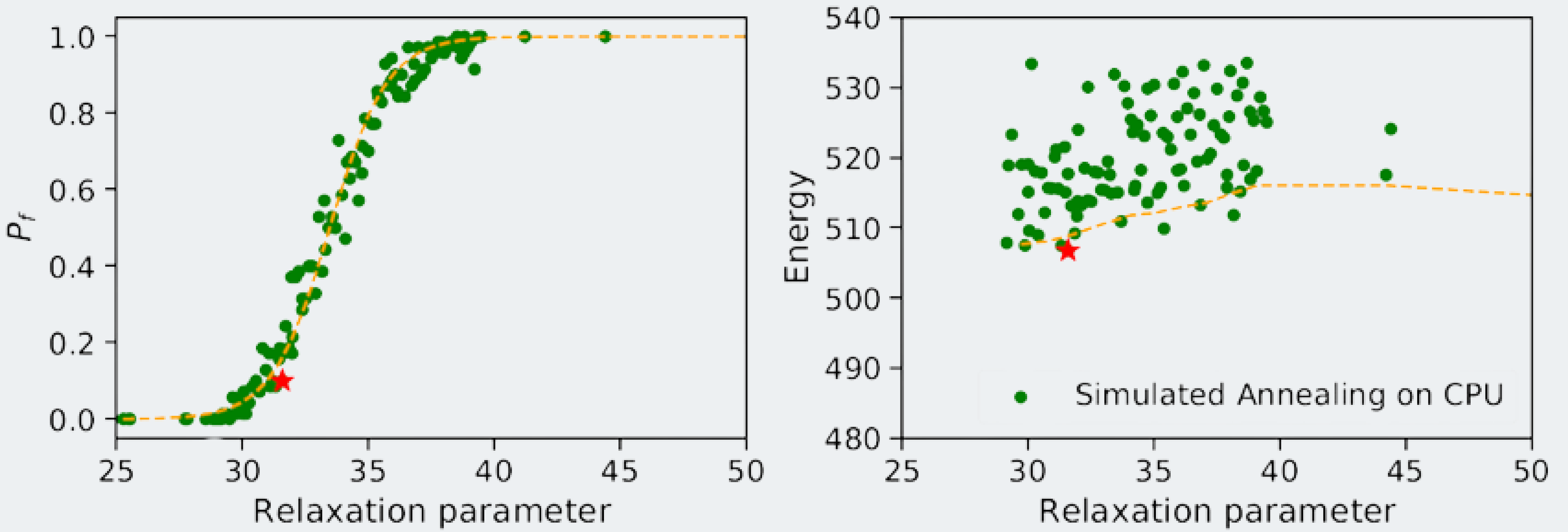
Significance of the Relaxation Parameter

The quality of the solutions returned by the QUBO solver is determined by the relaxation parameter value, depending on the choice of parameter, the feasibilty and optimality of the solution can vary. We have explored the relationship between feasibility and parameter value, and subsequently between solution objective energy and parameter value. Each point on the graph represents one of the 128 solutions provided by the QUBO solver.



