How data, synapses and neurons interact with each other: a variational principle marrying gradient ascent and message passing

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(Dated: November 19, 2019)

Unsupervised learning requiring only raw data is not only a fundamental function of the cerebral cortex, but also a foundation for a next generation of artificial neural networks. However, a unified theoretical framework to treat sensory inputs, synapses and neural activity together is still lacking. The computational obstacle originates from the discrete nature of synapses, and complex interactions among these three essential elements of learning. Here, we propose a variational mean-field theory in which only the distribution of synaptic weight is considered. The unsupervised learning can then be decomposed into two interwoven steps: a maximization step is carried out as a gradient ascent of the lower-bound on the data log-likelihood, and an expectation step is carried out as a message passing procedure on an equivalent or dual neural network whose parameter is specified by the variational parameter of the weight distribution. Therefore, our framework explains how data (or sensory inputs), synapses and neural activities interact with each other to achieve the goal of extracting statistical regularities in sensory inputs. This variational framework is verified in restricted Boltzmann machines with planted synaptic weights and learning handwritten digits.

I. INTRODUCTION

Searching for hidden features in raw data and thus a reasonable explanation of sensory data is a core function of natural intelligence [1]. Sensory cortical circuits are able to extract useful information from noisy sensory inputs because of unsupervised synaptic plasticity shaping well-organized synaptic connections [2, 3]. From a neural network perspective, this kind of unsupervised learning was modeled by a simple two-layer architecture, namely restricted Boltzmann machine (RBM) [4–6]. One layer is used to receive the sensory inputs, thereby being the visible layer; while the other layer serves as a hidden representation encoding features in the inputs. No lateral connections exist within each layer, which was designed to avoid costly sampling as in a fully-connected network. Synaptic plasticity thus refers to the learning process where the connection (weight) strengths between these two layers are adjusted to capture the hidden features in the input data.

In machine learning community, this learning process can be achieved by the popular truncated Gibbs sampling (also called contrast divergence algorithm [6]), which was particularly designed for continuous weight values, and thus a gradient ascent of the data log-likelihood is mathematically guaranteed [7]. However, to model unsupervised learning with energy-efficient computation using low-precision synapses (weights), the gradient-based method does not apply due to the discreteness of synapses. Several recent works paved the way along this line to understand computational principles of unsupervised learning with low-precision synapses [8–15]. Due to the complexity of analysis, these works either considered impractical network architectures or did not consider the constraint of arbitrarily many data samples, or their methods rely on Gibbs-sampling-based computations. These works thus failed to analyze the interaction among inputs, synaptic plasticity and neural activity within a unified framework. Therefore, how this interaction shapes the unsupervised learning process is still unknown, and moreover, because a typical learning procedure, occurring in both biological neural networks and artificial ones, should involve sensory inputs, synaptic plasticity and neural activity, understanding this interaction becomes a key to unlock the black box of unsupervised learning, which is a core principle of deep generative models widely used in real-world applications in the deep learning era [10], e.g., in the neuromorphic computing simulating brain computation [17].

Here, we propose a variational perspective that takes into account the uncertainty of weights given sensory inputs, which is neglected in previous modelings of unsupervised learning in a general setting. We model the learning process as a computation of the posterior on the weight parameters according to Bayesian principle. The variational perspective thus consists of finding the best approximation of the posterior within a tractable parametric family. Remarkably, even though in the presence of both a generic architecture and arbitrarily many sensory data, the learning process under the variational principle can be reduced to estimating equilibrium properties of an equivalent RBM whose parameters are determined by the variational parameters of the principle. According to this principle, rather than estimating the data log-likelihood in a direct way, the learning process improves a lower-bound on the data log-likelihood. Therefore, our variational principle opens a new path towards understanding how sensory data, synapses and neurons interact with each other during unsupervised learning.
In this study, we use the RBM defined above with arbitrarily many hidden neurons (the left panel of Fig. 1) to learn hidden features in $M$ input data samples, which are raw unlabeled data specified by $\{\sigma^a\}_{a=1}^M$. Each data sample is specified by an Ising-like spin configuration $\sigma = \{\sigma_i = \pm 1\}_{i=1}^N$ where $N$ is the size of an input sample (e.g., the number of pixels in an image). The synaptic weights are characterized by $\xi$, where each component takes a binary value ($\pm 1$). The number of hidden neurons is defined by $P$. The Boltzmann distribution of this RBM is given by Eq. (1):

