Measuring entropy using machine learning

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Efficient Entropy Evaluation Using Neural Network Estimator

INTRODUCTION

The calculation of the entropy of a physical system constitutes a critical stage in analyzing its thermodynamic properties. Much research has been carried out, endeavoring a general scheme for this calculation, yet current methods suffer from a high computational cost and inability to work on complex systems or apply to only specific systems. In our research, we developed a method based on a neural network estimator, which obtains the entropy of the physical system by an iterative calculation of the mutual information between its sub-systems.

Method

- The entropy of a system composed of two sub-systems – X_1, X_2 can be calculated by:

$$S(X_1,X_2) = S(X_1) + S(X_2) - MI(X_1,X_2)$$

- Recently, it was suggested that mutual information can be calculated using a neural network [1].
- We use a convolutional neural network to perform the mutual information estimation.
- By iteratively dividing our system, and calculating the mutual information between two sub-systems, we can calculate the entropy of the whole system.
- The entropy of the minimal sub-system (one spin for example), is calculated using simple methods.
- All the simulations were generated using a Monte Carlo simulation on 64x64 matrices of spins.

RESULTS

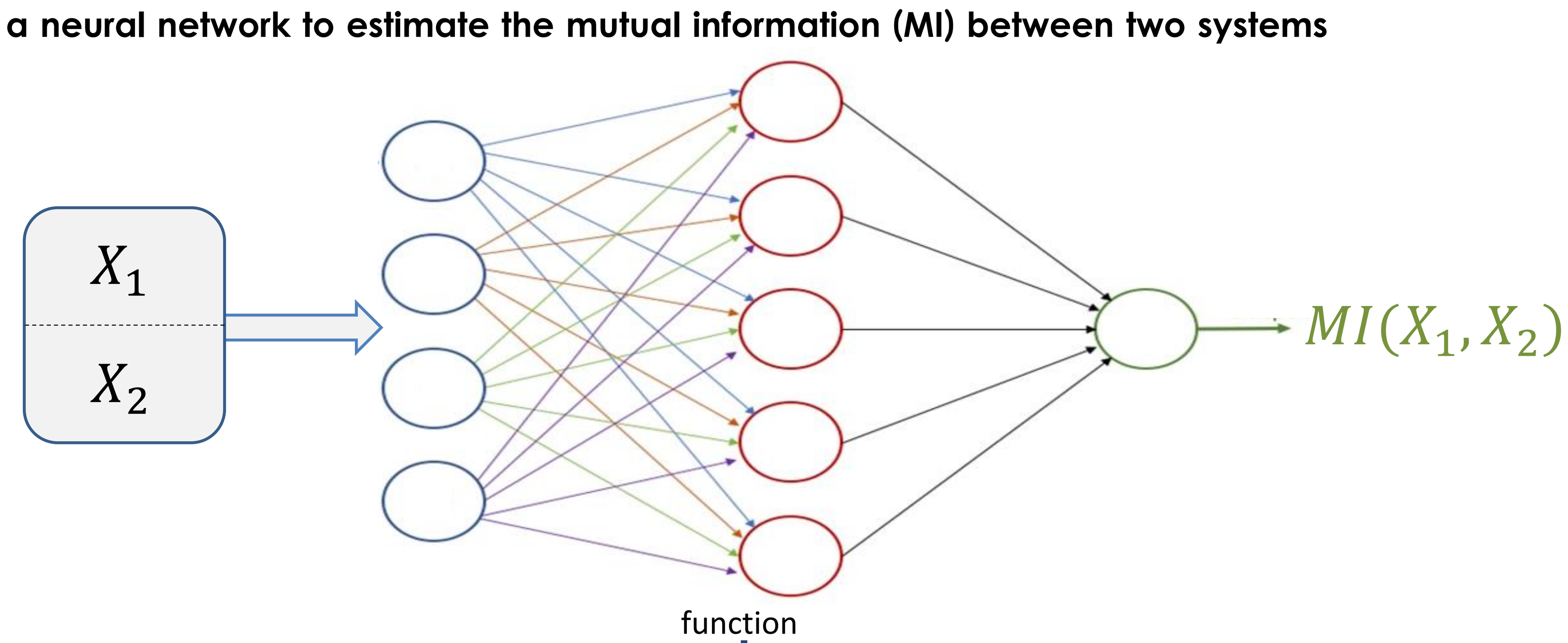
We tested our method on both discrete and continuous systems and showed that it allows for a precise calculation of the entropy with – at most – logarithmic running time. Compared to other methods, our method obtains high precision in calculating the entropy of the standard and the antiferromagnetic Ising models and the XY model with and without an external field.

