Neural-network based general method for statistical mechanics on sparse systems

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We propose a general method for solving statistical mechanics problems defined on sparse graphs, such as random graphs, real-world networks, and low-dimensional lattices. Our approach extract a small feedback vertex set of the sparse graph, converting the sparse system to a strongly correlated system with many-body and dense interactions on the feedback set, then solve it using variational method based on neural networks to estimate free energy, observables, and generate unbiased samples via direct sampling. Extensive experiments show that our approach is more accurate than existing approaches for sparse spin glass systems. On random graphs and real-world networks, our approach significantly outperforms the standard methods for sparse systems such as belief-propagation; on structured sparse systems such as two-dimensional lattices our approach is significantly faster and more accurate than recently proposed variational autoregressive networks using convolution neural networks.

Many systems in science and technology are sparse. These include physics models defined on 2D and 3D lattices; social systems such as networks that encode interactions of agents; mathematical systems such as satisfiability problems; information systems such as error correcting codes. Statistical mechanics defined on such systems are of great importance, it is used to formulate Bayesian inference, to describe dynamics of human behaviors, to compute number of solutions of constraint satisfaction problems, and to construct message passing algorithms for reconstructing signals in error correcting codes. Without loss of generality, in this work we consider statistical mechanics of $N$ spins sitting on a sparse graph, the joint probability distribution of a configuration $s \in \{+1, -1\}^N$ follows the Boltzmann distribution

$$p(s) = \frac{1}{Z} e^{-\beta E(s)},$$

where $\beta$ denotes inverse temperature, $E$ is the energy function and $Z$ denotes the partition function.

Since sparse systems that we are interested in are usually large, Markov-Chain Monte Carlo (MCMC) based sampling methods suffer from long mixing time, hence are not scalable. For systems with random sparsity, such as on random graphs and on-real-world large networks, approximations based on Bethe approximation, i.e. belief propagation (BP), have been widely applied. The key idea in the Bethe approximation, the conditional independence assumption, is exact when the system is a tree, and is usually a good approximation in random sparse systems. However, the approximation does not perform well when the system contain many short loops. Approximations such as Kikuchi loop expansions have been proposed to consider the effects of short loops, however it is still far from being optimal when the system has loops with different lengths such as lattice systems. In this kinds of structured sparse systems, tensor network based approaches are very powerful, however they do not apply when system has even few long range interactions.

Recently a more general variational method, the Variational Autoregressive Networks (VAN) is proposed for statistical mechanics problems. On dense systems, VAN uses multi-layered neural networks to describe a variational distribution, and achieves good performances in averaging and in sampling. However the VAN contains huge number of parameters to optimize hence is not designed for large sparse systems at the first place. On structured sparse systems such as lattices, VAN could resolve the issue by adopting convolution neural networks as a good structure prior of 2D lattices. But on random sparse systems it is an open question on how to propose efficient convolution-like network structures.

As a conclusion, existing methods such as BP do efficient computations by taking advantage of the sparsity. However one has to choose a specific treatment such as conditional independences or convolutions, to specific sparsity such as random or structured; we are still lack of an overall general methods for sparse systems.

In this work we propose a novel approach for the statistical mechanics problems on sparse graphs. Our approach converts a large sparse system equivalently to much smaller system composed of the (approximately) minimum Feedback Vertex Set (FVS) of the graph, which is densely connected, and contains complex many body interaction, then solve it using variational methods based on neural networks. At a first glance our idea converts the problem to a strongly correlated dense system which seems even harder than the original one. Indeed it is, in the sense that the converted system loses internal structure of the original sparse system. However our point is that the recently proposed neural-network based variational methods are particularly suitable for treating a small non-structured dense system by utilizing advanced computational techniques such as GPUs and recently developed machine learning techniques such as reinforcement learning, then finally give a large leavarge of performance on the large sparse systems.

