ЕВРОПЕЙСКИ СЪЮЗ
ЕВРОПЕЙСКИ ФОНД ЗА
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ОПЕРАТИВНА ПРОГРАМА
НАУКА И ОБРАЗОВАНИЕ ЗА
ИНТЕЛИГЕНТЕН РАСТЕЖ

Using machine learning for quantum annealing accuracy prediction

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ИКТ
ЦЕНТЪР ЗА ВЪРХОВИ ПОСТИЖЕНИЯ ПО
ИНФОРМАТИКА И ИНФОРМАЦИОННИ И
КОМУНИКАЦИОННИ ТЕХНОЛОГИИ

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  - Implementation
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Problem statement

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Background: quantum annealing

- Quantum annealing background
  - Quantum annealing (QA) uses quantum effects to find good quality solutions to Ising (**QUBO**) problems of the type

$$\text{minimize} \quad Q(x_1,\ldots,x_n) = \sum_{i=1}^{n}\sum_{j=i+1}^{n} J_{ij}x_ix_j + \sum_{i=1}^{n} h_ix_i\,, \quad x_i \in \{-1,1\}$$

(or $x_i \in \{0,1\}$),

  by mapping them to the Quantum Processing Unit, which seeks a minimum-energy quantum state that corresponds to a minimum value of function Q.

  - Many NP-hard problems can be easily formulated as QUBOs
    - **Maximum clique**, graph coloring, minimum vertex cover, maximum cut, knapsack, traveling salesman, graph partitioning, Boolean satisfiability (SAT), …

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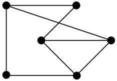
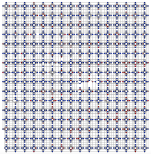
D-Wave quantum annealers



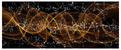
graph problem

$$\begin{pmatrix} -1 & 0 & 1 & 2 & -2 \\ 1 & 0 & 2 & 0 & -1 \\ 1 & 1 & 2 & 0 & -1 \\ 0 & 0 & 2 & -1 & -1 \\ 2 & -2 & 0 & 1 & 3 \end{pmatrix}$$

QUBO coefficients



map onto D-Wave



anneal

$$\begin{pmatrix} x_1 = 0 \\ x_2 = 1 \\ x_3 = 1 \\ x_4 = 0 \\ x_5 = 1 \end{pmatrix}$$

solutions

- D-Wave is a commercially available quantum annealer that solves optimization problems using the following steps:
  - Original problem formulated as a QUBO (or Ising);
  - QUBO mapped to D-Wave's hardware;
  - D-Wave performs a number of anneals and measures the qubits;
  - Results retrieved from D-Wave and transformed into a solution of the original problem.

How good is such a solution?

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Quality of D-Wave (DW) solutions

- DW returns a solution with low value (energy), but not necessarily the best.
- Quality depends on the problem's coefficients, annealing parameters, and the current state of the machine.
- There is no known method that can be used to determine how hard a particular problem will be for DW.

Our goal: use machine learning to predict problem's difficulty.

- This may help to
  - Allocate more resources (time) for solving harder problems;
  - Choose a (re)formulation that makes the problem easier for DW.

Methods

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Machine learning models

- Training set consists of random graphs of various densities.
- Problem solved is the Maximum Clique problem: find a *clique* (a set of maximally connected vertices) of maximum size, an NP-hard problem.
- Features include graph density, vertex degrees, # of triangles, eigenvalues, and annealing parameters.
- Two types of objective:
  - Can the problem be solved to optimality?
  - What is the size of the clique returned by D-Wave?
- Machine learning package used: *scikit-learn*.

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Computing ML model data

In a loop:

- Generate a random graph G;
- Compute QUBO coefficients matrix M for solving G;
- Get ML model feature vector F:
  - Get features using G, M, and D-Wave parameters;
- Get value v of ML target:
  - Use a classical solver to compute an optimal solution opt;
  - Send M to quantum annealer to get a solution sol;
  - Compare sol to opt to get $v \in \{yes, no\}$, for the classification version, or $v = sol$ for the regression;
- Add features+target vector (F, v) to training/testing set.

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Results

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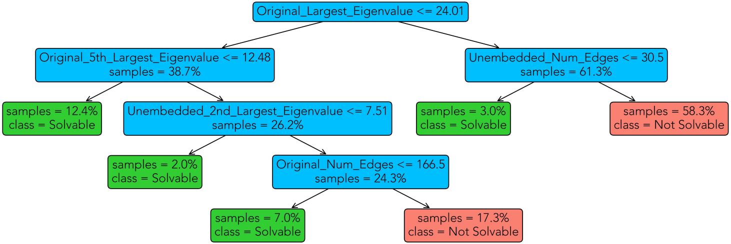
Results: Is the problem solvable to optimality on DW?

- Prediction results:

		Predicted	
		Not solvable	Solvable
Actual	Not solvable	3458	654
	Solvable	97	497

Accuracy: 0.84, Precision: 0.84, Recall (Sensitivity): 0.43

- Decision tree for classification:



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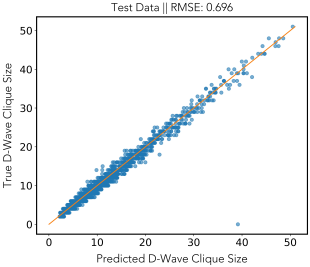
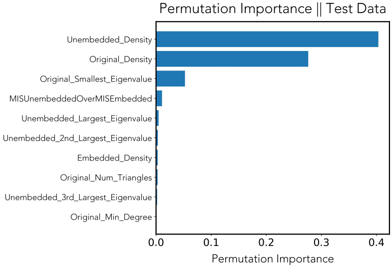
Results: What clique size is returned by DW?

- Prediction results:





Summary

- Predicting the outcome of quantum annealing is hard.
- Can be useful for estimating what resources to allocate for a particular problem.
- Machine learning works reasonably well (for the case of the maximum clique problem).
- Future work may target other optimization problems.

More details can be found in the paper:

A. Barbosa, E. Pelofske, G. Hahn and H. Djidjev, "Using machine learning for quantum annealing accuracy prediction," *Algorithms*, 14 (6), 187, 2021.

Thanks!