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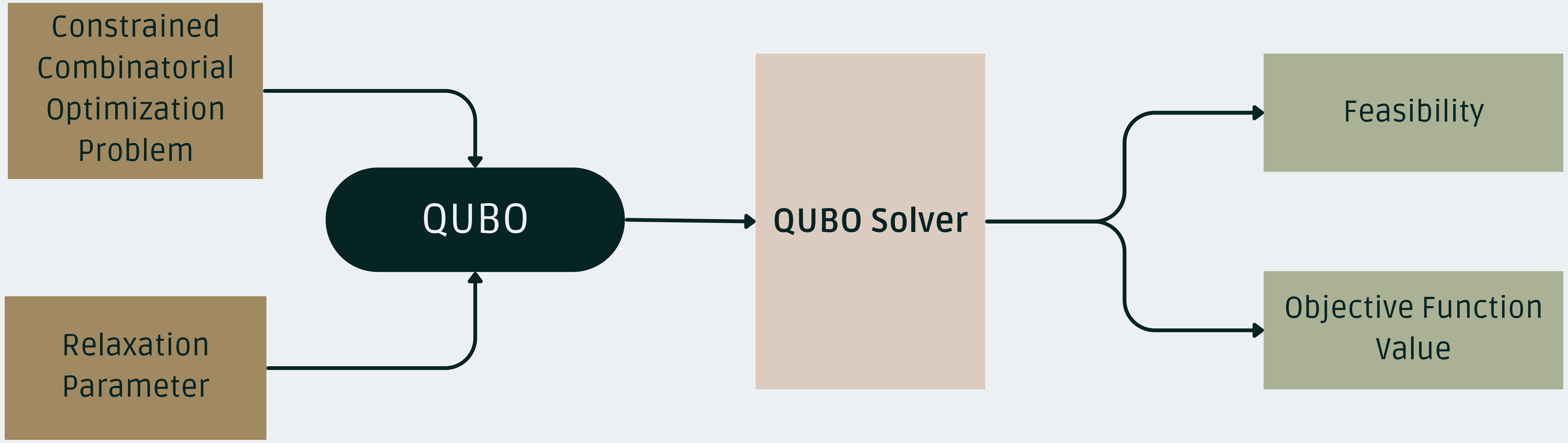
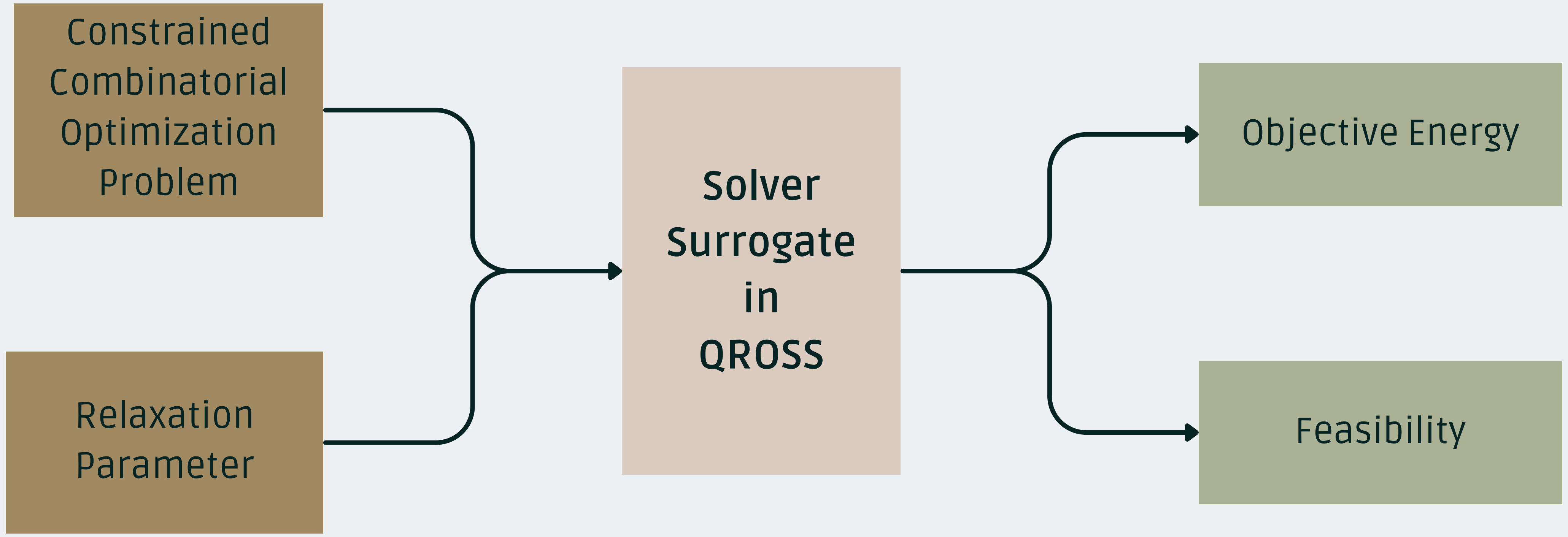
Picture Courtesy: QROSS paper

Goal of the Project



(a)



(b)

A deep learning surrogate model that learns from past solved instances by a QUBO solver and predicts probability of feasibility and fitness of solution of a relaxation parameter to a given problem instance. We capture the common structure of a problem and utilize the knowledge of the surrogate solver to propose optimal relaxation parameter while making fewer calls to a QUBO solver.

