

# A robust approach to QUBO on the chimera topology

Witold Jarnicki

BEIT

KQIS, October 5th, 2021

## The title

A robust approach to QUBO on the chimera topology

## The plan

- Bit graph topologies (“chimera topology”)
- QUBO problem statement (“QUBO”)
- Some applications
- Obstacles for hardware
- Understanding the hardware
- Our reference solution (“robust approach”)
- Scaling up

## Naming

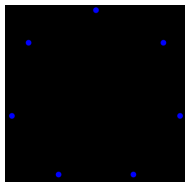
- $V$  — set of  $n := |V|$  variables (vertices, qubits).
- $K_V$  — complete graph on  $V$ .
- $E \subseteq K_V$  — topology of edges (couplings).
- $S := \{0, 1\}^n$  — bit states.

## Naming

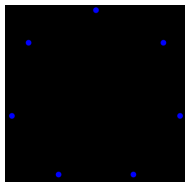
- $V$  — set of  $n := |V|$  variables (vertices, qubits).
- $K_V$  — complete graph on  $V$ .
- $E \subseteq K_V$  — topology of edges (couplings).
- $S := \{0, 1\}^n$  — bit states.

## Conventions

- $V = \{0, 1, \dots, n-1\}$ .
- $E = K_n := K_V$  — complete graph.
- $E = C_k$  — Chimera graph.
- $E = C_k^*$  — Chimera fragment.
- $E = P_k$  — Pegasus graph.



Complete graph  $K_7$



Complete graph  $K_7$

Chimera graph  $C_2$

Pegasus graph  $P_2$

## Weights

- $b : V \rightarrow \mathbb{R}$  — variable biases.
- $c : E \rightarrow \mathbb{R}$  — coupling weights.
- $2\beta \in \mathbb{R}_{>0}$  — Boltzmann distribution parameter.

## Weights

- $b : V \rightarrow \mathbb{R}$  — variable biases.
- $c : E \rightarrow \mathbb{R}$  — coupling weights.
- $\beta \in \mathbb{R}_{>0}$  — Boltzmann distribution parameter.

## State functions

- $E : S \rightarrow \mathbb{R}$  — state energy,

$$E(x) := \sum_{v \in V} b(v)x_v + \sum_{(f;g) \in E} c(f;g)x_f x_g$$

- $W : S \rightarrow \mathbb{R}_{>0}$  — state weight.
- $Z := \sum_{x \in S} W(x)$  — partition function.
- $p : S \rightarrow [0;1]$  — Boltzmann probability distribution.



## Boltzmann distribution weights

- $W(x) := e^{-E(x)}$ .
- Strongly prefers low energy states when sampling.
- May or may not find a global minimum.
- Used for Quantum Boltzmann Machines.

## Combinatorial problems

- Potentially lowest value of energy attained ( ) Boolean formula satisfied.
- SAT.
- Factorization.

# Some applications

## Combinatorial problems

- Potentially lowest value of energy attained ( ) Boolean formula satisfied.
- SAT.
- Factorization.

## Optimization problems

- Cost optimization.
- Max-variants of combinatorial problems e.g. MAX-SAT.

# Some applications

## Combinatorial problems

- Potentially lowest value of energy attained ( ) Boolean formula satisfied.
- SAT.
- Factorization.

## Optimization problems

- Cost optimization.
- Max-variants of combinatorial problems e.g. MAX-SAT.

## Boltzmann machines

“Here are some cats. Show me another cat.”

## Noisiness

- Low-order weights ignored in practice.
- No official data — needs experimental research.

# Obstacles for hardware

## Noisiness

- Low-order weights ignored in practice.
- No official data — needs experimental research.

## Topology

- Most problems cannot be directly embedded in target topology.
- Bit chaining required.

A 2-bit 2-bit 7! 4-bit factorization/multiplication circuit.  
Embedded into  $C_4$  — colors correspond to logical bits.

## Problems with bit chaining

- Low-priority chaining  $\Rightarrow$  solutions cannot be mapped to logical bits.
- High-priority chaining  $\Rightarrow$  non-solutions (noisiness).
- Strongly limits the number of bits e.g. 2048-bit  $C_{16}$  can embed at most a 65-bit clique.
- Attempts at hardware-level chaining to counter these issues (Pegasus).



## Questions

- How close to the ideal Boltzmann distribution are they?
- How close to the minimum energy they get?
- How noisy are they in general?

# Let us prove that 3 is prime

A 2-bit 2-bit 7! 4-bit factorization/multiplication circuit.

