

Optimisation via Adiabatic Quantum Computing

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Introduction

Main Research Question

- What instances characteristics of optimisation problems make them predisposed to being solved on a Quantum Computer?

Background

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- $|\psi(t)\rangle$ is our state vector, $H(t)$ is the time dependent Hamiltonian. A Hamiltonian of an n -qubit system $H(t)$ is given by $2^n \times 2^n$ matrix.

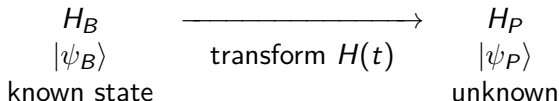
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$$\begin{array}{ccc} H_B & \xrightarrow{\hspace{1.5cm}} & H_P \\ |\psi_B\rangle & \text{transform } H(t) & |\psi_P\rangle \\ \text{known state} & & \text{unknown} \end{array}$$

- Loosely speaking, the adiabatic theorem tells us that if we vary from H_B to H_P *slowly enough* the system will remain in its ground state. This fact is a direct result of the Adiabatic Theorem.

Adiabatic Quantum Computing (AQC)

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- Where $g(t)$ is the difference between the first two smallest eigenvalues of $H(t)$

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- The basic SAT formulation can be described as follows: Given a boolean formula (AND \wedge , OR \vee , NOT \neg) over n variables (z_1, z_2, \dots, z_n) . Can one set z_i 's in a manner such that the Boolean formula is true?

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- A clause is an expression which the variables must satisfy. For example $z_1 \wedge z_2 \implies z_1 = z_2 = 1$

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- The 3-SAT problem in particular is a problem where each clause is comprised of 3 literals.

Mapping 3SAT to AQC

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- Farhi et al describes it very well.

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- Finally, complete measurement

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 1. Minimum Energy Gap g_{\min}
 2. Maximum Entropy of Entanglement

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- Ultimately, we can build a prediction model which maps instance features of different 3SAT instances to their inherent “Quantumness”

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- Given that we have access to IBM's Quantum Computer, we may also apply a discretized version of AQC, QAOA and produce results from a *real quantum computer*

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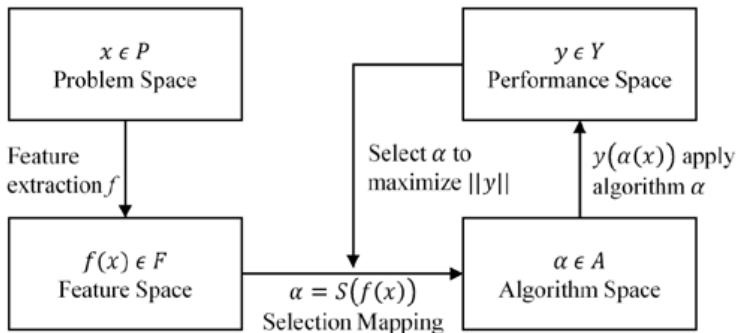
- Given that we have access to IBM's Quantum Computer, we may also apply a discretized version of AQC, QAOA and produce results from a *real quantum computer*
- This methodology can then be further extended to other optimisation problems that can be mapped to Quadratic Unconstrained Binary Optimisation (QUBO) problems.

Algorithm Selection

- Given a set of problem instances, predicting which algorithm is most likely to best perform was first explored by Rice [2].