Compressing the sparsity using the feedback vertex set. A feedback vertex set $\Omega$ of a graph is a set of vertices which intersects with every loop of the graph. With all vertices of the FVS removed, the graph becomes loop-free, hence is composed of trees, we denote the forest after removing FVS as
The free energy of the whole system thus can be written as

$$F = -\frac{1}{\beta} \ln \sum_{s \in \mathcal{T}} \sum_{t \in T} e^{-\beta E(s,t)} = -\frac{1}{\beta} \ln \sum_{s \in \Omega} e^{-\beta \tilde{E}(s)},$$  

(2)

where $\tilde{E}(s)$ is the effective energy of a configuration of vertices of FVS $s \in \Omega$:

$$\tilde{E}(s) = E_\Omega(s) + E_T(s).$$  

(3)

Here the effective energy has been divided into two parts: $E_\Omega(s)$ denotes the energy which only involves vertices in the FVS, and $E_T(s)$ is the energy of the forest $T$ given the configuration of FVS.

Observe that, once a configuration $s$ of the FVS is determined, what left in the graph is a forest with given boundary conditions. As a consequence, the summation over all variables in the forest as shown in Eq. (4) can be calculated in linear time easily, by i.e. taking a sequence from leaf vertices (a leaf vertex of the graph is a vertex which has only one attached edge) of the forest to the root vertices. A detailed example of how to calculate free energy of Ising model based on this method can be found in appendix.

There are many possible FVSes given a graph. Finding the smallest one, which is called the minimum feedback vertex set problem, belongs to the class of NP-hard problems. In this work we use an heuristic algorithm called CoreHD proposed in [5], which is a fast and simple heuristic method with $O(N)$ computation complexity. The sizes of the FVS for the graph instances of this work are about 20% – 33% of the original graph sizes. (It is possible to further reduce the FVS sizes through a message passing method [2].)

Eq. (2) converts partition-function-calculation of a sparse system to a system with much smaller size. Notice that the converting come with price: the effective energy of FVS indicates that they are densely connected with many-body interactions, thus good approximations on sparse graphs, i.e. Bethe approximation, fails in the FVS system. Actually it is really difficult to find good approximations or variational ansats for this dense and many-body interacting system in general.

**Solving the FVS system using neural-network based variational methods.** Fortunately a variational approach named Variational Autoregressive Networks [6] was proposed recently for statistical mechanics problems in general, and is particularly powerful for the densely connected structureless problems. The VAN adopts autoregressive distribution

$$q_\theta(s) = \prod_{i=1}^{N} q_\theta(s_i | s_1, \ldots, s_{i-1}),$$  

(5)

with all the conditional distributions parametrized by a neural network, with parameters being trained to optimize the variational free energy using a method closely related to reinforcement learning. One is able to generate samples according to the variational distribution by direct sampling. A short introduction to VAN can be found in the appendix, we also refer readers to [6] for more details. In this work we utilize the VAN to tackle the statistical mechanics defined on the FVS of the sparse graph. The advantage of VAN compared with conventional mean-field approximations such as Bethe, TAP for spin glasses, is that the neural-network model has much better representation power than the variational distributions used in classic mean-field approximations. This makes it suitable for the statistical mechanics problems defined on strong correlated systems such as our FVS system which is mapped from the original large sparse system by compressing all the sparse structures.

Our algorithm is thus described in detail as follows: (1) we extract a FVS $\Omega$ from the sparse graph using the CoreHD algorithm [5]. (2) We construct a neural network to express variational distribution $q_\theta(s)$ for $s \in \Omega$, and learn the parameters (i.e. weights of neural network) of the variational distribution by sampling $q_\theta(s)$. (3) We keep computing variational free energy using effective energy of every samples according to Eq. (3), and entropy, estimating gradient of the variational free energy with respect to the variational parameters using the REINFORCE algorithm [7], then updating the parameters until the algorithm converges.

**Numerical Experiments** To demonstrate the ability of our approach in computing free energy, and estimating physical quantities, in large sparse systems, and show superiority of our method against existing approaches, we perform extensive experiments in classic Ising spin model and spin glasses on sparse graphs. There are two kinds of sparse models: random sparsity including random graphs and real-world sparse networks and structured sparsity such as 2D and 3D lattices. For the random graphs and large real-world networks, Bethe approximation based methods such as belief propagation have been proved to be successful. On the lattice systems, recently proposed convolution networks based VAN have been shown to have better performance than mean-field approximations. We perform experiments in both kinds of sparse models.

