I. INTRODUCTION

The rise of machine learning in recent times has remarkably transformed science and society. The goal of machine learning is to get computers to act without being explicitly programmed [1, 2]. Some of the typical applications of machine learning are self-driving cars, efficient web search, improved speech recognition, enhanced understanding of the human genome and online fraud detection. This viral spread in interest has exploded to various areas of science and engineering, in part due to the hope that artificial intelligence may supplement human intelligence to understand some of the deep problems in science.

Philosophies in science can, in general, be delineated from the study of the science itself. Yet, in physics, the study of quantum foundations has essentially sprouted an enormously successful area called quantum information science. Quantum foundations tells us about the mathematical as well as conceptual understanding of quantum theory. Ironically, this area has potentially provided the seeds for future computation and communication, without at the moment reaching a consensus among all the physicists regarding how quantum theory tells us about the nature of reality [47].

In recent years, techniques from machine learning have been used to solve some of the analytically/numerically complex problems in quantum foundations. In particular, the methods from reinforcement learning and supervised learning have been applied for determining the maximum value of various Bell inequalities, the classification of experimental statistics in local/nonlocal sets, training AI for playing Bell nonlocal games, using hidden neurons as hidden variables for completion of quantum theory, and machine learning-assisted state classification [48–51].
II. MACHINE LEARNING

Machine learning is a branch of artificial intelligence which involves learning from data [1, 2]. The purpose of machine learning is to facilitate a computer to achieve a specific task without explicit instruction by an external party. According to Mitchel (1997) [3], “A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if the performance at tasks in T, as measured by P, improves with E.” Note that the meaning of the word “task” doesn’t involve the process of learning. For instance, if we are programming a robot to play Go, playing Go is the task. Some of the examples of machine learning tasks are following.

- Classification: In classification tasks, the computer program is trained to learn the appropriate function \( h : \mathbb{R}^m \to \{1, 2, \ldots, t\} \). Given an input, the learned program determines which of the \( t \) categories the input belongs to via \( h \). Deciding if a given picture depicts a cat or a dog is a canonical example of a classification task.

- Regression: In regression tasks, the computer program is trained to predict a numerical value for a given input. The aim is to learn the appropriate function \( h : \mathbb{R}^m \to \mathbb{R} \). A typical example of regression is predicting the price of a house given its size, location and other relevant features.

- Anomaly detection: In anomaly detection (also known as outlier detection) tasks, the goal is to identify rare items, events or objects that are significantly different from the majority of the data. A representative example of anomaly detection is credit card fraud detection where the credit card company can detect misuse of the customer’s card by modelling his/her purchasing habits.

- Denoising: Given a noisy example \( \tilde{x} \in \mathbb{R}^n \), the goal of denoising is to predict the conditional probability distribution \( P(x|\tilde{x}) \) over clean examples \( x \in \mathbb{R}^n \).

The measure of the success \( P \) of a machine learning algorithm depends on the task \( T \). For example, in the case of classification, \( P \) can be measured via the accuracy of the model, i.e., fraction of examples for which the model produces the correct output. An equivalent description can be in terms of error, i.e., fraction of examples for which the model produces the incorrect output. The goal of machine learning algorithms is to work well on previously unseen data. To get an estimate of model performance \( P \), it is customary to estimate \( P \) on a separate dataset called test set which the machine has not seen during the training. The data employed for training is known as the training set.

Depending on the kind of experience, \( E \), the machine is permitted to have during the learning process, the machine learning algorithms can be categorized into supervised learning, unsupervised learning, and reinforcement learning.

1. Supervised learning: The goal is to learn a function, that returns the label given the corresponding unlabeled data. A prominent example would be images of cats and dogs, with the goal to recognize the correct animal. The machine is trained with labeled example data, such that it learns to correctly identify datasets it has not seen before. The task of supervised learning is to infer \( P(Y = y|X = x) \) based on finitely many samples from the joint distribution \( P(Y, X) \).

2. Unsupervised learning: For this type of machine learning, data is given without any label. The goal is to recognize underlying structures in the data. The task of the unsupervised machine learning algorithms is to learn the probability distribution \( P(x) \) or some interesting properties of the distribution, when given access to several examples \( x \). It is worth stating that the distinction between supervised and unsupervised learning can be blurry. For example, given a vector \( x \in \mathbb{R}^m \), the joint probability distribution can be factorized (using the chain rule of probability) as

\[
P(x) = \prod_{i=1}^{m} P(x_i|x_1, \ldots, x_{i-1}).
\]  

The above factorization (1) enables us to transform a unsupervised learning task of learning \( P(x) \) into \( m \) supervised learning tasks. Furthermore, given the supervised learning problem of learning the conditional distribution \( P(y|x) \), one can convert it into the unsupervised learning problem of learning the joint distribution \( P(x, y) \) and then infer \( P(y|x) \) via

\[
P(y|x) = \frac{P(x, y)}{\sum_{y_1} P(x, y_1)}.
\]

