Instance Space Analysis on Quantum Algorithms

Vivek Katial

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Introduction

About Me

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 - PhD Candidate in School of Mathematics and Statistics

Talk Structure

 Introduction
 Adiabatic Quantum Computing (AQC)
 3SAT - Exact Cover 0000
 Instance Space Analysis 0000
 Current Literature 0000
 Research Council

- Background
- Overview of Literature
- Current Progress
- What's next?

Main Research Question

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

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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)

3SAT - Exact Cover

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- The basic SAT formulation can be described as follows: Given a boolean formula (AND \land , OR \lor , 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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- Exact Cover implies that clauses are "exclusive" and in the form of $z_i + z_i + z_k = 1$

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ullet Finally, complete measurement and our solution is our final state $|\psi(t=T)
angle$

Instance Space Analysis

Algorithm Selection

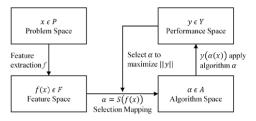
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 However, what we are interested in is probing the strengths and weaknesses of AQC for different instances of SAT.

Instance Space Methodology

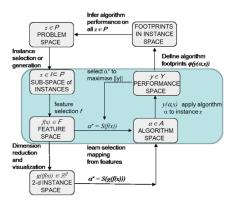
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- Their research indicated that as $N \to \infty$ the system is expected to lead to an exponentially small gap, and hence an exponential complexity.
- Farhi et al. [10] also investigated different evolution paths and their results suggested it is possible 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 [11].
- Hauke et al. [12] ran simulations of adiabatic quantum optimisation with n=16. Their results indicated that large entanglement entropy has little significance for the success probability of the optimisation task.

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- We are looking to investigate which types of instances are more pre-disposed to being solved on Quantum Computers. Currently, we have explored two types of instances:
 - Relaxed USA Instances
 - Generalised USA Instances

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- The algorithm portfolio $\mathcal A$ includes 16 algorithm parameter configurations for the run time T and also the time step Δt . We also are using a single path function $\lambda(t)$
- The performance metric $y \in \mathcal{Y}$ is the probability of success for the algorithm.

Research Overview - Generating GUSA Instances

Algorithm 1: Generalised USA Instances

```
Fix number of bits to n;
C = \{\}:
i = 0:
while While number of satisfying assignments > 0 do
    C_i = Three distinct bits randomly from a uniform distribution;
    i = i + 1;
    if number of satisfying assignments = 1 then
        return (n, \mathbf{C});
    else if number of satisfying assignments = 0 then
        restart:
    else if number of satisfying assignments has decreased then
        Add C_i into C;
end
Result: (n, \mathbf{C}): n variables with a set of clauses \mathbf{C}
```

Research Overview - Generating RUSA Instances

Algorithm 2: Relaxed USA Instances

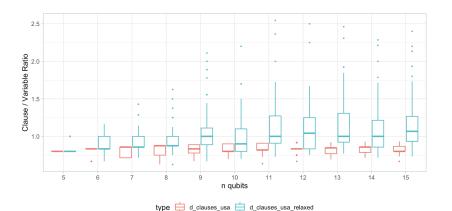
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Research Overview - f(x) Instance Characterstics

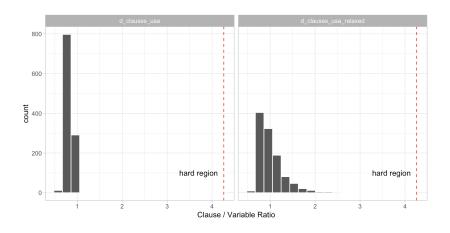
Feature Group	Feature
Problem Size	Number of variables: n
	Number of clauses: m
	Clause-to-Variable Ratio: $\frac{n}{m}$, $\frac{n}{m}^2$, $\frac{n}{m}^3$
	Inverse Clause-to-Variable Ratio: $\frac{m}{n}$, $\frac{m^2}{n}$, $\frac{m^3}{n}$
	Linearised Clause to Variable Ratio: $ 4.26 - \frac{n}{m} $, $ 4.26 - \frac{n}{m} ^2$,
	$ 4.26 - \frac{n}{m} ^3$
Variable Clause Graph	Variable Node Degree: mean, median, min, max
	Clause Node Degree : mean, median, min, max
Variable Graph	Node Degree : mean, median, min, max

