

Methods to Improve the Minimization of an Ising Objective Function

John E. Dorband, Ph.D.

University Of Maryland, Baltimore County

Dept. of Computer Science and Computer Engineering

Sept. 26, 2018

D-Wave Solution Goals

- Simulate quantum mechanical systems (physics/chemistry)
- Find the globally minimum solution of an objective function.
(Some may only be interested in a minimal solution.)

Objective function: $f(q) = \sum_i a_i + \sum_i \sum_j b_{ij} q_i q_j$

Towards the goal of finding the global minimum

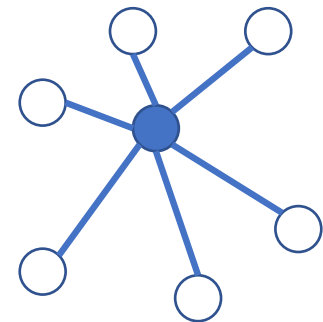
- Patch the values of bad qubits
- Find samples that are a local minimum of the objective function that correspond to each D-Wave sample
 - SQC – single qubit correction
- Find pseudo-tunnels that lead to the global minimum of the objective function
 - MQC – multiple-qubit correction
- Find a more minimal solution for an objective function with higher precision coefficients
 - HPE – high precision enhancement

Bad Qubit Value Patching

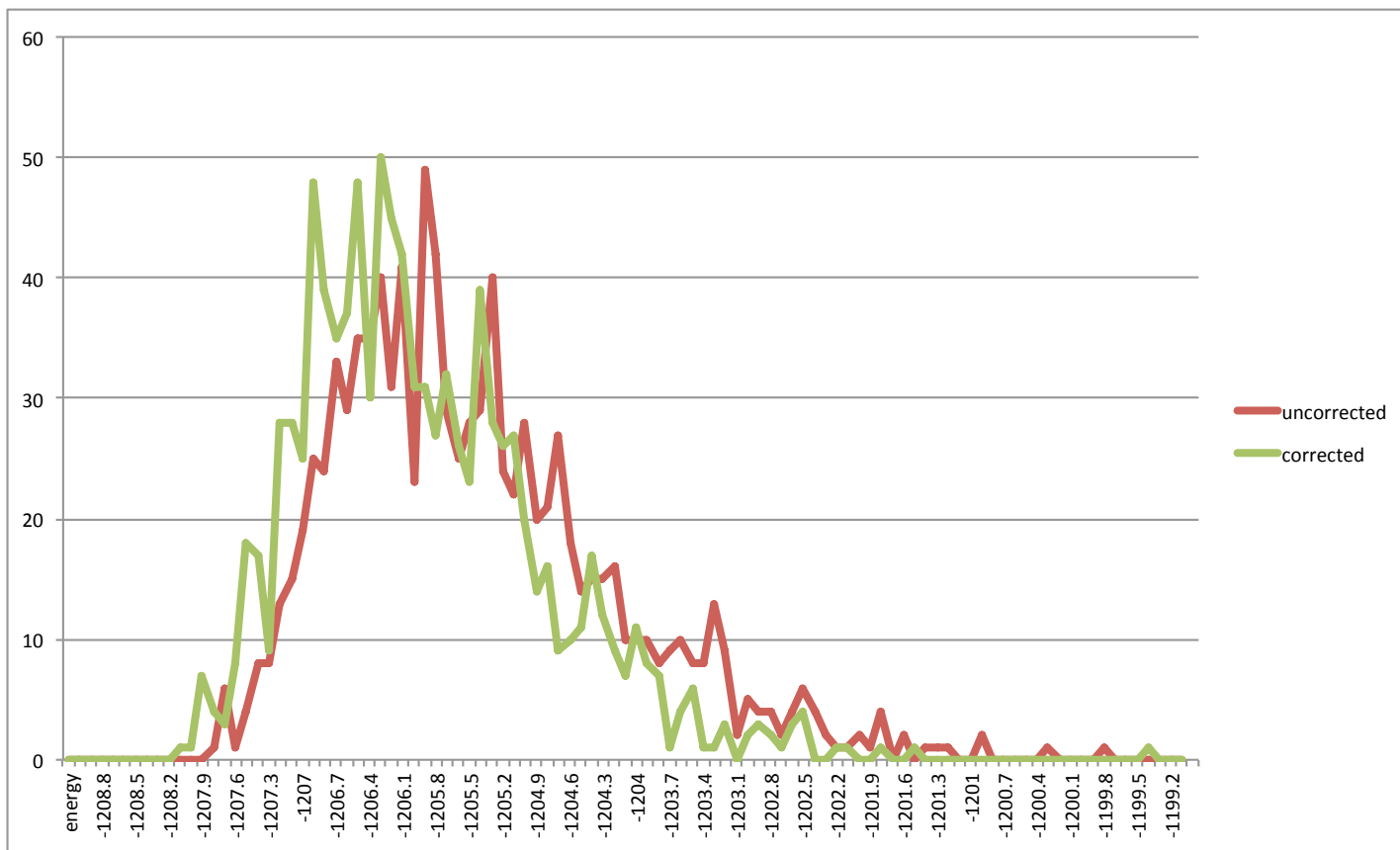
- Bad qubits are found in connected groups (of 1 or more qubits).
 - A connected group is a group of qubits that would have been connected if they were working
- For each sample a new value for the qubits of each bad qubit group is computed and included in the replacement sample.
- Given the values of the good qubits, the new values of a bad qubit group is calculated by exhaustively checking all possible set of values for the qubits of the group.
- The set of values for the bad qubits are chosen as the set of values that gives the lowest value of the objective function.