This last argument suggests that supervised and unsupervised learning are not entirely distinct. Yet, this distinction between supervised versus unsupervised is sometimes useful for the classification of algorithms.
3. Reinforcement learning: Here, neither data nor labels are available. The machine has to generate the data itself and improve this data generation process through optimization of a given reward function. This method is somewhat akin to a human child playing games: The child interacts with the environment, and initially performs random actions. By external reinforcement (e.g. praise or scolding by parents), the child learns to improve itself. Reinforcement learning has shown immense success recently. Through reinforcement learning, machines have mastered games that were initially thought to be too complicated for computers to master. This was for example demonstrated by DeepMind’s AlphaZero which has defeated the best human player in the board game, Go [54].

One of the central challenges in machine learning is to devise algorithms that perform well on previously unseen data. The learning ability of a machine to achieve a high performance \( P \) on previously unseen data is called generalization. The error measure on the training set is called training error. In contrast, the error measure on the test set is called generalization error or test error. Given an estimate of training error, how can we estimate test error? The field of statistical learning theory aptly answers this question. The training and test error is too big, the phenomenon is called over-fitting. The capacity of a machine learning model to fit a wide variety of functions is called model capacity. The model capacity of a machine learning algorithm determines if it is more likely to under-fit or over-fit the data. One of the ways to alter the model capacity of a machine learning algorithm is by constraining the class of functions that the algorithm is allowed to choose. This class is also known as the hypothesis class. For example, in linear regression, the hypothesis class is a set of linear functions.

### A. Artificial Neural Networks

Most of the recent advances in machine learning were facilitated by using artificial neurons. An artificial neuron (AN) is a real-valued function of the form,

\[
AN(x) = \phi \left( \sum_i w_i x_i \right) \quad \text{where} \quad x = (x_i) \in \mathbb{R}^k, \\
\quad w = (w_i) \in \mathbb{R}^k \quad \text{and} \quad \phi : \mathbb{R} \to \mathbb{R}. \tag{3}
\]

In equation\(^3\), the function \( \phi \) is usually known as activation function. Some of the well-known activation functions are

1. Threshold function: \( \phi(a) = 1 \) if \( a > 0 \) and \( 0 \) otherwise,
2. Sigmoid function: \( \phi(a) = \frac{1}{1 + \exp(-a)} \), and
3. Rectified Linear (ReLU) function: \( \phi(a) = \max(0,a) \).

The \( w \) vector in equation\(^3\) is known as weight vector. Many neurons can be combined together via communication links to perform complex computation. Such a graph structure \( G = (V,E) \), with the set of nodes \( V \) as artificial neurons and edges in \( E \) as connections, is known as an artificial neural network or neural network in short. A feedforward neural network is a directed acyclic graph. Apart from the feedforward neural network, some of the popular neural network architectures are convolutional neural networks (CNN), recurrent neural networks (RNN), generative adversarial network (GAN), Boltzmann machine and restricted Boltzmann machines (RBM). We provide a brief summary of RBM here. For a detailed understanding of various other neural networks, refer to [2].

An RBM is a bipartite graph with two kinds of binary-valued neuron units, namely visible \( \{v_i, v_2, \cdots \} \) and hidden \( \{h_1, h_2, \cdots \} \). The weight matrix \( W = (w_{ij}) \) encodes the weight corresponding to the connection between visible unit \( v_i \) and hidden unit \( h_j \). Let the bias weight (offset weight) for the visible unit \( v_i \) be \( a_i \) and hidden unit \( h_j \) be \( b_j \). For a given configuration of visible and hidden neurons \( (v,h) \), one can define an energy function \( E(v,h) \) as

\[
E(v,h) = -\sum_i a_i v_i - \sum_j b_j h_j - \sum_i \sum_j v_i w_{ij} h_j. \tag{4}
\]

At a given temperature \( T \), the probability of a configuration \( (v,h) \) is given by Boltzmann distribution,

\[
P(v,h) = \frac{\exp\left(\frac{-E(v,h)}{T}\right)}{Z}, \tag{5}
\]

where \( Z = \sum_{v,h} \exp\left(\frac{-E(v,h)}{T}\right) \) is a normalization factor, commonly known as partition function. The probability of visible units having configuration \( v \) is given by the marginalizing the joint probability in\(^5\), i.e.

\[
P(v) = \sum_h \frac{\exp\left(\frac{-E(v,h)}{T}\right)}{Z}. \tag{6}
\]

The input to the RBM can be encoded using the vector corresponding to \( v \). Given a set of training vectors \( v \in V \), the goal of RBM training is to evaluate

\[
\arg \max_w \prod_{v \in V} P(v), \tag{7}
\]

where \( W' \) includes weight matrix and biases corresponding to equation\(^4\) RBM-based representations of quantum states.
have been useful for various tasks in quantum many-body physics and quantum foundations [51, 55].

