Restricted Boltzmann Machine and Deep Belief Network: Tutorial and Survey

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Abstract

This is a tutorial and survey paper on Boltzmann Machine (BM), Restricted Boltzmann Machine (RBM), and Deep Belief Network (DBN). We start with the required background on probabilistic graphical models, Markov random field, Gibbs sampling, statistical physics, Ising model, and the Hopfield network. Then, we introduce the structures of BM and RBM. The conditional distributions of visible and hidden variables, Gibbs sampling in RBM for generating variables, training BM and RBM by maximum likelihood estimation, and contrastive divergence are explained. Then, we discuss different possible discrete and continuous distributions for the variables. We introduce conditional RBM and how it is trained. Finally, we explain deep belief network as a stack of RBM models. This paper on Boltzmann machines can be useful in various fields including data science, statistics, neural computation, and statistical physics.

1. Introduction

Centuries ago, the Boltzmann distribution (Boltzmann, 1868), also called the Gibbs distribution (Gibbs, 1902), was proposed. This energy-based distribution was found

to be useful for modeling the physical systems statistically (Huang, 1987). One of these systems was the Ising model which modeled interacting particles with binary spins (Lenz, 1920; Ising, 1925). Later, the Ising model was found to be able to be a neural network (Little, 1974). Hence, Hopfield network was proposed which modeled an Ising model in a network for modeling memory (Hopfield, 1982). Inspired by the Hopfield network (Little, 1974; Hopfield, 1982), which was itself inspired by the physical Ising model (Lenz, 1920; Ising, 1925), Hinton et. al. proposed Boltzmann Machine (BM) and Restricted Boltzmann Machine (RBM) (Hinton & Sejnowski, 1983; Ackley et al., 1985). These models are energy-based models (LeCun et al., 2006) and the names come from the Boltzmann distribution (Boltzmann, 1868; Gibbs, 1902) used in these models. A BM has weighted links between two layers of neurons as well as links between neurons of every layer. RBM restricts these links to not have links between neurons of a layer. BM and RBM take one of the layers as the layer of data and the other layer as a representation or embedding of data. BM and RBM are special cases of the Ising model whose weights (coupling parameters) are learned. BM and RBM are also special cases of the Hopfield network whose weights are learned by maximum likelihood estimation rather than the Hebbian learning method (Hebb, 1949) which is used in the Hopfield network.

The Hebbian learning method, used in the Hopfield network, was very weak and could not generalize well to unseen data. Therefore, backpropagation (Rumelhart et al., 1986) was proposed for training neural networks. Backpropagation was gradient descent plus the chain rule tech-

nique. However, researchers found out soon that neural networks cannot get deep in their number of layers. This is because, in deep networks, gradients become very small in the initial layers after many chain rules from the last layers of network. This problem was called vanishing gradients. This problem of networks plus the glory of theory in kernel support vector machines (Boser et al., 1992) resulted in the winter of neural networks in the last years of previous century until around 2006.

During the winter of neural networks, Hinton tried to save neural networks from being forgotten in the history of machine learning. So, he returned to his previously proposed RBM and proposed a learning method for RBM with the help of some other researchers including Max Welling (Hinton, 2002; Welling et al., 2004). They proposed training the weights of BM and RBM using maximum likelihood estimation. BM and RBM can be seen as generative models where new values for neurons can be generated using Gibbs sampling (Geman & Geman, 1984). Hinton noticed RBM because he knew that the set of weights between every two layers of a neural network is an RBM. It was in the year 2006 (Hinton & Salakhutdinov, 2006; Hinton et al., 2006) that he thought it is possible to train a network in a greedy way (Bengio et al., 2007) where the weights of every layer of network is trained using RBM training. This stack of RBM models with a greedy algorithm for training was named Deep Belief Network (DBN) (Hinton et al., 2006; Hinton, 2009). DBN allowed the networks to become deep by preparing a good initialization of weights (using RBM training) for backpropagation. This good starting point for backpropagation optimization did not face the problem of vanishing gradients anymore. Since the breakthrough in 2006 (Hinton & Salakhutdinov, 2006), the winter of neural networks started to end gradually because the networks could get deep to become more nonlinear and handle more nonlinear data.