We first consider the Ising $+J$ spin glasses on random graphs, with distribution of couplings following $P(J_{ij} = 1) = P(J_{ij} = -1) = 1/2$, the so-called Viena-Bray spin glass model [8]. We evaluate performance of our approach by comparing correlations obtained by our method to MCMC for a very long time ($5 \times 10^5 N$ steps, longer time simulation gives very similar results), which is considered to be very accurate. We also compare our results with correlations obtained by the BP algorithm which is a standard method for statistical mechanics and inferences on random graphs. The results are shown in Fig. 1. In Fig. 1a the graph is the regular random graph in which degree of every node is 3. We set $\beta = 0.9$ which locates at the spin glass phase. We see that the correlations given by our method is coincide with the MCMC results, while the BP results deviate significantly from the MCMC data. We see an analogous phenomenon on the spin glass model with $J$ following Gaussian distribution with unit variance, on an Erdős-Rényi random graphs as shown in Fig. 1b).
where the figure shows that while our method is very accurate but BP gives much worse results. In Fig. 1(c) and (d) we tested our algorithm on two classic real-world networks - Karate club network [9] and political blogs network [10].

On the Karate club we see that our method is almost identical to the exact results (exact results are given by enumerating all configurations of FVS, since the system size is quantitatively small). This is because the FVS size of the Karate club is very small, so our results is very accurate in describing the statistical mechanics on it. The figure also indicates that the BP results are much worse than those in random graphs. This is because that although average degree of Karate club \( c = 2.29 \) is small, the network contains many short loops, which make Bethe approximation less accurate than in random graphs. This effect turns out to be more serious for BP on the political blogs networks as shown in Fig. 1(d), due to the power-law degree distribution and relatively large average degree \( c = 11.21 \). Fortunately we see FVS is less affected by the large degree and gives much more accurate correlation estimate than the BP method.

Then we consider statistical mechanics on the graphs with structured sparsity. A classic example is the 2D ferromagnetic Ising model. Since it is on a planar graph, we can compute an exact solution of the free energy using e.g. the Kac-Ward formula [11] and use it to evaluate our algorithm. On this problem we set a baseline using variational auto-regressive network using convolution networks [6]. Convolution networks are originally proposed to extract relevant features of 2D data such as images [12, 13], and has been shown to give much better results than VAN without using convolution networks on the 2D Ising model [6]. In Fig. 2 we plot the variational free energy given by our method at different temperatures, compared with other methods. The relative error to the exact solution is plotted in the inset of the figure. We can see that in all temperature regime, our FVS method is significantly better than all the other methods. Particularly on the paramagnetic-ferromagnetic transition point with \( \beta = 0.4406868 \)...

![](https://i.imgur.com/2Q5Q5Q5.png)

**FIG. 1.** Correlations of spin glass models obtained by our method (FVS) and belief propagation (BP) compared with data given by MCMC running for a long time (5 \( \times \) 10⁵ N steps) on different graphs. (a) Viena-Bray spin glass model [8] on random regular graph, \( N = 1100 \), degree 3, \( \beta = 0.9 \), couplings \( J_{ij} = \{+1, -1\} \) with \( P(J_{ij} = 1) = P(J_{ij} = -1) = \frac{1}{2} \); (b) On the Erdős-Rényi random graph, \( N = 1100 \), average degree 3, \( \beta = 0.8 \) and couplings are Gaussian random variables with zero mean and unit variance; (c) The model is the same as that of (b) but on the real-world karate club network [9], with \( N = 34 \), average degree 2.29 and \( \beta = 0.54 \); (d) The same as in (b) but on the real-world political blogs network [10], with \( N = 1490 \), average degree 11.21 and \( \beta = 0.1 \).

