2D Ising model sampling using D-Wave quantum annealer

Sunkyu Lee
(CPNR Collaboration)

Center for Precision Neutrino Research
Department of Physics
Chonnam National University

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D-Wave Quantum Annealer I

- D-Wave is a quantum annealer specialized for searching low energy;
  - optimization - low energy
  - **probabilistic sampling** - samples from many low-energy states
- What is quantum annealing?

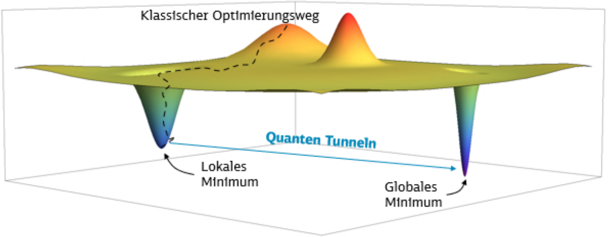


Figure: Quantum annealing in energy landscape
[https://bundesquantenallianz.de/Quantencomputing/Quantenannealer_en.shtml]

D-Wave Quantum Annealer II

- Qubit of D-Wave : superconducting loop (spin) - one or more Josephson junctions
- Zephyr topology : 20 connectivity

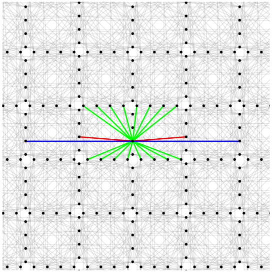


Figure: Zephyr topology; A black dot represents a qubit
[https://docs.dwavequantum.com/en/latest/quantum_research/topologies.html]

D-Wave Quantum Annealer III

Example : 2×2 2D Ising model

$$H_{\text{Ising}} = h \sum s_i + J \sum s_i s_j \tag{1}$$

$$H_{\text{QUBO}} = \sum x_i Q_{ij} x_j \tag{2}$$

under change of variable $s_i = 2x_i - 1$, $s_i \in [-1, 1]$, $x_i \in [0, 1]$

QUBO(Quadratic Unconstrained Binary Optimization) matrix
in upper triangular form

$$Q = \begin{pmatrix} 8+2h & -8 & -8 & 0 \\ 0 & 8+2h & 0 & -8 \\ 0 & 0 & 8+2h & -8 \\ 0 & 0 & 0 & 8+2h \end{pmatrix} \tag{3}$$

Motivation I

- Limitation of number of qubits and their connectivity.
  - maximized $L = 64$
  - for 2D Ising model with OBC [theoretically]
  - whereas $L =$11 or 12 with PBC
  - 4800 qubits D-Wave cloud (Zephyr topology)

$\Rightarrow$ Our idea : using D-Wave to update sub-lattice,
such as 32×32 ($l = 32$), iteratively
for larger size $L > 64$

Goal

Propose highly improved algorithm for 2D Ising model
using the **hybrid** MCMC algorithm with D-Wave annealer.

Brief steps

Brief steps are

1. **Estimate thermodynamic β from α of QUBO matrix**
   By comparing between enumeration and D-Wave sampling on sub-lattice $l \times l$

2. **D-Wave sampling + Metropolis-Hastings algorithm**
   Checkerboard method of $l \times l$ sub-lattices

3. **Measurement**
   Comparing their autocorrelations with other algorithm

β estimation I

2D Ising model Hamiltonian without external magnetic field ($h = 0$)

$$H = -J \sum_i \sum_j \left(s_{ij} s_{i+1\,j} + s_{ij} s_{i\,j+1} \right) \qquad T_c = \frac{2J}{\log(1+\sqrt{2})} \sim 2.269185J \tag{4}$$

We used 'Advantage2_system1' D-Wave cloud for this research.

