



Quantum annealing and its variants: Application to quadratic unconstrained binary optimization

Vrinda Mehta

IAS Series
Band / Volume 59
ISBN 978-3-95806-755-4

Forschungszentrum Jülich GmbH
Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

Quantum annealing and its variants: Application to quadratic unconstrained binary optimization

Vrinda Mehta

Schriften des Forschungszentrums Jülich
IAS Series

Band / Volume 59

ISSN 1868-8489

ISBN 978-3-95806-755-4

Contents

1. Introduction	1
1.1. A general overview	1
1.2. Gate-based quantum computing	3
1.2.1. Single-qubit state	3
1.2.2. Qubit as a two-level system	4
1.2.3. Multi-qubit state	5
1.2.4. Basic operations for gate-based quantum computing	5
1.3. Quantum annealing	6
1.3.1. The adiabatic theorem	7
1.3.2. The Landau-Zener theory	8
1.4. Problem sets	9
1.4.1. 2-SAT problems	10
1.4.1.1. Creation	10
1.4.1.2. Properties	11
1.4.1.3. Ising formulation	12
1.4.2. 2-SAT-derived problems	13
1.4.2.1. Random-g problems	14
1.4.2.2. Multiple-copies problems	14
1.4.3. Fully-connected QUBO problems	14
1.4.3.1. Random problems	14
1.4.3.2. Regular problems	15
1.4.3.3. Solving the fully-connected problems	15
1.5. Our focus	16
2. Numerical methods	17
2.1. Essential operations	17
2.1.1. Single-qubit operations	17
2.1.2. Two-qubit operators	18
2.2. Solving the TDSE	20
2.2.1. Crank-Nicolson algorithm	21
2.2.2. Suzuki-Trotter product formula algorithm	22
2.3. Lanczos algorithm for solving the spectrum	25
2.3.1. Repeated minimization in two-dimensional Krylov subspace	25
2.3.2. Minimization in L-dimensional Krylov subspace	26
3. Assessing the performance of the D-Wave systems	29
3.1. Solving optimization problems using D-Wave systems	30
3.1.1. Embedding of the problem Hamiltonian	30

3.1.2. D-Wave controls	31
3.2. Results	32
3.2.1. Benchmarking the D-Wave systems	32
3.2.1.1. 18-variable 2-SAT problems	32
3.2.1.2. Random-g problems	33
3.2.1.3. Multiple-copies problems	35
3.2.1.4. Fully-connected QUBO problems	37
3.2.2. Hardness of the QUBO problems	39
3.2.2.1. Hamming distance analysis	39
3.2.2.2. Scaling analysis	40
3.3. Summary	41
4. Fair sampling	43
4.1. Forward annealing	43
4.1.1. Simulation results	44
4.1.2. D-Wave results	47
4.1.3. Perturbation theory	48
4.2. Reverse annealing	50
4.2.1. Simulation results	50
4.2.2. D-Wave results	56
4.3. Summary	60
5. Adding the trigger Hamiltonian	63
5.1. 2-SAT problems	64
5.1.1. Standard Hamiltonian	64
5.1.2. Hamiltonian with the ferromagnetic trigger Hamiltonian	66
5.1.3. Hamiltonian with the antiferromagnetic trigger Hamiltonian	68
5.2. Nonstoquastic problem Hamiltonians	74
5.3. Summary	79
6. Scaling and distribution of quantifiers of quantum annealing	81
6.1. Analysis criteria	81
6.1.1. Minimum energy gap	82
6.1.2. Success probability	82
6.1.3. Time to solution	84
6.2. Numerical results	85
6.2.1. Minimum energy gaps	85
6.2.2. Success probability	87
6.2.3. TTS99	90
6.3. D-Wave results	91
6.3.1. Success probability	91
6.3.2. TTS99	92
6.4. Summary	94

7. Modifying the initial Hamiltonian	97
7.1. Choices for the initial Hamiltonian	97
7.2. Results	99
7.2.1. Minimum energy gaps	99
7.2.2. Success probability	100
7.2.3. Scaling	103
7.3. Summary	104
8. Summary	107
Appendices	113
A. Proof of the adiabatic theorem	114
B. Uniqueness of the ground state of the annealing Hamiltonian	121
C. Pseudo-code for the Kosaraju-Sharir's algorithm	123
D. Discretizing a quantum Hamiltonian in continuous space	125
E. Error bounds	127
E.1. Crank-Nicolson algorithm	127
E.2. Suzuki-Trotter product formula algorithm	128
E.2.1. First-order approximation	128
E.2.2. Second-order approximation	129
F. Quantum simulation	131
G. Distributions	133
Bibliography	135
List of publications	147
Eidesstattliche Erklärung	149
Acknowledgements	151

IAS Series
Band / Volume 59
ISBN 978-3-95806-755-4

Mitglied der Helmholtz-Gemeinschaft