SQC – Single Qubit Correction

- Each qubit has a region of influence and an influence value associated with the region.
- If one negates the value of a qubits the value of its influence is negated.
- If the influence value is positive and the qubit value is negated, then objective value decreases
- SQC repeatedly looks for qubits that have a positive value and negates them until no more qubit with positive influence can be found
- A local minimum of the objective function has been found.



1000 samples corrected with SQC (samples generated from a set of random coefficients)



Multi-qubit Correction

MQC

MQC Anchor Problem

Quantum Adiabatic Objective Function

$$\textit{Find Minimum of: } f(q) = \sum_i a_i + \sum_i \sum_j b_{ij} q_i q_j$$

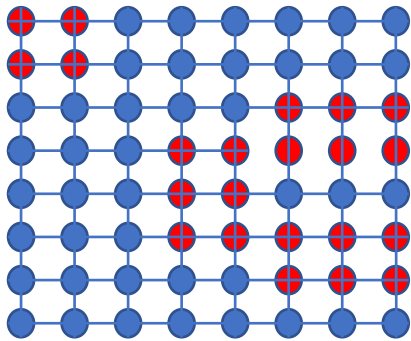
D-Wave finds small $f(q)$:

- Use D-Wave to find hints as what the minimum of $F(q)$ is.

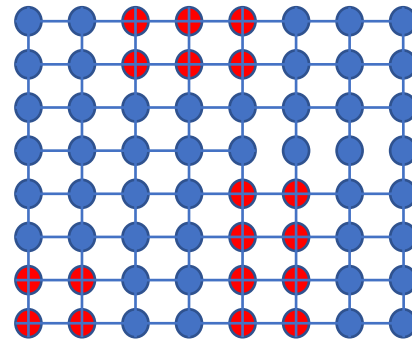
MQC Step 1

- Compare 2 samples

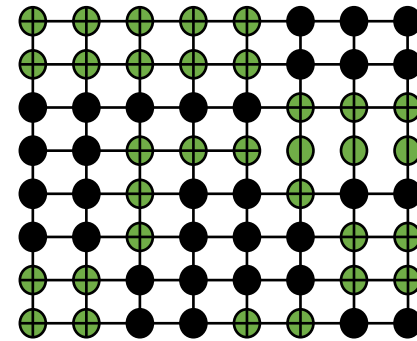
Sample 1



Sample 2



Difference flags



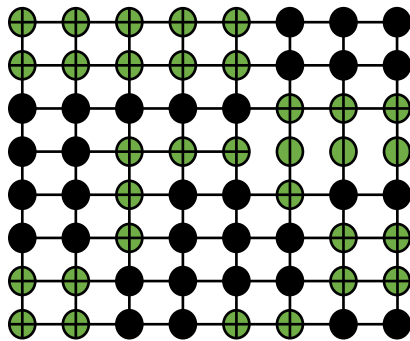
● true
● false

● same
● different

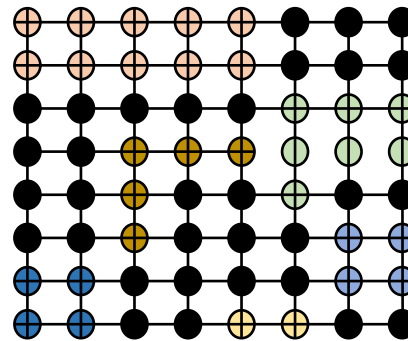
MQC Step 2

- Find independently connected groups of qubits (tunnels)

