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Certificates of many-body properties assisted by machine learning

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Computationally intractable tasks are ubiquitous in physics and optimization . Whereas variational approaches count amongst the most direct tools to find an optimal solution, they suffer from two main drawbacks: (i) non-convexity of the cost function and/or the feasible set and (ii) they provide only an inner bound to the optimal solution. On the other hand, relaxation techniques, which allow for more efficient methods, provide outer bounds to the optimal solution. Hence, the combination of both, variational ansatze and relaxations, provide bounded intervals which contain the optimal solution, thus allowing for control of the optimization error. We propose a novel approach combining the power of relaxation techniques with deep reinforcement learning (RL) to find the best possible relaxations given a limited computational budget. In many cases of interest, given an optimization problem, we consider a set of constraints that must be fulfilled by the solution. We can solve the resulting constrained optimization problem through semidefinite programming (SdP). Relaxing the constraints simplifies the problem, but it may yield looser bounds. At the same time, some smart relaxations may yield better bounds than others while using similar computational resources. Hence, it is paramount to find the best trade-off between accuracy and simplicity. Nevertheless, a successful search often relies upon specific insight about the problem at hand. Conversely, the analysis of an efficient proof is likely to reveal useful insight about the system's properties. We propose a systematic method to search for optimal sets of constraints given a computational budget. We illustrate the procedure in the context of ground state energy approximation. We showcase its validity in various scenarios where the ground states have different properties. Additionally, we benchmark the results against other optimization techniques and we study the effect of transfer learning. We highlight that our methods, while presented in the context of ground state energy approximation, are actually of much broader applicability, ranging, e.g. from entanglement witnesses optimization to device-independent quantum information processing tasks.

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