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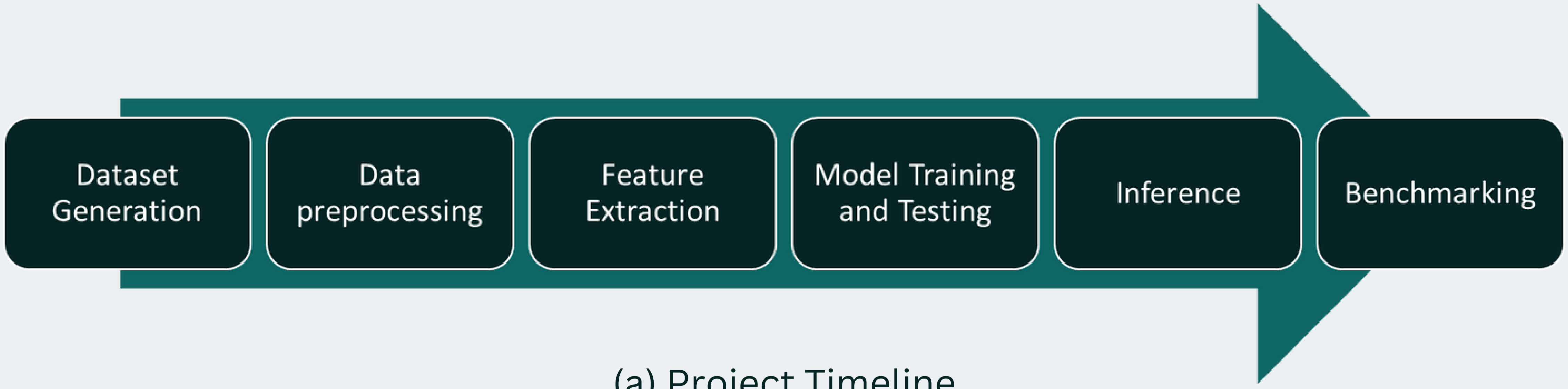
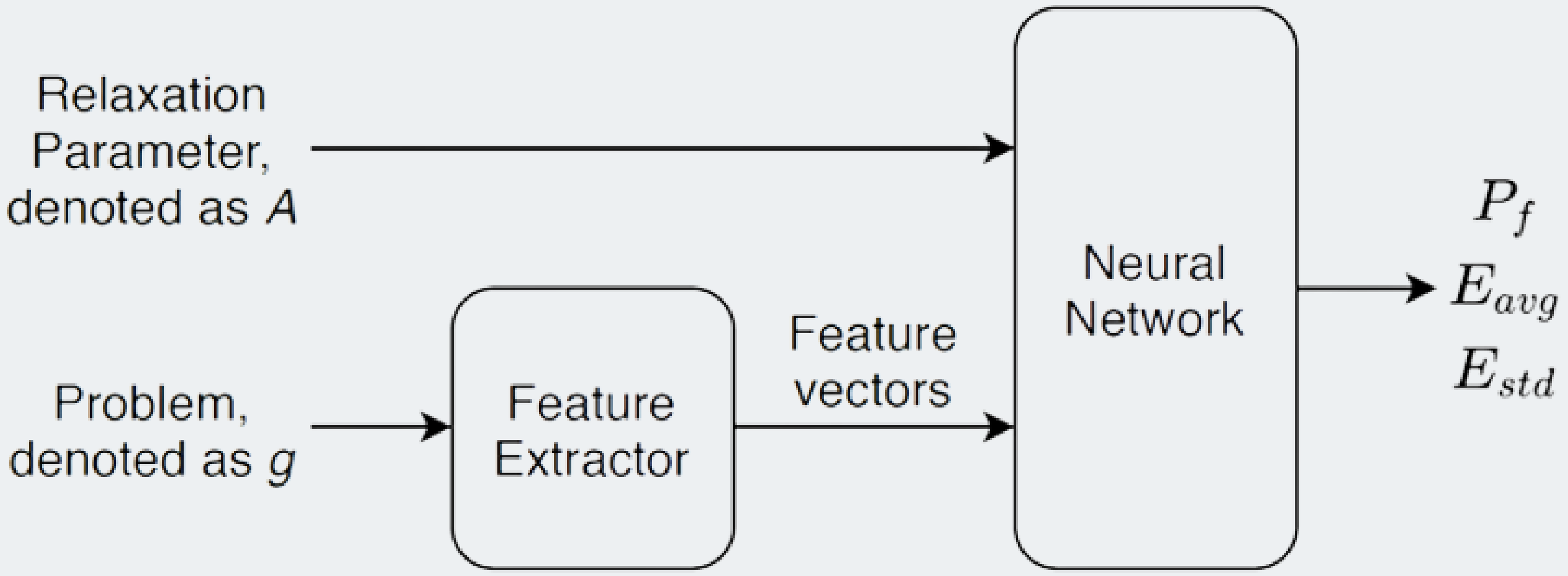
Project Description



