



Universiteit
Leiden
The Netherlands

Applications of quantum annealing in combinatorial optimization

Yarkoni, S.

Citation

Yarkoni, S. (2022, December 20). *Applications of quantum annealing in combinatorial optimization*. Retrieved from <https://hdl.handle.net/1887/3503567>

Version: Publisher's Version

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/3503567>

Note: To cite this publication please use the final published version (if applicable).

Applications of quantum annealing in combinatorial optimization

Proefschrift

ter verkrijging van
de graad van doctor aan de Universiteit Leiden,
op gezag van rector magnificus prof.dr.ir. H. Bijl,
volgens besluit van het college voor promoties
te verdedigen op dinsdag 20 december 2022
klokke 11.15 uur

door

Sheir Yarkoni

geboren te Tampa, FL, USA
in 1990

Promotores: Prof. Dr. T.H.W. Bäck
Prof. Dr. A. Laat

Co-promotor: Prof. Dr. F. Neukart

Promotiecommissie: Prof. Dr. K.J. Batenburg
Prof. Dr. M.M. Bonsangue
Prof. Dr. K. Michielsen (Jülich Supercomputing Center)
Prof. Dr. C. Linnhoff-Popien (LMU München)
Dr. H. Wang
Dr. V. Dunjko

Acknowledgements

I would like to thank my supervisors, colleagues, friends, and family who supported me throughout my studies. No work of science is ever truly done alone, and everyone in my life has a part in this thesis alongside me.

Contents

Acknowledgements	i
Glossary	
1 Introduction	1
1.1 Foundations of quantum computing	3
1.2 Definitions and notation	5
1.2.1 Problem complexity	5
1.2.2 Qubits and operators	8
1.2.3 Ising models and QUBO problems	9
1.3 Families of combinatorial optimization algorithms	10
1.4 Outline	11
2 Combinatorial optimization and quantum annealing	15
2.1 Adiabatic quantum computing and the adiabatic theorem	15
2.2 Theory of quantum annealing	17
2.3 Binary and combinatorial optimization	20
2.4 Generalizing QUBO and Ising	22
2.4.1 Constrained optimization	22
2.4.2 Discrete variables	24
2.4.3 Continuous variables	25
2.5 Quantum annealing in hardware	25
2.5.1 Minor-embedding for fixed topologies	26
2.5.2 Noise and mitigation strategies	27
2.5.3 Workflow of solving problems with QPUs	29
3 Annealing control parameters and tuning	32
3.1 Combinatorial optimization on a quantum annealing processor	32

3.1.1	The maximum independent set problem	33
3.1.2	Minor-embedding and parameter settings	34
3.1.3	Benchmarking quantum annealers against classical algorithms	39
3.2	Advanced annealing controls	44
3.2.1	Tunable annealing control parameters	44
3.3	Heuristic tuning of QPU controls	47
3.3.1	Covariance Matrix Adaptation Evolution Strategy for offset tuning	47
3.3.2	Solving optimization problems with parameter tuning . . .	52
4	Real-world combinatorial optimization	59
4.1	Combinatorial optimization with real-world constraints	60
4.1.1	The shipment rerouting problem (SRP)	60
4.1.2	Constructing a MIP for the SRP	63
4.1.3	From MIP to QUBO	64
4.2	Solving real-world QUBO models	68
4.2.1	Generating SRP QUBOs from data	68
4.2.2	Comparing QUBO and MIP solvers for the SRP	69
4.3	Adapting real-world optimization problems to known QUBOs . . .	73
4.3.1	The set cover problem	74
4.3.2	Time series reconstruction as a QUBO	75
4.4	Using QUBOs to perform classification	78
4.4.1	Classifying real-world time series data	80
4.4.2	Classification benchmarking	83
5	Hybrid quantum algorithms for real-world optimization	87
5.1	Motivating a real-world traffic optimization use-case	88
5.2	Building a quantum optimization service	90
5.2.1	Bus navigation Android app	91
5.2.2	Constructing live traffic-flow QUBOs from data	92
5.2.3	Solving the traffic-flow QUBOs with quantum annealing . .	93
5.2.4	Creating the live navigation service	95
5.3	Deploying a quantum optimization service	97
5.3.1	Initial tests: Wolfsburg	97
5.3.2	Final tests: Lisbon	98
5.3.3	Web Summit 2019: Live run	99
5.4	Motivating a better real-world optimization use-case	105

5.4.1	The paint shop optimization problem	106
5.4.2	Ising model representation of MCPS	108
5.5	Creating Ising models from paint shop data	109
5.5.1	Data sources	109
5.5.2	MCPS problem sizes	110
5.5.3	Classical, quantum, and hybrid solvers	111
5.6	Benchmarking solvers in the industrial limit	112
6 Conclusions and outlook		118
Bibliography		124
Summary		139
Samenvatting		143
About the Author		147

Glossary

\mathcal{T}	Universal Turing machine.
\mathcal{Q}	Universal quantum Turing machine.
\mathbb{R}	The field of real numbers.
\mathbf{B}	The domain of Boolean values, $\{0, 1\}$.
ψ	Wave function of a single qubit.
$ 0\rangle, 1\rangle$	Qubit computational basis states in bra-ket notation.
$\sigma_x, \sigma_y, \sigma_z$	The 2×2 Pauli-x, -y, and -z spin operators.
\mathcal{H}	Generic Hamiltonian operator.
\mathcal{H}_i	Initial Hamiltonian operator for Adiabatic Quantum Computing and quantum annealing.
\mathcal{H}_f	Final Hamiltonian operator for Adiabatic Quantum Computing and quantum annealing.
τ	Timescale of evolution for a time-dependent Hamiltonian.
x	Vector of N binary variables, $x_i \in \{0, 1\}$.
\mathbf{Q}	$N \times N$ QUBO matrix for binary variables.
s	Spin variable $s_i \in \{-1, 1\}$.
h_i	Linear weight for spin variable s_i (also known as bias).
J_{ij}	Quadratic interaction term for spin variables s_i and s_j (coupling strength).
$\mathcal{U}(a, b)$	The uniform random distribution between given points a and b .

CONTENTS

$\mathcal{N}(\mathbf{0}, \mathbf{I})$	The standard multivariate normal distribution.
\log	Natural logarithm.
\log_2	Natural logarithm (base 2).
${}_n C_k$	Binomial coefficient, “ n choose k ”.