Entropy Estimation of Ferromagnetic Models via Lossless Compression

Daniel Ribeiro [1] Stefano Martiniani [2]

[1]Department of Chemical Engineering and Materials Science–University of Minnesota

[2]Departments of Physics, Chemistry, and Mathematics–New York University

Abstract

Entropy calculations are essential for determining the level of randomness of a system. Numerical methods for entropy estimation of equilibrium systems is a developing field. We apply the Lempel-Ziv 77 lossless compression algorithm to the thermodynamically equilibrated 2-dimensional Ising model configurations generated via Markov-Chain Monte Carlo (MCMC) simulations, and show that the information content of the system, measured via its computable information density (CID), is directly proportional to the entropy of the system, thus providing accurate estimates for the thermodynamic entropy. This numerical method for entropy estimation can be further applied to systems for which analytical solutions are unknown.

Introduction

Many complex systems in physics undergo phase transitions at critical temperatures. Numerically estimating the entropy of a system gives insight into the level of order and disorder of a system, and therefore the amount of information necessary to fully describe it. In ferromagnetism, a phase transition is defined as a complete loss of magnetization at some critical temperature. One such models is the 2-dimensional Ising model[1], which undergoes a second-order phase transition at critical temperature T_c, where the system's correlation length diverges. The partition function of the 2-dimensional Ising model assuming no external magnetic field was solved in 1944 by Lars Onsager[2]. Although Onsager's results are limited to the thermodynamic limit, computing thermodynamic quantities as a function of simulation progress indicates whether the system has reached thermal equilibrium. The 2-dimensional Ising lattice Λ is a binary discrete rectangular lattice with sites i. At each lattice site, there is a spin σ_i such that

$$\sigma_i \in \{+1, -1\} \, \forall \, i \, \in \, \Lambda \tag{1}$$

Below the phase transition, the lattice develops a net magnetization, as shown by Fig. 1; however above the phase transition each spin is assigned a random state due to thermal fluctuations.

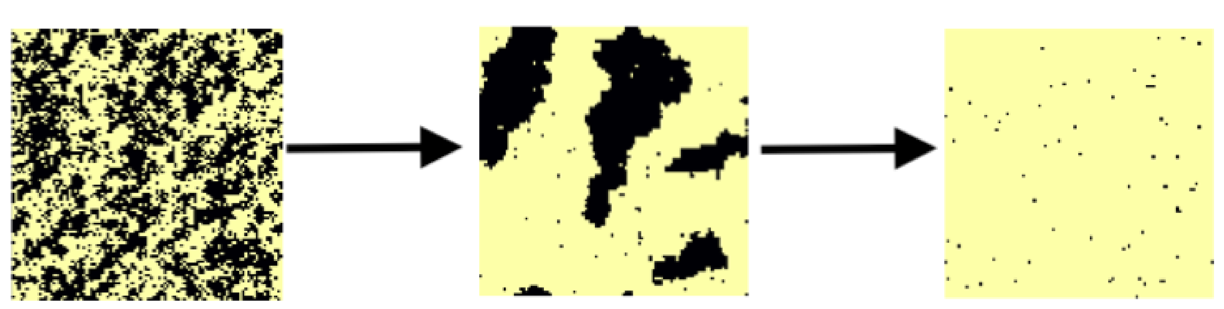

Figure 1. Thermal Equilibration for $T < T_c$

To measure the entropy of the 2-dimensional Ising model, it is necessary to generate thermally equilibrated lattice configurations. This is achieved via Markov-Chain Monte Carlo (MCMC) simulation of the system. MCMC techniques were developed to simulate systems with large configuration spaces[3]. During MCMC simulation, thermodynamic quantities are computed to track thermal equilibrium.

The average magnetization $\langle M \rangle$ is defined as

$$\langle M \rangle = \frac{\sum_{i=1}^{N} \sigma_i}{N} \tag{2}$$

The average internal energy $\langle U \rangle$ is defined as

$$\langle U \rangle = \frac{\sum_{\langle ij \rangle} \sigma_i \sigma_j}{N} \tag{3}$$

and the specific heat capacity is defined as

$$\langle C_v \rangle = \frac{\beta^2(\mathbb{E}(U^2) - \mathbb{E}(U)^2)}{N} \tag{4}$$

Generating Configurations via MCMC

Markov Chains

Thermally equilibrated configurations are generated via Markov-Chain Monte Carlo simulation of the 2-dimensional Ising model with periodic boundary conditions to minimize boundary effects. Specifically, the Metropolis single-spin flip algorithm is used[3]. Each time step of the simulation consists of a Markov state, and at every iteration, a transition probability P is used in determining whether to accept a move to a different state.

