

Provable learning of quantum states with graphical models

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The complete learning of any unknown many-body systems requires a number of samples exponentially in the particle number. Several works consider subclasses of physical meaningful states such as stabilizer states or high-temperature Gibbs states that can be learned in polynomial sample complexity. Others consider to learn states under special assumptions, such as PAC learning and shadow tomography. In this work, we consider learning many-body systems that can be approximately represented by restricted Boltzmann machines (RBMs). We exhibit robustness results for efficient provable two-hop neighborhood learning method for ferromagnetic and locally consistent RBMs. We consider the L_p norm as a distance measure, including both total variation distance and max-norm distance in the limit. We show that various quantum states can be learned with a sample complexity exponentially better than the naive state tomography. Our results establish a broader theoretical framework for the efficient learning of complex quantum many-body systems.

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I. INTRODUCTION

One of the fundamental questions in condensed matter physics revolves around probing the nature of quantum many-body systems. Quantum many-body system learning involves Hamiltonian learning, quantum process learning, and quantum state learning from measurements on ensembles of identical states [1–14]. Describing a general quantum many-body state requires a number of parameters exponential in the number of particles. In the worst case, this results in an exponential number of measurement samples for learning an arbitrary quantum many-body state. Interestingly, there are special many-body systems that can be efficiently learned in polynomial samples, such as stabilizer states [15]. Moreover, other than learning all the information about a quantum state, we can learn certain physically meaningful properties. One remarkable example is using shadow tomography (classical shadows) to estimate expectation values of many observables of a many-body system with an additive error [16–20].

Employing machine learning methodologies to investigate quantum many-body systems has been extensively studied [21–25]. Graphical models are useful tools and the restricted Boltzmann machine (RBM) is a well-studied example with latent (hidden) variables that has been proven to be a universal approximator for arbitrary functions [26]. At the interplay

between RBMs and quantum many-body systems, Carleo and Troyer represent quantum states with RBMs [27], and show that the so-called neural-network quantum (NNQ) state can efficiently represent the ground state of the Ising and Heisenberg models. This has been extended for certain topological states like toric code states and symmetry-protected topological cluster state by a local RBM [28]. Meanwhile, any local tensor network can be represented by a local NNQ state based on an RBM [29]. NNQ states have also been applied to quantum tomography [30–32] and explore many-body entanglement [33–35].

In the past few years, there has been considerable progress in efficient and provable learning algorithms for graphical models. In general, learning all parameters of a graphical model is hard [36]. Efficient algorithms can be constructed for special classes of graphical models and when considering not learning all parameters but only learning the structure of the graphical model, for example. An unconditional lower bound of $\log n$ holds for the learning of an n -spin Ising model [37]. For RBMs, Bresler *et al.* [38] proposed a classical efficient greedy algorithm for learning the structure in ferromagnetic cases, which can be used to simplify weight learning. Goel [39] provided a generalization to locally consistent cases. A fundamental question arises regarding the connection between these findings and the learning of quantum states. In particular, how close do quantum many-body states have to be to classes of RBMs such that the aforementioned algorithms can be effectively employed?

In this work, we focus on the provable learning of quantum states of quantum many-body systems; see Fig. 1 for an overview. We prove a robust version of an existing learning method, which allows us to efficiently learn the many-body systems that can be approximately represented by certain NNQ states. The procedure consists of two key steps. The first involves learning the underlying structure of the RBM

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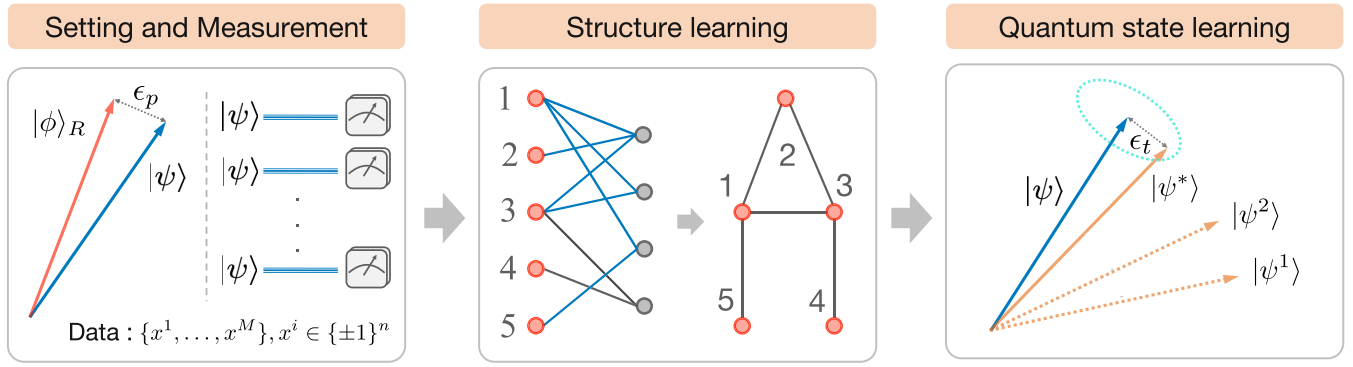


FIG. 1. Provable learning of quantum states with graphical models. (Left panel) Consider an unknown many-body system in the state $|\psi\rangle$. As there are many involved systems that can be represented by RBMs, our motivation here is to learn the many-body systems that can be approximately represented by RBMs, i.e., it is ϵ_p close to a neural network quantum state $|\phi\rangle_R$ based on RBMs defined in Eq. (3). For learning the unknown state, we perform the projection measurement on each copy in the computational basis, and obtain the measurement outcomes $x^i \in \{\pm 1\}^n$. (Middle panel) Based on the measurement results, we learn the two-hop neighborhood structure of the RBM corresponding to the state $|\phi\rangle_R$. An example of an RBM with five visible nodes and four hidden nodes is depicted. The two-hop edges of node 1 are shown in blue. The full two-hop neighborhood structure of the visible nodes is shown in the right figure. (Right panel) With the knowledge of the graphic structure, we can efficiently perform quantum state learning, here defined as finding parameters to estimate the magnitude of $|\psi\rangle$. We construct various hypothesis states $\{|\psi^1\rangle, \dots\}$ and choose the nearest one $|\psi^*\rangle$, which is ϵ_t close to $|\psi\rangle$, with $\text{poly}(n, 1/\epsilon_t)$ copies of the state. The sample complexity improves further when we learn any subsystems conditional on all the others.

representation by using algorithms in Refs. [38,39]. We establish a robust error bound on the L_p norm distance between the magnitudes of the true quantum state and those of a quantum state representable by an FRBM or a locally consistent RBM. The second step focuses on learning the full set of parameters that describe all the amplitudes of the quantum states. With the robustly learned structure, we employ the Alphasatron algorithm introduced in Ref. [40] as a subroutine. However, the task cannot be solved by a direct application of Alphasatron; instead, additional processing is required to reformulate the parameter learning problem into a form suitable for Alphasatron. The final error bounds and sample complexity also do not follow directly from Alphasatron's guarantees, but instead require additional analysis that combines the L_p -norm robustness, the error accumulation of adapting Alphasatron and repeating the algorithm n times. We demonstrate our results through numerical experiments, achieving a high fidelity of quantum state learning.

Main definitions

Any quantum many-body state can be represented by RBMs. An RBM is a two-layer (visible layer and hidden layer) neural network without connections among nodes within a layer [41,42], analogous to a weighted bipartite graph. An example can be seen in the middle panel of Fig. 1. Given an RBM with n visible nodes $\{X_i\}_{i \in [n]}$ and m hidden nodes $\{Y_k\}_{k \in [m]}$, the probability distribution for recovering a specific configuration $x \in \{\pm 1\}^n$ and $y \in \{\pm 1\}^m$ is given by

$$P(X = x, Y = y) = \frac{1}{Z} \exp(x^T J y + h^T x + g^T y), \quad (1)$$

where Z is the partition function, $[n] = \{1, 2, \dots, n\}$, the interaction matrix J , and external fields h and g are all real, i.e., $h \in \mathbb{R}^n$, $g \in \mathbb{R}^m$, and $J \in \mathbb{R}^{n \times m}$.

The RBM representation of the quantum state is then written as

$$|\phi\rangle = \sum_{x \in \{\pm 1\}^n} \phi(x) |x\rangle, \quad (2)$$

where $|\phi(x)|^2 = p(x)$ and $p(x)$ is the marginal distribution over the visible nodes of the RBM. In the classical definition of RBMs (as used in statistical physics and machine learning), the interaction matrix and external fields are restricted to real values, which ensures that $p(x)$ is strictly positive. In the quantum setting, however, it is natural to extend them to complex parameters, so that the RBM framework can represent quantum states with complex amplitudes.

It has shown that any n -qubit quantum state can be arbitrarily well approximated by an NNQ state based on RBM [29], associating each visible node with a qubit and having potentially an exponential number of hidden nodes. In this work, we consider a certain set of quantum states that can be represented or estimated by locally consistent RBMs. An RBM is locally consistent if for each hidden node $j \in [m]$, $J_{ij} \geq 0$ or $J_{ij} \leq 0$ for all $i \in [n]$.

Given an unknown state that can be estimated by a locally consistent RBM, we first learn the underlying structure of the RBM representation. The so-called two-hop neighborhood provides information about the underlying structure of an RBM. We say visible nodes i and j are two-hop neighbors of each other if they are connected via a hidden node in the graph representation. Let $\mathcal{N}_2(i)$ be the set for two-hop neighbors of visible node i . The two-hop degree of an RBM is defined as $d_2 := \max_{i \in [n]} \{|\mathcal{N}_2(i)|\}$. We call this interconnected arrangement among visible nodes the structure (underlying graph) of the RBM. For instance, in the middle panel of Fig. 1, we observe that $\mathcal{N}_2(1) = \{2, 3, 5\}$, $d_2 = 3$, and the structure is shown on the right-hand side.

To learn the underlying structure of an RBM, it is necessary to have both lower and upper bounds of the weights. We say an RBM is (α, β) *nondegenerate* if

- (1) for every $i \in [n]$ and $j \in [m]$, $|J_{ij}| \geq \alpha$ if $|J_{ij}| \neq 0$;
- (2) for every $i \in [n]$, $\sum_j |J_{ij}| + |h_i| \leq \beta$;
- (3) for every $j \in [m]$, $\sum_i |J_{ij}| + |g_j| \leq \beta$.

These assumptions are standard in the literature on learning Ising models and RBMs [38,43]. In physics, these bounds imply conditions on the temperature and the characteristic scales of the Hamiltonian of the Gibbs state in Eq. (1).

II. RESULTS

We begin with defining classes of quantum states. In this work, we consider NNQ states based on RBMs where the amplitudes are real and positive.

Definition 1 (Special RBM-NNQ states). Let $\mathcal{H}_n$ be the Hilbert space of an n -qubit system. Define $\mathcal{C} := \mathcal{C}(n, d_2, \alpha, \beta) \subset \mathcal{H}_n$ as the class of quantum states such that for each $|\phi\rangle_R \in \mathcal{C}$ there exists an (α, β) nondegenerate locally consistent RBM with two-hop degree d_2 with marginal probability distribution $p(x)$ and $|\phi\rangle_R = \sum_{x \in \{\pm 1\}^n} \sqrt{p(x)} |x\rangle$.

The main measure of closeness in this work is the L_p distance. Consider two n -qubit quantum states $|\psi\rangle = \sum_x \psi(x) |x\rangle$, with $|\psi(x)|^2 =: \tilde{p}(x)$ and $|\phi\rangle_R = \sum_x \phi_R(x) |x\rangle$, with $|\phi_R(x)|^2 =: p(x)$. Define L_p distance between the magnitudes of two states to be

$$L_p(|\phi\rangle_R, |\psi\rangle) := \left(\sum_{x \in \{\pm 1\}^n} |p(x) - \tilde{p}(x)|^p \right)^{1/p}. \quad (3)$$

We define a class of quantum states.

Definition 2 (ϵ_p -close states). Let $\mathcal{H}_n$ be Hilbert space of n qubits. Let $\epsilon_p \geq 0$. Define $\mathcal{C}(\epsilon_p) := \mathcal{C}(\epsilon_p, n, d_2, \alpha, \beta) \subset \mathcal{H}_n$ such that for each $|\psi\rangle \in \mathcal{C}(\epsilon_p)$ there exists at least a state $|\phi\rangle_R \in \mathcal{C}$ with L_p distance smaller than ϵ_p .

Even though $\mathcal{C}$ only considers quantum states with real and positive amplitudes, with $\mathcal{C}(\epsilon_p)$ it does allow us to probe quantum states with complex amplitudes. In the following, we will show that for quantum states belonging to this class, the magnitude of each amplitude is efficiently learnable under certain conditions. Since $\mathcal{C}$ is contained in $\mathcal{C}(\epsilon_p)$, the results translate to $\mathcal{C}$ obviously.

Structure learning. The key insight for efficient learning is that the structure of corresponding RBM can tell us certain properties of the unknown quantum states. For instance, if a quantum state can be represented by a local RBM, where hidden nodes are only connected to their geometrically local visible nodes, its entanglement entropy (Rényi entropy) satisfies the area law [44]. Based on nonlocal RBM, it can also represent quantum states efficiently, which exhibit volume-law entanglement [33].

Learning the two-hop neighborhood for each node can greatly reduce the sample complexity for finding parameters to recover the magnitudes of the amplitudes. We employ a greedy algorithm [39] to learn from the measurements and show that it is suitable to learn quantum states in $\mathcal{C}(\epsilon_p)$ for certain d_2 and ϵ_p . Recall Definitions 1 and 2.

Theorem 1 (Quantum state structure learning, informal). Let $\epsilon_p \in (0, 1)$. Suppose we are given many copies of an n -qubit unknown quantum state $|\psi\rangle$ in class $\mathcal{C}(\epsilon_p)$. Let $|\phi\rangle_R$ in class $\mathcal{C}$ be the state with L_p distance smaller than ϵ_p . If

ϵ_p is small enough (defined by a threshold depending on the parameters), then the two-hop neighborhood of the RBM associated with state $|\phi\rangle_R$ can be estimated with $\tilde{\mathcal{O}}(2^{4d_2} \log n)$ copies of $|\psi\rangle$ in time $\tilde{\mathcal{O}}(2^{4d_2} n^2)$ with constant success probability.

The formal version and the proof are given in Theorem B1 in Appendix B. The algorithm utilizes an observation that if nodes u and v are two-hop neighbors, their (classical) covariance can be lower bounded by a threshold value [39]. We show that this value is still valid for quantum states in $\mathcal{C}(\epsilon_p)$. Notice that if $d_2 = \log \log n$, the underlying structure can be estimated with $\text{poly}(\log n)$ samples. As we have no restriction on the physical local connection, the method also suits for learning quantum states which satisfy either area law or volume law, which also satisfies the constraints in our setting. This demonstrates that the entanglement property is not a constraint on the efficiency of the RBM representation.

Quantum state learning. With the two-hop structure of the RBM representation learned in the previous step, we can greatly reduce the sample complexity to find parameters to estimate the magnitudes of each amplitude. If the two-hop degree of the RBM representation of the state is bounded by d_2 , the magnitudes can be reconstructed using only $\mathcal{O}(n2^{d_2})$ parameters. Otherwise, we need exponentially many (in n) parameters in the worst case.

In general, the two-hop degree of the RBM representation of quantum states $|\psi\rangle \in \mathcal{C}(\epsilon_p)$ may not be bounded by d_2 , i.e., they may have more complex structures. We show that if ϵ_p is small enough, we can still well estimate magnitudes of the states with bounded degree d_2 . Also, to learn samples with intrinsic error, i.e., ϵ_p , we use a regression algorithm called Alphasatron.