Difference flags



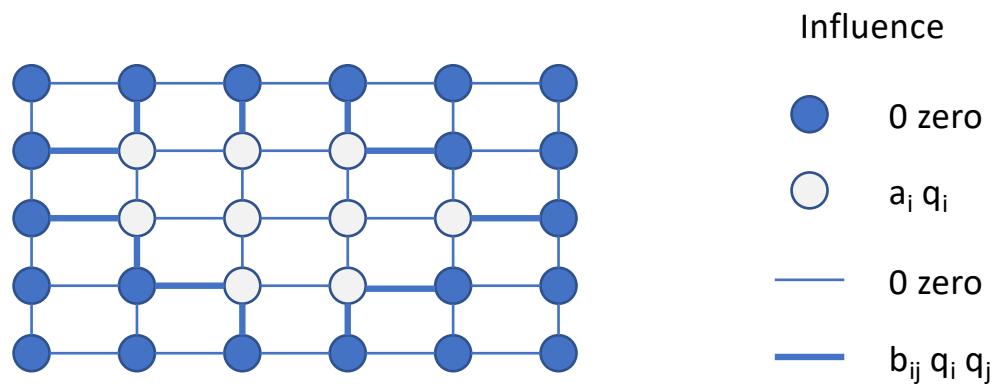
Independent Groups



- same
- different

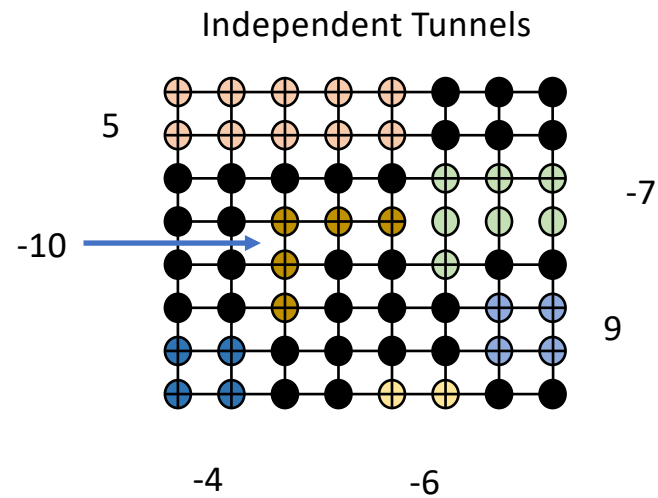
Transitively connected

MQC Tunnel Influence



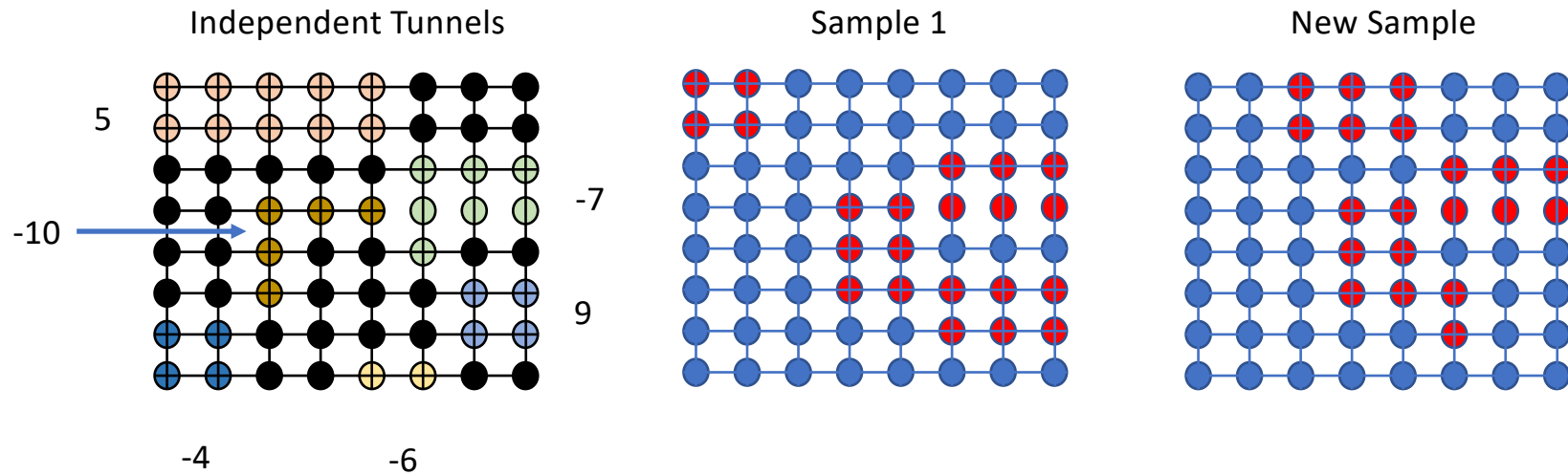
MQC Step 3

- Find which tunnels have a positive influence value.



MQC Step 4

- Flip qubits of tunnels with a positive influence value.