Last, our network studies the physical characteristics of the system and successfully uses the knowledge gained from one system for a fast entropy calculation of supplementary systems, of various temperatures.

[1] M.I. Belghazi, A. Baratin, S. Rajeshwar, S. Ozair, Y. Bengio, A. Courville & D. Hjelm. (2018). Mutual Information Neural Estimation. Proceedings of Machine Learning Research 80, 531-540

[2] R. Avinery, M. Kornreich & R. Beck. (2019). Universal and Accessible Entropy Estimation Using a Compression Algorithm. Phys. Rev. Lett. 123, 178102.

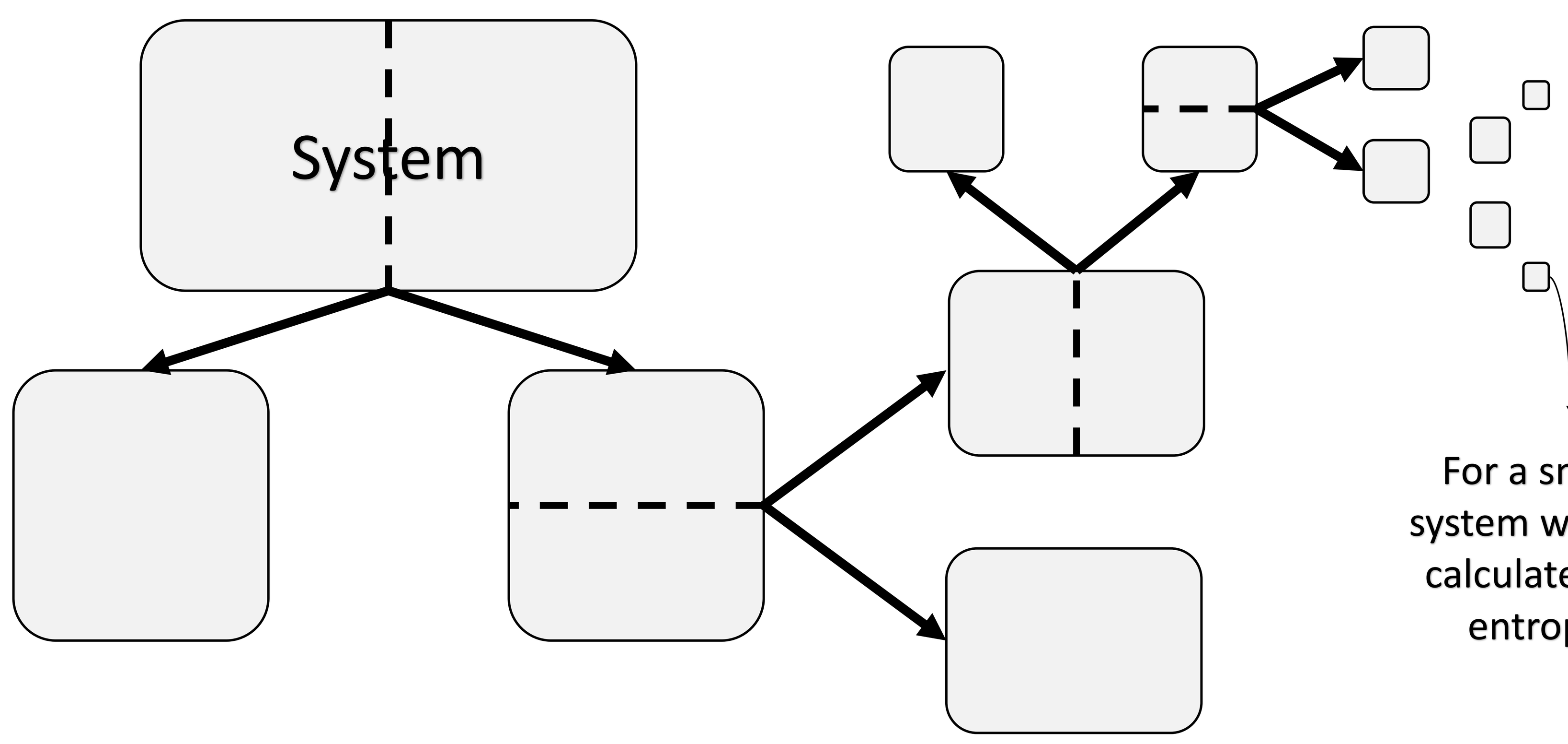
Using a neural network to estimate the mutual information (MI) between two systems