First, we show the learning of all parameters that represent the quantum state. We learn the parameters that provide efficient (query) access to unnormalized magnitudes $\propto \tilde{p}(x) = |\langle x | \psi \rangle|^2$ of the unknown quantum state, with $\mathcal{O}(2^{d_2} n^2)$ number of copies of the quantum state. Therefore, for $d_2 = \mathcal{O}(\text{poly}(\log n))$, we show a provable efficient learning result for a special class of quantum states. We remark that the unnormalized output does not directly provide us with query access to the normalized $\tilde{p}(x)$, as we do not compute the normalization. However, with our query access, one can use the Metropolis-Hastings algorithm to provide sampling access to the probability distribution.

Theorem 2 (Quantum state learning, informal). Let $\epsilon_p \in (0, 1)$. Suppose we are given many copies of an n qubit unknown quantum state $|\psi\rangle$ in class $\mathcal{C}(\epsilon_p)$, with magnitudes denoted as $\tilde{p}(x)$. Let $|\phi\rangle_R$ in class $\mathcal{C}$ be the state with L_p distance smaller than ϵ_p , and the underlying structure of the associated RBM of $|\phi\rangle_R$ is known. Let $\epsilon_t > 0$. If the number of copies is $\tilde{\mathcal{O}}(2^{d_2} n^2 / \epsilon_t^4)$ and ϵ_p is small enough, then we find a set of parameters that provide efficient query access to unnormalized versions of estimates $\tilde{p}^*(x)$ of the magnitudes of the quantum state $|\psi\rangle$, in time $\text{poly}(n)$ with a guarantee of $\sum_x |\tilde{p}(x) - \tilde{p}^*(x)| \in \mathcal{O}(\epsilon_t)$ with high probability.

The formal version of the theorem and the proof are given in Theorem D2 in Appendix D. Remarkably, if $d_2 = \log n$, we find that, for $p = 1$, $\epsilon_p = \epsilon_1$ scales as $1/n^2$, while, for $p > 1$, ϵ_p scales as $1/2^{n(1-1/p)}$.

Next, we discuss the partial learning of the quantum state in the same setting. We are given measurement results of only a subset of the qubits. Let $p(x)$ be related to $|\phi\rangle_R$ as before. For a single $u \in [n]$, it has been shown that the conditional probability depends only on the two-hop neighborhood as $p(x_u|x_{\neq u}) = p(x_u|x_{\mathcal{N}_2(u)})$ by the Markov property. For a set of nodes $J \subset [n]$, let $\mathcal{N}_2(J)$ be the set composed of two-hop neighbors of each node in J excluding the nodes in J itself, $\mathcal{N}_2(J) := (\bigcup_{u \in J} \mathcal{N}_2(u)) \setminus J$. With the complement $x_{\bar{J}}$, we have analogously that $p(x_J|x_{\bar{J}}) = p(x_J|x_{\mathcal{N}_2(J)})$. Our result is to provide estimates for the conditional probabilities $p(x_J|x_{\mathcal{N}_2(J)})$ involving $\mathcal{O}(|J|2^{d_2})$ parameters, which is significantly fewer than the naive representation of a quantum state that would require a number of parameters exponential in n .

Theorem 3 (Quantum state partial learning, informal).

Let $|\psi\rangle$ and $|\phi\rangle_R$ be as in Theorem 2, and the two-hop neighborhood for all visible nodes of the RBM associated with $|\phi\rangle_R$ be known. Let $J \subseteq [n]$ and consider its neighborhood $\mathcal{N}_2(J)$ and the set $J_{\text{tot}} = J \cup \mathcal{N}_2(J)$. Suppose we are given many copies of the qubits indexed by J_{tot} of the state $|\psi\rangle$. Let $\epsilon_c > 0$. If the number of copies is $\mathcal{O}(2^{d_2}|J|^2/\epsilon_c^4)$, there exists a small number $\epsilon_p \in (0, 1)$, such that we can find a set of parameters that can estimate the conditional probability $\tilde{p}(x_J|x_{\mathcal{N}_2(J)})$ with a bounded error ϵ_c in time $\text{poly}(n)$.

The formal version of this theorem is presented in Theorem D3. This result is especially useful if the size of the set J is $\log n$, which implies a sample complexity of $\text{poly}(\log n)$.

Ferromagnetic RBMs. We also explicitly consider a class of quantum states close to NNQ states based on ferromagnetic RBMs, which is a special case of the locally consistent RBMs, where both pairwise interactions and external fields are non-negative. We consider the same problem setting by replacing locally consistent RBMs with ferromagnetic RBMs. The sample complexity for the structure learning is much better on the lower and upper bound strength, i.e., α and β , achieved with a different algorithm [38]. Once we learn the structure, the sample complexity for quantum state learning is the same with locally consistent cases. Further details, along with related results and proofs, are provided in Appendix C 2.

III. NUMERICAL SIMULATION

To illustrate our results, we consider learning an unknown thermal pure state of a many-body quantum system with Hamiltonian

$$H = - \sum_{i=1}^{n-1} q_{i,i+1} \sigma_i^z \sigma_{i+1}^z - \sum_{i=1}^n q_i \sigma_i^z, \quad (4)$$

where $q_{i,i+1}$ denotes the interaction between the qubits i and $i+1$ and q_i is the external field of each qubit i , σ_i^z is the Pauli Z operator applying on qubit i . Suppose the system is in a thermal equilibrium state, which can be represented by many pure quantum states [45]. Observed that it can be a canonical thermal pure quantum state defined in [46]

$$|T, n\rangle = \frac{1}{Z} \sum_{x \in \{\pm 1\}^n} e^{-H/2T} |x\rangle, \quad (5)$$

where Z is the partition function. For simplicity, we set $T = 1$. We observed that $|T = 1, n\rangle = \frac{1}{Z} \sum_x e^{-E/2} |x\rangle$, where

$E = - \sum_{i=1}^{n-1} q_{i,i+1} x_i x_{i+1} - \sum_{i=1}^n q_i x_i$, which is the energy of a Markov random field (MRF) with a chain underlying structure. The definition of the MRFs can be found in the Appendixes. Here, we illustrate the present result with a quantum state that is close to the NNQ state based on a locally consistent RBM ($d_2 = 2$) in the Ising chain model in Eq. (4). It has been proved that the underlying structure of an RBM equals the induced MRF [38]. The probability distribution is given by $p(x) = \frac{1}{Z} e^{-E}$. We see that the distribution of the system can be an MRF and can also be the marginal probability of the corresponding RBM over the observed nodes.

We construct thermal pure states according to locally consistent RBM representation with errors where the error can be treated as a small transverse field $t_i \sigma_i^X$ for each qubit $i \in [n]$ added to the Hamiltonian in Eq. (4). Then, we verify the underlying structure and the magnitudes using our results with samples from the real probability distribution. Consider three cases of the chain model with varying system sizes, $n = 10, 15, 20$. There are n visible nodes and $n-1$ hidden nodes of the RBM representation, each hidden node connected to two neighboring visible nodes i and $i+1$. We set the threshold $\tau = 0.05$, each interaction (edge connects one visible node and one hidden node) being 1, and all external fields being -0.1 . We then construct the probability distribution $\tilde{p}(x)$ from the probability distribution $p(x)$ of the RBM by randomly changing each $p(x)$ within some range (bounded L_∞ distance). The next step is sampling from the distribution $\tilde{p}(x)$ and run the greedy algorithm to obtain the two-hop neighbors. We claim success when we achieve the same underlying structure as that of the RBM. We show the success probabilities along with the different number of samples of the two-hop neighbors learning in Fig. 2(a). With more samples, we achieve a higher success probability, for example, for $n = 20$, we achieve a success probability 1 with a sample size of 3700. For state learning, we use the Alphasat algorithm to obtain the parameters for magnitudes. As a result, we have the fidelities shown in Fig. 2(b). For $n = 20$, we achieve an average fidelity surpassing 0.99 for more than 2000 samples. These sample sizes are notably smaller than the exponential 2^{20} .

IV. DISCUSSION

We have presented a framework for learning quantum states that are well approximated by RBMs, using machine learning methods with provable guarantees. The sample complexity of our method scales polynomially with the number of qubits, which provides an exponential advantage over standard quantum state tomography that requires $\mathcal{O}(2^n)$ samples. This efficiency stems from the near-optimal sample complexity of the underlying classical algorithms for learning the structure of the corresponding RBM [38]. While the optimal sample complexity for the full quantum learning task (which includes estimating complex amplitudes) remains an open question, our work establishes a provably efficient and robust learning pipeline for a broad class of physically relevant quantum states.

We have discussed the learning of quantum states with RBMs using machine learning methods with provable guarantees. The technical contribution of this work is a robustness

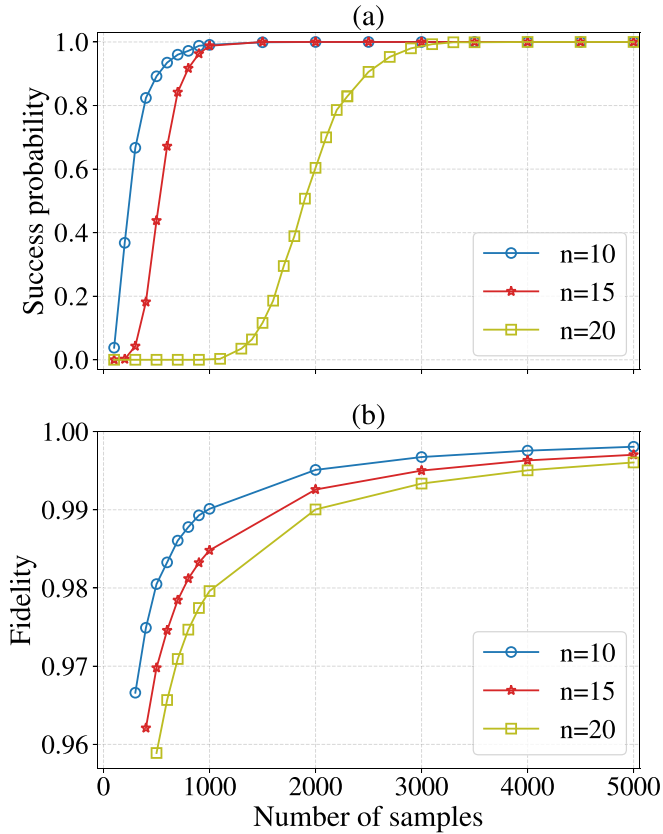


FIG. 2. Numerical results for learning from measurements of quantum states of a varying number of qubits. (a) The success probability of finding the two-hop neighborhood given a different number of samples. (b) Fidelity of the estimated state from learning from samples.

result for the RBM learning algorithms. This robustness implies that a much larger class of non-RBM quantum states can be efficiently represented by RBMs with bounded degrees. For such states, the sample complexity for learning them is $\text{poly}(n)$, in contrast to the 2^n dependency of naive tomography. Of course, other ways of tomography achieve better sample complexity than naive tomography for certain restricted classes of states, e.g., stabilizer states.

We have focused on learning partial information, specifically by learning the magnitudes while leaving the phases unexplored. We show that the amplitudes of these states can be learned efficiently both in terms of sample size and run-time. Notable methods for acquiring partial descriptions of quantum states include quantum PAC learning [47] and quantum shadow tomography [16]. Quantum PAC learning is generalized from classical learning theory, demonstrating that all quantum states are PAC learnable with $\mathcal{O}(n)$ samples. However, the time complexity remains an open problem. Quantum shadow tomography considers a set of positive semidefinite operators $\{E_i\}_{i \in [M]}$ and $\|E_i\| \leq 1$; the goal is to estimate each $\text{Tr}(\rho E_i)$ up to an additive error ϵ_s for a n -qubit quantum state ρ . The sample complexity of the quantum shadow tomography was first shown to be $\mathcal{O}(n \log^4 M / \epsilon_s^4)$ [48] and has been improved to $\mathcal{O}(n \log^2 M / \epsilon_s^4)$ [49].

Shadow tomography can be applied to the situation in the present work, where the measurement operators are the computation basis $\{|x\rangle\langle x|\}_{x \in \{\pm 1\}}$, and there are 2^n measurement operators. In this specific case, shadow tomography requires $\mathcal{O}(n^3 / \epsilon_s^4)$ samples where error bound ϵ_s is the infinity norm over the computation basis satisfying $|\hat{p}(x) - \text{Tr}(|\psi\rangle\langle\psi||x\rangle\langle x|)| < \epsilon_s$ for all $x \in \{\pm 1\}^n$, where $\hat{p}(x)$ is the empirical value obtained from shadow tomography. In our context, with a one-norm error bound ϵ_t over all $x \in \{\pm 1\}^n$, it requires $\mathcal{O}(n^3 / \epsilon_t^4)$ samples when $d_2 = \log n$. Moreover, for the case that $d_2 = \log \log d$, our method achieves a sample complexity of $\tilde{\mathcal{O}}(n^2 / \epsilon_t^4)$. Hence, our method obtains a polynomial improvement in n and is generally much better in the error dependency since the infinity norm is always bounded by the one norm for any vector.

Because of the definition of the ferromagnetic and locally consistent RBM, the probability $p(x)$ for each configuration $x \in \{1, -1\}^n$ must be strictly nonzero, since the interaction matrix elements and the external field elements real numbers, which makes the exponential strictly positive. Our algorithm also works for the quantum states where the magnitude $p(x)$ for some configurations is exactly 0. That is, the magnitudes of such a state are close to those of a state whose magnitudes can be represented by a ferromagnetic or locally consistent RBM. In such situations, the target state can still be well approximated by the magnitudes of a state representable by a ferromagnetic or locally consistent RBM and satisfies the ϵ_p distance. The norm distance bound in Theorem D2 is natural; for $p = 1$, the required accuracy scales only polynomial with n , while for $p > 1$, it scales exponential, consistent with the intrinsic amplitude scale of normalized many-body quantum states.

It would also be interesting to explore the relations with graphical model methods and tensor network-based methods, which have also been investigated for learning certain class of quantum states [50–54].

We believe our results show alternative ways of quantifying the learnability of quantum states. As our methods currently learn the magnitude of the quantum amplitudes, in future work, one can consider an extension to learning the magnitudes and phases of the quantum states.

V. METHODS

Consider Appendix A for general definitions, in particular the definitions of the conditional covariance and MRFs.

A. Schematic proof of Theorem 1

We consider estimating the underlying structure (the two-hop neighbor's structure) of the RBM representation of an unknown state in class $\mathcal{C}(\epsilon_p)$. We begin by demonstrating that if ϵ_p is sufficiently small, the difference between the average conditional covariance of the magnitude distributions of state $|\phi\rangle_R$ and that of the unknown state satisfies the inequality

$$|\text{Cov}^{\text{avg}}(u, v|S) - \widetilde{\text{Cov}}^{\text{avg}}(u, v|S)| \leq \frac{\tau}{8}, \quad (6)$$

where $u, v \in [n]$, $S \subset [n] \setminus \{u, v\}$, and τ is a threshold value. The definition of the conditional covariance can be found in the Appendixes. Then, we use the results in Ref. [39] that if

$v \in \mathcal{N}_2(u)$, then $\text{Cov}^{\text{avg}}(u, v|S) \geq 2\tau$. Conversely, if v is not a two-hop neighbor of u , we have $\text{Cov}^{\text{avg}}(u, v|S) = 0$. Additionally, if the number of samples satisfies a constraint, then with a high probability, we show that the difference between the average conditional covariance and the empirical one can be bounded as follows:

$$|\widetilde{\text{Cov}}^{\text{avg}}(u, v|S) - \widetilde{\text{Cov}}^{\text{avg}}(u, v|S)| \leq \tau/2. \quad (7)$$

Accordingly, we prove that

$$\begin{aligned} \widetilde{\text{Cov}}^{\text{avg}}(u, v|S) &> \tau, \text{ for any } v \in \mathcal{N}_2(u), \\ \widetilde{\text{Cov}}^{\text{avg}}(u, v|S) &< \tau, \text{ for } v \notin \mathcal{N}_2(u). \end{aligned} \quad (8)$$

This allows us to employ the greedy algorithm introduced in Ref. [39] to estimate the two-hop neighbors of each visible node of the underlying structure.