$$P(\sigma) = \frac{1}{Z(\xi)} \prod_\mu \cosh(\beta X_\mu),$$

where $\mu$ denotes the hidden neuron index, $X_\mu = \frac{1}{\sqrt{N}} \xi^\mu \cdot \sigma$, $\xi^\mu$ is also called the receptive field of the $\mu$-th hidden neuron, and $Z(\xi)$ is the partition function depending on the joint set of all receptive fields $\xi$. Note that the hidden neurons’ activities ($\pm 1$) have been marginalized out. The scaling factor $\frac{1}{\sqrt{N}}$ ensures that the argument is of the order of unity. Supposed that the data samples are generated from a RBM where the synaptic connections are randomly generated at first and then quenched. The inverse-temperature $\beta$ thus tunes the noise level of generated data samples from the planted RBM. Then one standard test of any learning algorithm is to learn the planted synaptic connection matrix from the supplied data samples.

To further model the learning process, we assume that the data samples are weakly-correlated, e.g., sampled with a large interval during sampling of the planted model. Therefore, we have the following data probability:

$$P(\{\sigma^a\}_{a=1}^M | \xi) = \prod_{a=1}^M \frac{1}{Z(\xi)} \prod_\mu \cosh(\beta X^a_\mu),$$

where the superscript $a$ in $X^a_\mu$ means that $\sigma$ in $X_\mu$ is replaced by $\sigma^a$. Finally, the learning process is modeled by estimating the posterior probability of the guessed synaptic weights according to the Bayes’ rule [9,15]:

$$P(\xi | \{\sigma^a\}_{a=1}^M) = \frac{\prod_\mu P(\sigma^a | \xi)}{\sum_\xi \prod_\mu P(\sigma^a | \xi)} = \frac{1}{\Omega} \exp \left( -M \ln Z(\xi) + \sum_{a,\mu} \ln \cosh (\beta X^a_\mu) \right),$$

where $\Omega$ is the partition function of the posterior, and a uniform prior for $\xi$ is assumed, i.e., we have no prior knowledge about the planted weights. For simplicity, we use the same temperature as that used to generate data. However, one obstacle to compute the posterior probability is the nested partition function $Z(\xi) \equiv \sum_\sigma \prod_\mu \cosh(\beta X_\mu)$ which involves an exponential computational complexity. Except for a few special cases of one or two hidden neurons as studied in previous works [8,9,12,15], the computation of the posterior is impossible, let alone understanding the learning process. This is the very motivation of this paper that proposes a new principled method to tackle this challenge for paving a way towards a scientific understanding of a generic unsupervised learning process.

FIG. 1: (Color online) The schematic illustration of the variational model. $N = 4$ in this example (say, $i,j,l$ and $l$). The hidden layer has $P = 3$ neurons. Note that $(N,P)$ can be arbitrarily finite numbers. (Left panel) The RBM architecture receives data of $M$ examples and encodes the hidden features of data into synaptic connections (weights) in an unsupervised way. Here, we take into account the weight uncertainty captured by a variational distribution $q_{\lambda_{\mu}}(\xi^\mu)$ where $\xi^\mu$ refers to the connection between sensory neuron $i$ and hidden neuron $\mu$, and $\lambda_{\mu}$ is the variational parameter. (Right panel) The equivalent RBM model where the connection becomes the variational parameter and the additional hidden bias is determined by the variance $(\Xi^\mu_\mu)$ of the weighted-sum input to a hidden neuron (see the main text). $z_\mu$ is a standard Gaussian random variable. The equilibrium properties of the equivalent RBM are used to adjust the variational parameter improving the lower-bound on the data log-likelihood.
III. A VARIATIONAL PRINCIPLE