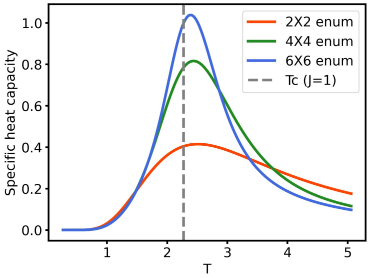
- Zephyr tolpology
- $N_{\text{qubit}} = 4800$ (4578, working Nqubit)
- annealing time $= 20\ \mu$s
- qubit temp $= 20 \pm 1$ mK
- programming thermalization time $= 1000\ \mu$s

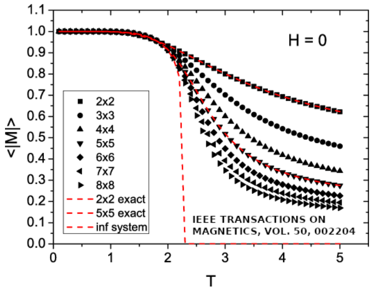
β estimation II

Firstly, we examine the maximized number, N_{block}, of $l^2 \times l^2$ blocks in QUBO matrix
(using PBC)

l	2	3	4	5	6	7	8	9	10	11
N_{block}	35	15	8	5	3	2	2	1	1	1

Chain break fraction is proportional to size of l, it is recommended to use appropriate l.





β estimation III

Estimation β from α as in

$$H = x^T Q x \; (x \in \{0,1\}), \qquad q \sim \exp\left(-\frac{\alpha\, H}{T_{\mathsf{QPU}}}\right) \tag{5}$$

For smaller $l (\leq 6)$, Boltzmann distribution p_i are given exactly by enumeration method. And for larger l, MCMC algorithms are used to estimate the probability distribution.

$$p_i = \frac{1}{Z} e^{-\beta E_i} \tag{6}$$

where Z is normalization factor and i denotes spin states $\{s_i\}$.

- KL divergence with enumeration method

$$D_{\mathsf{KL}}(p||q) = \sum_i p_i \log \frac{p_i}{q_i} \tag{7}$$

where p is from enumeration, q from D-Wave sampling

β estimation IV

- By minimizing KL divergence ($l = 4$ case)

$\alpha : 0.005$

$\beta_{\text{estimated}} : 0.040983$

$T_{\text{QPU}} : 0.122002$

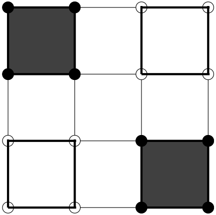
Observable	D-Wave	Exact
$\langle E \rangle$	-1.3174	-1.3174
$\langle \lvert M \rvert \rangle$	3.4548	3.4423

Energy	D-Wave Freq	Exact Prob
-24	0.12 %	0.13 %
-20	0.26 %	0.22 %
-16	1.29 %	1.21 %
-12	4.14 %	4.20 %
-8	13.85%	13.79%
-4	23.20%	23.74%
-0	31.01%	30.48%
4	17.14%	17.11%
8	6.98 %	7.16 %
12	1.6 %	1.57 %
16	0.36 %	0.33 %

- β Estimation from D-Wave is well done; But there is thermal fluctuations.

Hybrid algorithm I

Checkerboard of $l \times l$ sub lattice sampling
(ex. $L = 4$, $l = 2$ case; even ■ / odd □)



- β estimation : $(L/l)^2$s' $l \times l$ sub-lattices (OBC)
  We observe local thermal deviation on the chip
- Initialize whole lattice ($L \times L$) with D-Wave samples used for β estimation
- $n \times n$ sub-lattice update with fixed boundary condition

Hybrid algorithm II

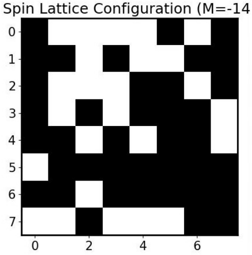
- Acceptance rate

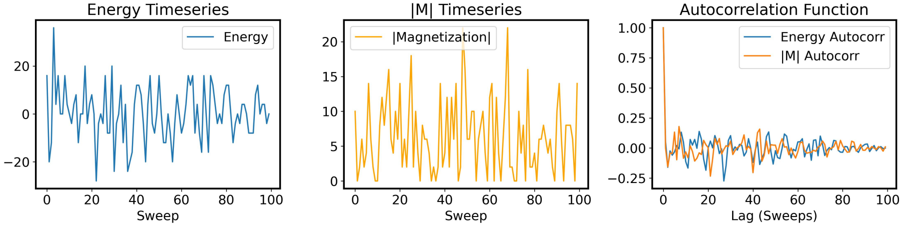
$$A(\text{old} \to \text{new}) = \text{min}\Big\{1, \exp\big[-(\beta_{\text{block},i} - \beta_{\text{avr}})\Delta E\big]\Big\} \qquad (8)$$