It has been proved that the marginal distribution on the visible nodes of an RBM with two-hop degree d_2 is a d_2 -wise Markov random field, e.g., used in Ref. [38,55]. In the other direction, Ref. [38] proves that every MRF can be converted to an equivalent RBM.

B. Schematic proof of Theorems 2 and 3

For the proof of Theorem 2, we assume the estimated underlying structure is known. Then an RBM can be learned by estimating the parameters of the induced MRF, where the definition can be found in the Appendixes. By using the Alphatron algorithm introduced in Ref. [40], the parameters can be learned with a bounded error. Specifically, for a node $u \in [n]$, we consider using the Alphatron algorithm to learn the parameters of the partial potential. Let $q_u(X) = \sum_I q_I x_I$ and $\tilde{q}_u(X) = \sum_J q_J x_J$ as the partial potential over node u of the MRF induced on the observed nodes corresponding to $|\phi\rangle_R$ and the unknown quantum state, respectively, where $I \subset \mathcal{N}_2(u)$, q_I represents the coefficients, and x_I is the product of x_i , for all $i \in I$. Note that $q_u(X)$ contains at most 2^{d_2} terms due to the bounded degree constraint, whereas $\tilde{q}_u(X_{\neq u})$ contains at most $\sum_{i=1}^{n-1} \binom{n}{i}$ terms, accounting for all possible monomials in a general MRF. Therefore, the partial potential $\tilde{q}_u(X_{\neq u})$ of the induced MRF representation of the unknown state can be divided into two parts, i.e.,

$$\tilde{q}_u(X_{\neq u}) = q_u(X_{\neq u}) + q_\epsilon(X_{\neq u}). \quad (9)$$

Assuming $\tilde{q}_u(X_{\neq u})$ consists of the same monomials as $q_u(X_{\neq u})$ but with different coefficients, and $q_\epsilon(X_{\neq u})$ can be treated as the error term, we demonstrate that the coefficients of $\tilde{q}_u(X_{\neq u})$ can be learned with bounded error. This is achieved by using the Alphatron algorithm in Ref. [40] with the knowledge of all two-hop neighbors of node u of the RBM representation of $|\phi\rangle_R$. By applying this method to all visible nodes, we can learn all the parameters of the induced MRF. Additionally, we prove that the 1-norm distance between the estimated magnitudes and the actual one of the unknown state can be bounded by a constant when ϵ_p is sufficiently small and the sample size is large enough.

The proof of Theorem 3 follows a similar approach to that of Theorem 2, wherein we focus solely on learning the parameters associated with a subset of nodes (subset $J \subset [n]$ and the neighbors), rather than all parameters. This targeted

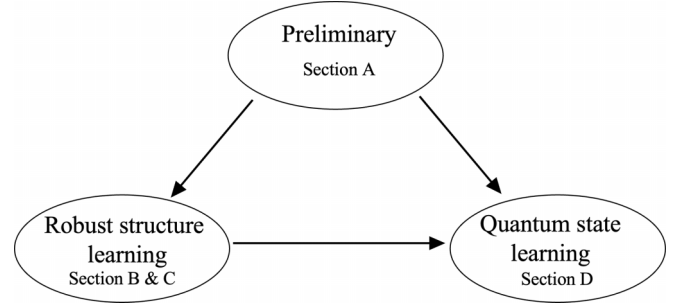


FIG. 3. Structure for the Appendixes.

approach significantly reduces the necessary sample size since we are only acquiring partial information.

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All authors contributed to the research and the writing of the manuscript.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIXES

These Appendixes provide technical details about the theorems discussed in the main paper. It is organized into three main parts, and the overall structure is illustrated in Fig. 3. The first part is preliminary, where we define the notations and review the necessary concepts related to the RBM and the MRF. Additionally, we review two greedy algorithms introduced in Refs. [38,56] for the convenience of the readers. The second part is dedicated to robust structure learning. In this part, we establish the robust version of classical learning algorithms and elucidate their application to learning the two-hop neighborhoods of the RBM representation of a quantum state in a certain class from measurement results. The last part is the quantum state learning. With the knowledge of the two-hop neighborhoods learned from measurements, we show that the magnitude of the quantum state can be recovered with a bounded error by using the Alphatron algorithm [40]. In particular, we also demonstrate the ability to estimate the distribution of the magnitude of a quantum state that involves a subset of the qubits, conditioned on the configu-

ration we have acquired through measurement results of the remaining qubits.

APPENDIX A: PRELIMINARIES

In this Appendix, we first introduce the notations used in this paper. Then, we review some important properties and results of the RBM. We also introduce two classical greedy algorithms for learning locally consistent and ferromagnetic RBMs for completeness. Then, we introduce a more general graph model called the MRF. We review the mapping relation between an RBM and the induced MRF proved in Ref. [38]. At last, we introduce the NNQ state, where the amplitudes are represented by a neural network.

1. Notation

Let $\mathbb{Z}_+$ denote the set of positive integers and $[N] = \{1, 2, \dots, N\}$. The set of real numbers is denoted by $\mathbb{R}$. For a set I , $|I|$ denotes the number of elements in the set. Let the sigmoid function be $\sigma(x) = 1/(1 + e^{-x})$ and the hyperbolic tangent function be $\tanh(x) = (e^x - e^{-x})/(e^x + e^{-x})$. For a random variable X , the probability for $X = x$ is given by $p(X = x)$. For simplicity, we sometimes write $p(x)$ with the same meaning. For a value a , we use $\hat{a}$ to represent its empirical version, i.e., estimated from samples. For a random variable b , we use $\mathbb{E}[b]$ to represent its expectation value and use $\hat{\mathbb{E}}[b]$ to represent its empirical expectation value estimated from samples.

2. Restricted Boltzmann machines

RBM is a class of graphical models with latent (hidden) variables that have many applications, such as dimension reduction [57], feature learning [58], and quantum many-body physics [27]. RBMs have also been proven to be universal approximators for arbitrary functions [26].

Definition A1 (Restricted Boltzmann machine). A restricted Boltzmann machine (J, h, g) with n visible nodes $\{X_i\}_{i \in [n]}$ and m hidden nodes $\{Y_j\}_{j \in [m]}$ is a weighted bipartite graph and the probability that the model assigns the configuration (x, y) , where $x \in \{\pm 1\}^n$, $y \in \{\pm 1\}^m$, is given by

$$P(X = x, Y = y) = \frac{1}{Z} \exp(x^T J y + h^T x + g^T y),$$

where Z is the partition function, $J \in \mathbb{R}^n \times \mathbb{R}^m$ is the interaction matrix, and vectors $h \in \mathbb{R}^n$, $g \in \mathbb{R}^m$ are external fields.

Locally consistent and ferromagnetic RBMs are the well-studied subclasses of RBMs, where the definitions are provided as follows. Notice that a ferromagnetic RBM is a special class of locally consistent RBM.

Definition A2 (Locally consistent RBM). An RBM is locally consistent if for each latent node $j \in [m]$, $J_{ij} \geq 0$ or $J_{ij} \leq 0$ for all visible nodes $i \in [n]$.

Definition A3 (Ferromagnetic RBM). An RBM is ferromagnetic if the pairwise interactions and external fields are all non-negative, i.e., $J_{ij} \geq 0$, $h_i \geq 0$, and $g_j \geq 0$, for all $i \in [n]$, $j \in [m]$.

In the following, for simplicity, we use FRBM instead of ferromagnetic RBM. RBM learning can be divided into structure learning and parameter learning. One purpose of structure

learning is to learn the two-hop neighbors of each visible node and use this information for parameter learning. Two visible nodes are two-hop neighbors with each other if they connect to at least one common hidden node. The definition of two-hop neighbors is shown in the following.

Definition A4 (Two-hop neighborhood [38]). Let $i \in [n]$ be a visible node for a fixed RBM (J, h, g) . Denote the two-hop neighborhood of i as $\mathcal{N}_2(i)$, which is the smallest set of visible nodes $S \subset [n] \setminus \{i\}$ such that conditioned on X_S , X_i is conditionally independent of X_j for all visible nodes $j \in [n] \setminus (S \cup \{i\})$. The two-hop degree of the RBM is defined as $d_2 = \max_{i \in [n]} |\mathcal{N}_2(i)|$.

To learn the underlying structure of an RBM, it is necessary to have both lower and upper bounds of the weights. We consider the (α, β) nondegenerate RBM as follows [38].

Definition A5. An RBM is (α, β) nondegenerate if

1. for every $i \in [n]$ and $j \in [m]$, $|J_{ij}| \geq \alpha$, if $|J_{ij}| \neq 0$.
2. for every $i \in [n]$, $\sum_j |J_{ij}| + |h_i| \leq \alpha$.
3. for every $j \in [m]$, $\sum_i |J_{ij}| + |g_j| \leq \beta$.

These assumptions are standard in the literature on learning Ising models and also allow for provable guarantees for the learning of RBMs [43].

3. Classical algorithms for RBM structure learning

In this Appendix, we review two classical greedy algorithms. Bresler *et al.* proposed an algorithm based on influence maximization for learning the two-hop neighborhoods of a visible node for FRBMs [38]. The algorithm takes nearly quadratic time with logarithmic sample complexity with respect to the number of visible nodes. The dependency on the maximum degree and upper-bounded strength are single exponential in the algorithm's run-time as well as in optimal sample complexity. Goel [39] on the other hand worked on locally consistent RBMs with arbitrary external fields and proposed an algorithm for learning two-hop neighborhoods on the maximization of conditional covariance, which relies on the Fortuin-Kasteleyn-Ginibre inequality. The run-time and sample complexity with respect to the number of visible nodes is the same with the FRBM case but the dependency on upper bound strength is doubly exponential. Note that since an FRBM is also a locally consistent RBM, the algorithm for learning the structure of a locally consistent RBM can be applied to FRBMs as well.

a. LRBM

It has been shown that for any two visible nodes that are the two-hop neighborhood of each other, the conditional covariance can be lower bounded for locally consistent RBMs [39]. Remind that external fields are h and g in Eq. (1). Based on this, the author introduced a classical greedy algorithm that maximizes covariance to learn the two-hop neighborhoods for any visible node of locally consistent RBMs (LRBMs) with arbitrary external fields.

Definition A6 (Conditional covariance). The conditional covariance for visible nodes u, v and a subset $S \subseteq [n] \setminus \{u, v\}$ is defined as

$$\begin{aligned} \text{Cov}(u, v | X_S = x_S) &:= \mathbb{E}[X_u X_v | X_S = x_S] \\ &\quad - \mathbb{E}[X_u | X_S = x_S] \mathbb{E}[X_v | X_S = x_S]. \end{aligned} \quad (\text{A1})$$

ALGORITHM 1. Greedy algorithm for structure learning of a locally consistent RBM [39].

Input: Samples $\{X^i\}_{i \in [M_2]}$, threshold τ , visible node u

- 1: Set $S := \emptyset$
- 2: Let $i^* = \arg \max_v \widehat{\text{Cov}}^{\text{avg}}(u, v|S)$, $\eta^* = \max_v \widehat{\text{Cov}}^{\text{avg}}(u, v|S)$
- 3: **if** $\eta^* \geq \tau$ **then**
- 4: $S = S \cup \{i^*\}$
- 5: **else**
- 6: go to step 2
- 7: **end if**
- 8: Go to step 2
- 9: pruning step: For each $v \in S$, if $\widehat{\text{Cov}}^{\text{avg}}(u, v|S) < \tau$, remove v

Output: S

The average conditional covariance is defined as

$$\text{Cov}^{\text{avg}}(u, v|S) := \mathbb{E}_{x_S}[\text{Cov}(u, v|X_S = x_S)]. \quad (\text{A2})$$

The following property of the average conditional covariance is proved in Ref. [39].

Lemma A1. Given node $u \in [n]$ and a subset $S \subseteq [n] \setminus \{u\}$ with configuration X_S , if node $v \in \mathcal{N}_2(u) \setminus S$, it satisfies

$$\text{Cov}^{\text{avg}}(u, v|S) \geq \alpha^2 \exp(-12\beta). \quad (\text{A3})$$

Given M samples of visible nodes $\{X^i \in \{\pm 1\}^n\}_{i \in [M]}$, the empirical average conditional covariance is defined as

$$\widehat{\text{Cov}}^{\text{avg}}(u, v|S) := \widehat{\mathbb{E}}_{x_S}[\widehat{\text{Cov}}(u, v|X_S = x_S)]. \quad (\text{A4})$$

Using Lemma A1, the author proposed a greedy Algorithm 1 by maximizing conditional covariance. The following theorem gives the number of samples required and the run-time of the algorithm.

Theorem A1 (Theorem 2 in Ref. [39]). Given M_2 samples of visible nodes $\{X^i \in \{\pm 1\}^n\}_{i \in [M_2]}$ of a (α, β) nondegenerate locally consistent RBM, for $\delta = \frac{1}{2}e^{-2\beta}$, $\tau = \frac{1}{2}\alpha^2 \exp(-12\beta)$, and $\gamma = \frac{8}{\tau^2}$, with probability $1 - \zeta$, the two-hop neighbours $\mathcal{N}_2(u)$ of a visible u can be obtained in time $O(M_2 n \gamma)$ by using Algorithm 1 as long as

$$M_2 \geq \Omega\left((\log(1/\zeta) + \gamma \log(n)) \frac{2^{2\gamma}}{\tau^2 \delta^{2\gamma}}\right).$$

Notice that $\gamma \geq d_2$, and $\delta < 1/2$ then we have $M_2 \geq \Omega((\log(1/\zeta) + d_2 \log(n)) \frac{2^{4d_2}}{\tau^2})$.

b. FRBMs

It has been shown that the two-hop neighbors of an FRBM can be learned by maximizing the influence function [38]. Given a visible node $u \in [n]$ and a subset $S \subset [n] \setminus \{u\}$ of an FRBM, as in the main paper, the discrete influence function is defined as

$$I_u(S) := \mathbb{E}[X_u|X_S = \{1\}^{|S|}]. \quad (\text{A5})$$

The discrete influence function is a monotone submodular function for any visible node $u \in [n]$, proved in Ref. [38]. The empirical discrete influence function is defined as

$$\hat{I}_u(S) := \hat{\mathbb{E}}[X_u|X_S = \{1\}^{|S|}], \quad (\text{A6})$$

ALGORITHM 2. Greedy algorithm for structure learning of an FRBM [38].

Input: Samples $\{X^i\}_{i \in [M_1]}$, threshold η , visible node u

- 1: Set $S_0 \leftarrow \emptyset$.
- 2: **for** $t = 0, \dots, k-1$ **then**
- 3: $j_{t+1} \leftarrow \arg \max_{j \in [n]} \hat{I}_u(S_t \cup \{j\})$.
- 4: $S_{t+1} \leftarrow S_t \cup \{j_{t+1}\}$.
- 5: **end for**
- 6: $\mathcal{N}_2(u) \leftarrow \{j \in S_k : \hat{I}_u(S_k) - \hat{I}_u(S_k \setminus \{j\}) \geq \eta\}$

Output: $\mathcal{N}_2(u)$

where $\hat{\mathbb{E}}$ denotes the empirical expectation based on samples from FRBM. Expanding the above equation gives us

$$\begin{aligned} \hat{I}_u(S) &= \frac{\sum_{x_u \in \{\pm 1\}} x_u \hat{p}(X_u = x_u, X_S = \{1\}^{|S|})}{\hat{p}(X_S = \{1\}^{|S|})} \\ &= \frac{2\hat{p}(X_{S \cup \{u\}} = \{1\}^{|S|+1})}{\hat{p}(X_S = \{1\}^{|S|})} - 1. \end{aligned} \quad (\text{A7})$$

The distribution probability for M samples can be obtained by

$$\hat{p}(X = x) = \frac{1}{M} \sum_{i=1}^M \mathbb{1}_{\{X^{(i)}=x\}}, \quad (\text{A8})$$

where $\mathbb{1}_{\{X^{(i)}=x\}}$ is equal to 1 when $X^{(i)} = x$, and 0 otherwise.