Rather than finding an approximate method to evaluate the posterior, we use a variational distribution belonging to the mean-field family \([19, 21]\), defined by \(q_\lambda(\xi)\), and find the best variational distribution to minimize the Kullback-Leibler (KL) divergence between \(q_\lambda(\xi)\) and \(P(\xi|D)\) where \(D\) denotes the data \(\{\sigma^a\}\), which is given by

\[
KL(q_\lambda(\xi)||P(\xi|D)) = \mathbb{E} \ln q_\lambda(\xi) - \mathbb{E} \ln P(\xi|D) = \mathbb{E} \ln q_\lambda(\xi) - \mathbb{E} \ln P(\xi, D) + \ln P(D) = -LB(\lambda) + \ln P(D),
\]

where \(KL(q||p) \equiv \langle \ln \frac{q}{p} \rangle\) for two distributions — \(q\) and \(p\), \(\mathbb{E}\) denotes the expectation under the variational probability \(q_\lambda\) where \(\lambda\) denotes the corresponding variational parameter, and \(P(\xi, D) = P(\xi|D)P(D)\). Because of the non-negativity of the KL divergence, the lower-bound on the data log-likelihood is given by

\[
LB(\lambda) \equiv \mathbb{E} \ln P(\xi, D) - \mathbb{E} \ln q_\lambda(\xi)
= \mathbb{E} \ln P(D|\xi) - KL(q_\lambda(\xi)||P(\xi)),
\]

where the argument of \(q_\lambda\) is omitted when it is clear, and \(P(\xi, D) = P(D|\xi)P(\xi)\) where \(P(\xi)\) can be treated as a prior probability of weights. The first term serves as the expected log-likelihood of the data, while the second term is a regularization term. The first term encourages the variational distribution to explain the observed data (maximizing the expected log-likelihood of the data), while the second term encourages the approximate posterior to match the prior. Therefore, the variational objective in Eq. (5) takes into account the balance between likelihood and prior \([21]\). The learning process is now interpreted as finding the variational parameter \(\lambda\) that improves the lower-bound on the data log-likelihood. It is clear that the lower-bound is tight once \(q_\lambda\) matches \(P(\xi|D)\).

To proceed, we assume a factorized (across individual weights) prior probability parameterized by \(m = \{m_{i,\mu}\}\):

\[
P(\xi) = \prod_{i,\mu} \left[ \frac{1+m_{i,\mu}}{2} \delta_{\xi_{i,\mu},+1} + \frac{1-m_{i,\mu}}{2} \delta_{\xi_{i,\mu},-1} \right]
\]

where \(\delta_{x,y}\) denotes the Kronecker delta function, and \(m_{i,\mu}\) defines the mean of synaptic strength from visible neuron \(i\) to hidden one \(\mu\) when the uncertainty is considered (Fig. 1) \([22, 23]\). For simplicity, we also parameterize the variational distribution in the same form but with different means specified by \(\lambda\). The variational distribution is given by

\[
q_\lambda(\xi) = \prod_{i,\mu} \left[ \frac{1+\lambda_{i,\mu}}{2} \delta_{\xi_{i,\mu},+1} + \frac{1-\lambda_{i,\mu}}{2} \delta_{\xi_{i,\mu},-1} \right].
\]

Hence the weight uncertainty can be explicitly captured by the variational distribution, in contrast to the point-estimate in a usual contrast divergence algorithm for continuous weights. This form was also recently used in supervised learning of perceptron models \([24, 25]\).

According to Eq. (2), we can write \(\ln P(D|\xi)\) explicitly and insert it into the lower-bound, then we get

\[
LB(\lambda) = -KL(q_\lambda(\xi)||P(\xi)) + \mathbb{E} \left[ \sum_{a,\mu} \ln \text{cosh}(\beta X_{\mu}^a) - M \ln Z(\xi) \right].
\]

The variational parameter \(\lambda\) is achieved by optimizing the lower-bound through gradient ascent, defined by

\[
\Delta \lambda = \eta \nabla_{\lambda} LB(q_\lambda(\xi))
\]

where \(\eta\) is a learning rate. Before evaluating the gradient, we need to calculate the regularization and log-likelihood terms. For the regularization term, due to the factorization assumption, it is easy to arrive at the following result:

\[
-\text{KL}(q_\lambda(\xi)||P(\xi)) = \sum_{x=\pm} \sum_{i,\mu} \left[ S \left( \frac{1 + \lambda_{i,\mu} x}{2}, \frac{1 + m_{i,\mu} x}{2} \right) - S \left( \frac{1 + \lambda_{i,\mu} x}{2}, \frac{1}{2} \right) \right],
\]

where \(S(z, y) \equiv z \ln y\).

