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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- 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 [1].

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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 $(z_1, z_2, ..., z_n)$. Can one set z_i's in a manner such that the Boolean formula is true?
- 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.

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- We then evolve our system with the following interpolation:
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- Finally, complete measurement and our solution is our final state $|\psi(t = T)\rangle$

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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 can also use this approach on QAOA and produce results from a *universal quantum computer*.
- This methodology can then be further extended to other optmisation problems that can be mapped to Quadratic Unconstrained Binary Optimisation (QUBO) problems.

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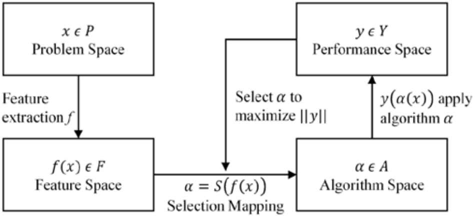

- However, what we are interested in is probing the strengths and weaknesses of AQC for different instances of SAT.

Instance Space Methodology

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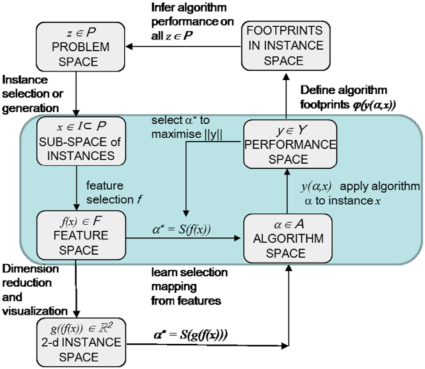

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2. Variable-Clause Graph Features
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5. Proximity to Horn Formula
6. Balance Features
7. DPLL Probing Features
8. Local Search Probing Features
9. LP-Based Features

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- Their research indicated that as $N \to \infty$ the system is expected to lead to an exponentially small gap, and hence an exponential complexity.
- Farhi et al. [13] also investigated different evolution paths and their results suggested it is possible to overcome the exponentially small minimum gap by selecting random initial Hamiltonians

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- However, their results also showed that for large N, the minimum gap scaling is exponential and can be associated with a *quantum phase transition* [14].
- Hauke et al. [15] ran simulations of adiabatic quantum optimization with $n = 16$. Their results indicated that large entanglement entropy has little significance for the success probability of the optimization task.

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- Gabor et al. [17] shows that the phase transition from 3SAT persists in some form (but possibly to a lesser extent) in AQC via **real experimental results** on D-WAVE.
- Most signficant for us is that none of this work approaches instances in a robust manner such as the MATILDA framework

Current Progress

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

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5. Provisioned all infrastructure required for above on Melbourne Research Cloud and SPARTAN
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2. Implement scripts to generate **hard** instances of 3SAT with respect to *instance characteristics*.
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

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    - PhD Candidate (Optimisation on Quantum Computers)

References

References I

1. Born M, Fock V (1928) Beweis des adiabatensatzes. *Zeitschrift für Physik* 51: 165–180.

2. Cook SA (1971) The complexity of theorem-proving procedures, In, *Proceedings of the third annual acm symposium on theory of computing*, ACM, 151–158.

3. Farhi E, Goldstone J, Gutmann S, et al. (2001) A quantum adiabatic evolution algorithm applied to random instances of an np-complete problem. *Science* 292: 472–475.

4. Smith-Miles K, Bowly S (2015) Generating new test instances by evolving in instance space. *Computers & Operations Research* 63: 102–113.

5. Smith-Miles K, Lopes L (2012) Measuring instance difficulty for combinatorial optimization problems. *Computers & Operations Research* 39: 875–889.

References II

6. 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.

7. Rice JR, others (1976) The algorithm selection problem. *Advances in computers* 15: 5.

8. Selman B, Mitchell DG, Levesque HJ (1996) Generating hard satisfiability problems. *Artificial Intelligence* 81: 17–29.

9. Xu L, Hutter F, Hoos HH, et al. (2008) SATzilla: Portfolio-based algorithm selection for sat. *Journal of artificial intelligence research* 32: 565–606.

10. 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.

References III

11. Hogg T (2002) Adiabatic quantum computing for random satisfiability problems. *Phys Rev A 67 022314 (2003)*.

12. Young AP, Knysh S, Smelyanskiy VN (2009) First order phase transition in the quantum adiabatic algorithm. *Phys Rev Lett 104, 020502 (2010)*.

13. Farhi E, Goldstone J, Gosset D, et al. (2009) Quantum adiabatic algorithms, small gaps, and different paths. *arXiv preprint arXiv:09094766*.

14. Latorre JI, Orús R (2004) Adiabatic quantum computation and quantum phase transitions. *Physical Review A* 69: 062302.

15. Hauke P, Bonnes L, Heyl M, et al. (2015) Probing entanglement in adiabatic quantum optimization with trapped ions. *Frontiers in Physics* 3: 21.

16. Choi V (2020) The effects of the problem hamiltonian parameters on the minimum spectral gap in adiabatic quantum optimization. *Quantum Information Processing* 19: 90.

References IV

17. Gabor T, Zielinski S, Feld S, et al. (2019) Assessing solution quality of 3SAT on a quantum annealing platform, In, *International workshop on quantum technology and optimization problems*, Springer, 23–35.