The two-hop neighborhoods of each visible node can be found by maximizing the empirical influence function, with the algorithm and theorem provided as follows.

Theorem A2 (Theorem 6.1 in Ref. [38]). Given M_1 samples $\{X^i \in \{\pm 1\}^n\}_{i \in [M_1]}$ of the visible nodes of a ferromagnetic restricted Boltzmann machine which is (α, β) nondegenerate, and has two-hop degree d_2 . For $\delta > 0$, if

$$M_1 \geq 2^{2k+3} (d_2/\eta)^2 (\log(n) + k \log(en/k)) \log(4/\delta), \quad (\text{A9})$$

where $\eta = \alpha^2 \sigma(-2\beta)(1 - \tanh(\beta))^2$, $k = d_2 \log(4/\eta)$, and $\sigma(x) = 1/(1 + e^{-x})$ for every visible node $u \in [n]$, then Algorithm 2 returns $\mathcal{N}_2(u)$ with probability $1 - \delta$ in time $O(M_1 kn)$.

The total run-time for all n visible nodes comes out to be $O(M_1 kn^2)$. Step 3 of Algorithm 2 is the most time-consuming part that requires $O(M_1 n)$. Note that the number of iterations k depends on the two-hop degree and the upper and lower bounds on the strengths of the RBM.

4. Markov random fields

An MRF with n variables can be represented by an undirected graph with n nodes, where the correlations among the variables can be described by the weights of the hyperedges (fully connected subgraph) in the graph.

Definition A7 (Markov random field). The probability distribution on $x \in \{\pm 1\}^n$ of an r -wise MRF of n variables can be expressed as

$$p(X = x) = \frac{1}{Z} \exp(q(x)), \quad (\text{A10})$$

where Z is the partition function and $q(x) = \sum_{I \subseteq [n]} q_I X_I$ is a multilinear polynomial referred to as the potential of the MRF, q_I is the coefficient for the subset I , and the monomial $X_I = \prod_{i \in I} X_i$ contains at most r variables.

Each monomial x_I in the potential $q(x)$ involves a fully connected subgraph. The fully connected subgraph means that each pair of nodes in the subgraph I are connected.

RBM is a subset of MRFs. Moreover, it has been proved that the marginal distribution on the visible nodes of an RBM with two-hop degree d_2 is a d_2 -wise Markov random field, e.g., used in Ref. [38,55]. In the other direction, Ref. [38] proves that every MRF can be converted to an equivalent restricted Boltzmann machine. A formal statement is provided as follows.

Theorem A3 (Theorem 4.4 in Ref. [38]). Consider an r -wise Markov random field on $\{\pm 1\}^n$. Suppose that the degree of the underlying structure of the MRF is d and the coefficients of each monomial of $q(x)$ are bounded by a constant M . Then, there is an RBM with n observable nodes and parameters (J, h, g) such that

- (1) The induced MRF of the RBM equals the original MRF, i.e., the marginal distribution of visible nodes equals the original MRF.
- (2) There are at most $O(n2^d)$ hidden nodes.
- (3) The degree of every hidden node is at most r .
- (4) The two-hop neighborhood of every visible node equals its original MRF neighborhood. The two-hop neighborhood degree d_2 equals the degree d of the structure graph of the MRF.

To learn the underlying structure of an MRF is to learn the neighbors of each node. There is an optimal algorithm for learning the underlying graph with $\log n$ samples in time $n^{O(t)}$ and learning the parameters with $n^{O(t)}$ samples [59].

5. Neural network quantum states

As mentioned in the main paper, it has been shown that any n -qubit quantum state can be arbitrarily well approximated by a neural network quantum state (NNQ state) based on RBM with potentially an exponential number of hidden nodes [29]. Suppose an NNQ state based on RBM is given by

$$|\phi\rangle_R = \sum_{x \in \{\pm 1\}^n} \phi(x)|x\rangle, \quad |\phi(x)|^2 = p(x), \quad (\text{A11})$$

where the magnitude $p(x)$ is the marginal probability distribution on the visible nodes of RBMs. For simplicity, in this paper, we focus on NNQ states whose amplitudes are real and positive, i.e., $\phi(x) = \sqrt{p(x)}$. We define a class named $\mathcal{C}$, which is defined in the main paper, Definition 1, and a subset of this class which is named $\mathcal{C}_F$. The formal definition is shown in the following.

Definition A8 (FRBM-NNQ states). Let $\mathcal{H}_n$ be the Hilbert space of an n -qubit system. Define $\mathcal{C}_F := \mathcal{C}(n, d_2, \alpha, \beta) \subset \mathcal{H}_n$ the class of quantum states based on (α, β) nondegenerate ferromagnetic RBM with two-hop degree d_2 .

With the L_p distance defined in Eq. (3), we define the following classes.

Definition A9 (ϵ_p -close classes). Let $\mathcal{H}_n$ be Hilbert space of n qubits. Let $\epsilon_p \geq 0$. Define two classes as follows:

- (1) $\mathcal{C}(\epsilon_p) \subset \mathcal{H}_n$ such that for each $|\psi\rangle \in \mathcal{C}(\epsilon_p)$ there exists a state $|\phi\rangle_R \in \mathcal{C}$ with L_p distance bounded by ϵ_p . (same as Definition 2).
- (2) $\mathcal{C}_F(\epsilon_p) \subset \mathcal{H}_n$ such that for each $|\psi\rangle \in \mathcal{C}_F(\epsilon_p)$ there exists a state $|\phi\rangle_R \in \mathcal{C}_F$ with L_p distance bounded by ϵ_p .

We say that a state $|\psi\rangle$ is associated with the NNQ state $|\phi\rangle_R$.

To distinguish with FRBM-NNQ states, sometimes we write LRBM-NNQ state to mean that the NNQ state is based on locally consistent RBMs, which corresponds to Definition 1 in the main paper.

APPENDIX B: LRBM-NNQ ROBUST STRUCTURE LEARNING

In this Appendix, we will show that if ϵ_p is small enough (bounded by α, β , and n), the difference of conditional covariance, defined in Definition A6, between $|\psi\rangle \in \mathcal{C}(\epsilon_p)$ and the associated NNQ state $|\phi\rangle \in \mathcal{C}$ can be bounded. Then we prove the robust structure learning, i.e., we can learn the underlying structure of the RBM representation of state $|\phi\rangle_R$ by giving many copies of $|\psi\rangle \in \mathcal{C}(\epsilon_p)$. We first prove the following two lemmas, which will be used later.

Lemma B1. Assume the probabilities $\tilde{p}(x)$ and $p(x)$ ($x \in \{\pm 1\}^n$) from the distributions $\tilde{\mathcal{D}}$ and $\mathcal{D}$, respectively, are ϵ_p close under the L_p distance described in Eq. (3). Then, for any subset $I \subseteq [n]$ and $x_I \in \{\pm 1\}^{|I|}$, we have

$$|p(x_I) - \tilde{p}(x_I)| \leq 2^{(n-|I|)(1-1/p)} \epsilon_p. \quad (\text{B1})$$

Proof. Let $\bar{I} = [n] \setminus I$ and $x_{\bar{I}} \in \{\pm 1\}^{|\bar{I}|}$. Let P_{x_I} be a vector of $p(x_I, x_{\bar{I}})$ over all configurations $x_{\bar{I}} \in \{\pm 1\}^{|\bar{I}|}$. Note that the dimension of P_{x_I} is $2^{|\bar{I}|}$. We define $\tilde{P}_{x_I}$ in a similar way. By definition of the marginal distribution, we have

$$\begin{aligned} |p(x_I) - \tilde{p}(x_I)| &= \left| \sum_{x_{\bar{I}}} p(x_I, x_{\bar{I}}) - \sum_{x_{\bar{I}}} \tilde{p}(x_I, x_{\bar{I}}) \right| \\ &\leq \sum_{x_{\bar{I}}} |p(x_I, x_{\bar{I}}) - \tilde{p}(x_I, x_{\bar{I}})| \\ &= \|P_{x_I} - \tilde{P}_{x_I}\|_1 \\ &\leq 2^{|\bar{I}|(1-1/p)} \|P_{x_I} - \tilde{P}_{x_I}\|_p \\ &\leq 2^{|\bar{I}|(1-1/p)} \epsilon_p = 2^{(n-|I|)(1-1/p)} \epsilon_p, \end{aligned} \quad (\text{B2})$$

where the first inequality is obtained by the triangle inequality, the second inequality comes from the Hölder's inequality, and the last inequality is obtained by the fact that $\|P_{x_I} - \tilde{P}_{x_I}\|_p$ is smaller than ϵ_p since x_I is fixed. Recall that by Hölder's inequality, for a vector $x \in \mathbb{R}^m$, we have

$$\|x\|_q \leq m^{1/q-1/p} \|x\|_p. \quad (\text{B3})$$

In this inequality, set $q = 1$ and $m = 2^{|\bar{I}|}$, we achieve the inequality above. ■

Lemma B2. If A, B are random variables following a distribution $\mathcal{D}$, and C, D are random variables following a distribution $\tilde{\mathcal{D}}$ on the same sample space, we have

$$\begin{aligned} |p(A|B) - \tilde{p}(C|D)| &\leq \frac{1}{p(B)} (|p(A, B) - \tilde{p}(C, D)| \\ &\quad + |p(B) - \tilde{p}(D)|). \end{aligned} \quad (\text{B4})$$

Proof. We expand the conditional probability by using Bayes' theorem and using an ancillary conditional probability

as following:

$$\begin{aligned}
& |p(A|B) - \tilde{p}(C|D)| \\
&= \left| \frac{p(A, B)}{p(B)} - \frac{\tilde{p}(C, D)}{p(B)} + \frac{\tilde{p}(C, D)}{p(B)} - \frac{\tilde{p}(C, D)}{\tilde{p}(D)} \right| \\
&\leq \left| \frac{p(A, B)}{p(B)} - \frac{\tilde{p}(C, D)}{p(B)} \right| + \left| \frac{\tilde{p}(C, D)}{p(B)} - \frac{\tilde{p}(C, D)}{\tilde{p}(D)} \right| \\
&= \left| \frac{p(A, B)}{p(B)} - \frac{\tilde{p}(C, D)}{p(B)} \right| + \frac{\tilde{p}(C, D)}{\tilde{p}(D)} \left| \frac{p(B) - \tilde{p}(D)}{p(B)} \right| \\
&\leq \frac{1}{p(B)} (|p(A, B) - \tilde{p}(C, D)| + |p(B) - \tilde{p}(D)|), \quad (\text{B5})
\end{aligned}$$

where the first inequality is obtained by using the triangle inequality and the last inequality results from $\frac{\tilde{p}(C, D)}{\tilde{p}(D)} = \tilde{p}(C|D) \leq 1$. ■

1. Bounds for covariance differences under L_p distance

Assume that we are given an n -qubit quantum state $|\psi\rangle$ in class $\mathcal{C}(\epsilon_p)$ as defined in Definition A9 and $|\phi\rangle_R \in \mathcal{C}$ is an associate NNQ state. The magnitudes of each amplitude in the

computational basis are $\tilde{p}(x)$ and $p(x)$, respectively. We show that the difference between the average conditional covariance of any $u, v \in [n]$ conditioned on a $S \subset [n] \setminus \{u, v\}$ of these two probability distributions can be bounded by a function of τ , if ϵ_p is small enough.

Lemma B3. If the probabilities $\tilde{p}(x)$ and $p(x)$ ($x \in \{\pm\}^n$), from the distributions $\tilde{\mathcal{D}}$ and $\mathcal{D}$, respectively, satisfy the L_p distance described in Eq. (3), and $\mathcal{D}$ is a distribution from a locally consistent RBM. Let $\text{Cov}^{\text{avg}}(u, v|S)$ and $\widetilde{\text{Cov}}^{\text{avg}}(u, v|S)$ as average conditional covariance of distributions $\mathcal{D}$ and $\tilde{\mathcal{D}}$, respectively. Let $\tau > 0$ and a constant $C > 0$, if the following constraint is satisfied:

$$\epsilon_p \leq \frac{\tau}{2^{2+n(1-1/p)}C}, \quad (\text{B6})$$

where $C > 0$ is constant, we have

$$|\text{Cov}^{\text{avg}}(u, v|S) - \widetilde{\text{Cov}}^{\text{avg}}(u, v|S)| \leq \frac{\tau}{C}. \quad (\text{B7})$$

Proof. Expand the average conditional covariance defined in Eq. (A4) as the following:

$$\begin{aligned}
\text{Cov}^{\text{avg}}(u, v|S) &= \mathbb{E}_{x_S}[\mathbb{E}[X_u X_v | X_S = x_S] - \mathbb{E}[X_u | X_S = x_S] \mathbb{E}[X_v | X_S = x_S]] \\
&= \sum_{x_u, x_v} x_u x_v p(x_u, x_v) - \sum_{x_u, x_v, x_S} x_u x_v p(x_u | x_S) p(x_v | x_S) p(x_S) \\
&= \sum_{x_u, x_v} x_u x_v p(x_u, x_v) - \sum_{x_u, x_v, x_S} x_u x_v p(x_u | x_S) p(x_v, x_S). \quad (\text{B8})
\end{aligned}$$

We consider the difference between the average conditional covariance $\text{Cov}^{\text{avg}}(u, v|S)$ and $\widetilde{\text{Cov}}^{\text{avg}}(u, v|S)$. Let $\mathcal{T}_1$ and $\mathcal{T}_2$ represent the first and second terms, respectively, of the above equation as follows:

$$\mathcal{T}_1 = \sum_{x_u, x_v} x_u x_v p(x_u, x_v), \quad \mathcal{T}_2 = \sum_{x_u, x_v, x_S} x_u x_v p(x_u | x_S) p(x_v, x_S), \quad (\text{B9})$$

and $\tilde{\mathcal{T}}_1$ and $\tilde{\mathcal{T}}_2$ represent the corresponding terms in $\widetilde{\text{Cov}}^{\text{avg}}(u, v|S)$. We have

$$|\text{Cov}^{\text{avg}}(u, v|S) - \widetilde{\text{Cov}}^{\text{avg}}(u, v|S)| = |\mathcal{T}_1 + \mathcal{T}_2 - \tilde{\mathcal{T}}_1 - \tilde{\mathcal{T}}_2| \leq |\mathcal{T}_1 - \tilde{\mathcal{T}}_1| + |\mathcal{T}_2 - \tilde{\mathcal{T}}_2|. \quad (\text{B10})$$

The first term can be divided into two parts: (1) the configurations of nodes v and u are identical; (2) the configurations of nodes v and u are different. We have

$$\begin{aligned}
|\mathcal{T}_1 - \tilde{\mathcal{T}}_1| &= \left| \sum_{x_u, x_v} x_u x_v p(x_u, x_v) - \sum_{x_u, x_v} x_u x_v \tilde{p}(x_u, x_v) \right| \\
&= \left| \sum_{x_u = x_v} (p(x_u, x_v) - \tilde{p}(x_u, x_v)) - \sum_{x_u \neq x_v} (p(x_u, x_v) - \tilde{p}(x_u, x_v)) \right| \\
&\leq \left| \sum_{x_u = x_v} p(x_u, x_v) - \tilde{p}(x_u, x_v) \right| + \left| \sum_{x_u \neq x_v} p(x_u, x_v) - \tilde{p}(x_u, x_v) \right|, \quad (\text{B11})
\end{aligned}$$

where the first inequality comes from the triangle inequality. By using Lemma B1 for set $I = \{u, v\}$, we have

$$|\mathcal{T}_1 - \tilde{\mathcal{T}}_1| \leq 2^{n(1-1/p)} \epsilon_p. \quad (\text{B12})$$