# Hardware sampling depends on more than energy

Factorize 3 by sampling the circuit 1000 times

Attempt	1	3 ( $E_{\min}$ )	3	1 ( $E_{\min}$ )	failed ( $> E_{\min}$ )
1		444		14	542
2		387		61	552
3		307		78	615
4		406		31	563
5		282		96	622
6		240		64	696
7		278		52	670
8		159		117	724
9		190		174	636
10		439		49	512

# Hardware sampling depends on more than energy

Use 10 rounds of random bit flips

Attempt	1	3 ( $E_{\min}$ )	3	1 ( $E_{\min}$ )	failed ( $> E_{\min}$ )
1		189		65	746
2		193		67	740
3		230		90	680
4		160		91	749
5		225		54	721
6		232		111	657
7		280		60	660
8		162		76	762
9		166		90	744
10		204		96	700

## Tailored example

- 2001 bits.
- Minimum theoretical energy 1000.
- 10000 samples.
- Sampled energy range [ 690; 538].
- Random bit flips do not help, either.

# Attaining minimum energy

## Tailored example

- 2001 bits.
- Minimum theoretical energy = 1000.
- 10000 samples.
- Sampled energy range [ 690; 538].
- Random bit flips do not help, either.

## However

- Not really a noisiness issue, as the theoretical energy distribution is binomial.
- Problem trivially solved by hybrid approaches involving local search.

## Boltzmann distribution

- $W : S \rightarrow \mathbb{R}_{>0}$  — state weight.
- $Z := \sum_{x \in S} W(x)$  — partition function.
- $p : S \rightarrow [0;1]$  — Boltzmann probability distribution.

## Boltzmann distribution

- $W : S \rightarrow \mathbb{R}_{>0}$   $e^{-E(x)}$  — state weight.
- $Z := \sum_{x \in S} W(x)$  — partition function.
- $p : S \rightarrow [0;1]$   $W(x)/Z$  — Boltzmann probability distribution.

## Experiment

- Set variable bias to 0.
- Sample variable 10000 times.
- Repeat 10 for 2000 qubits, resulting in 20000 frequencies.



## Boltzmann distribution

- $W : S \rightarrow \mathbb{R}_{>0}$  — state weight.
- $Z := \sum_{x \in S} W(x)$  — partition function.
- $p : S \rightarrow [0;1]$  — Boltzmann probability distribution.

## Experiment

- Set variable bias to 0.
- Sample variable 10000 times.
- Repeat 10 for 2000 qubits, resulting in 20000 frequencies.

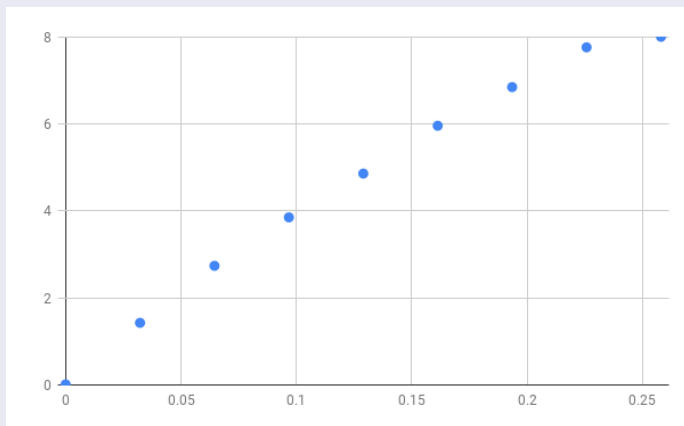
## Result

- Frequency ranging from 30% to 70%.
- Value of  $E = 0$  interpreted as one between  $[0.8; 0.8]$ .
- Resolution of  $E$  seems to be even integers, but no finer.

## Experiment

- Pick some bias values  $(b_1; \dots; b_m)$  spanning  $[0; 1]$ .
- Determine experimental probability  $p_j$  of getting value 1 by sampling multiple qubits with bias  $p_j$ ,  $j = 1; \dots; m$  (around half a million samples per  $j$ ).
- Throw away outliers with probabilities too close to 0 or 1.
- As  $p_j = \frac{1}{1 + e^{-b_j}}$ , determine the experimental value  $y_j$  of  $b_j$  by putting  $y_j := \ln\left(\frac{1-p_j}{p_j}\right)$ .
- Plot  $y_j$  as a function of  $b_j$  and use linear regression to determine  $\dots$ .

