Machine predicts quantum criticallity in the absence of direct exposure

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Quantum critical phases of matter are theoretically challenging to predict. Here we show that a physics guided machine can detect a quantum transition where the best unguided machine fails.

Introduction Breakthroughs in cold atom experiments, advances in quantum computing, developments in spin liquids, and the proliferating importance of quantum critical phenomena, in the shadow of the rapidly growing field of artificial intelligence compel the application of machine learning techniques to difficult quantum problems. The exponential complexity inherent to solving quantum problems dictates data should be used judiciously rather than be discarded. In an age where data can drive unparalleled discoveries, extremely-expensive-to-aquire data such as measurements of the D-wave machine or Bloch's cold atom chains can be used by the community to distill new information.

Here we have pioneered a method to predict quantum critical phenomena using machine learning in the absence of direct exposure to states on either side of the transition.

Although we only apply this to spin models, the general nature of the problem cannot be understated. We have developed

Methods The model we employ is the generalized transverse field Ising chain with a longitudinal field and periodic boundary conditions. The Hamiltonian is given by

$$H = J\sum_{i=0}^{N-1}\sigma_i^z\sigma_{i+1}^z - B_x\sum_{i=0}^{N-1}\sigma_i^x - B_z\sum_{i=0}^{N-1}\sigma_i^z, \qquad (1)$$

where the operators are understood to be the N fold

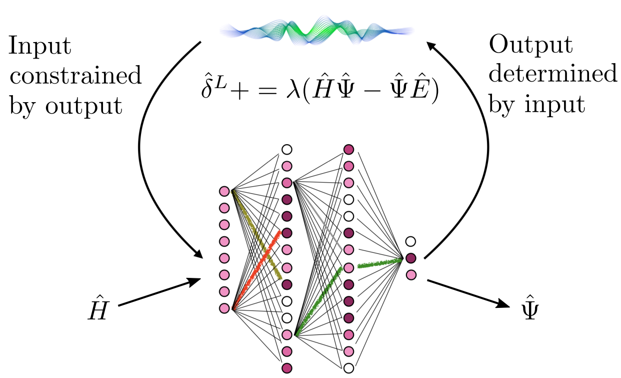

FIG. 1. Cartoon demonstrating the self-consistency between the inputs and outputs via the Schrödinger equation.

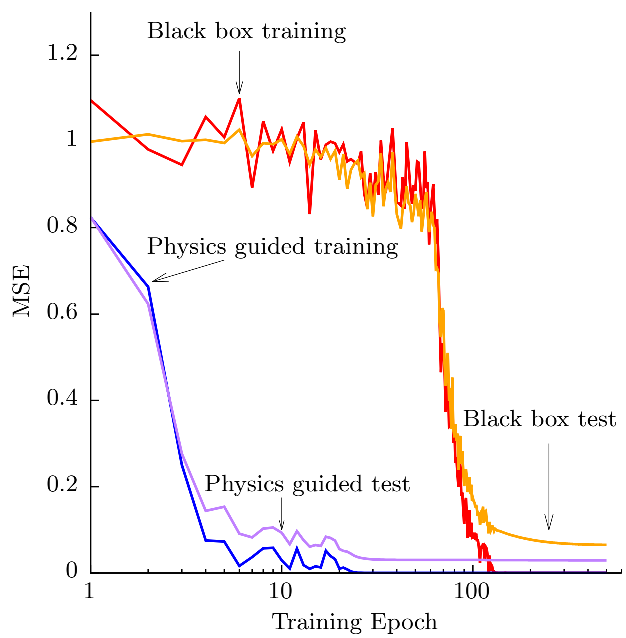

FIG. 2. **Efficacy of physics guided training on learning** The lines plot the mean square error for both the physics guided training and the black box training as a function of training epochs. It is clear that for the exact same network topology, the physics guided learning achieves better performance with less exposure than the black box.

product of Pauli space as

$$\sigma_i = \mathbf{1}\otimes ... \otimes \sigma \otimes \mathbf{1} ... \otimes \mathbf{1}; \qquad (2)$$

J, B_x, B_z are the coupling, transverse, and longitudinal fields respectively. The phase diagram of this model is has been studied recently [1] using exact diagonalization of spin chains up to 16 spins.

Results In all the following comparisons between the black box and the physics guided network, the two have the exact same topology, are initialized to identical states, and have identical inputs. The cost function is calculated identically as well. The only difference is the addition of the physics prior.