The expected log-likelihood term is still difficult to estimate without any approximations. However, based on the fact that the variational distribution \(q_\lambda\) is factorized, we assume that \(X_\mu^a\) involves a sum of a large number of nearly independent random variables and thus follows a Gaussian distribution \(\mathcal{N}(C_\mu^a, \Sigma_\mu^a)\), where the mean and variance can be easily computed respectively by

\[
C_\mu^a = \frac{1}{\sqrt{N}} \sum_{i \in \partial \mu} \lambda_{i,\mu} \sigma_i^a,
\]

\[
\Sigma_\mu^a = \frac{1}{N} \sum_{i \in \partial \mu} (1 - \lambda_{i,\mu}^2),
\]

where \(i \in \partial \mu\) denotes all incoming neurons into the \(\mu\)-th hidden neuron. Note that \(\lambda_{i,\mu}\) serves as the mean of synaptic strength \(\xi_{i,\mu}\). Therefore, the uncertainty of weights on the provided data \(D\) has been incorporated into this approximation using the central-limit-theorem for a large value of \(N\).
Given one sensory input, say $\sigma^a$, it is reasonable to assume that the weighted-sum $X^n_a$ is conditionally independent (this is also the working mechanism of contrast divergence [6]). It then follows that the expected log-likelihood can be approximated by a Monte-Carlo estimation [29]:

$$
\mathbb{E} \left[ \sum_{a,\mu} \ln \cosh(\beta X^n_a) - M \ln \mathcal{Z}(\xi) \right] = \frac{1}{B_1} \sum_{a,\mu, s} \ln \cosh \left( \beta G^n_\mu + \beta \Xi^s_\mu z^s_\mu \right) - \frac{M}{B_2} \sum_{s} \ln \prod_{\mu} \cosh \left( \beta G^n_\mu + \beta \Xi^s_\mu z^s_\mu \right),
$$

where $s$ denotes the index for Monte-Carlo samples, $z^s_\mu$ is a standard Gaussian random variable, $B_1$ and $B_2$ denote the number of Monte-Carlo samples, and are not necessarily equal, and $G^n_\mu$ is defined by $G^n_\mu$ without the symbol $a$. A careful inspection of the second term in Eq. (9) reveals that the partition-function part of the expected log-likelihood reduces to an equivalent RBM model (the right panel of Fig. 1) whose synaptic connections are now replaced by the variational parameter $\lambda$ scaled by $\sqrt{N}$, and an additional random bias is introduced for each individual hidden neuron as $\Xi^s_\mu z^s_\mu$ due to the fluctuation of the weighted-sum. This surprising transformation makes estimation of the original computational hard partition function tractable, as the cavity method developed for a RBM [18] can be directly applied. Another benefit is that the resulting expression in Eq. (9) is amenable to variational inference, i.e., gradient estimation.

Next, we briefly summarize the mean-field estimation of the partition function of the equivalent model as follows. Technical details to derive these results based on the cavity method have been given in a series of works [9, 18]. This estimation provides a practical procedure called message passing working on single instances of the RBM, which is efficient for a practical learning. First, the interaction between visible and hidden neurons is of the order $O(m \log NM)$, thus weak, then the cavity approximation taking only correlations around a factor in the product (see Eq. (9)) leads to the following self-consistent cavity iteration:

$$
m_{i \rightarrow \nu} = \tanh \left( \sum_{\mu \in \partial i \setminus \nu} u_{\mu \rightarrow i} \right),
$$

$$
u \leftarrow i = \tanh^{-1} \left( \tanh(\beta \chi_{\mu \rightarrow i} + \beta H_{\mu}) \tanh(\beta \lambda_{i\mu}/\sqrt{N}) \right),
$$

where $\mu \in \partial i \setminus \nu$ indicates all factors around the visible neuron $i$ excluding the factor indexed by $\nu$. $m_{i \rightarrow \nu}$ is the cavity magnetization interpreted as the message passing from visible neuron to hidden neuron (Fig. 1), while $u_{\mu \rightarrow i}$ denotes the cavity bias interpreted as the message passing from hidden neuron to visible neuron. $\chi_{\mu \rightarrow i} \equiv \frac{1}{\sqrt{N}} \sum_{j \in \partial \mu \setminus i} \lambda_{j\mu} m_{j \rightarrow \mu}$ collecting all messages except those from $i$ around the factor $\mu$ weighted by their corresponding variational parameters, and $H_{\mu}$ denotes the random hidden bias expressed as $\Xi^s_\mu z^s_\mu$.