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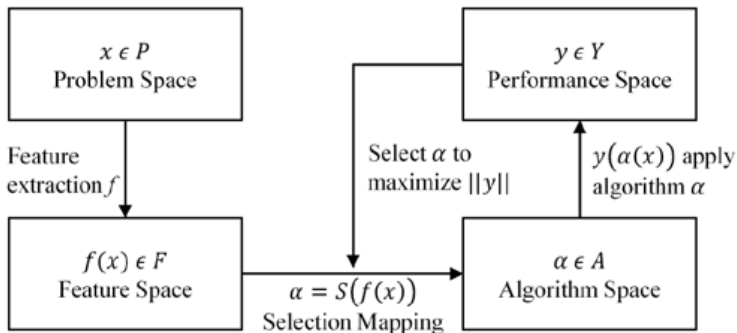
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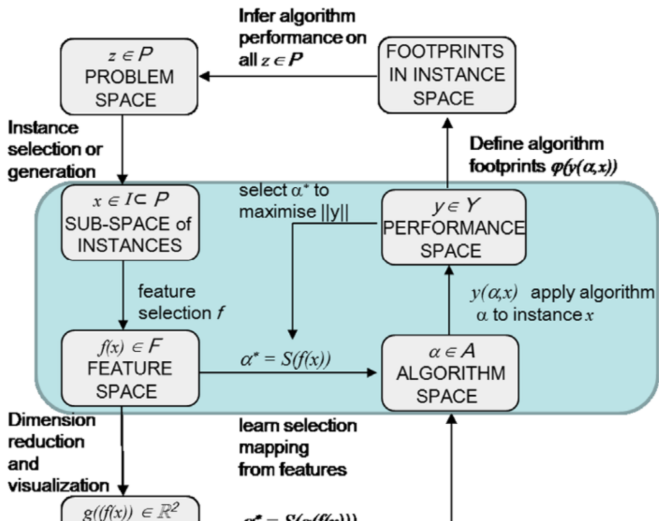
- However, what we are interested in is probing the strengths and weaknesses of AQC for different instances of SAT.

Instance Space Methodology

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2. Variable-Clause Graph Features
3. Variable Graph Features
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|-----------------------------------|----------------------------------|
| 1. Problem Size Features | 6. Balance Features |
| 2. Variable-Clause Graph Features | 7. DPLL Probing Features |
| 3. Variable Graph Features | 8. Local Search Probing Features |
| 4. Clause Graph Features | 9. LP-Based Features |
| 5. Proximity to Horn Formula | |

Quantum Computing Research into Hard SAT problems

- Different Paths (Farhi 2009)
- Hamiltonian Parameters (Choi)
- Volks group research on SAT

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3. Developed working environment, set up GitHub, scripts, organizational tools enabling an efficient working environment.

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6. Developed a working implementation of Adiabatic Quantum Computing on different instances of 3SAT.

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3. Apply Instance Space Methodology from MATILDA to find decision boundaries for *Entanglement Entropy* and *Minimum Energy Gap*

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8. Extend research to look at other optimisation problems

About Me

- Vivek Katial (vkatial@student.unimelb.edu.au)
 - PhD Candidate (Optimisation on Quantum Computers)
- Check out the slides at
<https://tinyurl.com/vkatial-preconfirmation>

References

References I

1. Cook SA (1971) The complexity of theorem-proving procedures, In, *Proceedings of the third annual acm symposium on theory of computing*, ACM, 151–158.
2. Rice JR, others (1976) The algorithm selection problem. *Advances in computers* 15: 5.
3. Smith-Miles K, Bowly S (2015) Generating new test instances by evolving in instance space. *Computers & Operations Research* 63: 102–113.
4. Smith-Miles K, Lopes L (2012) Measuring instance difficulty for combinatorial optimization problems. *Computers & Operations Research* 39: 875–889.

References II

5. Smith-Miles K, Baatar D, Wreford B, et al. (2014) Towards objective measures of algorithm performance across instance space. *Computers & Operations Research* 45: 12–24.
6. Selman B, Mitchell DG, Levesque HJ (1996) Generating hard satisfiability problems. *Artificial Intelligence* 81: 17–29.
7. Xu L, Hutter F, Hoos HH, et al. (2008) SATzilla: Portfolio-based algorithm selection for sat. *Journal of artificial intelligence research* 32: 565–606.
8. Nudelman E, Leyton-Brown K, Hoos HH, et al. (2004) Understanding random sat: Beyond the clauses-to-variables ratio, In: Wallace M (Ed.), *Principles and practice of constraint programming – cp 2004*, Berlin, Heidelberg, Springer Berlin Heidelberg, 438–452.