**FIG. 2.** Free energy (per spin) of the Ising model on 16 \( \times \) 16 lattice with open boundary condition obtained by various method, and their relative errors to the exact solution [11]. The vertical dashed line in the inset represents the phase transition point of an infinite system (\( \beta = 0.4406868 \)).
FIG. 3. (a) Evolution of the variational free energy through training. Solid lines represent mean of $E(s) + \frac{1}{\beta} \ln q_\theta(s)$, and shaded areas represent standard derivation. In the inset, a longer time scale of 5000 epochs is illustrated; (b) Time used for one epoch (training step) in seconds. Each point is averaged 100 instances.

networks and structured sparsity such as lattices in the same way, by extracting a small feedback vertex cover set, mapping the original problem to the statistical mechanics on the FVS, then solving it using neural-network based variational method. Numerical experiments show that our method significantly outperforms belief propagation on random graphs, and convolution-neural-network based methods in 2D lattices.

An interesting application of our approach would be optimization and constraint satisfaction problems defined on sparse graphs, such as vertex cover [14] and satisfiability problems [15], and statistical inference problems where the Bayesian inference formula corresponds to the Boltzmann distribution. We will put this into future work.

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[1] H. Bethe, Proc. R. Soc. London A 150, 552 (1935).
[2] J. Yedidia, W. Freeman, and Y. Weiss, in International Joint Conference on Artificial Intelligence (IJCAI) (2001).
[3] R. Kikuchi, Physical review 81, 988 (1951).
[4] H.-J. Zhou, The European Physical Journal B 86, 455 (2013).
[5] L. Zdeborová, P. Zhang, and H.-J. Zhou, Scientific reports 6, 37954 (2016).
[6] D. Wu, L. Wang, and P. Zhang, Physical Review Letters 122, 080602 (2019).
[7] R. J. Williams, Machine learning 8, 229 (1992).
[8] L. Viana and A. Bray, J. Phys. C 18, 3037 (1985).
[9] W. W. Zachary, Journal of anthropological research 33, 452 (1977).
[10] L. A. Adamic and N. Glance, in Proceedings of the 3rd international workshop on Link discovery (ACM, 2005) pp. 36–43.
[11] M. Kac and J. C. Ward, Physical Review 88, 1332 (1952).
[12] I. Goodfellow, Y. Bengio, and A. Courville, Deep learning (MIT press, 2016).
[13] A. van den Oord, N. Kalchbrenner, and K. Kavukcuoglu, in International Conference on Machine Learning (2016) pp. 1747–1756.
[14] P. Zhang, Y. Zeng, and H. Zhou, Phys. Rev. E 80, 021122 (2009).
[15] M. Mézard, G. Parisi, and R. Zecchina, Science 297, 812 (2002).
[16] D. J. MacKay, Information theory, inference and learning algorithms (Cambridge university press, 2003).
[17] H. Zhou, “Spin glass and message passing,” (2015).
[18] D. P. Kingma and J. Ba, arXiv preprint arXiv:1412.6980 (2014).
Variational autoregressive networks

The variational mean field methods approximate the Boltzmann distribution using some tractable variational distributions from certain families. Due to the limitations of computing the variational free energy, the variational distributions are usually not very representative. The recent developments of deep neural networks may be very helpful to give a much more representative variational distribution. The universal approximation theorem [12] ensures that a neural network containing a large-enough hidden layer can approximate any continuous functions. This means that a deep neural network might be used to approximate the Boltzmann distribution very accurately. This idea has recently been used in VAN for building a neural-network-based variational mean-field method for statistical mechanics problems [6].

VANs factorize the variational distribution by writing the joint probability as the product of conditional probabilities

$$q(s) = \prod_{i=1}^{N} q(s_i|s_{<i}) , \quad (6)$$

where $s_{<i}$ represents the state of all variables with index less than $i$. Here we can see, for variable of index $i$, its state will be determined by previous variables but independent of all variables behind it. This is called autoregressive property in the machine learning community. From the views of graphical models, Eq. (6) connects all variables through their indices to a complete directed graph (suppose each variable is represented by a vertex). This connection pattern is universal for all graphical models but it makes no conditional independence assumptions about the variables.