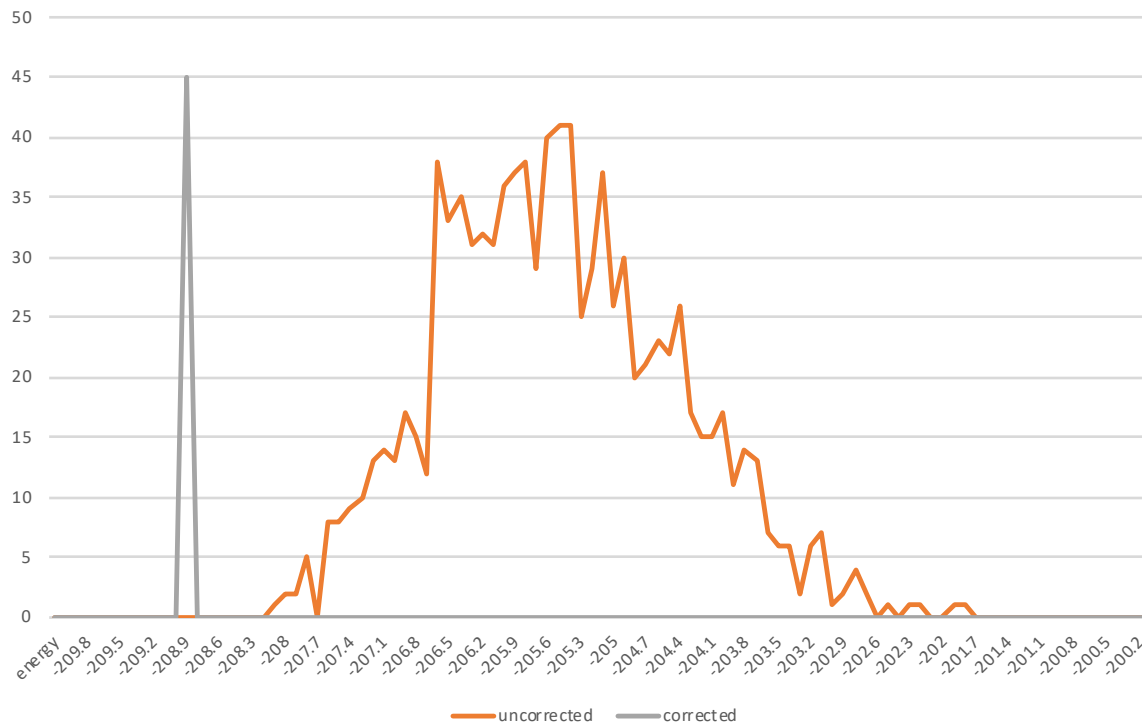


The new sample has a lower value than either sample 1 or 2.

MQC Final Reduction (for n samples)

- Pair up the n samples and form $n/2$ new samples
- Pair up the $n/2$ new samples and form $n/4$ newer samples
- Repeat until only one sample is left
- This final sample is equal to or less than the value of any of the initial samples.

1000 samples corrected with MQC
(samples generated from a set of random coefficients)