  where $(\beta_{\text{block},i} - \beta_{\text{avr}})$ term corrects thermal deviation(local) and fluctuation(time) of the chip.
- β update per 20 sweeps (fixed boundary condition)
  considering thermal fluctuation of the chip during calculation
- To stabilize β fluctuation from the same α, we use sufficiently large `num_reads`(=5000) and choose averaged β after repeat 3 times β estimation.

Measurement I

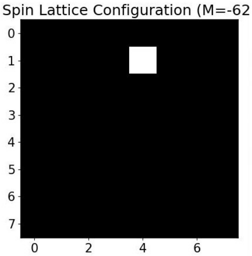
- $\beta = 0.010565$ from $\alpha = 0.001$
  $T = 94.6$ (hot)

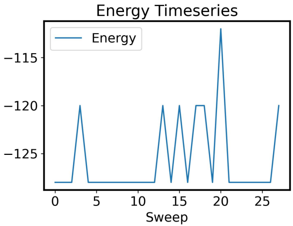


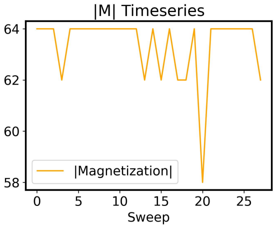


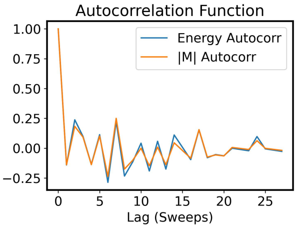
Measurement II

- $\beta = 0.728445$ from $\alpha = 0.1$
  $T = 1.37$ (cold)
  (Early stopped)









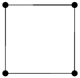
Future work I

2D Ising model

- Estimate the variance of T_{QPU} for local position on the chip over time.
- Reduce the fluctuation (dynamic embedding, Hamiltonian invariant transformation) to improve acceptance rate
- Larger size $L = 64, 128, \ldots$ with larger $l = 32$

Application to more complex theory

- Z_2 gauge theory
  - confinement



$$H = \sum s_{ij} \times s_{ij+1} \times s_{i+1j+1} \times s_{i+1j}$$

- SU(3) EFT in strong coupling limit
  - sign problem
  - finite temperature

D-Wave application to experiment I

- It can be used for DL model learning on experiment
- Through optimization of loss function
- But now it plays an assistant role; not a whole DL model training, but a part of it; because of its performance limitation.
- I'm staying tuned.

Appendix I

Target distribution is

$$\pi(x) = \frac{1}{Z_{\text{target}}} \exp\left[-\beta_{\text{target}} E(x)\right] \tag{9}$$

And the probability of QPU-proposed configuration y from x, $g(x \to y)$ is *independent* on the previous configuration x

$$g(x \to y) = p_{\text{QPU}} = \frac{1}{Z_{\text{QPU}}} \exp\left[-\beta_{\text{QPU}} E(x)\right] \tag{10}$$

Accept probability

$$p_{\text{accept}} = \min\left[1, \frac{\pi(y)g(y \to x)}{\pi(x)g(x \to y)}\right] \tag{11}$$

$$= \min\left\{1, \exp\left[-(\beta_{\text{target}} - \beta_{\text{QPU}})\Delta E\right]\right\} \tag{12}$$

Appendix II

Detailed balance

$$\pi(x)P(x \to y) = \pi(y)P(y \to x) \tag{13}$$

where $P(x \to y) = g(x \to y)A(x \to y)$