Certificates of many-body quantum properties assisted by machine learning

Borja Requena[1], Gorka Muñoz-Gil[1], Maciej Lewenstein[1,2], Vedran Dunjko[3], Jordi Tura[4,5]

[1]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Av. Carl Friedrich Gauss 3, 08860 Castelldefels (Barcelona) Spain

[2]ICREA, Pg. Lluis Companys 23, 08010 Barcelona, Spain

[3]LIACS, Leiden University, Niels Bohrweg 1, 2333 CA Leiden, Netherlands

[4]Max-Planck Institut für Quantenoptik, Hans-Hopfermann-Str. 1, 85748 Garching, Germany

[5]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

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).

$$\begin{aligned} E_0 = \quad & \min_{\rho_i} \sum_i \mathrm{Tr}\left[\rho_i H_i\right] \\ \text{s.t.} \quad & \rho_i \geq 0 \\ & \mathrm{Tr}\left[\rho_i\right] = 1 \\ & +\rho_i \text{ compatibility constraints} \end{aligned}$$

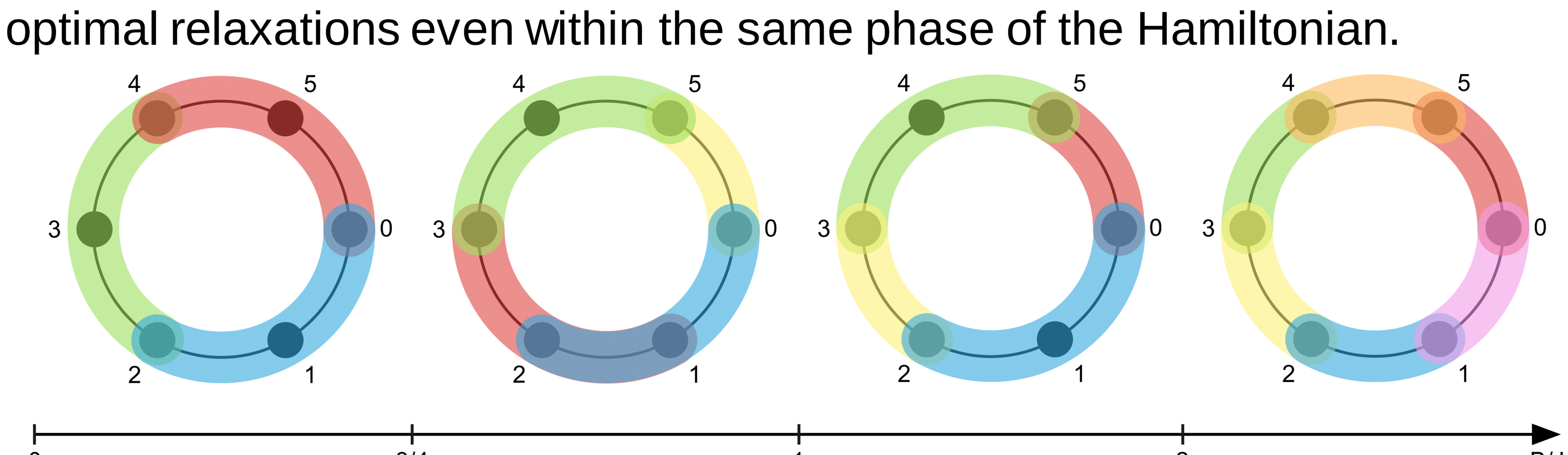
Compatibility constraints can be strengthened or loosened yielding different relaxations. Stronger constraints tend to yield better certificates, although, some provide high quality at a lower cost. We propose a scheme in which a RL agent finds the optimal relaxation within a computational budget.

RESULTS

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

$$H = J\sum_i \sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + B\sum_i \sigma_i^z$$

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.

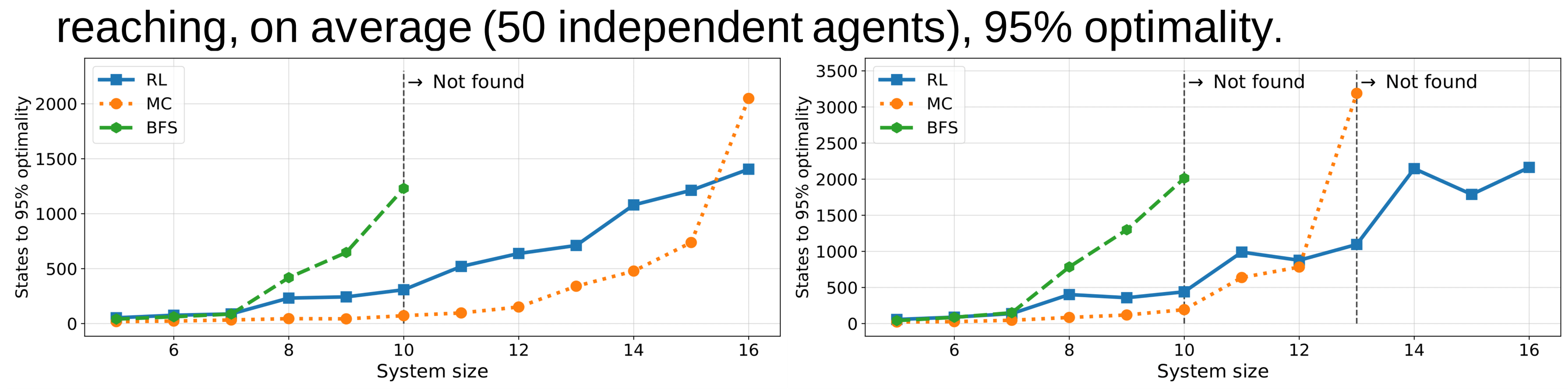


CONCLUSIONS

- 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).