Machine learning with deep neural networks has accomplished many significant milestones, such as mastering various games, image recognition, self-driving cars, and so forth. Its impact on the physical sciences is just about to start [46, 51].

B. Relation with Artificial Intelligence

The term “artificial intelligence” was first coined in the famous 1956 Dartmouth conference [56]. Though the term was invented in 1956, the operational idea can be traced back to Alan Turing’s influential “Computing Machinery and Intelligence” paper in 1950, where Turing asks if a machine can think [57]. The idea of designing machines that can think dates back to ancient Greece. Mythical characters such as Pygmalion, Hephaestus and Daedalus can be interpreted as some of the legendary inventors and Galatea, Pandora and Hephaestus can be thought of as examples of artificial life [2]. The field of artificial intelligence is difficult to define, as can be seen by four different and popular candidate definitions [58]. The definitions start with “AI is the discipline that aims at building ...”

1. (Reasoning-based and human-based): agents that can reason like humans.
2. (Reasoning-based and ideal rationality): agents that think rationally.
3. (behavior-based and human-based): agents that behave like humans.
4. (behavior-based and ideal rationality): agents that behave rationally.

Apart from its foundational impact in attempting to understand “intelligence,” AI has reaped practical impacts such as automated routine labour and automated medical diagnosis, to name a few among many. The real challenge of AI is to execute tasks which are easy for people to perform, but hard to express formally. An approach to solve this problem is by allowing machines to learn from experience, i.e. via machine learning. From a foundational point of judgment, the study of machine learning is vital as it helps us understand the meaning of “intelligence”. It is worthwhile mentioning that deep learning is a subset of machine learning which can be thought of as a subset of AI (see Fig 1).

III. QUANTUM FOUNDATIONS

The mathematical edifice of quantum theory has intrigued and puzzled physicists, as well as philosophers, for many years. Quantum foundations seek to understand and develop the mathematical as well as conceptual understanding of quantum theory. The study concerns the search for non-classical effects such as nonlocality, contextuality and different interpretations of quantum theory. This study also involves the investigation of physical principles that can put the theory into an axiomatic framework, together with an exploration of possible extensions of quantum theory. In this survey, we will focus on non-classical features such as Bell nonlocality, contextuality and quantum steering in some detail.

An interpretation of quantum theory can be viewed as a map from the elements of the mathematical structure of quantum theory to physical phenomena. Most of the interpretations of quantum theory seek to explain the famous measurement problem. Some of the brilliant interpretations are the Copenhagen interpretation, quantum Bayesianism [59], the many-world formalism [60, 61] and the consistent history interpretation [62]. The axiomatic reconstruction of quantum theory is generally categorized into two parts: the generalized probabilistic theory (GPT) approach [63] and the black-box approach [64]. The physical principles underlying the framework for axiomatizing quantum theory are non-trivial communication complexity [65, 66], information causality [67], macroscopic locality [68], negating the advantage for non-local computation [69], consistent exclusivity [70] and local orthogonality [71]. The extensions of the quantum theory include collapse models [72], quantum measure theory [73] and acausal quantum processes [74].

A. Bell Nonlocality

According to John Bell [75], any theory based on the joint assumptions of locality and realism must be at variance with experiments conducted by space-like separated parties involving shared entanglement. The phenomenon, as discussed before, is known as Bell nonlocality [76]. Apart from its significance in understanding foundations of quantum theory, Bell nonlocality is a valuable resource for many emerging device-independent quantum technologies like quantum key distribution (QKD), distributed computing, randomness certification and self-testing [77–79]. The experiments which can potentially manifest Bell nonlocality are known as Bell
experiments. A Bell experiment involves \( N \) space-like separated parties \( A_1, A_2, \ldots, A_N \). Each party receives an input \( x_1, x_2, x_3, \ldots, x_N \in \mathcal{X} \) and gives an output \( a_1, a_2, a_3, \ldots, a_N \in \mathcal{A} \). For various input-output combinations one gets the statistics of the following form:

\[
\mathcal{P} = \{ P(a_1, a_2, \ldots, a_N | x_1, x_2, \ldots, x_N) \}_{x_1, \ldots, x_N \in \mathcal{X}, a_1, \ldots, a_N \in \mathcal{A}}.
\]

(8)

We will refer to \( \mathcal{P} \) as behavior. A Bell experiment involving \( N \) space-like separated parties, each party having access to \( m \) inputs and each input corresponding to \( k \) outputs is referred to as \( (N, m, k) \) scenario. The famous Clauser-Horn-Shimony-Holt (CHSH) experiment is a \( (2, 2, 2) \) scenario, and it is the simplest scenario in which Bell nonlocality can be demonstrated. A behavior \( \mathcal{P} \) admits local hidden variable description if and only if

\[
P(a_1, a_2, \ldots, a_N | x_1, x_2, \ldots, x_N) = \sum_\lambda P(\lambda) P(a_1 | x_1, \lambda) \cdots P(a_n | x_n, \lambda).
\]