Because of weak interactions, this message passing equation is able to converge even in a few steps. Then the log-partition-function (so-called free energy) can be readily constructed based on the visible neuron’s contribution $F_i$ and the factor’s contribution $F_\mu$, as $\ln Z = \sum_i F_i \equiv \left( N - 1 \right) \sum_i F_i$ where the subtraction removes the double counting of the contribution from the first term [27]. $F_i$ and $F_\mu$ are given respectively by

$$
F_i = \sum_{\mu \in \partial i} \left[ \beta^2 \Lambda^2_{\mu \rightarrow i}/2 + \ln \cosh \left( \beta \chi_{\mu \rightarrow i} + \beta H_{\mu} + \beta \lambda_{i\mu}/\sqrt{N} \right) \right] + \ln \left( 1 + \prod_{\mu \in \partial i} e^{-2u_{\mu \rightarrow i}} \right),
$$

$$
F_\mu = \beta^2 \Lambda^2_{\mu}/2 + \ln \cosh \left( \beta \chi_{\mu} + \beta H_{\mu} \right),
$$

where $\Lambda^2_{\mu \rightarrow i} \equiv \frac{1}{N} \sum_{j \in \partial \mu \setminus i} \lambda_{j\mu} \Lambda^2_{j \rightarrow \mu}$ (1-2), $\Lambda^2_{\mu} \equiv \frac{1}{N} \sum_{j \in \partial \mu} \lambda_{j\mu} \Lambda^2_{j \rightarrow \mu}$, and $\chi_{\mu} \equiv \frac{1}{\sqrt{N}} \sum_{i \in \partial \mu} \lambda_{i\mu} m_{i \rightarrow \mu}$. Note that $\chi_{\mu}$ and $G_{\mu}$ are intrinsically different, because the former describes the equilibrium properties of the equivalent RBM with fixed $\lambda_{i\mu}$ (the right panel of Fig. 1), while the latter captures the statistics under the variational distribution given the sensory input (the left panel of Fig. 1).

Finally, let us evaluate the gradient of the lower-bound. First, the gradient of the regularization term with respect to the variational parameter is obtained as

$$
- \frac{\partial}{\partial \lambda_{i\mu}} \text{KL}(q_{\lambda}(\xi) || P(\xi)) = \sum_{x = \pm 1} \frac{x}{2} \left( \ln \frac{1 + x m_{i\mu}}{1 + x \lambda_{i\mu}} - 1 \right).
$$

It is clear that this term vanishes when the variational distribution is exactly matched to the prior. Second, the
gradient of the first term in the expected log-likelihood (Eq. 9) can be written as
\[
\frac{\partial}{\partial \lambda_{i\mu}} \mathbb{E} \left[ \sum_{a,\mu} \ln \cosh(\beta X_{\mu}^a) \right] \approx \frac{\beta}{B_1 \sqrt{N}} \sum_{a,s} \sigma_i^s \tanh(\beta G_{\mu}^a + \beta \Xi_{\mu} z_{\mu}^s) \\
- \frac{\beta^2 \lambda_{i\mu}}{N B_1} \sum_{a,s} \left[ 1 - \tanh^2 (\beta G_{\mu}^a + \beta \Xi_{\mu} z_{\mu}^s) \right].
\]
(13)