Table 1: Instance Features for 3SAT Exact Cover

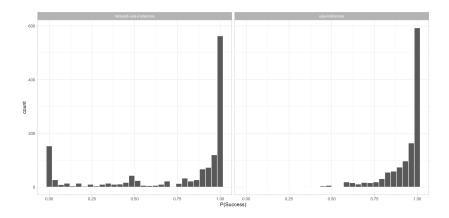
Research Overview - Distribution of Features

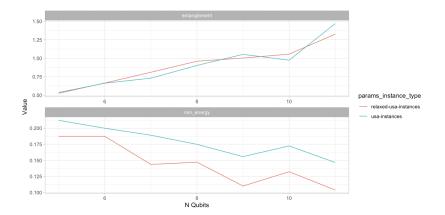


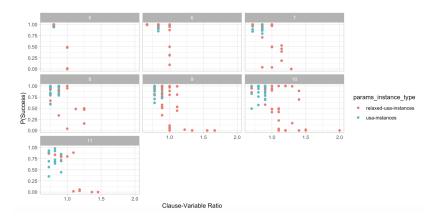
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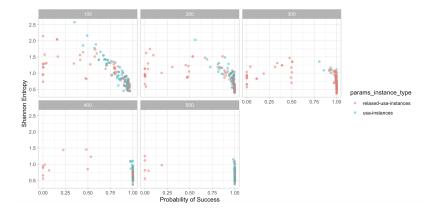
Results



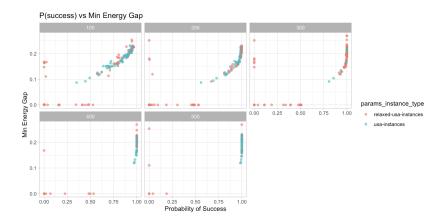


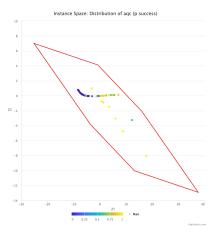


Research Overview - Entropy

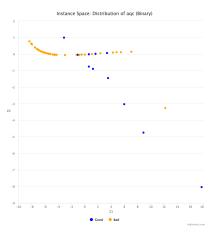


Research Overview - Minimum Energy Gap





• We set a threshold $\tau = 0.95$ for "good" or easy instances.



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- 4. Investigate the effects of randomising initial Hamiltonians

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- Apply ISA to results from QAOA and run QAOA on Universal Quantum Computer
- 8. Extend research to look at other QUBO problems

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. Rice JR, others (1976) The algorithm selection problem. *Advances in computers* 15: 5.
- 5. Smith-Miles K, Bowly S (2015) Generating new test instances by evolving in instance space. *Computers & Operations Research* 63: 102–113.

References II

- 6. Smith-Miles K, Lopes L (2012) Measuring instance difficulty for combinatorial optimization problems. *Computers & Operations Research* 39: 875–889.
- 7. 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.
- 8. Hogg T (2002) Adiabatic quantum computing for random satisfiability problems. *Phys Rev A 67 022314 (2003)*.
- 9. Young AP, Knysh S, Smelyanskiy VN (2009) First order phase transition in the quantum adiabatic algorithm. *Phys Rev Lett 104, 020502 (2010)*.
- 10. Farhi E, Goldstone J, Gosset D, et al. (2009) Quantum adiabatic algorithms, small gaps, and different paths. *arXiv preprint* arXiv:09094766.

References III

- 11. Latorre JI, Orús R (2004) Adiabatic quantum computation and quantum phase transitions. *Physical Review A* 69: 062302.
- 12. Hauke P, Bonnes L, Heyl M, et al. (2015) Probing entanglement in adiabatic quantum optimization with trapped ions. *Frontiers in Physics* 3: 21.
- 13. Lucas A (2014) Ising formulations of many np problems. *Frontiers in Physics* 2: 5.
- 14. Mandrà S, Katzgraber HG (2017) A deceptive step towards quantum speedup detection. *Quant Sci Technol 3, 04LT01 (2018)*.
- 15. 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.
- 16. Li RY, Gujja S, Bajaj SR, et al. (2019) Unconventional machine learning of genome-wide human cancer data. *arXiv preprint arXiv:190906206*.

References IV

17. Inoue D, Okada A, Matsumori T, et al. (2020) Traffic signal optimization on a square lattice using the d-wave quantum annealer. arXiv preprint arXiv:200307527.