Similarly, we divide the second term in Eq. (B10) into two parts: whether the configurations of nodes u and v are the same or not. For simplicity, we consider the case when $x_u = x_v$. We have

$$\begin{aligned}
& \left| \sum_{x_S} \sum_{x_u=x_v} (p(x_u|x_S)p(x_v, x_S) - \tilde{p}(x_u|x_S)\tilde{p}(x_v, x_S)) \right| \\
&= \left| \sum_{x_S} \sum_{x_u=x_v} p(x_u|x_S)(p(x_v, x_S) - \tilde{p}(x_v, x_S)) + p(x_u|x_S)\tilde{p}(x_v, x_S) - \tilde{p}(x_u|x_S)\tilde{p}(x_v, x_S) \right| \\
&= \left| \sum_{x_S} \sum_{x_u=x_v} p(x_u|x_S)(p(x_v, x_S) - \tilde{p}(x_v, x_S)) + \tilde{p}(x_v, x_S)(p(x_u|x_S) - \tilde{p}(x_u|x_S)) \right| \\
&\leq \sum_{x_S} \sum_{x_u=x_v} p(x_u|x_S) |p(x_v, x_S) - \tilde{p}(x_v, x_S)| + \tilde{p}(x_v, x_S) |p(x_u|x_S) - \tilde{p}(x_u|x_S)| \\
&\leq \sum_{x_S} \sum_{x_u=x_v} |p(x_v, x_S) - \tilde{p}(x_v, x_S)| + (|p(x_u, x_S) - \tilde{p}(x_u, x_S)| + |p(x_S) - \tilde{p}(x_S)|) \tilde{p}(x_v|x_S) \\
&\leq \sum_{x_S} \sum_{x_u=x_v} |p(x_v, x_S) - \tilde{p}(x_v, x_S)| + |p(x_u, x_S) - \tilde{p}(x_u, x_S)| + |p(x_S) - \tilde{p}(x_S)|, \tag{B13}
\end{aligned}$$

where the first inequality is obtained by using the triangle inequality, the second inequality is the result of the fact that the conditional probability is always bounded by 1 and Lemma B2. Combine with the case $x_u = -x_v$, we have

$$|\mathcal{T}_2 - \tilde{\mathcal{T}}_2| \leq 3 \times 2^{n(1-1/p)} \epsilon_p. \tag{B14}$$

Combine all these together, we have

$$\begin{aligned}
& |\text{Cov}^{\text{avg}}(u, v|S) - \widetilde{\text{Cov}}^{\text{avg}}(u, v|S)| \\
&\leq 2^{n(1-1/p)} \epsilon_p + 3 \times 2^{n(1-1/p)} \epsilon_p \\
&\leq 2^{2+n(1-1/p)} \epsilon_p. \tag{B15}
\end{aligned}$$

For a constant $C > 0$, set $2^{2+n(1-1/p)} \epsilon_p \leq \frac{\tau}{C}$ and we prove the lemma. ■

2. LRBM robust two-hop neighbor estimation

Assume we are given many copies of an unknown state $|\psi\rangle \in \mathcal{C}(\epsilon_p)$. We show that if ϵ_p is small enough for $|\psi\rangle$ with its associate NNQ state $|\phi\rangle_R \in \mathcal{C}$, we prove that for a visible $v \in [n] \setminus (S \cup \{u\})$ in the RBM representation of $|\phi\rangle_R$, τ can be a threshold to distinguish whether node v is a two-hop neighborhood of node u or not.

The following theorem is the formal version of Theorem 1 in the main manuscript.

Theorem B1 (Error threshold for neighborhood identifiability). Let us be given M_2 copies of a n -qubit unknown quantum state in the class $\mathcal{C}(\epsilon_p)$ defined in Definition A9, τ, γ as in Theorem A1. Denote the average conditional covariance of the RBM representation of the unknown state as $\widetilde{\text{Cov}}^{\text{avg}}(u, v|S)$ and the empirical average conditional covariance as $\text{Cov}^{\text{avg}}(u, v|S)$ for $u, v \in n$ and $S \subset [n] \setminus \{u, v\}$. If M_2 satisfies the constraint in Theorem A1 and the constraint is satisfied, i.e.,

$$L_p : \epsilon_p \leq \frac{\tau}{2^{n(1-1/p)+5}}, \tag{B16}$$

we have

$$\begin{aligned}
& \widetilde{\text{Cov}}^{\text{avg}}(u, v|S) > \tau, \text{ for any } v \in \mathcal{N}_2(u), \\
& \widetilde{\text{Cov}}^{\text{avg}}(u, v|S) < \tau, \text{ for } v \notin \mathcal{N}_2(u). \tag{B17}
\end{aligned}$$

Then, we can learn the underlying structure of the RBM representation in time $\tilde{O}(M_2 n^2)$ using the greedy Algorithm 1.

Proof. Given two nodes u, v and a subset $S \subseteq [n] \setminus \{u, v\}$ with $|S| \leq \gamma$, it has been proved in Ref. [56] that if the number of samples satisfies the constraint in Theorem A1, then with probability $1 - \rho$, we have

$$|\widetilde{\text{Cov}}^{\text{avg}}(u, v|S) - \text{Cov}^{\text{avg}}(u, v|S)| \leq \tau/2. \tag{B18}$$

By using Lemma B3, if the constraints in Eq. (B16) are satisfied, the difference between the average conditional covariance of the RBM representation of state $|\phi\rangle_R$ [which we denote as $\widetilde{\text{Cov}}^{\text{avg}}(u, v|S)$] and the one of state $|\psi\rangle$ [which we denote as $\text{Cov}^{\text{avg}}(u, v|S)$] is bounded as follows:

$$|\text{Cov}^{\text{avg}}(u, v|S) - \widetilde{\text{Cov}}^{\text{avg}}(u, v|S)| \leq \frac{\tau}{8}. \tag{B19}$$

Here, we set constant $C = 8$. Combining with Eqs. (B19) and (B18), we have

$$\begin{aligned}
& |\widetilde{\text{Cov}}^{\text{avg}}(u, v|S) - \text{Cov}^{\text{avg}}(u, v|S)| \\
&\leq |\widetilde{\text{Cov}}^{\text{avg}}(u, v|S) - \widetilde{\text{Cov}}^{\text{avg}}(u, v|S)| \\
&\quad + |\widetilde{\text{Cov}}^{\text{avg}}(u, v|S) - \text{Cov}^{\text{avg}}(u, v|S)| \\
&\leq \frac{\tau}{2} + \frac{\tau}{8}. \tag{B20}
\end{aligned}$$

From Corollary 1 in Ref. [39], we have

$$\begin{aligned}
& \text{Cov}^{\text{avg}}(u, v|S) \geq 2\tau, \quad \text{if } v \in \mathcal{N}_2(u), \\
& \text{Cov}^{\text{avg}}(u, v|S) = 0, \quad \text{if } v \notin \mathcal{N}_2(u). \tag{B21}
\end{aligned}$$

Combining with Eq. (B20), we have

$$\begin{aligned}\widetilde{\text{Cov}}^{\text{avg}}(u, v|S) &\geq 2\tau - \frac{\tau}{8} - \frac{\tau}{2} > \tau, \quad \text{if } v \in \mathcal{N}_2(u) \\ \widetilde{\text{Cov}}^{\text{avg}}(u, v|S) &\leq \frac{\tau}{8} + \frac{\tau}{2} < \tau, \quad \text{if } v \notin \mathcal{N}_2(u).\end{aligned}\quad (\text{B22})$$

APPENDIX C: FRBM-NNQ ROBUST STRUCTURE LEARNING

In this Appendix, we first show that the difference of the discrete influence functions, defined in Eq. (A5), between $|\psi\rangle \in \mathcal{C}_F(\epsilon_p)$ and the associated FRBM-NNQ state can be bounded if their L_p distance is close enough. Then we prove the robust structure learning, i.e., we can learn the underlying structure of the RBM representation of state $|\phi\rangle_R$ by giving many copies of $|\psi\rangle \in \mathcal{C}_F(\epsilon_p)$.

1. Bounds for the influence difference under L_p distance

Assume that we are given an n -qubit quantum state $|\psi\rangle$ in class $\mathcal{C}_F(\epsilon_p)$ as defined in Definition A9 and $|\phi\rangle_R \in \mathcal{C}_F$ is an associate FRBM-NNQ state, and the magnitudes in the computational basis are $\tilde{p}(x)$ and $p(x)$, respectively. We show that the difference between the discrete influence functions of these two probability distributions (magnitudes) can be bounded by $O(\eta)$ if ϵ_p is small enough.

Lemma C1. If the probabilities $\tilde{p}(x)$ and $p(x)$ ($x \in \{\pm\}^n$), from the distributions $\tilde{\mathcal{D}}$ and $\mathcal{D}$, respectively, satisfy the L_p distance described in Eq. (3), and $\mathcal{D}$ is a distribution from a ferromagnetic RBM. Let $\tilde{I}_u(S \cup \{j\})$ and $I_u(S \cup \{j\})$ as the influence function of distributions $\tilde{\mathcal{D}}$ and $\mathcal{D}$, respectively, and $\eta > 0$, $|S| = s \leq k$. For a constant $C > 0$, if the following constraint

$$\epsilon_p \leq \frac{\eta}{2^{(n-k-1)(1-1/p)+k+3}C} \quad (\text{C1})$$

is satisfied, we have

$$|I_u(S \cup \{j\}) - \tilde{I}_u(S \cup \{j\})| \leq \frac{\eta}{C}. \quad (\text{C2})$$

Proof. By the definition of the influence in Eq. (A5), we have

$$\begin{aligned}&|I_u(S \cup \{j\}) - \tilde{I}_u(S \cup \{j\})| \\ &= |\mathbb{E}[X_u | X_{S \cup \{j\}} = \{1\}^{s+1}] - \tilde{\mathbb{E}}[X_u | X_{S \cup \{j\}} = \{1\}^{s+1}]| \\ &= 2|p(X_u = 1 | X_{S \cup \{j\}} = \{1\}^{s+1}) \\ &\quad - \tilde{p}(X_u = 1 | X_{S \cup \{j\}} = \{1\}^{s+1})|,\end{aligned}\quad (\text{C3})$$

where $s = |S|$ is the number of nodes contained in set S . For the sake of convenience, let

$$\begin{aligned}a &:= p(X_u = 1, X_{S \cup \{j\}} = \{1\}^{s+1}), \\ b &:= p(X_{S \cup \{j\}} = \{1\}^{s+1}), \\ \tilde{a} &:= \tilde{p}(X_u = 1, X_{S \cup \{j\}} = \{1\}^{s+1}), \\ \tilde{b} &:= \tilde{p}(X_{S \cup \{j\}} = \{1\}^{s+1}).\end{aligned}\quad (\text{C4})$$

From Eq. (C3), we have

$$\begin{aligned}&|I_u(S \cup \{j\}) - \tilde{I}_u(S \cup \{j\})| \\ &= 2 \left| \frac{a}{b} - \frac{\tilde{a}}{\tilde{b}} \right| \leq \frac{2}{b} (|a - \tilde{a}| + |b - \tilde{b}|),\end{aligned}\quad (\text{C5})$$

where the first inequality is obtained by using Lemma B2. From Lemma B1, the distance $|I_u(S \cup \{j\}) - \tilde{I}_u(S \cup \{j\})|$ can be upper bounded by

$$\begin{aligned}&\frac{2}{b} (|a - \tilde{a}| + |b - \tilde{b}|) \\ &\leq \frac{2(2^{n-s-2})^{(1-1/p)}\epsilon_p + 2(2^{n-s-1})^{(1-1/p)}\epsilon_p}{2^{-(s+1)}} \\ &\leq (2^{n-s-1})^{(1-1/p)}2^{k+3}\epsilon_p,\end{aligned}\quad (\text{C6})$$

where we use $b \geq 2^{-(s+1)}$ (because in a ferromagnetic model, $x_s = \{1\}^s$ is the most possible configuration to observe for X_s), the inequality of the inequality is obtained from the facts that $|a - \tilde{a}| < (2^{n-s-2})^{(1-1/p)}\epsilon_p$, $|b - \tilde{b}| < (2^{n-s-1})^{(1-1/p)}\epsilon_p$, and $b \geq 2^{-(s+1)}$. Then, for a constant $C \geq 0$, if it satisfies that

$$\begin{aligned}&(2^{n-s-1})^{(1-1/p)}2^{k+3}\epsilon_p \\ &\leq \frac{\eta}{C}, \text{ i.e.,} \\ \epsilon_p &\leq \frac{\eta}{C(2^{n-s-1})^{(1-1/p)}2^{k+3}} \\ &\leq \frac{\eta}{C2^{(n-k-1)(1-1/p)+k+3}},\end{aligned}\quad (\text{C7})$$

then Eq. (C2) is satisfied. $\blacksquare$

2. FRBM robust two-hop neighbor estimation

In Appendix C1, we have shown that if the L_p distance between two distributions $\mathcal{D}$ and $\tilde{\mathcal{D}}$ is small enough, we can bound the influence function distance between these two distributions when $\mathcal{D}$ is from a ferromagnetic RBM. In this Appendix, we prove the robust structure learning, i.e., we can learn the underlying structure of the RBM representation of state $|\phi\rangle_R$ by giving many copies of state $|\psi\rangle \in \mathcal{C}_F(\epsilon_p)$.

Assume we are given a quantum state $|\psi\rangle$ close to an FRBM-NNQ state $|\phi\rangle_R$. We will show that the difference between the theoretical and empirical influence function of the magnitude probability distribution of state $|\psi\rangle$ can be bounded with enough samples and for any subset $S \subset [n]$ with size $|S| \leq k$, the following constraint is satisfied:

$$|\tilde{p}(X_S = \{1\}^s) - p(X_S = \{1\}^s)| \leq \xi, \quad (\text{C8})$$

where $\xi \geq 0$, $p(\cdot)$, and $\tilde{p}(\cdot)$ are the distribution probability corresponding to $|\phi\rangle_R$ and $|\psi\rangle$, respectively. Assuming $|\phi\rangle_R$ is an FRBM-NNQ state, we have the following lemma.