Lastly, the gradient of the second term in the expected log-likelihood can be derived as
\[
\frac{\partial}{\partial \lambda_{i\mu}} \mathbb{E} \ln Z(\lambda) \approx \frac{\beta}{\sqrt{N} B_2} \sum_s \langle \sigma_i \tanh(\beta G_{\mu}^a + \beta \Xi_{\mu} z_{\mu}^s) \rangle \\
- \frac{\beta \lambda_{i\mu}}{N B_2} \sum_s \left[ \frac{z_{\mu}^s}{\Xi_{\mu}} \tanh (\beta G_{\mu}^a + \beta \Xi_{\mu} z_{\mu}^s) \right],
\]
(14)

where the expectation \( \langle \cdot \rangle \) means an average under the Boltzmann measure of the equivalent model \( \mathcal{P}_\text{eq}(\sigma) = \frac{1}{Z} \prod_{a,\mu} \cosh (\beta G_{\mu}^a + \beta \Xi_{\mu} z_{\mu}^s) \), \( C_{i\mu} \) and \( \bar{m}_\mu \) thus define the correlation between visible and hidden neurons, and mean activities of hidden neurons, respectively. Interestingly, these two macroscopic thermodynamic quantities can be evaluated from the fixed point of the message passing equation (Eq. (10)). Interested readers can find technical details in our previous work [18]. Here we summarize the result as follows,
\[
m_i = \tanh \left( \sum_{\mu \in \partial i} u_{\mu \rightarrow i} \right),
\]
(15a)
\[
\bar{m}_\mu = \int Dz \tanh(\beta \tilde{\chi}_\mu + \beta H_{\mu} + \beta \tilde{\Lambda}_\mu z),
\]
(15b)
\[
C_{i\mu} = \bar{m}_{i\mu} m_i + \frac{\beta \lambda_{i\mu}}{\sqrt{N}} (1 - m_i^2) A_{\mu},
\]
(15c)
\[
A_{\mu} = 1 - \int Dz \tanh^2 (\beta \tilde{\chi}_\mu + \beta H_{\mu} + \beta \tilde{\Lambda}_\mu z),
\]
(15d)

where \( Dz \equiv e^{-z^2/2} / \sqrt{2\pi} dz \), \( \tilde{\chi}_\mu \equiv \frac{1}{\sqrt{N}} \sum_{i \in \partial \mu} \lambda_{i\mu} m_i \), and \( \tilde{\lambda}_\mu^2 \equiv \frac{1}{N} \sum_{i \in \partial \mu} \lambda_{i\mu}^2 (1 - m_i^2) \).

Collecting all three parts of the gradient, we arrive at the gradient ascent formula to update the variational parameter as \( \lambda_{i\mu}^{t+1} = \lambda_{i\mu}^t + \eta \Delta_{i\mu} \), where \( t \) denotes the learning step, and \( \Delta_{i\mu} \) is given by
\[
\Delta_{i\mu} = \sum_{x = \pm 1}^x \left( \ln \frac{1 + x m_{i\mu}}{1 + x \lambda_{i\mu}} - 1 \right) + \frac{\beta}{B_1 \sqrt{N}} \sum_{a,s} \sigma_i^s \tanh(\beta G_{\mu}^a + \beta \Xi_{\mu} z_{\mu}^s) \\
- \frac{\beta^2 \lambda_{i\mu}}{N B_1} \sum_{a,s} \left[ 1 - \tanh^2 (\beta G_{\mu}^a + \beta \Xi_{\mu} z_{\mu}^s) \right] - \frac{M \beta}{\sqrt{N} B_2} \sum_s \left[ C_{i\mu} - \frac{\lambda_{i\mu} z_{\mu}^s}{\sqrt{N \Xi_{\mu}}} \bar{m}_\mu \right].
\]
(16)

Note that \(|\lambda_{i\mu}| \leq 1\), and \( \xi_{i\mu}^t \) can be decoded as \( \xi_{i\mu}^t = \text{sgn}(\lambda_{i\mu}) \). We remark that this variational principle combines coherently the gradient ascent of the variational parameter \( \lambda \) with the probabilistic inference of message passing given \( \Lambda \). This mimics an Expectation-Maximization procedure [28]: the gradient ascent behaves as an M-step at the synaptic activity level, while the message passing behaves as an E-step at the neural activity level. This also explains why the aforementioned \( \chi_{\mu} \) and \( G_{\mu} \) are intrinsically different. These two steps parameterized by probability distributions interact with each other and iteratively improve the lower-bound on the log-likelihood of the data, explaining how data, synapses and neurons shape the unsupervised learning based only on raw sensory inputs. Interestingly, this variational principle marrying gradient ascent and message passing shares the similar spirit with the free-energy principle proposed for explaining action, perception and learning in the brain [29].