$$MI_\theta(X_1,X_2) = sup E_{P_{X_1X_2}}[T_\theta] - \log(E_{P_{X_1}\otimes P_{X_2}}[e^{T_\theta}])$$

joint distribution — marginal distribution

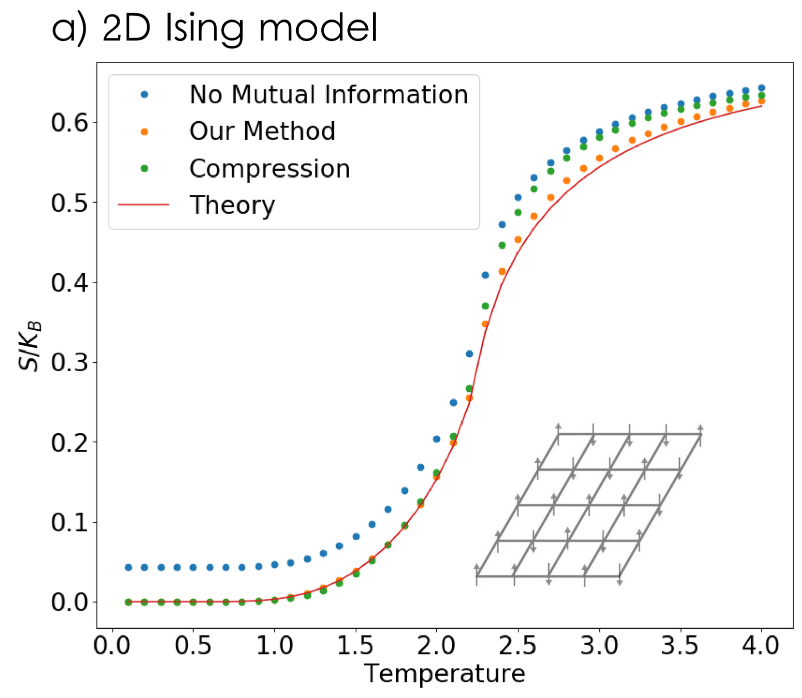
Using the calculated mutual information to calculate the system's entropy



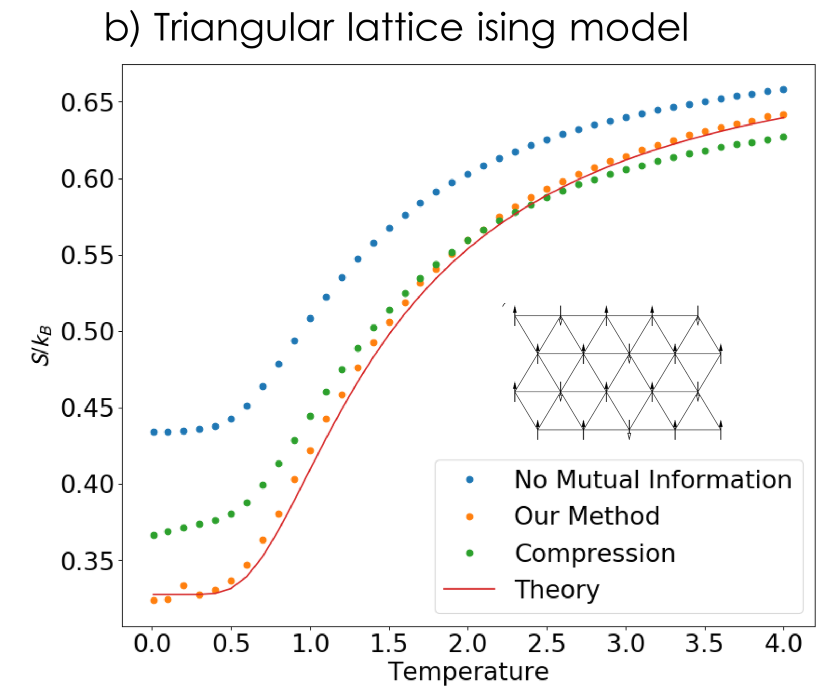
For a small system we can calculate the entropy

Calculating entropy of various systems – our method in comparison to a compression-based method[2].

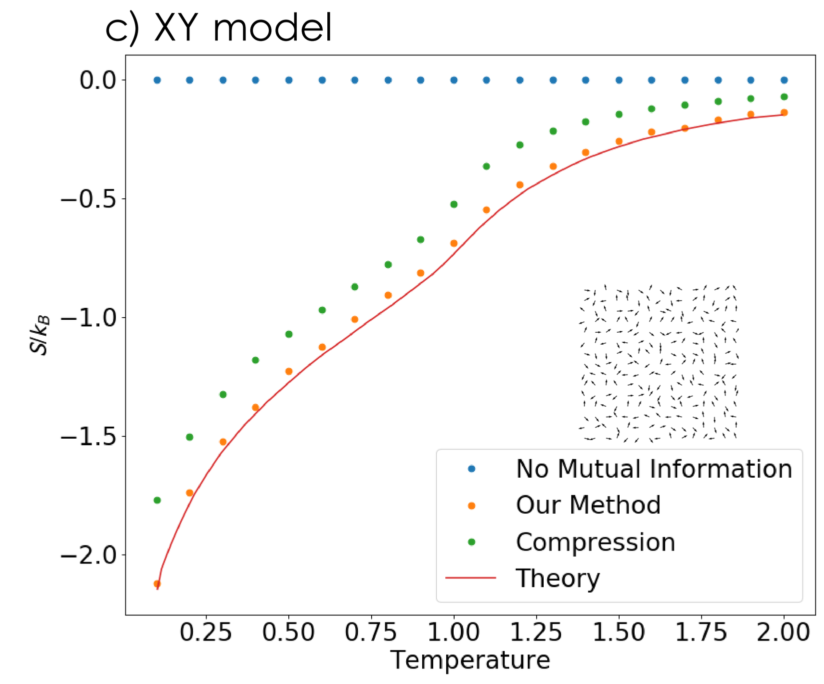
a) 2D Ising model



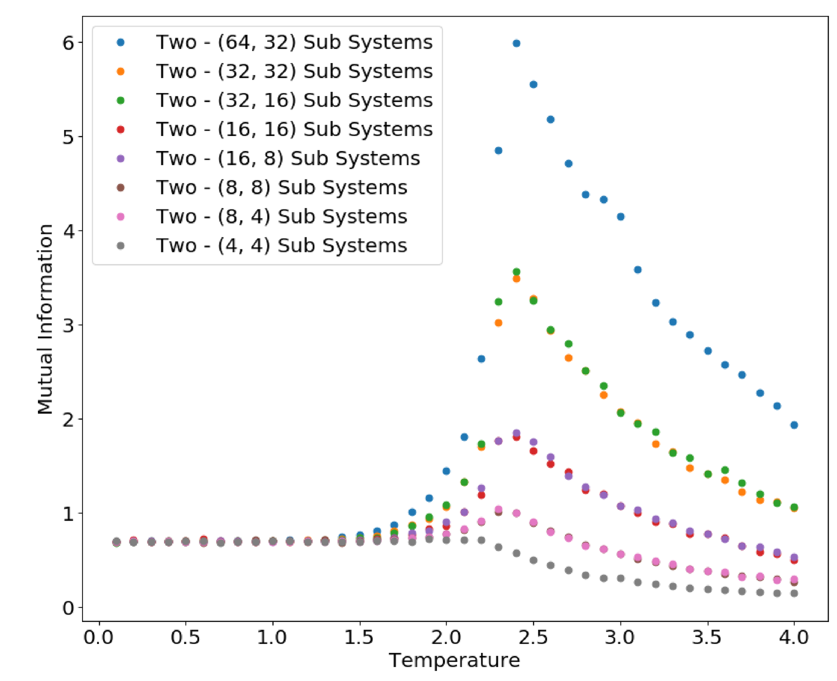
b) Triangular lattice ising model



c) XY model

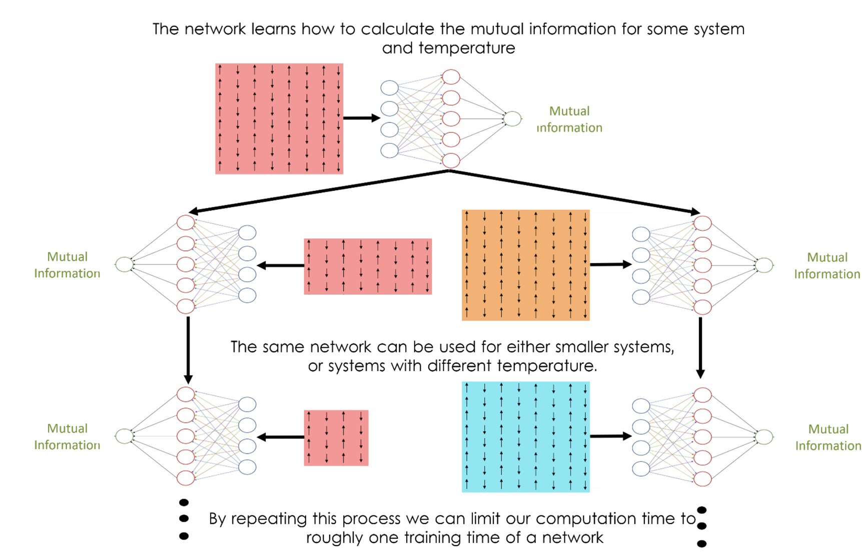


Mutual information between sub systems of different sizes

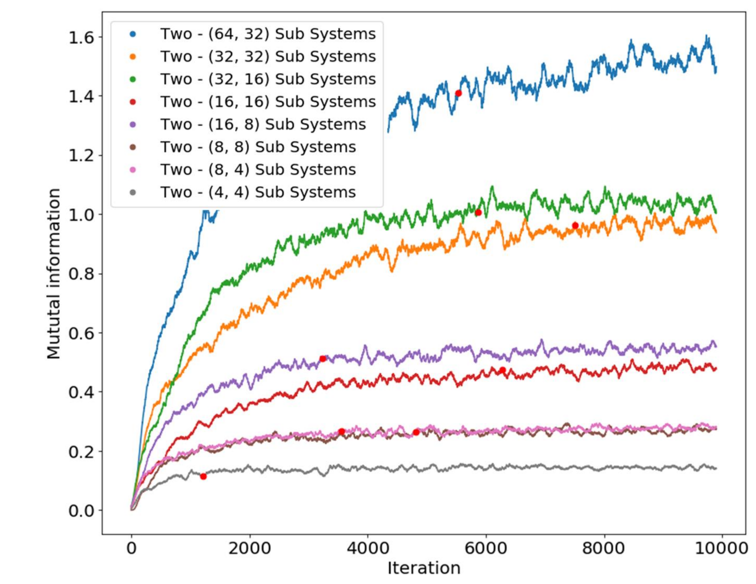


Monte-Carlo simulations on 64x64 matrix of spins