(9)

Such a behavior is known as local behavior. The set of local behaviors \( \{ \mathcal{P} \} \) forms a convex polytope, and the facets of this polytope are Bell inequalities. In quantum theory, Born rule governs probability according to

\[
P(a_1, a_2, \ldots, a_N | x_1, x_2, \ldots, x_N) = \text{Tr} \left[ M_{a_1|x_1} \otimes \cdots \otimes M_{a_N|x_N} \rho \right],
\]

(10)

where \( \{ M_{a_i|x_i} \}_i \) are positive-operator valued measures (POVMs) and \( \rho \) is a shared density matrix. If a behavior satisfying Eq.(10) falls outside \( \mathcal{L} \), then it violates at least one Bell inequality, and such behavior is said to manifest Bell nonlocality. The set of behaviors considered so far is convex. However, in experiments such as entanglement swapping, which comprises three separated parties sharing two independent sources of quantum states, the local set admits the following form and the set is non-convex,

\[
P(a_1, a_2, a_3) = \sum_{\lambda_1, \lambda_2} P(\lambda_1) P(\lambda_2) P(a_1 | x_1, \lambda_1) P(a_2 | x_2, \lambda_2) P(a_3 | x_3, \lambda_3).
\]

(11)

Here, non-convexity emerges from the independence of the sources i.e. \( P(\lambda_1, \lambda_2) = P(\lambda_1) P(\lambda_2) \). In this case, the Bell inequalities are no longer linear. Characterizing the set of classical as well as quantum behaviors gets complicated for such scenarios \([80, 81]\).

### B. Contextuality

Contextuality is one of the profound ways to capture non-classicality of quantum theory. Bell nonlocality is regarded as a particular case of contextuality where the space-like separation of parties involved creates "context" \([82, 83]\). The study of contextuality has led not only to insights into the foundations of quantum mechanics, but it also offers practical implications as well \([84, 85]\). Mathematical techniques involving sheaf theory, graph theory, hypergraphs, algebraic topology and probabilistic couplings have been developed to understand contextuality better \([85]\). There are several frameworks for contextuality including sheaf-theoretic framework \([89]\), graph and hypergraph framework \([82, 100]\), contextuality-by-default framework \([101, 103]\) and operational framework \([104]\). A scenario exhibits contextuality if it does not admit the non-contextual hidden variable (NCHV) model \([105]\).

### C. Quantum Steering

Correlations produced by steering lie between the Bell nonlocal correlations and those generated from entangled states \([106, 107]\). A state that manifests Bell nonlocality for some suitably chosen measurement settings also exhibits steering \([108]\). Furthermore, a state which exhibits steering must be entangled. A state demonstrates steering if it does not admit "local hidden state (LHS)" model \([107]\). We discuss this formally here.

Alice and Bob share some unknown quantum state \( \rho^{AB} \). Alice can perform a set of POVM measurements \( \{ M_a^{AB} \}_a \). The probability of her getting outcome \( a \) after choosing measurement \( x \) is given by

\[
P(a|x) = \text{Tr} \left[ (M_a^{AB} \otimes I) \rho^{AB} \right] = \text{Tr} \left( \rho_{a|x}^{B} \right),
\]

(12)

where \( \rho_{a|x}^{B} = \text{Tr}_A \left[ (M_a^{AB} \otimes I) \rho^{AB} \right] \) is Bob’s residual state upon normalization. A set of operators \( \{ \rho_{a|x}^{B} \}_a \) acting on Bob’s space is called an assemblage if

\[
\sum_a \rho_{a|x}^{B} = \sum_a \rho_{a|x'}^{B} \quad \forall x \neq x'
\]

(13)

and

\[
\sum_a \text{Tr} \left[ \rho_{a|x}^{B} \right] = 1 \quad \forall x.
\]

(14)

Condition (13) is the analogue of the no-signalling condition. An assemblage \( \{ \rho_{a|x}^{B} \}_a \) is said to admit LHS model if there exists some hidden variable \( \lambda \) and some quantum state \( \rho_\lambda \) acting on Bob’s space such that

\[
\rho_{a|x}^{B} = \sum \lambda P(\lambda) P(a|x, \lambda) \rho_\lambda.
\]

(15)

A bipartite state \( \rho^{AB} \) is said to be steerable from Alice to Bob if there exist measurements for Alice such that the corresponding assemblage does not satisfy equation (15). Determining whether an assemblage admits LHS model is a semidefinite program (SDP). The concept of steering is asymmetric by definition, i.e. even if Alice could steer Bob’s state, Bob may not be able to steer Alice’s state.
IV. NEURAL NETWORK AS ORACLE FOR BELL NONLOCALITY

The characterization of the local set for the convex scenario via Bell inequalities becomes intractable as the complexity of the underlying scenario grows (in terms of the number of parties, measurement settings and outcomes). For networks where several independent sources are shared among many parties, the situation gets increasingly worse. The local set is remarkably non-convex, and hence proper analytical and numerical characterization, in general, is lacking. Applying machine learning technique to tackle these issues were studied by Canabarro et al. [49] and Krivachy et al. [48]. In the work by Canabarro et al., the detection and characterization of nonlocality is done through an ensemble of multilayer perceptrons blended with genetic algorithms (see [VA]).