## Result



Value of  $y_j$  '  $b_j$  as a function of  $b_j$ . Experimentally, ' 32.

## Experiment

- Generate a QUBO instance on  $C_{6;16}$  choosing biases and couplings uniformly among even numbers in  $[-30;30]$ .
- Compute the minimum energy value and its probability using the exact reference solver.
- Sample 100 thousand points from the hardware implementation.

## Experiment

- Generate a QUBO instance on  $C_{6;16}$  choosing biases and couplings uniformly among even numbers in  $[-30;30]$ .
- Compute the minimum energy value and its probability using the exact reference solver.
- Sample 100 thousand points from the hardware implementation.

## Result

- The exact minimum energy of  $-12000$  has probability  $0.09$  in the Boltzmann distribution, assuming the value of  $\beta = 32$  applied to the normalized biases.
- Sampling 100 thousand points failed to produce the minimum energy value. The minimum energy attained was  $-11992$ .

## Questions

- How close to the ideal Boltzmann distribution are they?
- How close to the minimum energy they get?
- How noisy are they in general?

## Questions

- How close to the ideal Boltzmann distribution are they?
- How close to the minimum energy they get?
- How noisy are they in general?

## Answers

- Even in random cases, the probabilities seem to be off by many orders of magnitude.
- Sometimes the minimum is not found, even if the theoretical probability guarantees that.
- The noise of  $E$  seems to be on the level of 0.8, but rounding  $E$  to even integers still produces results that we cannot explain.

## Methods

- Dynamic programming on bounded treewidth graphs.
- Cannot do full  $C_{16}$ .
- Uses some ideas by Alex Selby (minimum energy value).
- Computes much more using our new approach.



# Our QUBO exact reference solver

Current state for  $C_k$ : ( $k; \cdot \geq N, k \cdot$ )

Capability	CPU	GPU
Maximum $k$	7	8
Typical runtime	1 minute	10 seconds
Minimum energy value	$O(\cdot 2^{4k})$	
Minimum energy probability	—	$O(\cdot 2^{4k})$
Minimum energy state	$O(\cdot 2^{4k})$	$O(\cdot 2^{24k})$
Boltzmann sample	—	$O(\cdot 2^{24k})$
$m$ Boltzmann samples	$O(k \cdot m + \cdot 2^{24k})$	

# Our QUBO exact reference solver

**4x16 Chimera QUBO Solver - demo version**

About us  
Our Work  
Our Code  
QUBO Solver  
Our Team  
Career  
Contact

```
512 112
0 0 0.3870967741935484
1 1 0.7060774193548387
22 22 0.25806451612903225
3 3 0.4193548387096774
4 4 0.9354838709677419
5 5 0.9632258064516129
6 6 0.89677419354838709677419
7 7 0.3870967741935484
8 8 0.3225806451612903
9 9 -0.06451612903225806
10 10 0.67419354838709677419
11 11 0.4483870967741935
12 12 0.5806451612903225
13 13 0.25806451612903225
14 14 0.967741935483871
15 15 0.219354838709677419
128 128 0.5161290322580645
129 129 0.16129032258064516
130 130 0.483870967741935
```

Submit

**Energy:**  
-10.129032135009765

**Qubits:**  
{ 0,0, 1,1, 2,2, 3,3, 4,4, 5,5, 6,6, 7,7, 8,8, 9,9, 10,10, 11,11, 12,12, 13,13, 14,14, 15,15, 128,1, 129,1, 130,0, 131,0, 132,1, 133,0, 134,1, 135,1, 136,1, 137,1, 138,1, 139,1, 140,0, 141,1, 142,0, 143,1 }

**4x16 Chimera QUBO Solver - demo version**

About us  
Our Work  
Our Code  
QUBO Solver  
Our Team  
Career  
Contact

**USAGE**

A QUBO problem description should be composed of an optional header:  
(number\_of\_qubits) (number\_of\_lines)

Followed by a content with a list of node ids and their energy values:  
(node\_id) (node\_id) (value)

**Example**

```
512 8
0 0 -1
3 3 -2
4 4 1
7 7 2
0 4 -1
3 4 -0.5
0 7 0.5
3 7 1
```

**DISCLAIMER**

THE SERVICE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT. IN NO EVENT SHALL THE AUTHORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.

Online QUBO solver demo:  
finds minimum energy value and state on  $C_{4,16}$ .

- Our exact solver does not scale that well.
- It can be used to validate hardware platforms or other heuristics.
- Biggest hope lies in hybrid local-search or MCMC solutions.

Thank you for your attention