Certificates of many-body quantum properties assisted by machine learning

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In physics and optimization, computationally intractable tasks are often encountered. Among the various approaches to tackle such problems, relaxation techniques have been proposed to approximate the feasible set from outside, leveraging efficient descriptions of the relaxed set, thus providing bounds to the optimal solution. In this work, we propose a novel approach combining the power of relaxation techniques with deep reinforcement learning to find the best possible bounds within a limited computational budget. We illustrate the viability of the method in the context of finding the ground state energy of many-body quantum systems, a paradigmatic problem in quantum physics. We benchmark our approach against other classical optimization algorithms and we characterize the effect of transfer learning to find it may be indicative of phase transitions, with a completely unsupervised approach. Finally, we provide the tools to generalize the approach to other common applications in the field of quantum information processing.

INTRODUCTION

We propose a scheme combining Reinforcement Learning (RL) with relaxation techniques. We illustrate the process in the context of approximating the ground state energy of local Hamiltonians, which can be expressed as a semi-definite program (SDP).

\[ E_0 = \min \rho \sum_j \text{Tr}[\rho H_j] \]

subject to:

- \( \rho \geq 0 \)
- \( \text{Tr}[\rho] = 1 \)
- \( \rho \) compatibility constraints

Compatibility constraints can be strengthened or loosened yielding different relaxations. Stronger constraints tend to yield better certificates, although, some provide high quality at a lower cost. We propose a scheme in which a RL agent finds the optimal relaxation within a computational budget.

RESULTS

We showcase the applicability of the proposed framework with the 1D Heisenberg model with periodic boundary conditions.

\[ H = J \sum_j \sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + B \sum_j \sigma^z_j \]

The model presents a phase transition at \( B/J=2 \). We emphasize that the RL agent is never provided with explicit information about the physical problem at hand, being a completely unsupervised approach. Already for such a simple model, we find a wide plethora of different optimal relaxations even within the same phase of the Hamiltonian.

CONCLUSIONS

- Meta-optimization applicable to other areas of quantum information based on finding outer approximations to convex sets.
- Non-trivial solutions even in simple and reduced systems.
- Transfer learning can be leveraged to infer properties of the physical system at hand (completely unsupervised).

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