Conditional probabilities $q(s_i|s_{<i})$ then will be parametrized by carefully designing neural networks to represent the many-body interactions of variables. Without loss of generality, for the simplest case of one layer autoregressive network without bias, the outputs can be write as

$$s'_i = \sigma(\sum_{j<i} W_{ij} s_j) ,$$

where $\sum_{j<i} W_{ij}$ is achieved by adding mask at weights $W_{ij}$. Since the sigmoid function $\sigma(\cdot)$ limits outputs to be in the range of $(0, 1)$, outputs can be naturally deemed as probability. In this case, the conditional probability can be written as

$$q(s_i|s_{<i}) = s'_i^{s_i}(1 - s'_i)^{1-s_i} , \quad (7)$$

which is a Bernoulli distribution, with $s'_i = p(s_i = +1|s_{<i})$. And the variational joint distribution becomes

$$q_\theta(s) = \prod_{i=1}^{N} q_\theta(s_i|s_{<i}) , \quad (8)$$

where $\theta$ are network parameters like weights and bias.

For variation methods, they adjust parameters to make $q_\theta(s)$ close enough to the Boltzmann distribution. The distance between two distributions is usually quantified by Kullback-Leibler (KL) divergence [16]

$$D_{KL}(q||p) = \sum_s q(s) \ln \left( \frac{q(s)}{p(s)} \right) = \beta (F_q - F) \quad (9)$$

where

$$F_q = \sum_s q_\theta(s) \left[ E(s) + \frac{1}{\beta} \ln q_\theta(s) \right] , \quad (10)$$

is the variational free energy and $F$ is the true free energy. Since KL divergence is positive, minimizing KL divergence is equivalent to minimizing $F_q$ to its lower bound $F$. Thus variational free energy is set to be loss function for VANs. Here $E(s)$ is energy function determined by models and $\ln q_\theta(s)$ can be calculated combining Eq. (7) and Eq. (8)

$$\ln q_\theta(s) = \sum_{i=1}^{N} \left[ s_i s'_i + (1 - s_i)(1 - s'_i) \right] . \quad (11)$$

Minimizing $F_q$ requires optimization over network parameters $\theta$, here score function estimator [7] is adopted to calculate gradient of the variational free energy with respect to network parameters

$$\nabla_\theta F_q = \sum_s q_\theta(s) \left[ \left( E(s) + \frac{1}{\beta} \ln q_\theta(s) \right) \nabla_\theta \ln q_\theta(s) \right] . \quad (12)$$

Using Adam optimizer [13] to minimize the loss function will make the variational free energy closer to its lower bound. After training, the variational distribution $q_\theta(s)$ will be a good approximation to the Boltzmann distribution $p(s)$.

The work flow of a VAN is shown in Fig. 4. At first, an autoregressive network needs to be constructed according to factorization of the joint probability. Then we need to get samples from the autoregressive network that obey variational distribution through vertex by vertex sampling in a given ordering, the probability of next vertex given former vertices is determined by previous variables but independent of all variables behind it. This is called autoregressive property in the machine learning community. From the views of graphical models, Eq. (6) connects all variables through their indices to a complete directed graph (suppose each variable is represented by a vertex). This connection pattern is universal for all graphical models but it makes no conditional independence assumptions about the variables.

Replacing $E(s)$ with $E(s; \theta)$, the entropy $\ln q_\theta(s)$ and variational free energy $F_q$ will propagate back to change network parameters $\theta$ according to Eq. (12).
Calculation example of Ising model

Suppose here we consider the classic Ising spin glasses as representative models, in which the energy function is defined as

$$E(\sigma) = - \sum_{(ij) \in E} J_{ij} \sigma_i \sigma_j - \sum_i \sigma_i \theta_i ,$$

(13)

where $\sigma$ is the joint state of state of FVS $s$ and state of forest $t$, $E$ denotes set of edges, $J_{ij}$ is couplings of the Ising model and $\theta_i$ is the external field acting on the node $i$.