BENCHMARKING

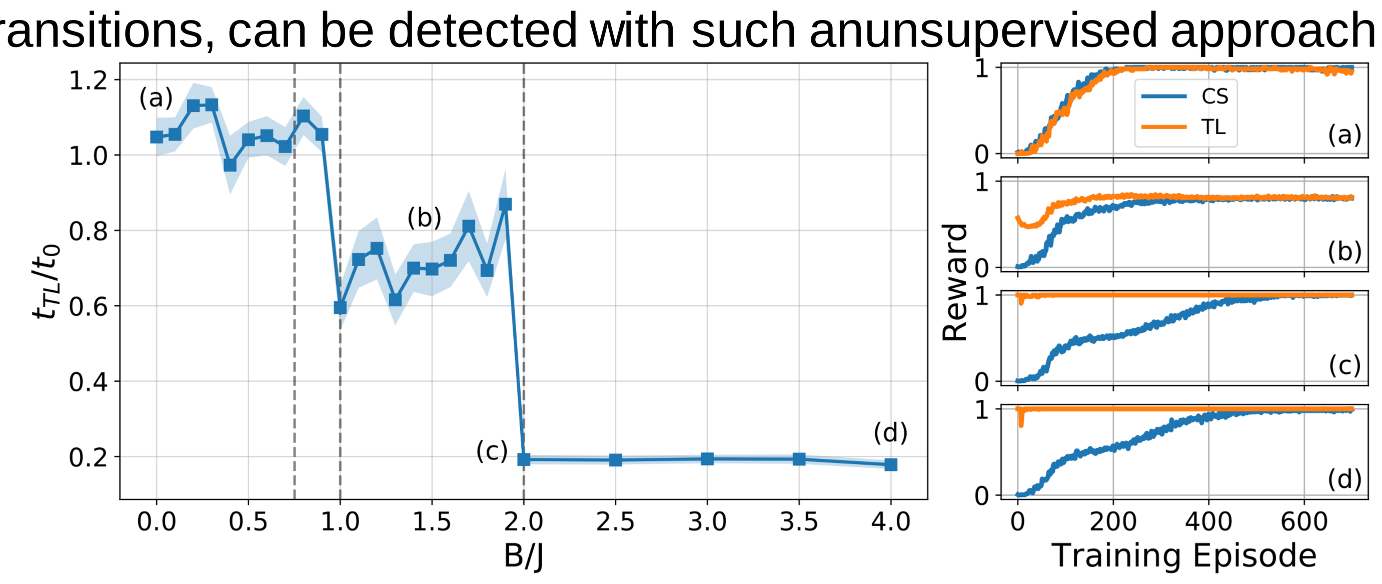
Following our case of study with the 1D XY Heisenberg model, in order to evaluate the RL results, we use two informative points of reference: breadth first search (BFS) and Monte Carlo (MC) optimization. To perform the evaluation, we track the number of new states evaluated before reaching, on average (50 independent agents), 95% optimality.



The benchmark is conducted with two different computational budgets. On the left, the budget is small and, thus, the search space is reduced. On the right, the budget is doubled, significantly increasing the search space. The RL agent thrives in large spaces, where the overhead of learning is overcome by the complexity of the space.

TRANSFER LEARNING

In a final experiment, we study the effect of transfer learning across phases of the same Hamiltonian. We observe a significant speedup in the source phase (B/J>2) that is sharply reduced beyond the phase transition B/J=2. Results suggest that changes in the ground state, some due to phase transitions, can be detected with such anunsupervised approach.



REFERENCES

[1] M. Navascués, S. Pironio, A. Acín. Phys. Rev. Lett. **98** (1), 010401 (2007).

[2] V. Mnih et al. Nature **518**(7540), 529-533 (2015).

[3] E. P. L. van Nieuewenburg et al. Nat. Phys. **13**(5), 435-439 (2017).

ACKNOWLEDGMENTS

B. R., G. MG. And M. L. acknowledge financial support from ERC AdG NOQIA, Spanish Ministry MINECO and State Research Agency AEI (FIDEUA PID2019-106901GB-I00/10.13039 / 501100011033, SEVERO OCHOA No. SEV-2015-0522 and CEX2019-000910- S, FPI), European Social Fund, Fundació Cellex, Fundació Mir-Puig, Generalitat de Catalunya (AGAUR Grant No. 2017 SGR 1341, CERCA program, QuantumCAT _U16-011424 , co-funded by ERDF Operational Program of Catalonia 2014-2020), MINECO-EU QUANTERA MAQS (funded by State Research Agency (AEI) PCI2019-111828-2 / 10.13039/501100011033), EU Horizon 2020 FET-OPEN OPTOLogic (Grant No 899794), and the National Science Centre, Poland-Symfonia Grant No. 2016/20/W/ST4/00314.

Trustees:

Supported by:

Member of: