Phase Diagram of the Semiclassical Boltzmann Machine at T = 0

Nicolás A. C. Carpio[1], Tiago de S. Farias[1], Celso J. Villas-Bôas[1]

Departamento de Física, Universidade Federal de São Carlos[1]

Quantum machine learning is an emerging branch that combines principles of quantum computing and machine learning, with the goal of developing algorithms that take advantage of the unique properties of quantum systems. Among these properties are entanglement, superposition, interference and tunneling , which can potentially speed up certain computations and allow the handling of data on scales that would be unattainable for classical algorithms. One of the most promising quantum machine learning architectures is the Quantum Boltzmann Machine (QBM)[1]. The QBM is an extension of the Classical Boltzmann Machine (CBM), which is a stochastic neural network model used to model complex probability distributions. While the CBM uses thermal fluctuations to explore state configurations, the QBM uses Thermal and Quantum fluctuations, which opens up new possibilities for state exploration and optimization of objective functions in high-dimensional spaces.

The study of the phase diagram of a neural network, whether classical or quantum, is crucial to understand the dynamics of the system under different conditions, optimize the network parameters to improve its performance and stability, predict how the network will respond to changes in external or internal conditions, and compare classical and quantum approaches. The learning phase is typically found at the transition between ordered and disordered phases[2], where the network can better explore and generalize real world data configurations. In this transition region, the system is flexible enough to adjust to new data configurations (disordered phase) while maintaining sufficient structure not to over fit (ordered phase).

In this study, we analyzed the phase diagram at the zero temperature limit ($T = 0$ K) for a Quantum Boltzmann Machine. Using the Suzuki-Trotter decomposition, we transformed the quantum Hamiltonian into a classical effective Hamiltonian. With the classical Hamiltonian at hand we use the replica formalism with the semiclassical and static approximations (in the Trotter direction) to analytically derive the order parameter equations in order to study the properties of the system.

We found that, in the absence of an external field, the behavior of the QBM(in the Semi classical approximation) mirrors that of the Classical Boltzmann Machine, but with quantum fluctuations playing a role analogous of thermal fluctuations. In addition, we perform an analysis of the stability of the solutions, observing a restoration of the replica symmetry, whose effect may be due to quantum tunneling between the "trapped" states, separated by infinitely high barriers in the free energy landscape[3]. In the thermodynamic limit, we also know that these barriers become much narrow as the system grows, since we have a finite area where tunneling is possible.

[1] Mohammad H. Amin, Evgeny Andriyash, Jason Rolfe, Bohdan Kulchytskyy, and Roger Melko. Quantum boltzmann machine. *Phys. Rev. X*, 8:021050, May 2018.

[2] Giancarlo Fissore. *Generative modeling : statistical physics of Restricted Boltzmann Machines, learning with missing information and scalable training of Linear Flows.* Theses, Université Paris-Saclay, March 2022.

[3] Mukherjee Sudip. Role of quantum fluctuation in inducing ergodicity in the spin glass phase and its effect in quantum annealing. *Phil. Trans. R. Soc.*, 38, Jan 2023.