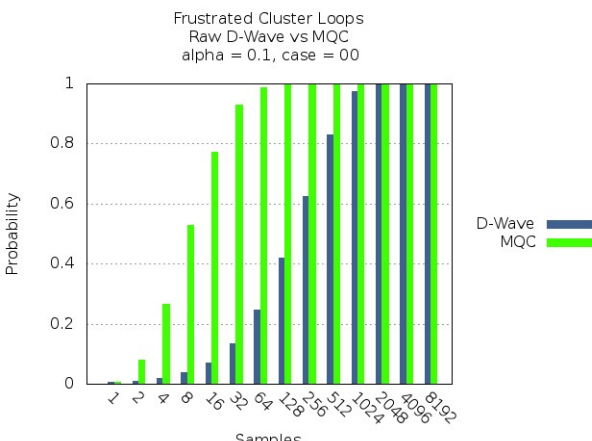
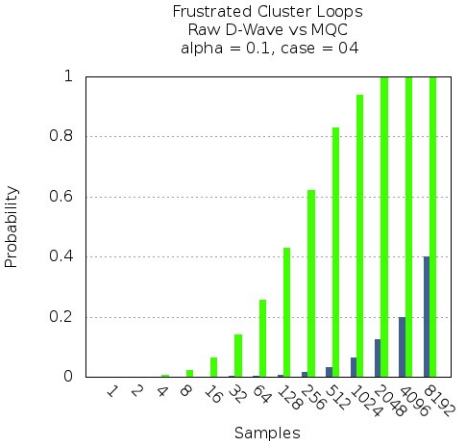
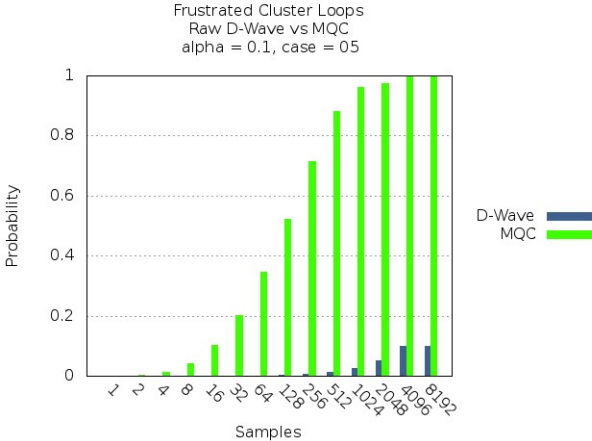
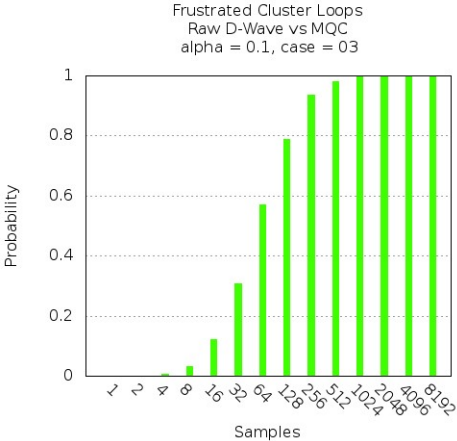
Multi-qubit Correction (MQC)

- MQC
 - Finds groups of independent groups of qubits (tunnels) that can potentially reduce the value of the objective function.
 - Determines the influence of each tunnel.
 - Finds a lower value of the objective function through lower energy tunnels.
- Use cases
 - Random objective function coefficients
 - Over 1000 cases improved the objective function value in more than 99% of the cases
 - Boltzmann machine
 - Was trained more rapidly than using the D-Wave without MQC
 - Virtual Qubits (qubit chains)
 - Verified that for all case, MQC found the global minimum

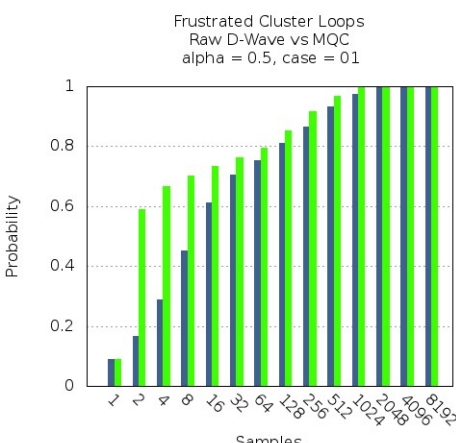
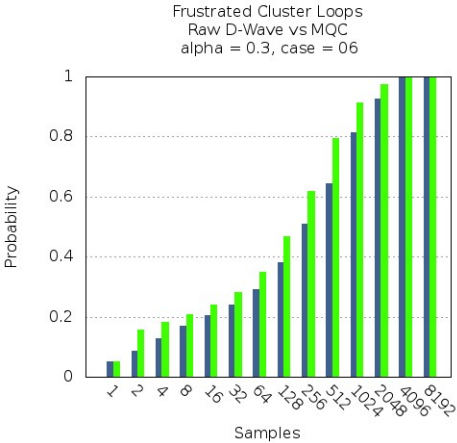
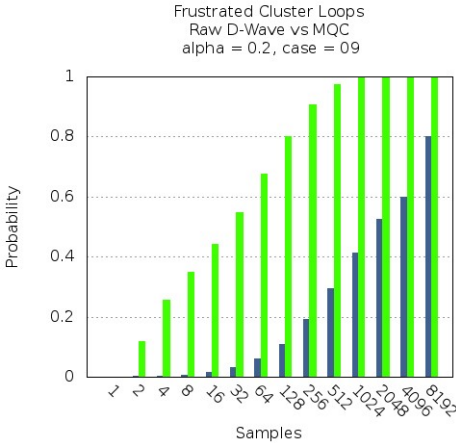
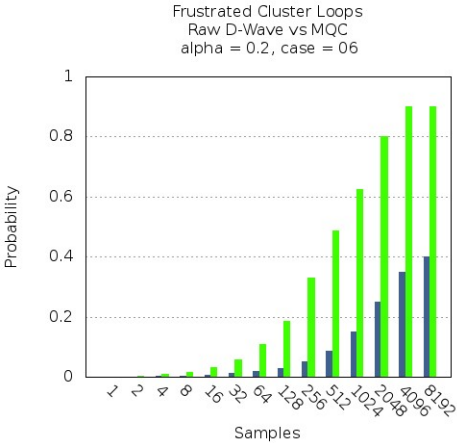
Frustrated Cluster Loops (FCL)