The lower-bound \( \mathcal{L}(q_\Lambda) \) can be estimated using Eqs. (1, 7, 8) and (17). This bound we try to optimize is nevertheless highly non-convex in the variational parameter space. Using the trick of adding momentum [28, 30] helps acceleration of learning towards meaningful regions. In the next section, we first prove the effectiveness of the variational mean-field framework on planted RBM models. Then the framework is applied to a structured dataset, in order to illustrate how unsupervised learning with our current framework works in practice, and furthermore explain mechanisms of the interaction among data, synapses and neural activity.
IV. RESULTS AND DISCUSSIONS

We first test our variational framework on planted RBM models. More precisely, we first generate a RBM model whose synaptic weights are randomly generated with a specified correlation level \( q \). The correlation-free case of \( q = 0 \) corresponds to the orthogonal weight vectors of hidden neurons. Based on this RBM model with planted ground truth, a collection of data samples is prepared from Gibbs samplings of the model [15]. These data samples are finally used as sensory inputs to our variational learning algorithm, with the goal of reconstructing the ground truth. The ground truth is the hidden feature/rule embedded in the data samples with a certain level of variability (controlled by the inverse-temperature \( \beta \)). The learning performance is naturally characterized by the overlap between predicted and planted weights, defined as \( Q^\mu \) where \( \mu \) is the hidden neuron’s index.

As shown in Fig. 2 (a), the variational learning framework is able to recover the ground truth, confirming that the variational mean-field theory is capable of capturing the complex interaction among sensory inputs, synaptic plasticity and neural activities during a typical learning process. Most interestingly, there appears a permutation-symmetry-broken phenomenon in inferred synaptic weights, which is shown by the observation that when we carry out a permutation operation to receptive fields at an intermediate step (e.g., 50-th step), the overlap with the ground truth can have a significant quantitative change (Fig. 2 (a), the case of \( q = 0.3 \)). The permutation-symmetry-broken phase indeed exists as proved in a recent work [15]. The simulation results of our new variational framework add further evidence to this fundamental phenomenon. This symmetry can only be spontaneously broken when the amount of data reaches a certain threshold. The inset of Fig. 2 (a) shows that the KL divergence grows with learning, demonstrating that our variational principle is able to search for a biased probability of weights. Note that in the algorithm we do not assume any prior knowledge about the weight vectors, or \( m_{i\mu} = 0 \) for all \((i\mu)\). However, the algorithm itself takes the variability of the data samples into account, driving the update of the variational parameter towards the ground truth. Therefore, we observe that the KL divergence grows until saturation.

Our current work goes beyond the two-hidden-neuron case. As shown in Fig. 2 (b), the variational mean-field method is able to recover the true/planted synaptic weights in a RBM with three hidden neurons. Remarkably, we observe the permutation-symmetry-broken phenomenon once again in this more complex model (the posterior in Eq. (3) is previously thought to be very difficult to handle, and even out of reach), by using our variational mean-field method, which is illustrated by the sudden switch of the overlap. Apart from the KL divergence, the inset also shows the lower-bound on the data log-likelihood, which is observed to grow with learning, suggesting that the variational mean-field framework indeed improves the bound, while the KL divergence is driven away from the uniform prior. The learning is achieved by an Expectation-Maximization-like procedure.

Typical behavior of the proposed variational mean-field framework is shown in Fig. 3 (a). It is clear that in the correlation-free case, the learning threshold does not depend on the number of hidden neurons \((P = 3 \text{ or } P = 2)\), in accord with the recent theoretical work [15] which explained that the underlying physics is the partition function factorization. Furthermore, the correlation level decreases the threshold, as also verified in simulation results of the current framework. Below the threshold, a random-guess phase \((\lambda = 0)\) dominates the learning such that the fluctuation (of the order \( \mathcal{O}(\frac{1}{N}) \)) dominates the inference accuracy. Above the threshold, there appears spontaneous symmetry breaking corresponding to concept-formation in unsupervised learning [8, 9].