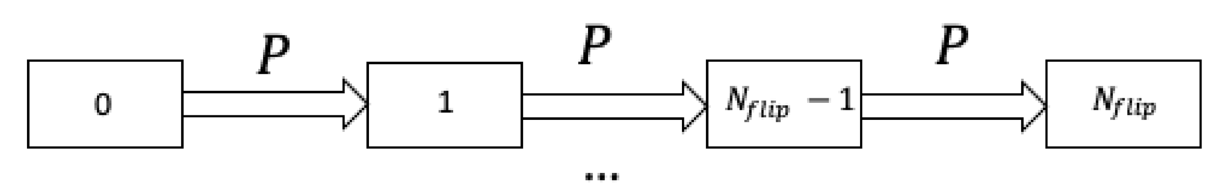

Figure 2. Illustration of a Markov chain of states

Metropolis Algorithm

In the Metropolis algorithm, a spin is selected and flipped at random, thus generating a new configuration. The acceptance probability of the new configuration is a function of the change in internal energy ΔU and temperature T

$$P(\Delta U, T) = \begin{cases} 1 & \text{if } \Delta U \leq 0 \\ \exp -\frac{\Delta U}{T} & \text{if } \Delta U > 0 \end{cases} \tag{5}$$

Hilbert Space Filling Curve

In order to compute the entropy of the lattice, a Hilbert space filling curve is used in the vectorization of the lattice to capture 2D spatial correlations.

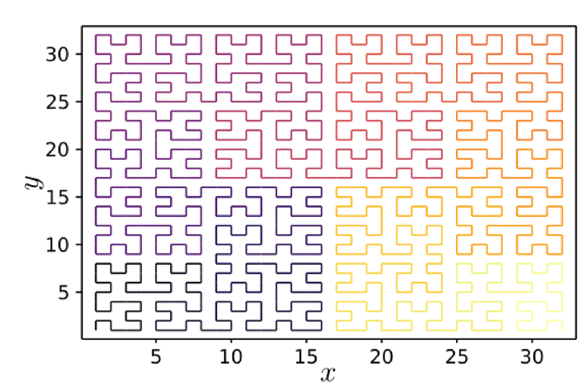

Figure 3. Hilbert space filling curve for lattice of size $L = 2^5$ x 2^5

Thermodynamic Equilibration

Thermodynamic quantities are computed during MCMC simulation to track system equilibration. Once the thermodynamic variables approximate Onsager's result, the system has reached thermodynamic equilibrium.

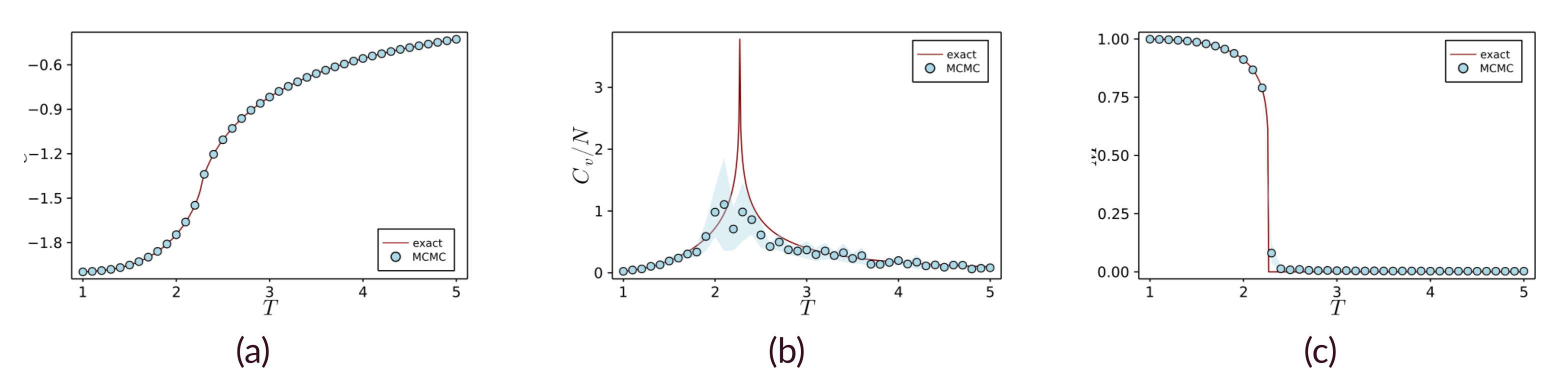

Figure 4. (4a) shows the internal energy normalized by the number of spins in the lattice for a size $L = 2^9$ x 2^9 averaged over 5 realizations. Each realization had 1 x 10^8 steps. The normalized heat capacity and magnetization are shown in (4b) and (4c) respectively. The light blue shading is the standard deviation of each thermodynamic property.

After thermodynamic equilibrium for all temperatures has been verified, it is possible to compute the CID of the lattice configurations via lossless compression, which applies the *sweetsourcod*[4] library, developed by Martiniani et al.

