Benchmarking Quantum Boltzmann Machines on physical Gibbs states

Enrico Rinaldi, Yuta Kikuchi, Matthias Rosenkranz
Quantinuum

Ryuji Sakata
Panasonic Holdings Corporation

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Gibbs states play central roles in understanding the equilibrium properties of quantum many-body systems, and also find applications in optimization [1] and machine learning [2, 3], where they are known as quantum Boltzmann machines (QBMs). The Gibbs state represents the canonical ensemble, specified by the Hamiltonian H and inverse temperature β, and describes a thermal system attached to a thermal bath. A thermal state for a quantum many-body system is described by a density matrix,

$$\rho_\beta := \frac{\mathrm{e}^{-\beta H}}{Z} = \frac{\sum_n \mathrm{e}^{-\beta E_n} |E_n\rangle \langle E_n|}{Z}, \qquad Z := \mathrm{Tr}[\mathrm{e}^{-\beta H}] = \sum_n \mathrm{e}^{-\beta E_n} \tag{1}$$

where $\{E_n, |E_n\rangle\}_n$ are the pairs of eigenvalue and eigenstate for the Hamiltonian H, i.e, $H|E_n\rangle = E_n|E_n\rangle$. The Gibbs state (1) is given by a sum of energy eigenstates $|E_n\rangle\langle E_n|$ weighted with the Boltzmann factor $\mathrm{e}^{-\beta E_n}$. The state is normalized by the partition function Z so that $\mathrm{Tr}[\rho_\beta] = 1$ is satisfied.

We investigate the performance of a parameterized QBM, used as a quantum generative model [2, 3]. More specifically, provided access to the target distribution η, we attempt to learn this target by training the QBM model, with the goal of being able to later sample from it. The expressivity of the model relies on the form of the Hamiltonian H that we choose. The fact that the model Hamiltonian may contain non-commuting terms can make QBM more expressive than the classical Boltzmann machine [3, 4]. We emphasize that, in stark contrast to many other quantum machine learning models, training the QBM with an appropriate choice of objective function does not suffer from the vanishing gradient problem, dubbed Barren Plateaus in quantum machine learning community [5], as shown in [6].

We numerically investigate the performance of QBMs for different target Gibbs states, model Hamiltonians, training parameters, and training strategies. We have developed a software package [7] that performs the QBM training with various combinations of target, model, and parameters using exact diagonalization on classical computers. Using this software, we can conveniently benchmark the QBM training performance of different models and on different Gibbs states, and the GitHub repository [7] contains results for the 1D transverse-field Ising (TFI) model, the 1D Heisenberg model, the 1D Hubbard model, the 2D Hubbard model, and the 1D J_1-J_2 model.

We consider a quantum Boltzmann machine defined in the form

$$\rho_\theta = \frac{\mathrm{e}^{H_\theta}}{Z}, \qquad H_\theta = \sum_{i=1}^{m} \theta_i h_i, \tag{2}$$

where the parameterized Hamiltonian H_θ has m real parameters θ_i and bounded orthogonal Hermitian operators h_i acting on a 2^n-dimensional Hilbert space.

Target Gibbs states and QBM models are given in the forms of $\mathrm{e}^{-\beta H}/\mathrm{Tr}[\mathrm{e}^{-\beta H}]$ (1) and $\mathrm{e}^{H_\theta}/\mathrm{Tr}[\mathrm{e}^{H_\theta}]$ (2), respectively, where β is the inverse temperature and θ stands for a set of training parameters. The Hamiltonians H can be selected from an existing list in our package or can be coded up easily to extend the package (We welcome pull requests on this open source package).

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