(a) Project Timeline

	A	B	C	D	E
1	Relaxation Parameter	Probability P_f	E_avg	E_std	E_min
2	2187	0.0234375	25254.25	1985.421	20580.56
3	2208.88	0.03125	25724.15	2542.224	20259.88
4	2230.76	0.0390625	25811.81	2184.521	21776.53
5	2252.64	0.0625	26027.42	2359.88	21455.23
6	2274.52	0.0703125	26139.4	2167.194	21477.82
7	2296.4	0.0625	25898.6	2294.125	21599.05
8	2318.28	0.0625	26539.89	2723.839	19677.53
9	2340.16	0.109375	26217.78	2458.692	21469.5
10	2362.04	0.140625	26533.87	2218.745	21123.97
11	2383.92	0.078125	27032.79	2467.733	21309.12
12	2405.8	0.078125	26351.17	2060.215	21786.58
13	2427.68	0.1328125	27216.57	2386.709	21710.6
14	2449.56	0.1171875	26873.78	2650.289	21473.07
15	2471.44	0.2421875	27484.07	2589.501	20955.35
16	2493.32	0.1796875	27461.86	2611.089	21993.73
17	2515.2	0.109375	27326.93	2473.589	20638.42
18	2537.08	0.203125	27246.02	2378.375	22738.85
19	2558.96	0.2109375	27296.31	2626.62	22217.64
20	2580.84	0.21875	27753.75	2676.995	21901.99

(b) Dataset



(c) Structure of solver surrogate

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Work done/Progress so far

Created a pipeline to read and analyze data from TSPLIB dataset.

Implemented QUBO formulation of TSP using PyQUBO.

Used D-Wave neal to solve instances from TSPLIB and study the relation between relaxation parameter, the problem instance, feasibility and the objective energy.

Explored different ways for selecting the range of parameters for each instance based on the feasibility of the solutions returned by solver.

Generated a training dataset for surrogate model consisting of 300 instances and 30000 parameter values, taking an approximate compute time of 180 hours to generate.

Currently exploring feature extraction methods for TSP and VRP instances, such as using Graph Convolutional Neural Network or Reinforcement Learning.