Lossless Compression and Entropy

Given an ensemble of microstates X, it is possible to determine the information entropy of the system as[5]

$$S = -\sum_{x \in X} p(x) \log p(x) \tag{6}$$

Shannon's entropy formula however is unfeasible for calculating the entropy of large ensembles. It becomes impossible to apply Eq. 6 if the probability of a microstate $p(x)$ is not known.

The CID is then used in the numerical computation of the thermodynamic entropy. The CID of a sequence is the size of the compressed sequence divided by the length of the sequence. Martiniani et. al. showed that the CID can be used to compute the thermodynamic entropy of a system[6]. The thermodynamic entropy is computed via

$$S = \frac{CID_{\text{lattice}}}{CID_{\text{Bernoulli}}} \tag{7}$$

A 2-dimensional Ising lattice with system size $L = 2^9$ x 2^9 was simulated using the Metropolis algorithm, and configurations were generated after thermodynamic equilibrium had been achieved and scanned with a Hilbert space filling curve. The entropy was computed using Eq. (7). Results are shown on Fig. 5.

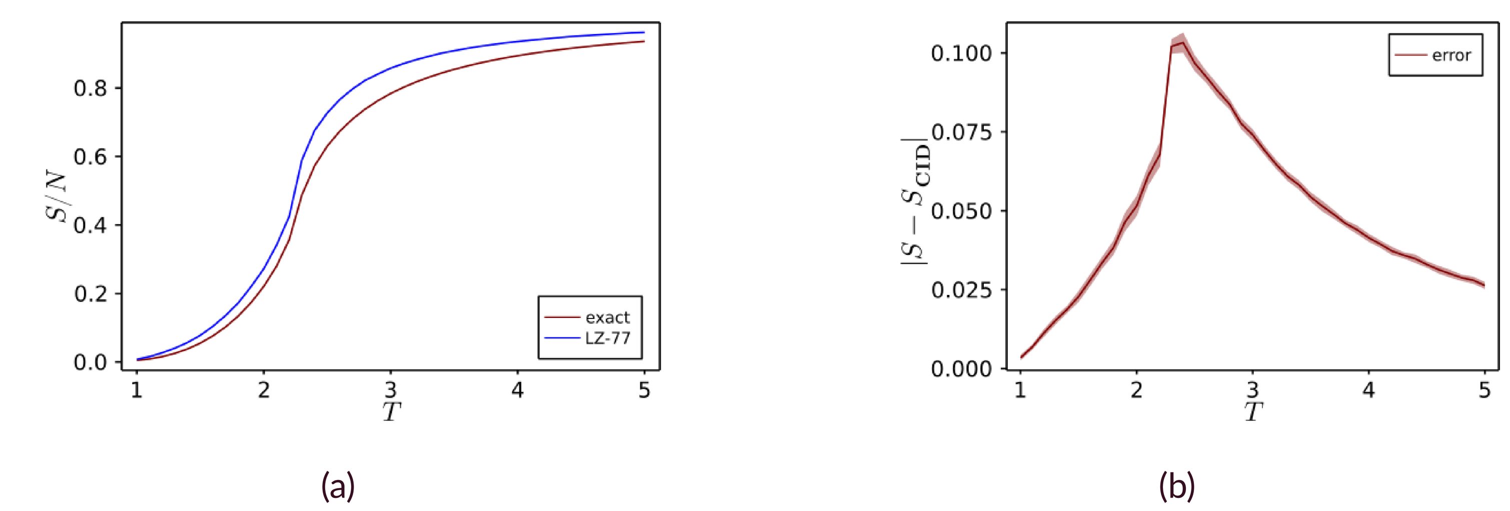

Figure 5. (5a) shows the entropy computed using Eq. 7 and the exact entropy of the 2D Ising model. The absolute error is shown in (5b)

Lossless compression of a $L = 2^7$ x 2^7 yielded a good numerical approximation of the true entropy per spin of the 2D Ising model. Lossless compression proves to be a useful technique for numerical entropy estimation.

Conclusion and Future Work

We have demonstrated that numerical entropy estimation via lossless compression is feasible for the 2-dimensional Ising model. This technique can be further applied to systems for which analytical solutions have not been derived. Lossless compression has proven a useful numerical method for entropy estimation.

References

[1] Ising E. Beitrag zur theorie des ferromagnetismus. *Z. Phys.*, 31(1):253–258, 1925.

[2] Onsager L. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Physical Review*, 65(3-4):117–149, 1944.

[3] Metropolis N., Rosenbluth A., Rosenbluth M., Teller A., and Teller E. Equation of state calculations by fast computing machines. *J. Chem. Phys.*, 21(6):1088–1092, 1952.

[4] Martiniani S. Sweetsourcod. `https://github.com/martiniani-lab/sweetsourcod`, 2018.

[5] Shannon C. A mathematical theory of communication. *The Bell System Technical Journal*, 27(3):379–423, 1948.

[6] Martiniani S., Chaikin P., and Levine D. Quantifying hidden order out of equilibrium. *Physical Review X*, 9(1):011031, 2019.