- An FCL is a set of qubits and corresponding coupler that form a closed loop.
- The qubit coefficients are given a value zero.
- The all couplers are given a value of -1, except one which is given a value of 1.
- Multiple loops are randomly generated ($\alpha * L_c$).
- They are added to give the final set of qubit and coupler coefficients.
- L_c Refers to a partial virtual D-Wave of size $c * c$ cells or $c * c * 8$ qubits

Comparison of Raw vs MQC FCL results



Comparison of Raw vs MQC FCL results (more)

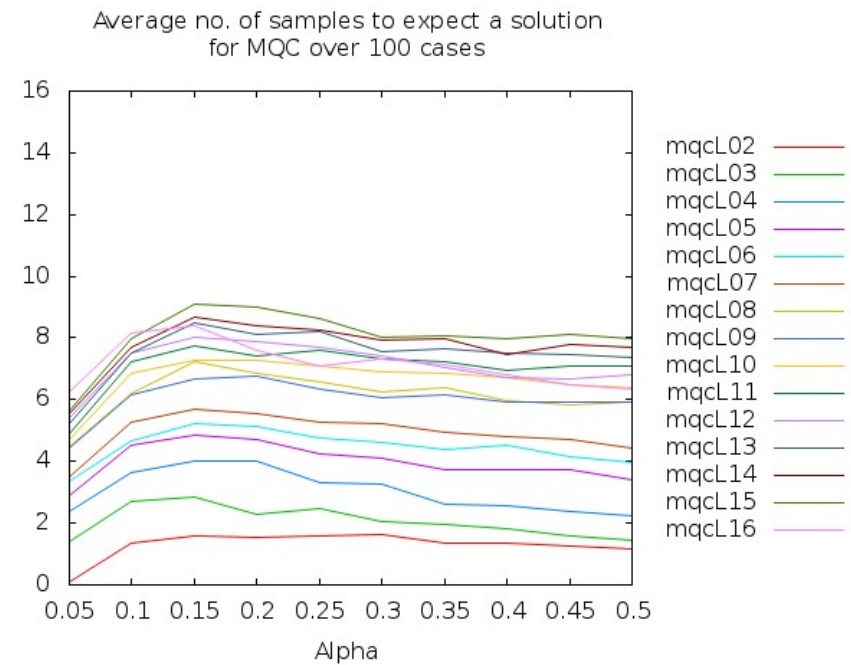
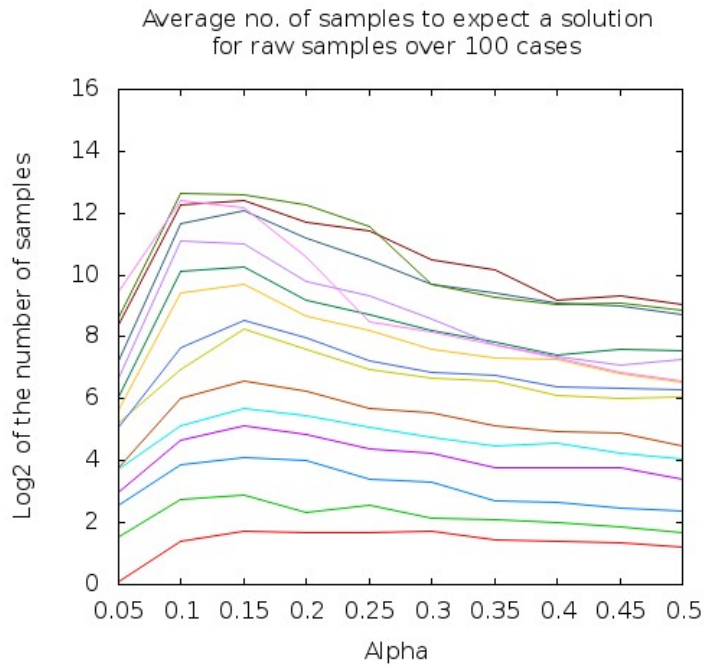