A. Machine Learning Nonlocal Correlations

Given a behavior, deciding whether it is classical or non-classical is an extremely challenging task since the underlying scenario grows in complexity very quickly. Canabarro et al. [49] use supervised machine learning with an ensemble of neural networks to tackle the approximate version of the problem (i.e. with a small margin of error) via regression. The authors ask “How far is a given correlation from the local set.” The input to the neural network is a random correlation vector. For a given behavior, the output (label) is the distance of the feature vector from the classical, i.e. local set. The nonlocality quantifier of a behavior \( q \) is the minimum trace distance, denoted by \( \text{NL}(q) \) [109]. For the two-party scenario, the nonlocality quantifier is given by

\[
\text{NL}(q) \equiv \frac{1}{2|\mathcal{X}|} \min_{p \in \mathcal{L}} \sum_{a,b,x,y} |q - p|, 
\]

(16)

where \( \mathcal{L} \) is the local set and \(|\mathcal{X}| = |\mathcal{Y}| = m \) is the input size for the parties. The training points are generated by sampling the set of non-signalling behaviors randomly and then calculating its distance from the local set via equation 16. Given a behavior \( q \), the distance predicted by the neural network is never equal to the actual distance, i.e. there is always a small error \( \varepsilon \neq 0 \). Let us represent the learned hypothesis as \( f : q \rightarrow \mathbb{R} \). The performance metric of the learned hypothesis \( f \) is given by

\[
\mathcal{P}(f) \equiv \frac{1}{N} \sum_{i=1}^{N} |\text{NL}(q_i) - f(q_i)|. 
\]

(17)

Canabarro et al. train the model for convex as well as non-convex scenarios. They also train the model to learn post-quantum correlations. The techniques studied in the paper are valuable for understanding Bell nonlocality for large quantum networks, for example those in quantum internet.

B. Oracle for Networks

Given an observed probability distribution corresponding to scenarios where several independent sources are distributed over a network, deciding whether it is classical or non-classical is an important question, both from practical as well as foundational viewpoint. The boundary separating the classical and non-classical correlations is extremely non-convex and thus a rigorous analysis is exceptionally challenging. In reference [48], the authors encode the causal structure into the topology of a neural network and numerically determine if the target distribution is “learnable”. A behavior belongs to the local set if it is learnable. The authors harness the fact that the information flow in feedforward neural networks and causal structures are both determined by a directed acyclic graph. The topology of the neural network is chosen such that it respects the causality structure. The local set corresponding to even elementary causal networks such as triangle network is profoundly non-convex, and thus analytical characterization of the same is a notoriously tricky task. Using the neural network as an oracle, Krivachy et al. [48] convert the membership in a local set problem to a learnability problem. For a neural network with adequate model capacity, a target distribution can be approximated if it is local. The authors examine the triangle network with quaternary outcomes as a proof-of-principle example. In such a scenario, there are three independent sources, say \( \alpha, \beta \) and \( \gamma \). Each of the three parties receives input from two of the three sources and process the inputs to provide outputs via fixed response functions. The outputs for Alice, Bob and Charlie will be indicated by \( a, b, c \in \{0, 1, 2, 3\} \). The scenario as discussed here can be characterized by the probability distribution \( P(a,b,c) \) over the random variables \( a, b \) and \( c \). If the network is classical, then the distribution can be represented by a directed acyclic graph known as a Bayesian network (BN). Assuming the distribution \( P(a,b,c) \) over the random variables \( a, b \) and \( c \) to be classical, it is assumed without loss of generality that the sources send a random variable drawn uniformly from the interval 0 to 1. A classical distribution for such a case admits the following form:

\[
P(a,b,c) = \int_{0}^{1} d\alpha d\beta d\gamma P_A(a|\beta, \gamma) P_B(b|\gamma, \alpha) P_C(c|\alpha, \beta). 
\]

(18)

The neural network is constructed such that it can approximate the distribution of type Eq.18. The inputs to the neural network are \( \alpha, \beta \) and \( \gamma \) drawn uniformly at random and the outputs are the conditional probabilities i.e. \( P_A(a|\beta, \gamma), P_B(b|\gamma, \alpha) \) and \( P_C(c|\alpha, \beta) \). The cost function is chosen to be any measure of the distance between the target distribution \( P \) and the network’s output \( P_M \). The authors employ the techniques to a few other cases, such as the elegant distribution and a distribution proposed by Renou et al. [110]. The application of the technique to the elegant distribution suggests that the distribution is indeed nonlocal as conjectured in [111]. Furthermore, the distribution proposed by Renou et al. appears to have nonlocal features for some parameter regime.
V. MACHINE LEARNING-ASSISTED DETECTION OF BELL NONLOCALITY IN QUANTUM MANY BODY SYSTEMS