Lemma C2. Let $\delta, \epsilon, k > 0$, probability $p(x)$ and $\tilde{p}(x)$ is from distribution $\mathcal{D}$ and $\tilde{\mathcal{D}}$ of an RBM with n visible nodes, respectively, $\mathcal{D}$ is from a ferromagnetic RBM, and Eq. (C8) is satisfied for any $S \subset [n]$. Assume we have many samples from distribution $\tilde{\mathcal{D}}$, to estimate the $\tilde{I}_u(S)$ with additive precision ϵ , i.e., $|\tilde{I}_u(S) - \tilde{\tilde{I}}_u(S)| \leq \epsilon$, for all $S \subset [n]$ satisfying $|S| = s \leq k$, with probability at least $1 - \delta$, it suffices to take

T many samples with

$$T \geq \frac{2}{\epsilon^2(2^{-k} - \xi)^2} \left(\log(n) + k \log\left(\frac{en}{k}\right) \right) \log\left(\frac{4}{\delta}\right). \quad (\text{C9})$$

Proof. The proof is partially based on the previous work [38]. Observe that for an FRBM with non-negative external fields, the configuration $X_S = 1^S$ is the most probable. We have

$$p(X_S = \{1\}^S) \geq 2^{-S}. \quad (\text{C10})$$

From Eq. (C8), we obtain

$$\tilde{p}(X_S = \{1\}^S) \geq 2^{-S} - \xi. \quad (\text{C11})$$

Additionally, notice that the total number of possible sets S is bounded by $\sum_{j=0}^k \binom{n}{j} \leq (en/k)^k$. Now, consider taking T samples. For each S , we define T_S as the number of samples where $X_S = \{1\}^S$. Applying Hoeffding's inequality, we have

$$\tilde{p}(T_S - \mathbb{E}[T_S] \leq -t) \leq e^{-2t^2/T}. \quad (\text{C12})$$

Since $\mathbb{E}[T_S] \geq (2^{-k} - \xi)T$ for $|S| \leq k$,

$$p\left(T_S < \frac{2^{-k} - \xi}{2} T\right) \leq e^{-\frac{1}{2}T(2^{-k} - \xi)^2}. \quad (\text{C13})$$

Using the conventional rejection sampling argument, we see that the samples where $X_S = \{1\}^S$ are independent and identically distributed samples drawn from the conditional law. One way to comprehend this is to regard each sample as generated by first sampling X_S and then subsequently sampling the remaining spins conditioned on X_S . Therefore, through another utilization of Hoeffding's inequality, we can deduce that for a specific selection of u and S , we obtain the following:

$$p(|\tilde{I}_u(S) - \tilde{I}_u(S)| \geq \epsilon |T_S|) \leq 2e^{-2T_S^2 \epsilon^2 / T_S} \leq 2e^{-2T_S \epsilon^2}. \quad (\text{C14})$$

Then, employing the law of total expectation, we obtain

$$\begin{aligned} p(|\tilde{I}_u(S) - \tilde{I}_u(S)| \geq \epsilon) &= \mathbb{E}[p(|\tilde{I}_u(S) - \tilde{I}_u(S)| \geq \epsilon |T_S)] \\ &\leq 2\mathbb{E}[e^{-2T_S \epsilon^2}] \\ &= 2\mathbb{E}[(\mathbf{1}_{T_S < (2^{-k-1} - \frac{\xi}{2})T} + \mathbf{1}_{T_S \geq (2^{-k-1} - \frac{\xi}{2})T})e^{-2T_S \epsilon^2}] \\ &\leq 4e^{-2T(2^{-k-1} - \frac{\xi}{2})^2 \epsilon^2}. \end{aligned} \quad (\text{C15})$$

By the union bound, the probability that $|\tilde{I}_u(S) - \tilde{I}_u(S)| \geq \epsilon$ for some u, S is at most $n(\frac{en}{k})^k \times 4e^{-\frac{1}{2}T(2^{-k} - \xi)^2 \epsilon^2}$. Therefore, if we take $T \geq \frac{2}{(2^{-k} - \xi)^2} (1/\epsilon^2)(\log(n) + k \log(en/k)) \log(4/\delta)$, the result follows. ■

We now prove that if given enough samples of a quantum state in the class $\mathcal{C}_F(\epsilon_p)$, we can estimate the structure of the state (two-hop neighborhoods of each visible node) if ϵ is small enough.

Theorem C1 (FRBM error threshold for neighborhood identifiability). Let us be given T_2 copies of a quantum state in the class $\mathcal{C}_F(\epsilon_p)$ defined in Definition A9, k, η, δ, d_2 as in Theorem A2. Denote the influence function of the RBM representation of the unknown state as $\tilde{I}_u(S)$ and the empirical influence function as $\tilde{I}(S)_u$ for $u \in [n]$ and $S \subset [n] \setminus \{u\}$.

Assume the following constraint is satisfied,

$$L_p \text{ distance} : \epsilon_p \leq \frac{\eta}{2^{(n-k-1)(1-1/p)+k+6}}, \quad (\text{C16})$$

and the number of copies satisfies

$$T \geq 2^{2k+5} (d_2/\eta)^2 (\log(n) + k \log(en/k)) \log(4/\delta), \quad (\text{C17})$$

we have

$$\begin{aligned} |\tilde{I}_u(S) - \tilde{I}_u(S \setminus \{j\})| &> \eta, \text{ if } j \in \mathcal{N}_2(u), \\ |\tilde{I}_u(S) - \tilde{I}_u(S \setminus \{j\})| &< \eta, \text{ if } j \notin \mathcal{N}_2(u). \end{aligned} \quad (\text{C18})$$

Proof. We first show that if we choose $\xi \leq 2^{-k-1}$ in Lemma C2, the constraints in Eq. (C8) can be satisfied under conditions of the L_p distance. By Lemmas C1 and B1 and set $C = 8$, we have

$$\begin{aligned} |\tilde{p}(X_S = \{1\}^S) - p(X_S = \{1\}^S)| \\ \leq 2^{(n-k)(1-1/p)} \frac{\eta}{2^{(n-k-1)(1-1/p)+k+6}} \leq 2^{-k-1}. \end{aligned}$$

By using Lemma C2, and setting $\xi = 2^{-k-1}$, $\epsilon = \frac{\eta}{4d_2}$ in Eq. (C9), we have

$$T \geq 2^{2k+5} (d_2/\eta)^2 (\log(n) + k \log(en/k)) \log(4/\delta). \quad (\text{C19})$$

Now we turn to prove Eq. (C18). By using Lemma C2, as we set $\epsilon = \frac{\eta}{4d_2}$ in Eq. (C9), we have

$$|\tilde{I}_u(S) - \tilde{I}_u(S)| \leq \eta/(4d_2) \leq \eta/4. \quad (\text{C20})$$

From Lemma 6.3 in Ref. [38], for any two-hop neighbours $j \in S$, $j \in \mathcal{N}_2(u)$ we have

$$|I_u(S) - I_u(S \setminus \{j\})| \geq 2\eta. \quad (\text{C21})$$

If j is not a two-hop neighbourhood of u , i.e., $j \notin \mathcal{N}_2(u)$, then

$$|I_u(S) - I_u(S \setminus \{j\})| = 0. \quad (\text{C22})$$

Then, by using Lemma C1, if the constraints in Eq. (C16) is satisfied, the difference between the influence of state $|\phi\rangle_R$ as $I_u(S \cup \{j\})$ and the one of state $|\psi\rangle$ (which we denote as $\tilde{I}_u(S \cup \{j\})$) is bounded as follows:

$$|I_u(S \cup \{j\}) - \tilde{I}_u(S \cup \{j\})| \leq \frac{\eta}{8}. \quad (\text{C23})$$

By the triangle inequality, we have

$$\begin{aligned} |I_u(S) - I_u(S \setminus \{j\})| \\ \leq |I_u(S) - \tilde{I}_u(S)| + |\tilde{I}_u(S) - \tilde{I}_u(S)| + |\tilde{I}_u(S) \\ - \tilde{I}_u(S \setminus \{j\})| + |\tilde{I}_u(S \setminus \{j\}) - \tilde{I}_u(S \setminus \{j\})| \\ + |\tilde{I}_u(S \setminus \{j\}) - I_u(S \setminus \{j\})|. \end{aligned} \quad (\text{C24})$$

Combining Eqs. (C20), (C21), and (C23), for any $j \in \mathcal{N}_2(u)$, we have

$$\begin{aligned} |\tilde{I}_u(S) - \tilde{I}_u(S \setminus \{j\})| \\ \geq 2\eta - 2 \times \frac{\eta}{4} - 2 \times \frac{\eta}{8} \geq 2\eta - \frac{\eta}{2} - \frac{\eta}{4} > \eta. \end{aligned} \quad (\text{C25})$$

On the other hand, if $j \notin \mathcal{N}_2(u)$, combining Eqs. (C20), (C21), and (C22), we will obtain

$$|\tilde{I}_u(S) - \tilde{I}_u(S \setminus \{j\})| \leq 2 \times \frac{\eta}{4} + 2 \times \frac{\eta}{8} < \eta. \quad (\text{C26})$$

With the threshold η , we can distinguish whether a node j is a two-hop neighborhood of u . ■

Notice that in our robust setting, the number of copies of state required here is slightly bigger than the number of samples required in Ref. [38].

APPENDIX D: ROBUST QUANTUM STATE LEARNING

In this Appendix, we demonstrate the process of quantum state learning with the estimated two-hop neighborhood structure. We prove that we can learn magnitudes of each amplitude $\tilde{p}(x)$ of the unknown quantum state $|\psi\rangle$ with good precision. The main idea is to learn the parameters of the induced MRF, introduced in Sec. A 4.

For a quantum state $|\psi\rangle \in \mathcal{C}(\epsilon_p)$ and its associate NNQ state $|\phi\rangle_R \in \mathcal{C}$, we say that the underlying structure of $|\phi\rangle_R$ is an estimate of the underlying structure of $|\psi\rangle$. As described above, the magnitude of a quantum state can be represented by the marginal probability distribution on the visible nodes of an RBM. In Sec. A 4, we mentioned that for an RBM, there is always an induced MRF, indicating that we can learn the marginal probability distribution of an RBM by learning the induced MRF instead. Since we use an estimated structure to approximate the unknown quantum state, there will be a mitigation error between the magnitude we estimate and the magnitude of the actual quantum state. To learn with the mitigation error, we employ an algorithm called Alphatron [40] to find parameters that recover the magnitudes with $\text{poly}(n)$ samples. Additionally, we can also learn the conditional probability of a set of qubits J conditioned on the remaining qubits, with $\text{poly}(|J|)$ samples if d_2 is equal to $\log |J|$.

The results are achieved by employing the Alphatron algorithm described in the following.

Theorem D1 (Alphatron [40]). Let $\mathcal{K}$ be a kernel function corresponding to feature map ϕ such that for all variable X' in an input domain $\mathcal{X}$, $\|\phi(X')\| \leq B_1$. Consider samples $(X'_i, Y'_i)_{i=1}^M$ drawn independent and identically distributed, from distribution $\mathcal{D}$ on $\mathcal{X} \times [0, 1]$ such that $\mathbb{E}[Y'|X'] = \mathcal{U}(\langle v, \phi(X') \rangle + \epsilon(X'))$ where $\mathcal{U} : \mathbb{R} \rightarrow [0, 1]$ is a known L -Lipschitz nondecreasing function, $\epsilon : \mathbb{R}^n \rightarrow [-\epsilon_1, \epsilon_1]$, for $\epsilon_1 > 0$ such that $\mathbb{E}[\epsilon(X')^2] \leq \epsilon_b$ and $\|v\| \leq B_2$. Then for $\delta \in (0, 1)$, with probability $1 - \delta$, Alphatron with $\lambda = 1/L$, the number of iterations $T = CBL\sqrt{M/\log(1/\delta)}$ and data size $N = C'M \log(T/\delta)$ for large enough constants $C, C' > 0$, outputs a hypothesis h such that,

$$\begin{aligned} & \mathbb{E}_{X', Y'}[(h(X') - \mathbb{E}[Y'|X'])^2] \\ & \leq \mathcal{O}\left(L\sqrt{\epsilon_b} + L\epsilon_1\sqrt{\frac{\log(1/\delta)}{M}} + B_1B_2L\sqrt{\frac{\log(1/\delta)}{M}}\right), \end{aligned} \quad (\text{D1})$$

in time $\text{poly}(n, \log(1/\delta), t_\phi)$, where t_ϕ is the time required to compute the kernel function $\mathcal{K}$.

Consider an unknown quantum state that $|\psi\rangle \in \mathcal{C}(\epsilon_p)$, and $|\phi\rangle_R$ is the associated NNQ state. Let $q(X)$ and $\tilde{q}(X)$ be

the potential of the MRF induced on the observed nodes corresponding to $|\phi\rangle_R$ and the unknown quantum state, respectively, and the partial derivative over node u as $\tilde{q}_u(X_{\neq u}) = \partial_u \tilde{q}(X)$ and $q_u(X_{\neq u}) = \partial_u q(X)$. Observe that $q_u(X)$ contains at most 2^{d_2} terms because of the bounded degree constraint, while $\tilde{q}_u(X_{\neq u})$ contains at most $m_u = \sum_{i=1}^{n-1} \binom{n}{i}$ terms because there are m_u possible monomial containing nodes u for a general MRF. Therefore, we can divide the partial potential $\tilde{q}_u(X_{\neq u})$ of the MRF representation of the unknown state into two parts, i.e.,

$$\tilde{q}_u(X_{\neq u}) = q_u(X_{\neq u}) + q_\epsilon(X_{\neq u}), \quad (\text{D2})$$

where $q_u(X_{\neq u})$ contains the monomials from subset in $\mathcal{N}_2(u)$, and we treat $q_\epsilon(X_{\neq u})$ as the error term. We show that we can learn the parameters by using the Alphatron algorithm in Ref. [40] with the knowledge of the underlying graph of the induced MRF, which is the two-hop neighbor structure of the corresponding RBM. Particularly, for a node $u \in [n]$, we consider using the Alphatron algorithm to learn the parameters of the partial potential with the knowledge of $\mathcal{N}_2(u)$.

Lemma D1. Let $p(X)$ be the marginal probability distribution from a distribution $\mathcal{D}$, which is over the visible node from an (α, β) nondegenerate RBM, $\tilde{p}(X)$ from distribution $\tilde{\mathcal{D}}$ as the probabilities distribution which is close to $p(X)$, such that $\max_{u \in [n]} \{|\mathbb{E}_{\mathcal{D}}[X_u|X_{\neq u}] - \mathbb{E}_{\tilde{\mathcal{D}}}[X_u|X_{\neq u}]\} =: \epsilon$ and $\epsilon > 0$. Let $q(X)$ and $\tilde{q}(X)$ be the corresponding potentials of the induced MRFs, respectively. For a node u , the partial potential $\tilde{q}_u(X)$ and $q_u(X)$ of the MRFs satisfy

$$|\tilde{q}_u(X_{\neq u}) - q_u(X_{\neq u})| \leq \epsilon', \quad (\text{D3})$$

$$|\tilde{q}_u(X_{\neq u})| \leq \beta + \epsilon', \quad (\text{D4})$$

where $\epsilon' = \epsilon/(1 - (\tanh(\beta) + \epsilon)^2)$.