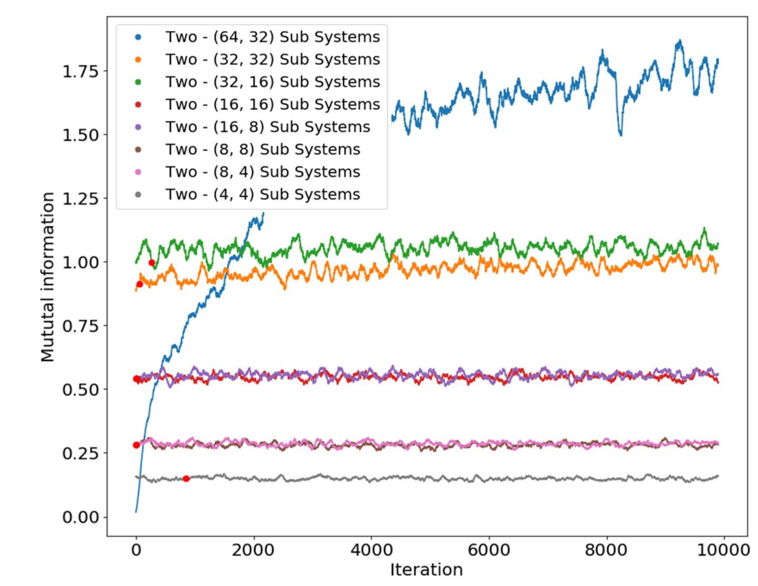
Transfer learning process



Learning process as function of iteration for 2D Ising model of various sub-systems



Without using knowledge learned on one sub-system to the next



Using transfer learning from one sub-system to another

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