Several methods from machine learning have been adopted to tackle intricate quantum many-body problems \[51, 55, 112, 113\]. Dong-Ling Deng \[51\] employs machine learning techniques to detect quantum nonlocality in many-body systems using the restricted Boltzmann machine (RBM) architecture. The key idea can be split into two parts:

- The Bell operator for fixed measurement settings for convex scenarios is mapped to an appropriate Hamiltonian, and the problem of finding the ground state of the Hamiltonian is then mapped to the problem of finding the maximum violation of the underlying Bell inequality for a set of fixed measurement settings.

- Finding ground state of a quantum Hamiltonian is QMA-hard and thus in general difficult. However, using heuristic techniques involving RBM architecture, the problem is recast into the task of finding the approximate answer in some cases.

Techniques like density matrix renormalization group (DMRG) \[114\], projected entangled pair states (PEPS) \[115\] and multiscale entanglement renormalization ansatz (MERA) \[116\] are traditionally used to find (or approximate) ground states of many-body Hamiltonians. But these techniques only work reliably for optimization problems involving low-entanglement states. Moreover, DMRG works well only for systems with short-range interactions in the one-dimensional case. As evident from references \[55\], RBM can represent quantum many-body problems beyond 1-D and low-entanglement.

VI. AI FOR BELL NONLOCAL GAMES

Prediction of winning strategies for (classical) games and decision-making processes with reinforcement learning (RL) has made significant progress in game theory in recent years. Motivated partly by these results, the authors in Bharti et al. \[50\] have looked at a game-theoretic formulation of Bell inequalities (known as Bell games) and applied machine learning techniques to it. To violate a Bell inequality, both the quantum state as well as the measurements performed on the quantum states have to be chosen in a specific manner. The authors transform this problem into a decision making process. This is achieved by choosing the parameters in a Bell game in a sequential manner, e.g. the angles of the measurement operators, the angles parameterizing the quantum states, or both. Using RL, these sequential actions are optimized for the best configuration corresponding to the optimal/near-optimal quantum violation (see Fig. 2). The authors train the RL agent with a cost function that encourages high quantum violations via proximal policy optimization - a state-of-the-art RL algorithm that combines two neural networks. The approach succeeds for well known convex Bell inequalities, but it can also solve Bell inequalities corresponding to non-convex optimization problems, such as in larger quantum networks. So far, the field has struggled solving these inequalities; thus, this approach offers a novel possibility towards finding optimal (or near-optimal) configurations.

![FIG. 2: Playing Bell games with AI: In [50], the authors train AI agent to play various Bell nonlocal games.](image)

Furthermore, an approach to investigate Bell inequalities applicable to noisy near-term quantum computers is shown. The quantum state is parameterized by a set of single-qubit rotations and CNOT gates acting on neighbouring qubits arranged in a one-dimensional line. Both the gates and the measurement angles are chosen in a sequential manner by the RL agent and are optimized using a variational hybrid classical-quantum algorithm, where the classical optimization is performed by RL.

As an example, the training progress for optimizing a many-body Bell inequality is shown in Fig. 3 for a quantum circuit with two (left) and three layers (right). Initially, the RL agent chooses actions at random, and the average expectation value is below the classical and quantum bounds. Over the course of the training, the agent improves itself by learning from experience. For two layers, the RL agent can violate the classical bound, whereas, for three layers, the maximal quantum violation is approximately reached. After reaching a certain high reward, sudden drops and revivals in the reward are observed. This is an indication that the RL algorithm is not perfectly stable and better methods or hyperparameter tuning are needed.

VII. MACHINE LEARNING-ASSISTED STATE CLASSIFICATION

A crucial problem in quantum information is identifying the degree of entanglement within a given quantum state. A \(n\)-partite state \(\rho_{\text{sep}}\) is called separable if it can be represented...
as a convex combination of product states i.e.
\[ \rho_{\text{sep}} = \sum_i p_i \rho_1^i \otimes \rho_2^i \otimes \cdots \otimes \rho_n^i, \]

where \( 0 \leq p_i \leq 1 \) and \( \sum_i p_i = 1 \). A quantum state \( \rho \) is entangled if it is not separable. For Hilbert space dimensions up to 6, one can use Peres-Horodecki criterion, also known as positive partial transpose criterion (PPT) to distinguish entangled and separable states. However, there is no generic observable or entanglement witness as it is in fact a NP-hard problem \[117\]. Thus, one must rely on heuristic approaches. This poses a fundamental question: Given partial or full information about the state, are there ways to classify whether it is entangled or not? Machine learning has offered a way to find new answers to this question.