Proof. Observe that for MRFs with distribution $p(x)$, we have $\mathbb{E}[X_u|X_{\neq u}] = \tanh(q_u(X_{\neq u}))$. Since $|\mathbb{E}_{\mathcal{D}}[X_u|X_{\neq u}] - \mathbb{E}_{\tilde{\mathcal{D}}}[X_u|X_{\neq u}]| \leq \epsilon$ for $\epsilon > 0$, we obtain

$$|\tanh(q_u(X_{\neq u})) - \tanh(\tilde{q}_u(X_{\neq u}))| \leq \epsilon. \quad (\text{D5})$$

Now, we turn to calculate the bound of the partial potential $\tilde{q}_u(X_{\neq u})$ by using the bound of $|q_u(X_{\neq u})|$. Using Lemma 6.1 in Ref. [38], we have $|q_u(X_{\neq u})| < \beta$. We now consider the following two cases. First, if $|\tilde{q}_u(X_{\neq u})| \leq |q_u(X_{\neq u})|$, straightforwardly we obtain $|\tilde{q}_u(X_{\neq u})| \leq \beta$. Therefore, in the following we consider the case that $|\tilde{q}_u(X_{\neq u})| \geq |q_u(X_{\neq u})|$. Note that $\text{arctanh}(x) = \frac{1}{2} \ln \frac{1+x}{1-x}$ is a monotonic increasing function for $x \in (-1, 1)$, and the derivative function $\frac{d}{dx} \text{arctanh}(x) = 1/(1-x^2)$. For $x, y \in (-1, 1)$ and $x > y$, we also have

$$\text{arctanh}(x) - \text{arctanh}(y) \leq \frac{1}{1-x^2}(x-y). \quad (\text{D6})$$

With this, we can show that

$$\begin{aligned} |\tilde{q}_u(X_{\neq u}) - q_u(X_{\neq u})| &= |\text{arctanh}(\tanh(\tilde{q}_u(X_{\neq u}))) - \text{arctanh}(\tanh(q_u(X_{\neq u})))| \leq \max \left\{ \frac{1}{1 - \tanh^2(\tilde{q}_u(X_{\neq u}))}, \frac{1}{1 - \tanh^2(q_u(X_{\neq u}))} \right\} \\ &\quad \times |\tanh(\tilde{q}_u(X_{\neq u})) - \tanh(q_u(X_{\neq u}))| \leq \frac{\epsilon}{1 - (\tanh(\beta) + \epsilon)^2} := \epsilon'. \end{aligned} \quad (\text{D7})$$

If $\tilde{q}_u(X_{\neq u})q_u(X_{\neq u}) \geq 0$, by using Eq. (D6) with $x = \tanh(|\tilde{q}_u(X_{\neq u})|)$, $y = \tanh(|q_u(X_{\neq u})|)$, we have

$$\begin{aligned} |\tilde{q}_u(X_{\neq u})| - |q_u(X_{\neq u})| &\leq \frac{1}{1 - \tanh(|\tilde{q}_u(X_{\neq u})|)^2} (\tanh(|\tilde{q}_u(X_{\neq u})|) - \tanh(|q_u(X_{\neq u})|)) \\ &= \frac{1}{1 - \tanh(|\tilde{q}_u(X_{\neq u})|)^2} |\tanh(\tilde{q}_u(X_{\neq u})) - \tanh(q_u(X_{\neq u}))| = \frac{\epsilon}{1 - (\tanh(\beta) + \epsilon)^2} = \epsilon'. \end{aligned} \quad (\text{D8})$$

If $\tilde{q}_u(X_{\neq u})q_u(X_{\neq u}) \leq 0$, we have

$$\begin{aligned} &\tanh(|\tilde{q}_u(X_{\neq u})|) - \tanh(|q_u(X_{\neq u})|) \\ &= |\tanh(\tilde{q}_u(X_{\neq u})) + \tanh(q_u(X_{\neq u}))| \\ &\leq |\tanh(\tilde{q}_u(X_{\neq u})) - \tanh(q_u(X_{\neq u}))| \leq \epsilon, \end{aligned} \quad (\text{D9})$$

where the first inequality arises from the property that $\tanh(\cdot)$ is an odd function. Combining these two cases together, we obtain

$$\begin{aligned} |\tilde{q}_u(X_{\neq u})| &\leq \frac{\epsilon}{1 - \tanh^2(|\tilde{q}_u(X_{\neq u})|)} + |q_u(X_{\neq u})| \\ &\leq \frac{\epsilon}{1 - (\tanh(\beta) + \epsilon)^2} + \beta = \epsilon' + \beta. \end{aligned} \quad (\text{D10})$$

Lemma D2. Let $p(X)$, $\tilde{p}(X)$, $\mathcal{D}$, $\tilde{\mathcal{D}}$, $q_u(X_{\neq u})$, $\tilde{q}_u(X_{\neq u})$ as the same setting with Lemma D1. Suppose $q_u(X_{\neq u})$ contains at most d_2 nodes, for any $u \in [n]$. Given M samples from distribution $\tilde{\mathcal{D}}$, we can find a polynomial $\tilde{q}_u^*(X_{\neq u})$, which is an estimation of $\tilde{q}_u(X_{\neq u})$, by using Alphasatron algorithm with probability at least $1 - \delta$ such that

$$\|\tilde{q}_u^* - \tilde{q}_u\|_2^2 \leq \mathcal{O}\left(\frac{\text{err}}{2^{d_2}\sigma(-2\beta')^{d_2}(1 - \tanh^2(\beta'))^2}\right) \quad (\text{D11})$$

where $\text{err} = \epsilon' + \epsilon' \sqrt[4]{\frac{\log(1/\delta)}{M}} + \beta 2^{d_2/2} \sqrt{\frac{\log(1/\delta)}{M}}$, $\beta' = \beta + \epsilon'$, $\tilde{q}_u$, and $\tilde{q}_u^*$ are the vectors of coefficient of monomial $\tilde{q}_u(X_{\neq u})$ and $\tilde{q}_u^*(X_{\neq u})$, respectively.

Proof. We use the Alphasatron algorithm as in Theorem D1 with the following setting. Set $X' = (\prod_{s \in S} x_s)_{S \subset \mathcal{N}_2(u)}$ and $Y' = X_u$. Note that $\|X'\|_2 \leq 2^{d_2/2}$ as there are 2^{d_2} terms at most

in X' , i.e., $B_1 = 2^{d_2/2}$. Set the function $\mathcal{U}(x) = \tanh(x)$, which is a 1-Lipschitz function, i.e., $L = 1$. Since $|q_u(X_{\neq u})| \leq \beta$, by using Parseval's theorem, we have $\|q_u\|_2 \leq \beta$. Note that q_u corresponds to the vector v and $B_2 = \beta'$ in the Alphasatron algorithm. By using Eq. (D2), we have

$$\mathcal{U}(\tilde{q}_u(X_{\neq u})) = \tanh(q_u(X_{\neq u}) + q_\epsilon(X_{\neq u})). \quad (\text{D12})$$

From Lemma D1, we have $\epsilon_1 \leq \epsilon'$, $\epsilon_b \leq \epsilon'^2$. Under this setting, the Alphasatron algorithm returns $\tilde{q}_u^*$ such that

$$\begin{aligned} &\mathbb{E}[(\tanh(\tilde{q}_u^*(X)) - \tanh(\tilde{q}_u(X)))^2] \\ &\leq \mathcal{O}\left(\epsilon' + \epsilon' \sqrt[4]{\frac{\log(1/\delta)}{M}} + \beta 2^{d_2/2} \sqrt{\frac{\log(1/\delta)}{M}}\right) \\ &:= \mathcal{O}(\text{err}), \end{aligned} \quad (\text{D13})$$

with probability $1 - \delta$. This is from Theorem 6.8 in Ref. [38]. Since the derivative of $\tanh$ on $[-\beta', \beta']$ is lower bounded by $1 - \tanh^2(\beta')$ and it is monotonically increasing, we obtain

$$\mathbb{E}[(\tilde{q}_u^*(X) - \tilde{q}_u(X))^2] = \mathcal{O}\left(\frac{\text{err}}{(1 - \tanh^2(\beta'))^2}\right) \quad (\text{D14})$$

By using similar proof in Lemma 6.1 in Ref. [38], we see $\tilde{p}(x_u) = \sigma(2\tilde{q}_u) \geq \sigma(-2\beta')$. Iterating using the proof for d_2 nodes, we have $\tilde{p}(x_{\mathcal{N}(u)}) \geq \sigma(-2\beta')^{d_2}$. By using Lemma 6.9 in Ref. [38], we can obtain $\sigma(-2\beta')^{d_2} = \frac{\delta}{2^{d_2}}$, with $\delta = 2^{d_2}(\sigma(-2\beta')^{d_2})$,

$$\|\tilde{q}_u^* - \tilde{q}_u\|_2^2 \leq \mathcal{O}\left(\frac{\text{err}}{2^{d_2}\sigma(-2\beta')^{d_2}(1 - \tanh^2(\beta'))^2}\right). \quad (\text{D15})$$

1. Quantum state learning

By employing an iterative application of the Alphasatron algorithm to each visible node, we can estimate the coefficients of the potential polynomial of the induced MRF. Subsequently, we can recover the probability distribution using these parameters, ensuring bounded errors. When shifting the probability δ to $\delta' = \delta/n$ in Lemma D2, the overall success probability remains at δ by the union bound. We can obtain $\tilde{q}^*$ by selecting the coefficient of a monomial x_S equal to (arbitrarily chosen) the corresponding coefficient of $x_{S \setminus \{u\}}$ in $\tilde{q}_u^*$ for some u within the set S . Finally, we have

$$\|\tilde{q}^* - \tilde{q}\|_2^2 = \mathcal{O}\left(\frac{\text{err}(n)}{2^{d_2}(\sigma(-2\beta')^{d_2})(1 - \tanh^2(\beta'))^2}\right), \quad (\text{D16})$$

where $\text{err}(n) = \epsilon' + \epsilon' \sqrt[4]{\frac{\log(n/\delta)}{M}} + \beta 2^{d_2/2} \sqrt{\frac{\log(n/\delta)}{M}}$.

Based on the L_2 norm distance between the estimated and the true coefficients of the potential of the induced MRF, we show that the L_1 distance between the estimated magnitude and the actual magnitude of a state can be bounded as follows.

Lemma D3. Given M copies of an unknown n -qubit quantum state close to a quantum state based on an (α, β) nondegenerate LRBM with two-hop degree d_2 . Given M copies of this state, we can learn the distribution probability $\tilde{p}(x)$ of the unknown quantum state by Alphasatron algorithm with probability at least $1 - \delta$ such that

$$\sum_x |\tilde{p}(x) - \tilde{p}^*(x)| = \mathcal{O}\left(\frac{\sqrt{n}\sqrt{\text{err}(n)}}{\sigma(-2\beta')^{d_2/2}(1 - \tanh^2(\beta'))} + (\sqrt{n}2^{d_2} + n)\epsilon'\right), \quad (\text{D17})$$

where $\tilde{p}^*(x)$ is the estimation of $\tilde{p}(x)$ and ϵ' is defined in Lemma D1, $\text{err}(n) = \epsilon' + \epsilon' \sqrt[4]{\frac{\log(n/\delta)}{M}} + \beta 2^{d_2/2} \sqrt{\frac{\log(n/\delta)}{M}}$.

Proof. After obtaining the coefficients of the induced MRF's potential, we can obtain the probability distribution of the quantum state. We now analyze the distance between the actual and the estimated probabilities.

First, we bound the distance between the actual and the estimated potential as follows:

$$|\tilde{q}(x) - \tilde{q}^*(x)| = \sum_I |\tilde{q}_I^* - q_I| x_I + n\epsilon(x) \leq \sum_I |\tilde{q}_I^* - q_I| + n\epsilon' \quad (\text{D18})$$

$$\begin{aligned} &\leq \sqrt{n2^{d_2}} \|\tilde{q}^* - q\|_2 + n\epsilon' \leq \sqrt{n2^{d_2}} \|\tilde{q}^* - \tilde{q} + \tilde{q} + q\|_2 + n\epsilon' \\ &\leq \sqrt{n2^{d_2}} (\|\tilde{q}^* - \tilde{q}\|_2 + \|q\|_2) + n\epsilon' \leq \sqrt{n2^{d_2}} (\|\tilde{q}^* - \tilde{q}\|_2 + \epsilon') + n\epsilon', \end{aligned} \quad (\text{D19})$$

where $I \subset [n]$ with size at most $d_2 + 1$, then there are $n2^{d_2}$ monomials of $\tilde{q}^*(x)$ and $q(x)$, the right side of the first line is obtained using the triangle inequality and the second last inequality is according to the fact that $\|x\|_1 \leq \sqrt{n}\|x\|_2$ for a vector x with dimension n .

Let the partition functions $\tilde{Z} := \sum_x e^{\tilde{q}(x)}$ and $\tilde{Z}^* := \sum_x e^{\tilde{q}^*(x)}$. First, assume $\tilde{Z} \geq \tilde{Z}^*$, then we have

$$\begin{aligned} \sum_x |\tilde{p}(x) - \tilde{p}^*(x)| &= \sum_x \left| \frac{e^{\tilde{q}(x)}}{\tilde{Z}} - \frac{e^{\tilde{q}^*(x)}}{\tilde{Z}^*} \right| = \sum_x \left| \frac{e^{\tilde{q}(x)}}{\tilde{Z}} - \frac{e^{\tilde{q}^*(x)}}{\tilde{Z}} + \frac{e^{\tilde{q}^*(x)}}{\tilde{Z}} - \frac{e^{\tilde{q}^*(x)}}{\tilde{Z}^*} \right| \\ &\leq \frac{1}{\tilde{Z}} \sum_x |e^{\tilde{q}(x)} - e^{\tilde{q}^*(x)}| + \left| \frac{1}{\tilde{Z}} - \frac{1}{\tilde{Z}^*} \right| \sum_x e^{\tilde{q}^*(x)}, \end{aligned} \quad (\text{D20})$$

where the inequality is obtained by using the triangle inequality. We now focus on the second term of Eq. (D20),

$$\left| \frac{1}{\tilde{Z}} - \frac{1}{\tilde{Z}^*} \right| \sum_x e^{\tilde{q}^*(x)} = \left| \frac{1}{\tilde{Z}} - \frac{1}{\tilde{Z}^*} \right| \tilde{Z}^* = \left| \frac{\tilde{Z}^* - \tilde{Z}}{\tilde{Z}} \right| = \frac{1}{\tilde{Z}} \left| \sum_x (e^{\tilde{q}^*(x)} - e^{\tilde{q}(x)}) \right| \leq \frac{1}{\tilde{Z}} \sum_x |e^{\tilde{q}(x)} - e^{\tilde{q}^*(x)}|, \quad (\text{D21})$$

where the inequality is obtained by using the triangle inequality. Combining Eq. (D20), we have

$$\begin{aligned} \sum_x |\tilde{p}(x) - \tilde{p}^*(x)| &\leq \frac{2}{\tilde{Z}} \sum_x |e^{\tilde{q}(x)} - e^{\tilde{q}^*(x)}| \leq \frac{2}{\tilde{Z}} \sum_x \max\{e^{\tilde{q}(x)}, e^{\tilde{q}^*(x)}\} |\tilde{q}(x) - \tilde{q}^*(x)| \\ &\leq \frac{2}{\tilde{Z}} \sqrt{n2^{d_2}} \|\tilde{q}^* - \tilde{q}\|_2 \sum_x \max\{e^{\tilde{q}(x)}, e^{\tilde{q}^*(x)}\} \leq \frac{2 \sum_x \max\{e^{\tilde{q}(x)}, e^{\tilde{q}^*(x)}\}}{\frac{1}{2}(\tilde{Z} + \tilde{Z}^*)} (\sqrt{n2^{d_2}} (\|\tilde{q}^* - \tilde{q}\|_2 + \epsilon') + n\epsilon') \\ &\leq 4\sqrt{n2^{d_2}} (\|\tilde{q}^* - \tilde{q}\|_2 + \epsilon') + 4n\epsilon', \end{aligned} \quad (\text{D22})$$

where the right side of the second line is obtained by using the Cauchy inequality for a convex function $f = e^x$, which is $f'(b) \leq \frac{f(a)-f(b)}{a-b} \leq f'(a)$, for $a > b$. The third inequality results from Eq. (D19), and the last inequality is obtained by using the fact that $\tilde{Z} \geq \tilde{Z}^*$ and $\sum_x \max\{e^{\tilde{q}(x)}, e^{\tilde{q}^*(x)}\} \leq \sum_x (e^{\tilde{q}(x)} + e^{\tilde{q}^*(x)})$. Similarly, when $\tilde{Z} \leq \tilde{Z}^*$, we can obtain the same bound in Eq. (D22). Therefore, by using Eq. (D16), we have

$$\sum_x |\tilde{p}(x) - \tilde{p}^*(x)| \leq 4\sqrt{n2^{d_2}} (\|\tilde{q}^* - \tilde{q}\|_2 + \epsilon') + 4n\epsilon' = \mathcal{O}\left(\frac{\sqrt{n} \sqrt{\text{err}(n)}}{\sigma(-2\beta')^{d_2/2} (1 - \tanh^2(\beta'))} + (\sqrt{n2^{d_2}} + n)\epsilon'\right), \quad (\text{D23})$$

where $\text{err}(n) = \epsilon' + \epsilon' \sqrt{\frac{\log(n/\delta)}{M}} + \beta 2^{d_2/2} \sqrt{\frac{\log(n/\delta)}{M}}$ and $\beta' = \beta + \epsilon'$. ■

As the error ϵ' is related to ϵ in Lemma D1, we now show that ϵ can be bounded under the L_p distance constraint.