Figure 2 shows the mean square error as a function of training epochs during the training phase for a four site generalized Ising ring with infinitesimal longitudinal field, and varying transverse field. The training data lies

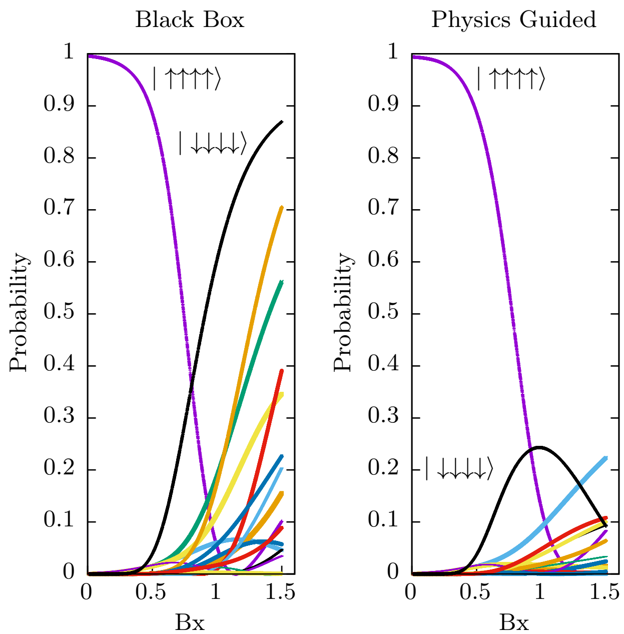

FIG. 3. **Efficacy of physics guided training on predictions** The line plot the square of the coefficients of the ground state wavefunction, representative of the probability of obtaining a certain magnetic order. Across the phase transition boundary $B_x = 1$, the physics guided machine makes better predictions.

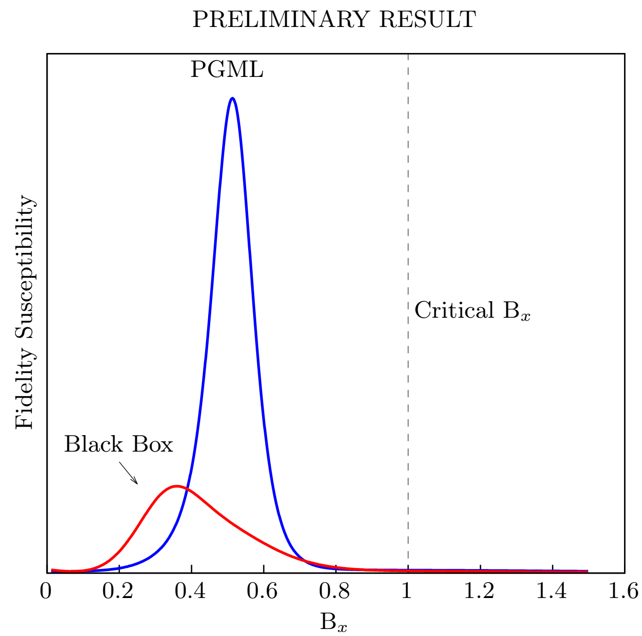

FIG. 4. **Efficacy of physics guided training on quantum observable** The line plot the quantum fidelity. The physics guided machine more accurately predicts the critical field strength.

exclusively in the ferromagnetically ordered phase, whilst the testing data contains points in both the ferromagnetic phase and the disordered phase. The training and testing datasets are composed of strictly mutually exclusive samplings of the phase diagram. The inputs to the network are the elements of the Hamiltonian operator, and the output is the ground state wavefunction. What can be noticed in Fig 2 is that the learning happens much faster in the physics guided model than in the black box model. Concomitantly the final mean square error is lower in the physics guided than in the black box. This is surprising given the two networks are more the same than different.

Figure 3 shows the predictions of the square of the coefficients of the ground state wavefunction. The lines plot each of the coefficients as a function of increasing longitudinal field. The transverse field Ising chain is known to have a quantum phase transition as a function of transverse field strength at $B_x = 1$, if the energy scale is set by the Ising coupling $J = 1$. Here the magnetization of the model is determined by the difference in the square of the first coefficient less the sixteenth. The transition is identified by going from finite magnetization to zero magnetization. In the left panel, with learning unguided by a prior, the magnetization becomes zero near $B_x = 0.7$. In the right panel, the magnetization dies out near $B_x = 0.9$. This is already an improvement towards predicting the thermodynamic limit, but is not the most important feature. Comparing the physics guided to the unguided model, the physics guided correctly identifies that the probability of obtaining an ordered state should go to zero across the transition, whereas the unguided model has no such inkling. Additionally, the physics guided machine more correctly preserves the normalization condition, that the sum of the squares of the coefficients should be one. The black box machine completely violates this.

Discussion

Conclusion We have demonstrated that the addition of an intelligence prior can greatly improve the learning capabilities and predictive power of soft computational intelligence engines. In the most rudimentary of circumstances, the improvements are vast. With the ever increasing importance of precipitating valuable information from effecitvely infinite amounts of chaotic data, succint training routines for neural networks are critical. Although we have demonstrated the efficacy of this approach as applied to quantum phase transitions in model systems, the basic premise is widely applicable to any system that follows known laws of motion in the generalized sense. This strongly suggests the art of machine intelligence should be refined to include the aformentioned precepts, and we suspect that leveraging this technique will find application accross many areas of physics and engineering.

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Appendix

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