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Future Plans

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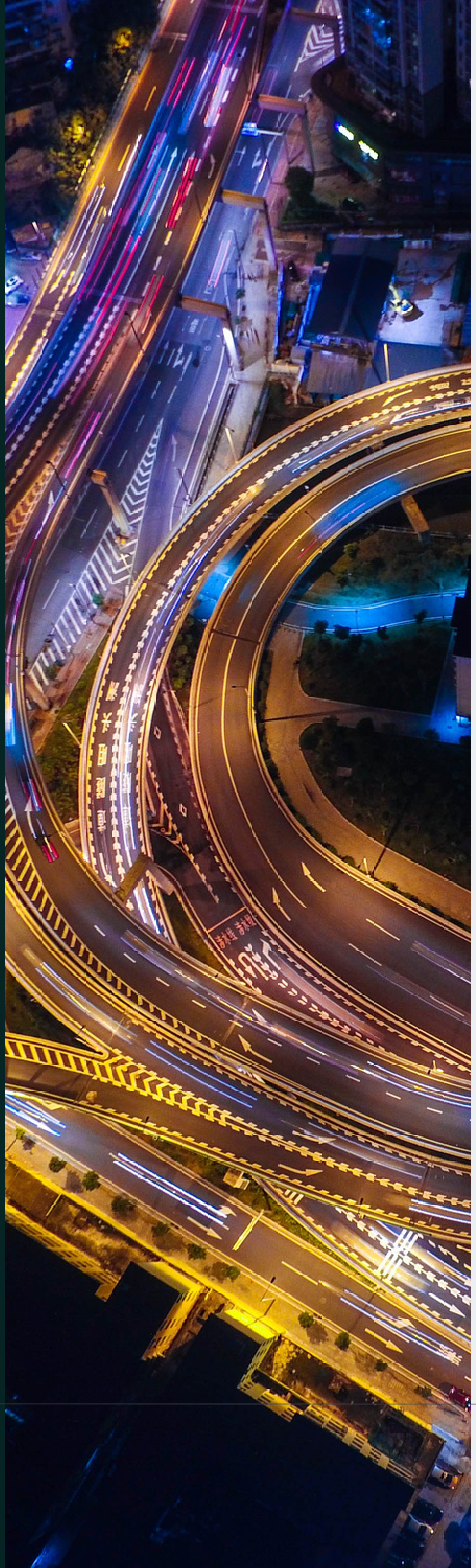
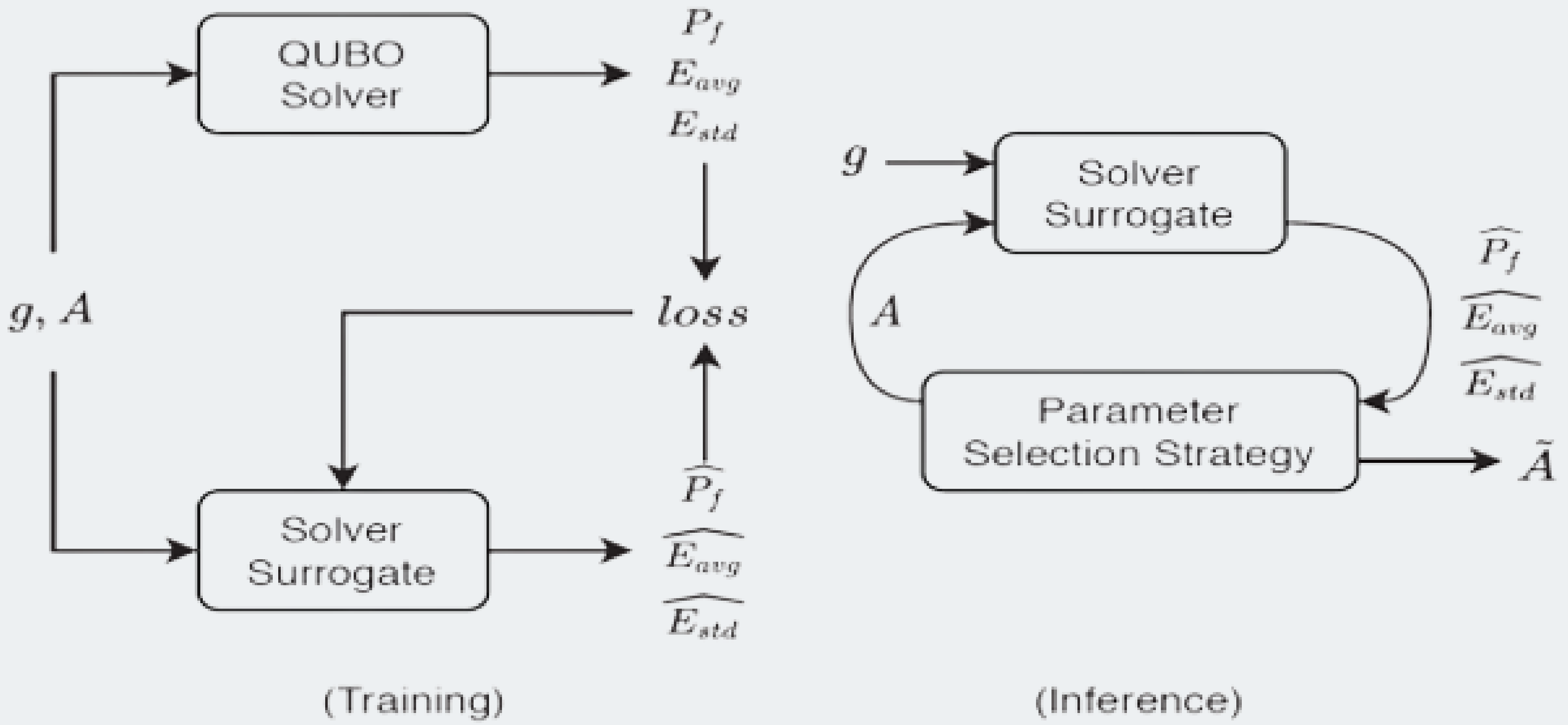


- Data preprocessing and postprocessing: We need to minimize variance in data i.e., move or shift different problem instances into same order of magnitude so that learning and inference becomes easier. Normalization helps in convergence of training curve.
- Training and testing of the Neural Network of Surrogate Model.
- Inference: In order to exploit the knowledge in the surrogate we will implement three strategies, two of which are offline i.e., do not require a call to QUBO solver.
- Benchmarking & comparison



Challenges and Obstacles

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- Solving 300 instances over a wide range of parameter takes a lot of time and memory space. Estimated time for generating the dataset is 180hours on a single runtime. We are experimenting with running multiple runtimes at once, but the out of memory errors and crashes become common.

- We are currently limited to simulated annealing due to lack of quantum annealer runtime.

Conclusion

Goal:
To create an AI-driven application that would allow us to obtain promising solutions to problems of similar structure with minimum number of calls to a solver. Minimizing time and cost required in performance critical operations.

Current Stage:
We are currently in the process of designing feature extraction layer that can vectorize problem instance using graph convolutional neural network.

Short term plans:

- Design the feature extraction layer
- Optimize the dataset generation process
- Implement the QROSS model

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Surrogate Optimization for QUBO solvers using QROSS method

Ashmit Gupta
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http://dssconf.pl/user.html#!/lecture/DSS23-daf9/rate

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Thank you for watching!

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