Given the configuration of FVS $s$, external field FVS vertices exert on the forest will be

$$h_i^0 = \sum_{j \in E_{\Omega}(i)} \beta(J_{ij}s_j + \theta_j s_j) ,$$

(14)

where $n(i)$ is the set of neighbors of vertex $i$. Then the energy of forest $T$ will be

$$E(t) = - \sum_{(ij) \notin E_T} J_{ij} t_j t_j - \sum_{i \in T} t_i h_i .$$

(15)

Here $E_T$ denotes edges of forest $T$ and $h_i = \theta_i + h_i^0$ is the overall external field vertex $i$ feels.

When performing leaf removal (which removes all leaves of this graph recurrently), the whole forest will be hierarchized to levels with leaves on top and roots on bottom. Our leaf removal ordering is constructed by appending these levels from top to bottom to ensure after removing vertices in upper level, vertices in the next level will all be leaves.

When a leaf $i$ is removed from the forest, the partition function of $T$ can be written as

$$Z(s) = \sum_{t \in T} e^{-\beta E(s,t)} = \sum_{t_i} e^{\beta h_i t_i} \sum_{t_{\Omega}(i)} e^{-\beta E_\Omega(t_{\Omega})}$$

$$= 2 \cosh \beta(J_{ij} t_j + h_i) \sum_{t_{\Omega}} e^{-\beta E_\Omega(t_{\Omega})}$$

$$= 2 \sqrt{\cosh \beta(J_{ij} + h_i) \cosh \beta(-J_{ij} + h_i)} \exp \left[ \frac{s_j}{2} \ln \left( \frac{\cosh \beta(J_{ij} + h_i)}{\cosh \beta(-J_{ij} + h_i)} \right) \right] \sum_{t_{\Omega}} e^{-\beta E_\Omega(t_{\Omega})}$$

$$= 2 \sqrt{\cosh \beta(J_{ij} + h_i) \cosh \beta(-J_{ij} + h_i)} \sum_{t_{\Omega}} e^{\beta h_j t_j} e^{-\beta E_\Omega(t_{\Omega})}$$

$$= 2 \sqrt{\cosh \beta(J_{ij} + h_i) \cosh \beta(-J_{ij} + h_i) Z_{\Omega}},$$

(16)

where $E_\Omega(t_{\Omega})$ represents energy with vertex $i$ and its interaction excluded, $E_{ij}(t_{ij}) = E_{ij}(t_{\Omega}) - h_j t_j$ and $h_j'$ is the external field that combines the original external field of vertex $j$ and a external field vertex $i$ exert on $j$.

Thus when a leaf vertex $i$ be removed from the graph, it will give a factor $2 \sqrt{\cosh \beta(J_{ij} + h_i) \cosh \beta(-J_{ij} + h_i)}$ to the partition function and change the external field of its neighbor $j$ will be

$$h_j' = h_j + \frac{1}{2\beta} \ln \left( \frac{\cosh \beta(J_{ij} + h_i)}{\cosh \beta(-J_{ij} + h_i)} \right).$$

(17)

While for root vertex $k$ the factor will be $2 \cosh \beta h_k$ since it has no neighbors when removed.

Multiplying these factors together and combining Eq. (3) and Eq. (4), the effective energy of the FVS can be analytically expressed as

$$\tilde{E}(s) = E_\Omega(s) + \frac{1}{\beta} \sum_{(ij) \notin E_T} \ln \sqrt{4 \cosh \beta(J_{ij} + h_i)}$$

$$+ \sum_{(ij) \notin E_T} \ln \sqrt{4 \cosh \beta(-J_{ij} + h_i) + \sum_{j \in R} \ln(2 \cosh(\beta h_j))}$$

(18)

Here $R$ denotes set of roots of the remaining forest, and $h_i$ is the effective field acting on vertex $i$ when $j$ is a neighbor of $i$.

Experimental settings

On the first experiment, we compare correlations of three methods based on spin glass model. MCMC results are deemed as the base line. Hyperparameter settings are roughly the same as the first experiment, so we will not specify it here. Connected correlations calculation of MCMC is trivial since samples obey Boltzmann distribution have already gotten. Thus here we only introduce how to calculate connected correlations of other two methods.