Distribution of the no. of cases solved with no. of samples

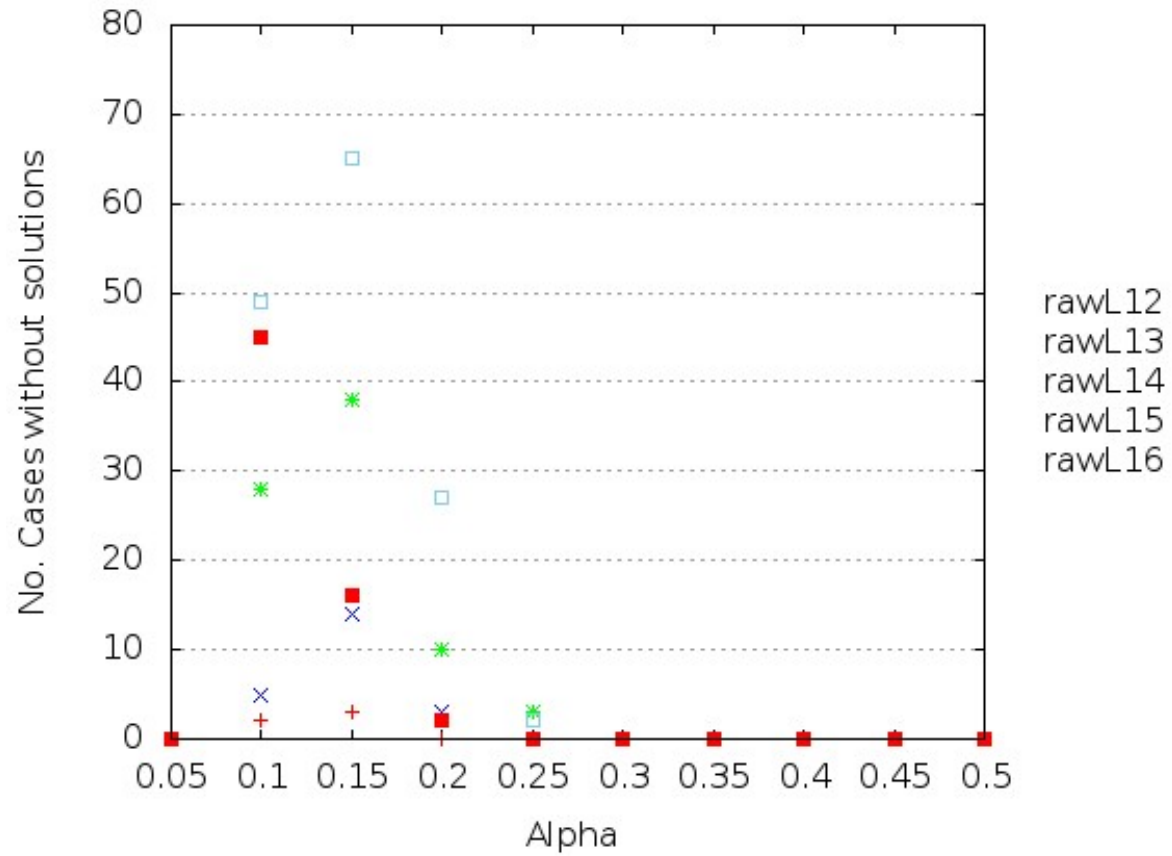
Raw samples for L_{16} and unlimited loop overlap																
No. of samples	1	2	4	8	16	32	64	128	256	512	1024	2048	4096	8192	unsolved	
Alpha = 0.05 --	0	0	0	0	0	4	5	14	32	20	16	5	2	2	0	0
Alpha = 0.10 --	0	0	0	0	0	0	0	0	0	0	7	8	12	28	0	45
Alpha = 0.15 --	0	0	0	0	0	0	0	0	0	0	14	20	20	30	0	16
Alpha = 0.20 --	0	0	0	0	0	0	0	4	13	28	30	10	6	7	0	2
Alpha = 0.25 --	0	0	0	0	0	0	4	22	43	24	5	2	0	0	0	0
Alpha = 0.30 --	0	0	0	0	0	0	4	30	45	17	4	0	0	0	0	0
Alpha = 0.35 --	0	0	0	0	0	1	15	42	28	12	2	0	0	0	0	0
Alpha = 0.40 --	0	0	0	0	0	3	26	47	18	5	1	0	0	0	0	0
Alpha = 0.45 --	0	0	0	0	1	9	38	38	13	1	0	0	0	0	0	0
Alpha = 0.50 --	0	0	0	0	3	17	36	35	9	0	0	0	0	0	0	0