A. Classification with Bell Inequalities

In reference \[118\], the authors blend Bell inequalities with a feed-forward neural network to use them as state classifiers. The goal is to classify states as entangled or separable. If a state violates a Bell inequality, it must be entangled. However, Bell inequalities cannot be used as a reliable tool for entanglement classification i.e. even if a state is entangled, it might not violate an entanglement witness based on the Bell inequality. For example, the density matrix \( \rho = \rho \ket{\psi_+} \bra{\psi_+} + (1-p) \frac{1}{4} \)
violates the CHSH inequality only for \( p > \frac{1}{\sqrt{2}} \), but is entangled for \( p > \frac{1}{2} \). Moreover, given a Bell inequality, the measurement settings that witness entanglement of a quantum state (if possible) depend on the quantum state. Motivated by these issues, the authors ask if they can transform Bell inequalities into a reliable separable-entanglement states classifier. For example, for fixed measurement settings corresponding to CHSH inequality, is it possible to get better performance compared with the values \((1, -1, 1, 1, 2)\)? Is it possible to improve the optimization using hidden layers? The main challenge to answer such questions in a supervised learning setting is to get labelled data that is verified to be either separable or entangled.

To train the network, the correlation vector corresponding to the appropriate Bell inequality was chosen as a feature vector with the state being entangled or separable \((1 \text{ versus } 0)\) as corresponding output. The performance of the network improved as the model capacity was increased, which hints that the hypothesis which separates entangled states from separable ones must be sufficiently “complex.” The authors also trained a neural network to distinguish bi-separable and bound-entangled states.

B. Classification by Representing Quantum States with Restricted Boltzmann Machines

Harney et al. \[119\] use reinforcement learning with RBMs to detect entangled states. RBMs have demonstrated being capable of learning complex quantum states. The authors modify RBMs such that they can only represent separable states. This is achieved by separating the RBM into \( K \) partitions that are only connected within themselves, but not with the other partitions. Each partition represents a (possibly) entangled sub-space, that however is not entangled with the other partitions. This choice enforces a specific \( K \)-separable Ansatz of the wavefunction. This RBM is trained to represent a target state. If the training converges, it must be representable by the Ansatz and thus be \( K \)-separable. However, if the training does not converge, the Ansatz is insufficient and the target state is either of a different \( K' \)-separable form or fully entangled.

C. Classification with Tomographic Data

Can tools from machine learning help to distinguish entangled and separable states given the full quantum state \( \text{e.g. obtained by quantum tomography} \) as an input? Two recent studies address this question.

In Lu et al. \[120\], the authors detect entanglement by employing classic \( \text{i.e. non-deep learning} \) supervised learning. To simplify data generation of entangled and separable states, the authors approximate the set of separable states by a convex hull (CHA). States that lie outside the convex hull are assumed to be most likely entangled. For the decision process, the authors use ensemble training via bootstrap aggregating (bagging). Here, various supervised learning methods are trained on the data, and they form a committee together that decides whether a given state is entangled or not. The algorithm is trained with the quantum state and information encoding the position relative to the convex hull as inputs. The authors show that accuracy improves if bootstrapping of machine learning methods is combined with CHA.

In a different approach Goes et al. \[121\], the authors present an Automated Machine Learning approach to classify random states of two qutrits as separable (SEP), entangled with positive partial transpose (PPTES) or entangled with negative
partial transpose (NPT). For training, the authors elaborate a way to find enough samples to train on. The procedure is as follows: A random quantum state is sampled, then using the General Robustness of Entanglement (GR) and PPT criterion, it is classified to either SEP, PPTES or NPT. The GR measures the closeness to the set of separable states. The authors compare various supervised learning methods to distinguish the states. The input features fed into the machine are the components of the quantum state vector and higher-order combinations thereof, whereas the labels are the type of entanglement. Besides, they also train to estimate the GR with regression techniques and use it to validate the classifiers.

VIII. NEURAL NETWORKS AS “HIDDEN” VARIABLE MODELS FOR QUANTUM SYSTEMS

Understanding why deep neural networks work so well is an active area of research. The presence of the word “hidden” for hidden variables in quantum foundations and hidden neurons in deep learning neurons may not be that accidental. Using conditional Restricted Boltzmann machines (a variant of Restricted Boltzmann machines), Steven Weinstein provides a completion of quantum theory in reference [122]. The completion, however, doesn’t contradict Bell’s theorem as the assumption of “statistical independence” is not respected. The statistical independence assumption demands that the complete description of the system before measurement must be independent of the final measurement settings. The phenomena where apparent nonlocality is observed by violating statistical independence assumption is known as “nonlocality without nonlocality” [123].