For belief propagation, we adopt the scheme of [17] by propagating cavity fields $h_{i \rightarrow j}$. As long as cavity fields reaching their fixed point, we can calculate physical quantities based on them. The magnetism of vertex $i$ is

$$m_i = \sum_{j \notin \partial i} \text{arctanh} \left( \frac{\tanh(\beta J_{ij}) \tanh(\beta h_{j \rightarrow i}))}{\cosh(\beta J_{ij}) + \cosh(\beta h_{j \rightarrow i})} \right)$$

(19)

where $\partial i$ represents all neighbors of vertex $i$.

And the connected correlation of $i$ and $j$ is

$$\langle s_i s_j \rangle_C = \frac{e^{\beta J_{ij} \cosh \beta h_{ij} - e^{-\beta J_{ij} \cosh \beta h_{ij}^c}} - m_i m_j}{e^{\beta J_{ij} \cosh \beta h_{ij}^c} + e^{-\beta J_{ij} \cosh \beta h_{ij}^c}}$$

(20)

where $h_{ij}^c = h_{i \rightarrow j} + h_{j \rightarrow i}$ and $h_{ij}^c = h_{i \rightarrow j} - h_{j \rightarrow i}$.

For our method, calculations can be a little obscure since we only have samples of FVS vertices but correlations of all edges are needed. But we can start from the definition of correlations

$$\langle s_i s_j \rangle = \sum_{s_i s_j} s_i s_j p(s_i s_j)$$

$$= \frac{\sum_{s_i s_j} s_i s_j e^{-\beta E(s)}}{Z}$$

$$= \frac{\sum_{s_i s_j} \sum_{s_{\Omega}(i)} s_i s_j e^{-\beta E(s_{\Omega})}}{Z}$$

$$= \frac{Z_{++} + Z_{-+} - Z_{+-} - Z_{-\cdot}}{\sum_{s_{\Omega}(i)} e^{-\beta E(s_{\Omega})}}$$

(21)
where $s_{\text{aug}} = s_{\text{fvs}+ij}$ is the state of FVS vertices plus vertex $i$ and $j$, $Z_{++} = \sum_{s_{\text{fvs}}} e^{-\beta E(s_{\text{fvs}}|s_i=+1,s_j=+1)}$. Then both the numerator and denominator can be calculated using our method, $\langle s_i \rangle$ can be calculated similarly thus we can use expressions above to calculate connected correlations of entire graph.

| Table I. Hyperparamters of Fig. 2 |
|-----------------------------------|
|                                   |
| Dense   | Convolution | FVS    |
| Batch   | $1 \times 10^3$ | $1 \times 10^3$ | $1 \times 10^3$ |
| Net depth | 3           | 3       | 2       |
| Net width | 4           | 64      | 3       |
| Max step | $1 \times 10^4$ | $1 \times 10^4$ | $1 \times 10^4$ |
| Learning rate | $1 \times 10^{-3}$ | $1 \times 10^{-3}$ | $1 \times 10^{-3}$ |
| Number of parameters | 1577216 | 714113 | 22532 |

$^a$ For convolution, this number represent channels.

$^b$ This quantity is not a hyperparamter, but we list it here for comparison.

On the second experiment, our method, two architectures from original version of VAN and belief propagation are implemented on a $16 \times 16$ 2D ferromagnetic Ising model with open boundary conditions. For dense and convolution architectures, we borrow hyperparameter settings from [6]. All hyperparameters used in this experiment are listed in Table I. Since all these methods have been fine-tuned for their best performance, there are some differences on the hyperparameter settings. We can clearly see that our approach achieves better performance over others with less hyperparameters, which proves the superiority of our construction.

On the third experiment in the main text, two methods are implemented on random regular graphs to compare their running times and convergence speeds. Hyperparamters like batch, net depth, net width and learning rate used in Fig. 3(a) are all the same for both methods in order to compare the differences in performance. The resulting numbers of trainable parameters differ a lot: 63503 for the FVS and 1002000 for the dense VAN, for a random graph of size $N = 1000$. We see our method massively decreases the number of hyperparameters.

The hyperparameters of Fig. 3(b) are similar to Fig. 3(a), with the only difference on the number of vertices.