MQC samples for L_{16} and unlimited loop overlap																
No. of samples	1	2	4	8	16	32	64	128	256	512	1024	2048	4096	8192	unsolved	
Alpha = 0.05 --	0	0	0	0	3	19	54	21	3	0	0	0	0	0	0	0
Alpha = 0.10 --	0	0	0	0	0	0	2	28	48	20	2	0	0	0	0	0
Alpha = 0.15 --	0	0	0	0	0	0	0	18	51	27	4	0	0	0	0	0
Alpha = 0.20 --	0	0	0	0	0	0	10	53	30	5	2	0	0	0	0	0
Alpha = 0.25 --	0	0	0	0	0	1	28	53	17	1	0	0	0	0	0	0
Alpha = 0.30 --	0	0	0	0	0	0	23	50	23	4	0	0	0	0	0	0
Alpha = 0.35 --	0	0	0	0	0	2	36	43	16	2	1	0	0	0	0	0
Alpha = 0.40 --	0	0	0	0	1	10	40	36	11	2	0	0	0	0	0	0
Alpha = 0.45 --	0	0	0	0	3	20	38	33	6	0	0	0	0	0	0	0
Alpha = 0.50 --	0	0	0	0	5	26	34	31	4	0	0	0	0	0	0	0

The Average of samples that are need to solve a case



Cases where D-Wave found no solutions.
(out of 8192 samples)



Enhanced D-Wave Coefficient Precision (HPE-Higher Precision Enhancement)

Base Expression:
$$F(q) = \sum_i a_i q_i + \sum_{ij} b_{ij} q_i q_j$$

Version Expressions:
$$F_k(q) = \sum_i c_k a_i q_i + \sum_{ij} c_k b_{ij} q_i q_j$$

$$d = \max_{ij}(\text{abs}(a_i), \text{abs}(b_{ij}))$$

$$c_0 = \frac{1}{8 * d}$$

$$c_k = c_{k-1} \sqrt{2} = c_0 (\sqrt{2})^k$$

Note: $F(q)$ and $F_k(q)$ have the same minima.

HPE-Higher Precision Enhancement Method

- Step 1: D-Wave generates samples for each version of objective function.
 - $F^k \rightarrow S^k$ where $k = 0 \dots k_{max}$
- Step 2: Create sample groups.
 - $s_h^k \in S^k$ where $h = 0 \dots samples$
 - $s_h^k \in T^h$
- Step 3: Reduce samples groups to single samples.
 - $MQC(T^h, F) = t_h$
- Step 4: Reduce single samples to a single sample group.
 - $t_h \in H$
 - $MQC(H, F) = h$
- h is the result sample from HPE for F

Enhanced D-Wave Coefficient Precision

Version constants

- c_k is intended to scale the coefficients, a_i and b_{ij} , from all being near zero for c_0 to all being either 1 or -1 for c_{max}
- As k increments from 0 to k_{max} , c_k increases by factors of $\sqrt{2}$ which is in effect a half a bit of resolution
- d = the maximum of the absolute values, a_i and b_{ij} of F

HPE Method

- 1) Create multiple versions (k=20) of the 'Base expression'.
- 2) Use D-Wave to solve each version (1000 result samples each).
- 3) Use MQC to collapse the sample results into a single result.

Bexp	Vexp	Cases	Samples	Raw<HPE	MQC<HPE	MQC=HPE	HPE<MQC
9	3	1000	1000	9	775	106	119
9	3	100	10000	1	56	28	16
17	3	100	10000	0	59	30	11
25	3	100	10000	0	56	34	10
33	3	100	10000	0	52	38	10

Base Precision(Bexp) vs. Pseudo-Hardware(Vexp) Test cases.

Bexp	Vexp	Cases	Samples	Raw<HPE	MQC<HPE	MQC=HPE	HPE<MQC
9	9	100	1000	0	0	37	63
17	9	100	1000	0	0	48	52
25	9	100	1000	0	0	45	55
33	9	100	1000	0	0	45	55
41	9	100	1000	0	0	44	56
49	9	100	1000	0	0	48	52

Base Precision(Bexp) vs. D-Wave(Vexp) Test cases.

Bexp	Vexp	Cases	Samples	Raw<HPE	MQC<HPE	MQC=HPE	HPE<MQC
dbl	dbl	100	1000	0	0	39	61

Unconstrained Base Precision vs. Unconstrained D-Wave Test cases.

References

- 2017 J. E. Dorband, "Improving the Accuracy of an Adiabatic Quantum Computer", eprint arXiv:1705.01942, May 2017.
- 2018 J. E. Dorband, "A Method of Finding a Lower Energy Solution to a QUBO/Ising Objective Function", eprint arXiv:1801.04849, Jan. 2018.
- 2018 J. E. Dorband, "Extending the D-Wave with support for Higher Precision Coefficients", eprint arXiv:1807.05244, July 2018.

Acknowledgements

- I would like thank the following for their support for this research:
 - NASA Advanced Information Systems Technology Office for grant NNH16ZDA001N-AIST16-0091
 - D-Wave through CHMPR program for time on their QPU at Burnaby, BC
 - ORNL for some of their time on the QPU at Burnaby , BC
 - NASA for time on the QPU at NASA Ames

Questions?