

Quantum Scalar Field Theoretic Extension of Boltzmann Machines to Solve a Class of Moment Matching Problems

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Background

The Boltzmann machine is a generative machine learning model originated from the toy model of magnetic materials in statistical mechanics. It can approximate a probability distribution by adjusting the set of potential parameters and the number of units. In particular, over the last decade, there has been a significant amount of research on approximating ground state wave functions of quantum many-body systems via the Boltzmann machine. However, in order to achieve high expressive power, it is inevitable to increase the number of units. The computational complexity of the total variation distance between a target distribution and the Boltzmann machine is known to be NP-hard [1], hence we have to develop alternative methods to obtain the scalability. In this research, I generalize the Boltzmann machine and prove that it gives a solution of some moment matching problems without increasing the number of units, by utilizing the result of constructive quantum field theory.

My contribution

Firstly, we introduce the Scalar Field Machine (SFM) as a generalization of the Boltzmann machine, originated from ϕ^4 scalar field model in constructive quantum field theory:

$$\gamma_N^{\beta, m, J} = \frac{1}{Z_N} \exp \left[- \sum_{i=1, \dots, N} \beta_i \left(\phi_i^2 - m_i \right)^2 + \sum_{i=1, \dots, N-1} J_{i,i+1} \phi_i \phi_{i+1} \right]$$

The main modifications from ordinal Boltzmann machines are as follows:

- We extend the spin variable ϕ from $\{0, 1\}$ values to \mathbb{R} values.
- The reference measure is not limited to the Gaussian, allowing for multimodality.
- If the distribution to be approximated is N -dimensional, the number of units in the learning model is also fixed at N .

Our main theorem is as follows. The proof utilizes techniques cultivated in rigorous statistical mechanics and constructive quantum field theory.

Theorem. Let $C_i > 0$, $C_N = 0$, $M_i > 0$ for $i = 1, \dots, N$ and $\{X_i\}_{i=1, \dots, N}$ be the set of random variables distributed from the target N -dimensional two-modal symmetric distribution μ such that

$$\mathbb{E}[\mu] \left[X_i^2 \right] = M_i, \quad \mathbb{E}[\mu] \left[X_i X_{i+1} \right] = C_i.$$

Then, there exists a SFM $\gamma_N^{\beta, m, J}$ that satisfies the all above-mentioned conditions.

Application (Approximation of entangled dynamics).

As an application, we demonstrate that short-time entangled behavior of the dynamically decoupling quantum harmonic oscillators can be approximated by the SFM. The dynamics is constructed via the stochastic quantization, which is equivalent to the canonical quantization [2]. However, for long-time dynamics, the SFM approximation begins to break down, hence it needs to update the distribution successively. The optimal update rule for this is currently under investigation.

References

- [1] A. Bhattacharyya, S. Gayen, et al. "Computational explorations of total variation distance," ICLR 2025.
- [2] N. C. Petroni and L. M. Morato, "Entangled states in stochastic mechanics," J. Phys. A. 33, 5833 (2000).

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