In a Bell-experiment corresponding to CHSH scenario, the detector settings \( \alpha \in \{a,a'\} \) and \( \beta \in \{b,b'\} \), and the corresponding measurement outcomes \( x_\alpha \in \{1, -1\} \) and \( x_\beta \in \{1, -1\} \) for a single experimental trial can be represented as a four-dimensional vector \( \{\alpha, \beta, x_\alpha, x_\beta\} \). Such a vector can be encoded in a binary vector \( V = (v_1, v_2, v_3, v_4) \) where \( v_i \in \{0, 1\} \). Here, \((+1)/(-1)\) has been mapped to \(0/(+1)\). The four-dimensional binary vector \( V \) represents the value taken by four visible units of an RBM. The dependencies between the visible units is encoded using sufficient number of hidden units \( H = (h_1, h_2, \cdots, h_j) \). With four hidden neurons, the authors could reproduce the statistics predicted by EPR experiment with high accuracy. For example, say the vector \( V = (0, 1, 1, 0) \) occurs in 3% of the trials, then after training the machine would associate \( P(V) \approx 0.03 \). Quantum mechanics gives us only the conditional probabilities \( P(x_\alpha, x_\beta | \alpha, \beta) \) and thus learning joint probability using RBM is resource-wasteful. The authors harness this observation by encoding the conditional statistics only in a conditional RBM (cRBM).

The difference between a cRBM and RBM is that the units corresponding to the conditioning variables (detector settings here) are not dynamical variables. There are no probabilities assigned to conditioning variables, and thus the only probabilities generated by cRBM are conditional probabilities. This provides a more compact representation compared to RBM.

IX. CONCLUSION AND FUTURE WORK

In this survey, we discussed the various applications of machine learning for problems in the foundations of quantum theory such as determination of the quantum bound for Bell inequalities, the classification of different behaviors in local/nonlocal sets, using hidden neurons as hidden variables for completion of quantum theory, training AI for playing Bell nonlocal games, ML-assisted state classification, and so forth. Now we discuss a few open questions at the interface. Some of these open questions have been mentioned in references [48, 51].

Witnessing nonlocality in many-body systems is an active area of research [51, 124]. However, designing experimentally friendly many-body Bell inequalities is a difficult task. It would be interesting if machine learning could help design optimal Bell inequalities for scenarios involving many-body systems. In reference [51], the author used RBM based representation coupled with reinforcement learning to find near-optimal quantum values for various Bell inequalities corresponding to various convex Bell scenarios. It is well known that optimization becomes comparatively easier once the representation gets compact. It would be interesting if one can use other neural networks based representations such as convolutional neural networks for finding optimal (or near-optimal) quantum values.

As mentioned in reference [49], it is an excellent idea to deploy techniques like anomaly detection for the detection of non-classical behaviors. This can be done by subjecting the machine to training with local behaviors only.

In reference [50], the authors used reinforcement learning to train AI to play Bell nonlocal games and obtain optimal (or near-optimal) performance. The agent is offered a reward at the end of each epoch which is equal to the expectation value of the Bell operator corresponding to the state and measurement settings chosen by the agent. Such a reward scheme is sparse and hence it might not be scalable. It would be interesting to come up with better reward schemes. Furthermore, in this approach only a single agent tries to learn the optimization landscape and discovers near-optimal (or optimal) measurement settings and state. It would be exciting to extend the approach to multi-agent setting where every space-like separated party is considered a separate agent. It is worth mentioning that distributing the actions and observations of a single agent into a list of agents reduces the dimensionality of agent inputs and outputs. Furthermore, it also dramatically improves the amount of training data produced per step of the environment. Agents learn better if they tend to interact as compared to the case of solitary learning.

Finding quantum Bell inequalities is an interesting and challenging problem [125, 126]. However, one can aim to obtain the approximate expression by supervised learning with the quantum Bell inequalities being the boundary separating the quantum set from the post-quantum set. Moreover, it is interesting to see if it is possible to guess physical principles by simply opening the neural-network black box.

Driven by the success of machine learning in Bell nonlocality, it is genuine to ask if the methods could be useful to
solve problems in quantum steering and contextuality. Recently, ideas from the exclusivity graph approach to contextuality were used to investigate problems involving causal inference [127]. Ideas from quantum foundations could further assist in developing a deeper understanding of machine learning or in general artificial intelligence.

In artificial intelligence, one of the tests to distinguish between humans and machines is the famous “Turing Test (TT)” due to Alan Turing [68, 128]. The purpose of TT is to determine if a computer is linguistically distinguishable from a human. In TT, a human and a machine are sealed in different rooms. A human jury who does not know which room contains a human and which room not, asks questions to them, by email, for example. Based on the returned outcome, if the judge cannot do better than fifty-fifty, then the machine in question is said to have passed TT. The task of distinguishing the humans from machine based on the statistics of the answers (say output $a$) given questions (say input $x$) is a statistical distinguishability test assuming the rooms plus its inhabitants as black boxes. In the black-box approach to quantum theory, experiments are regarded as a black box where the experimentalist introduces a measurement (input) and obtains the outcome of the measurement (output). One of the central goals of this approach is to deduce statements regarding the contents of the black box based on input-output statistics [64]. It would be nice to see if techniques from the black-box approach to quantum theory could be connected to TT.

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