Finally, we apply the proposed framework to the MNIST dataset [31], as shown in Fig. 3 (b). We clearly see that the original uniform prior is not preferred, thus the KL divergence increases until a highly biased (non-uniform) probability of weight configurations is reached. Meanwhile, the lower-bound on the data log-likelihood increases until saturation. Due to the weight discreteness, there does not exist efficient or valid methods of training RBM with low-precision weights. One main reason is that the gradient of the data log-likelihood is mathematically ill-defined. The variational distribution of weights is used instead here to get around this computational difficulty. Furthermore, the framework explains the interaction among three essential elements of a typical learning process, i.e., data, synapses and neural activity. Therefore, our framework is promising in studying structured real dataset, especially testing hypotheses or predictions drawn from theoretical studies of random models of unsupervised learning.

V. CONCLUSION

Although training and understanding of neural networks with low-precision weights and activations becomes increasingly important [24, 32], a unified theoretical framework to treat sensory inputs, synapses and neural activity together is still lacking, and thus the conceptual advance contributed by our variational mean-field theory provides a route towards an in-depth understanding of unsupervised learning in a principled probabilistic framework. In this framework, the synaptic weight is no longer treated to be deterministic, but rather, it is subject to a variational distribution where the variation parameter, mean synaptic activity level, is adjusted by an expectation-maximization-like mechanism. The M-step at the synaptic activity level is carried out by a gradient ascent of the lower-bound on the...
FIG. 2: (Color online) Inference performance in planted RBM models with sensory inputs of \( N = 100 \) dimensionality. The amount of data for training is given by \( M = 500 \). The inverse temperature \( \beta = 1 \). (a) Learning trajectories of RBM models with \( P = 2 \) and planted correlation levels—\( q = 0 \) and \( q = 0.3 \). Each learning step indicates all synapses are updated once. The inset shows the evolution of the Kullback-Leibler divergence. (b) Learning trajectories of RBM models with \( P = 3 \) and orthogonal planted receptive field vectors of three hidden neurons. The lower-bound of the data log-likelihood in the inset has been subtracted by its starting value.

FIG. 3: (Color online) (a) Typical learning performance in planted RBM models with sensory inputs of \( N = 100 \) dimensionality, as a function of data density \( \alpha \) (defined as the data sample per input neuron). The inverse temperature \( \beta = 1 \). The learning performance is estimated at the 200-th step. Each marker in the plot indicates the average over ten independent realizations of the model, with the error bar characterizing the standard deviation. (b) Learning trajectories of RBM models with \( P = 4 \) for structured (handwritten digits, thus \( N = 784 \)) inputs. The inverse temperature \( \beta = 1 \), and \( M = 2000 \). The lower-bound of the data log-likelihood in the inset has been subtracted by its starting value.

Despite the crude mean-field approximation used to derive this conceptual framework, the extensive numerical simulations on planted RBM models confirm the validity of the variational framework. The result is also consistent with theoretical predictions of simple toy models [9, 15]. Moreover, the method goes beyond the limitation of previous theoretical models, providing a promising and valid path towards understanding mechanisms of unsupervised learning.
in a generic architecture. We remark here that unsupervised learning is not only a fundamental function of cerebral cortex, but also a foundation for a next generation of artificial neural networks [33]. To propose a principled framework for unsupervised learning, as a motivation of this paper, is urgent and will undoubtedly accelerate the theoretical studies of unsupervised learning. The variational mean-field theory for challenging discrete synapses in unsupervised learning proposed in this paper encourages several future directions. First, a more expressive variational Ansatz can be used to improve the computational power of the framework. Second, noisy estimates of gradients using stochastic optimization can be applied. The studies on the framework itself would shed light on developing theory-grounded neuromorphic algorithms on neural networks with low-precision yet robust synapses and activations. Last but not the least, this framework opens a new way to test the hypothesis that unsupervised learning can be interpreted as breaking different types of inherent symmetry in a data-driven spontaneous manner [15], in a general setting, i.e., neural network architectures with arbitrarily many hidden neurons, and hidden layers.

Acknowledgments

This research was supported by the start-up budget 74130-18831109 of the 100-talent- program of Sun Yat-sen University, and the NSFC (Grant No. 11805284).

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