Lemma 10. Let $\tilde{p}(x)$ be the probability distribution of state $|\psi\rangle \in \mathcal{C}(\epsilon_p)$ and $p(x)$ is the distribution probability of an associate NNQ state $|\phi\rangle_R$. Suppose $p(x)$, $\tilde{p}(x)$, and ϵ satisfy the setting in Lemma D1, then the following constraint is satisfied for state $|\psi\rangle$,

$$\epsilon \leq \frac{2^{(n-1)(1-1/p)+2} \epsilon_p}{\sigma(-2\beta)^{d_2}}. \quad (\text{D24})$$

Proof. By using Lemmas B2 and D1, we have

$$\begin{aligned} \epsilon &= \max_{u \in [n]} \{|\mathbb{E}_{\mathcal{D}}[X_u | X_{\neq u} = x_{\neq u}] - \mathbb{E}_{\tilde{\mathcal{D}}}[X_u | X_{\neq u} = x_{\neq u}]\}| = \max_{u \in [n]} \{2|p(X_u = 1 | x_{\neq u}) - \tilde{p}(X_u = 1 | x_{\neq u})|\} \\ &\leq \max_{u \in [n]} \left\{ \frac{2}{p(x_{\neq u})} |p(X_u = 1, x_{\neq u}) - \tilde{p}(X_u = 1, x_{\neq u})| + |\tilde{p}(x_{\neq u}) - p(x_{\neq u})| \right\}. \end{aligned} \quad (\text{D25})$$

If the two terms can be bounded by L_p norm, we have $|\tilde{p}(x_{\neq u}) - p(x_{\neq u})| \leq 2^{(n-1)(1-1/p)}\epsilon_p$ and $|\tilde{p}(X_u = 1, x_{\neq u}) - p(X_u = 1, x_{\neq u})| \leq 2^{(n-1)(1-1/p)}\epsilon_p$. And we have $p(x_{\neq u}) \geq \sigma(-2\beta)^{d_2}$. After simple calculation, we can then obtain Eq. (D24). ■

Now, we show that the magnitude of a quantum state in class $\mathcal{C}(\epsilon_p)$ can be estimated if ϵ_p is small enough.

Theorem D2 (Quantum state learning). Suppose we are given M copies of an unknown n -qubit quantum state in the class $\mathcal{C}(\epsilon_p)$ Defined in Definition A9, and the estimated two-hop neighbor's structure of the RBM representation be known. Let $\vartheta = \sigma(-2\beta)^{2d_2}(1 - \tanh(\beta)^2)^3$, if the probability distribution satisfies the following constraint:

$$L_p \text{ distance : } \epsilon_p = \mathcal{O}\left(\frac{\vartheta \epsilon_t^2}{(\sqrt{n}2^{d_2} + n)^2 2^{(n-1)(1-1/p)}}\right) \quad (\text{D26})$$

and

$$M = \mathcal{O}\left(\frac{\beta^2 2^{d_2} n^2 \log(1/\delta)}{\vartheta (1 - \tanh^2(\beta)) \epsilon_t^4}\right) \quad (\text{D27})$$

we can find a polynomial $\tilde{q}^*$ with probability $1 - \delta$ such that

$$\sum_x |\tilde{p}(x) - \tilde{p}^*(x)| = \mathcal{O}(\epsilon_t), \quad (\text{D28})$$

where $p(x) = \frac{e^{q(x)}}{Z}$.

Proof. By using Theorem D1, if we require

$$\sum_x |\tilde{p}(x) - \tilde{p}^*(x)| \in \mathcal{O}\left(\frac{\sqrt{n}\sqrt{2\epsilon'} + 2\epsilon' \sqrt[4]{\frac{\log(n/\delta)}{M}} + \beta 2^{d_2/2} \sqrt[4]{\frac{\log(n/\delta)}{M}}}{\sigma(-2\beta')^{d_2/2}(1 - \tanh^2(\beta'))} + (\sqrt{n}2^{d_2} + n)\epsilon'\right) = \mathcal{O}(\epsilon_t), \quad (\text{D29})$$

where $\beta' = \beta + \epsilon'$. Let $\chi = \sigma(-2\beta')^{d_2/2}(1 - \tanh^2(\beta'))$. By using the fact that $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ for $a, b > 0$, then each one of the following inequality should be satisfied:

$$\max\left\{\frac{\sqrt{2n\epsilon'}}{\chi}, \frac{\sqrt{2n\epsilon'} \sqrt[4]{\frac{\log(n/\delta)}{M}}}{\chi}, \frac{\sqrt{n\beta} 2^{d_2/2} \sqrt[4]{\frac{\log(n/\delta)}{M}}}{\chi}, (\sqrt{n}2^{d_2} + n)\epsilon'\right\} = \mathcal{O}(\epsilon_t). \quad (\text{D30})$$

Using a similar approach as in the proof of Theorem D3, we can conclude that the above inequality holds if Eq. (D26) satisfied, and the number of samples satisfies

$$M \geq \tilde{\mathcal{O}}\left(\frac{2^{d_2} \beta^2 n^2 \log(1/\delta)}{\sigma(-2\beta)^{2d_2}(1 - \tanh^2(\beta))^4 \epsilon_t^4}\right). \quad (\text{D31})$$

■

2. Quantum state partial learning

Next, we show that, under certain conditions, with just $O(\log n)$ copies of a quantum state (from the class in Theorem D2), we can learn the conditional probability of a subset of qubits relative to the remaining qubits with good precision. Let $J \subset [n]$ and $\bar{J} = [n] \setminus J$. As discussed before, the conditional probability $p(x_J | x_{\bar{J}}) = p(x_J | x_{\mathcal{N}_2(J)})$, where $\mathcal{N}_2(J)$ is the visible node set composed of two-hop neighbors of each node in J but excluding the nodes in J . Let $J_t = J \cup \mathcal{N}_2(J)$, and $q(X_{J_t})$ to be a polynomial which is a part of polynomial $q(X)$, where each monomial in $q(X_{J_t})$ contain at least one node in J . Naturally we also define $\tilde{q}(X_{J_t}) = q(X) - q(X_{J_t})$. Denote the coefficient vector of $q(X_{J_t})$ as $q(J_t)$. We have the following theorem.

Theorem D3 (Quantum state partial learning). Let an unknown n -qubit quantum state as in Theorem D2, and the estimated two-hop neighborhood structure of the RBM representation be known. Let $J \subseteq [n]$, set $J_t = J \cup \mathcal{N}_2(J)$, and $\vartheta = \sigma(-2\beta)^{2d_2}(1 - \tanh(\beta)^2)^3$, $\epsilon_c, \delta \in (0, 1)$. Suppose we are given M_c copies of the qubits indexed by J_{tot} of the state. If the following constraint is satisfied for state $|\psi\rangle$,

$$L_p \text{ distance : } \epsilon_p = \mathcal{O}\left(\frac{\vartheta \epsilon_c^2}{(\sqrt{2^{d_2}|J|} + |J|)^2 2^{(n-1)(1-1/p)}}\right); \quad (\text{D32})$$

and the number of samples satisfies

$$M_c = \mathcal{O}\left(\frac{\beta^2 2^{d_2} |J|^2 \log(1/\delta)}{\vartheta (1 - \tanh^2(\beta)) \epsilon_c^4}\right), \quad (\text{D33})$$

we can find a polynomial $q^*(X_{J_t})$ with probability $1 - \delta$ such that

$$|\tilde{p}(x_J|x_{\mathcal{N}_2(J)}) - \tilde{p}^*(x_J|x_{\mathcal{N}_2(J)})| = \mathcal{O}(\epsilon_c), \quad (\text{D34})$$

where $p(x_J|x_{\bar{J}}) = \frac{\exp(q(x_{J_t}))}{\sum_{x_J} \exp(q(x_{J_t}))}$.

Proof. The proof is similar to that of Theorem D2. First, by expanding the condition probability by using Bayes' law and the marginal probability, we have

$$p(x_J|x_{\bar{J}}) = \frac{p(x_J, x_{\bar{J}})}{\sum_{x_J} p(x_J, x_{\bar{J}})} = \frac{\exp(q(x_{J_t}) + \bar{q}(x_{J_t}))}{\sum_{x_J} \exp(q(x_{J_t}) + \bar{q}(x_{J_t}))} = \frac{\exp(q(x_{J_t}))}{\sum_{x_J} \exp(q(x_{J_t}))} = \frac{1}{1 + \sum_{k_J \neq x_J} \exp(q(k_{J_t}) - q(x_{J_t}))}, \quad (\text{D35})$$

where $x_J, k_J \in \{\pm 1\}^{|J|}$.

Then, we bound the difference between the estimated conditional probability and the real conditional probability as follows:

$$\begin{aligned} |\tilde{p}(x_J|x_{\bar{J}}) - \tilde{p}^*(x_J|x_{\bar{J}})| &= \left| \frac{1}{1 + \sum_{k_J \neq x_J} \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))} - \frac{1}{1 + \sum_{k_J \neq x_J} \exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t}))} \right| \\ &= \left| \frac{\sum_{k_J \neq x_J} \exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})) - \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))}{(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})))} \right| \\ &\leq \frac{\sum_{k_J \neq x_J} |\exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})) - \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))|}{(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})))}, \end{aligned} \quad (\text{D36})$$

$$\leq \frac{\sum_{k_J \neq x_J} \max\{\exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})), \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))\} |(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})) - (\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))|}{(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})))}, \quad (\text{D37})$$

$$\leq \frac{\sum_{k_J \neq x_J} \max\{\exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})), \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))\} (|\tilde{q}^*(k_{J_t}) - \tilde{q}(k_{J_t})| + |\tilde{q}^*(x_{J_t}) - \tilde{q}(x_{J_t})|)}{(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})))}, \quad (\text{D38})$$

where Eqs. (D36) and (D38) are obtained by using the triangle inequality, while in Eq. (D37) we use the property of a convex function $f = e^x$, which is $f'(b) \leq \frac{f(a)-f(b)}{a-b} \leq f'(a)$ for $a > b$. By using Eq. (D2) and Lemma D1, we have

$$\begin{aligned} |\tilde{q}^*(k_{J_t}) - \tilde{q}(k_{J_t})| &\leq |\tilde{q}^*(k_{J_t}) - q(k_{J_t})| + |q(k_{J_t}) - \tilde{q}(k_{J_t})| \leq \sum_{I \subset J_t} |\tilde{q}_I^* - q_I| + |J|\epsilon' \\ &\leq \sqrt{|J|2^{d_2}} \|\tilde{q}^*(J_t) - q(J_t)\|_2 + |J|\epsilon' \leq \sqrt{|J|2^{d_2}} \|\tilde{q}^*(J_t) - \tilde{q}(J_t) + q_\epsilon(J_t)\|_2 + |J|\epsilon' \\ &\leq \sqrt{|J|2^{d_2}} (\|\tilde{q}^*(J_t) - \tilde{q}(J_t)\|_2 + \|q_\epsilon(J_t)\|_2) + |J|\epsilon' \leq \sqrt{|J|2^{d_2}} (\|\tilde{q}^*(J_t) - \tilde{q}(J_t)\|_2 + \epsilon') + |J|\epsilon', \end{aligned} \quad (\text{D39})$$

for any $k_J \in \{\pm 1\}^{|J|}$, where the first inequality is obtained by using the triangle equality and Eq. (D2), and the second inequality is according to the fact that there are at most $|J|2^{d_2}$ monomials in polynomial $q(X_{J_t})$ and $\|x\|_1 \leq \sqrt{n}\|x\|_2$ for a vector x with dimension n . For the last two inequalities, we use triangle inequality and the fact that $\|q_\epsilon(J_t)\|_2 \leq |q_\epsilon(J_t)| \leq \epsilon'$.

Additionally, we divided the sum of $\max\{\cdot\}$ in Eq. (D38) into two parts, one part only containing terms from learning results (with $*$ sign), and the other part containing only the terms from the real distribution. Then, we see

$$\frac{\sum_{k_J \neq x_J} \max\{\exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})), \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))\}}{(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}(k_{J_t}) - \tilde{q}(x_{J_t}))(1 + \sum_{k_J \neq x_J} \exp(\tilde{q}^*(k_{J_t}) - \tilde{q}^*(x_{J_t})))} < 2. \quad (\text{D40})$$

Combining Eqs. (D38)–(D40), we can obtain

$$|\tilde{p}(x_J|x_{\bar{J}}) - \tilde{p}^*(x_J|x_{\bar{J}})| \leq 4(\sqrt{|J|2^{d_2}} (\|\tilde{q}^*(J_t) - \tilde{q}(J_t)\|_2 + \epsilon') + |J|\epsilon'). \quad (\text{D41})$$

The polynomial $q(X_{J_t})$ can be obtained by performing the Alphasat algorithm for all nodes $u \in J$. Let $\chi = \sigma(-2\beta')^{d_2/2}(1 - \tanh^2(\beta'))$. By using Lemma D2, we have

$$|\tilde{p}(x_J|x_{\bar{J}}) - \tilde{p}^*(x_J|x_{\bar{J}})| = \mathcal{O}\left(\frac{\sqrt{|J|}\sqrt{\text{err}(|J|)}}{\chi} + (\sqrt{|J|2^{d_2}} + |J|)\epsilon'\right), \quad (\text{D42})$$

where $\text{err}(|J|) = \epsilon' + \epsilon' \sqrt{\frac{\log(|J|/\delta)}{M}} + \beta 2^{d_2/2} \sqrt{\frac{\log(|J|/\delta)}{M}}$.

By using the fact that $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$, for $a, b > 0$, the following inequality should be satisfied:

$$\begin{aligned} & \max \left\{ \frac{\sqrt{\epsilon'|J|}}{\chi}, \frac{\sqrt{\epsilon'|J|} \sqrt[4]{\frac{\log(|J|/\delta)}{M_c}}}{\chi}, \frac{\sqrt{\beta 2^{d_2/2} |J|} \sqrt[4]{\frac{\log(|J|/\delta)}{M_c}}}{\chi}, (\sqrt{|J| 2^{d_2}} + |J|) \epsilon' \right\} \\ &= \max \left\{ \frac{\sqrt{\epsilon'|J|}}{\chi}, \frac{\sqrt{\beta 2^{d_2/2} |J|} \sqrt[4]{\frac{\log(|J|/\delta)}{M_c}}}{\chi}, (\sqrt{|J| 2^{d_2}} + |J|) \epsilon' \right\} \leq \max \left\{ \frac{\sqrt{\epsilon'(\sqrt{|J| 2^{d_2}} + |J|)}}{\chi}, \frac{\sqrt{\beta 2^{d_2/2} |J|} \sqrt[4]{\frac{\log(|J|/\delta)}{M_c}}}{\chi} \right\}. \end{aligned} \quad (\text{D43})$$

For the first term in Eq. (D43), as $\epsilon' = \frac{\epsilon}{1 - (\tanh(\beta) + \epsilon)^2}$, we have

$$\frac{\epsilon'(\sqrt{|J| 2^{d_2}} + |J|)^2}{\chi^2} \leq \frac{\epsilon(\sqrt{|J| 2^{d_2}} + |J|)^2}{\chi^2(1 - (\tanh(\beta) + \epsilon)^2)}. \quad (\text{D44})$$

If we restrict the conditional probability distance as Eq. (D34), combining with Lemmas D1 and 10, Eq. (D32) should be satisfied.

For the second term of Eq. (D43), the constraint in Eq. (D34) is satisfied if

$$M_c = \tilde{\mathcal{O}}\left(\frac{\beta^2 2^{d_2} |J|^2 \log(1/\delta)}{\chi^4 \epsilon_c^4}\right). \quad (\text{D45})$$

We see if $d_2 = \mathcal{O}(\log \log n)$, $|J| = \log n$, it requires $M_c \in \mathcal{O}(\text{poly}(\log n))$ samples in terms of the number of qubits. ■

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