DBN was used in different applications including speech recognition (Mohamed et al., 2009; Mohamed & Hinton, 2010; Mohamed et al., 2011) and action recognition (Taylor et al., 2007). Hinton was very excited about the success of RBM and was thinking that the future of neural networks belongs to DBN. However, his research group proposed two important techniques which were the ReLu activation function (Glorot et al., 2011) and the dropout technique (Srivastava et al., 2014). These two regularization methods prevented overfitting (Ghojogh & Crowley, 2019) and resolved vanishing gradients even without RBM pre-training. Hence, backpropagation could be used alone if the new regularization methods were utilized. The success of neural networks was found out more (LeCun et al., 2015) by its various applications, for example in in image recognition (Karpathy & Fei-Fei, 2015).

This is a tutorial and survey paper on BM, RBM, and DBN.

The remainder of this paper is as follows. We briefly review the required background on probabilistic graphical models, Markov random field, Gibbs sampling, statistical physics, Ising model, and the Hopfield network in Section 2. The structure of BM and RBM, Gibbs sampling in RBM, training RBM by maximum likelihood estimation, contrastive divergence, and training BM are explained in Section 3. Then, we introduce different cases of states for units in RBM in Section 4. Conditional RBM and DBN are explained in Sections 5 and 6, respectively. Finally, Section 7 concludes the paper.

Required Background for the Reader

This paper assumes that the reader has general knowledge of calculus, probability, linear algebra, and basics of optimization. The required background on statistical physics is explained in the paper.

2. Background

2.1. Probabilistic Graphical Model and Markov Random Field

A Probabilistic Graphical Model (PGM) is a grpah-based representation of a complex distribution in the possibly high dimensional space (Koller & Friedman, 2009). In other words, PGM is a combination of graph theory and probability theory. In a PGM, the random variables are represented by nodes or vertices. There exist edges between two variables which have interaction with one another in terms of probability. Different conditional probabilities can be represented by a PGM. There exist two types of PGM which are Markov network (also called Markov random field) and Bayesian network (Koller & Friedman, 2009). In the Markov network and Bayesian network, the edges of graph are undirected and directed, respectively. BM and RBM are Markov networks (Markov random field) because their links are undirected (Hinton, 2007).

2.2. Gibbs Sampling

Gibbs sampling, firstly proposed by (Geman & Geman, 1984), draws samples from a d-dimensional multivariate distribution $\mathbb{P}(X)$ using d conditional distributions (Bishop, 2006). This sampling algorithm assumes that the conditional distributions of every dimension of data conditioned on the rest of coordinates are simple to draw samples from.

In Gibbs sampling, we desire to sample from a multivariate distribution $\mathbb{P}(X)$ where $X \in \mathbb{R}^d$. Consider the notation $\mathbb{R}^d \ni \boldsymbol{x} := [x_1, x_2, \dots, x_d]^\top$. We start from a random d-dimensional vector in the range of data. Then, we sample the first dimension of the first sample from the distribution of the first dimension conditioned on the other dimensions. We do it for all dimensions, where the j-th dimension is

sampled as (Ghojogh et al., 2020):

$$x_j \sim \mathbb{P}(x_j \mid x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_d).$$
 (1)

We do this for all dimensions until all dimensions of the first sample are drawn. Then, starting from the first sample, we repeat this procedure for the dimensions of the second sample. We iteratively perform this for all samples; however, some initial samples are not yet valid because the algorithm has started from a not-necessarily valid vector. We accept all samples after some burn-in iterations. Gibbs sampling can be seen as a special case of the Metropolis-Hastings algorithm which accepts the proposed samples with probability one (see (Ghojogh et al., 2020) for proof). Gibbs sampling is used in BM and RBM for generating visible and hidden samples.

2.3. Statistical Physics and Ising Model

2.3.1. BOLTZMANN (GIBBS) DISTRIBUTION

Assume we have several particles $\{x_i\}_{i=1}^d$ in statistical physics. These particles can be seen as randome variables which can randomly have a state. For example, if the particles are electrons, they can have states +1 and -1 for counterclockwise and clockwise spins, respectively. The *Boltzmann distribution* (Boltzmann, 1868), also called the *Gibbs distribution* (Gibbs, 1902), can show the probability that a physical system can have a specific state. i.e., every of the particles has a specific state. The probability mass function of this distribution is (Huang, 1987):

$$\mathbb{P}(x) = \frac{e^{-\beta E(x)}}{Z},\tag{2}$$

where E(x) is the energy of variable x and Z is the normalization constant so that the probabilities sum to one. This normalization constant is called the *partition function* which is hard to compute as it sums over all possible configurations of states (values) that the particles can have. If we define $\mathbb{R}^d \ni \boldsymbol{x} := [x_1, \dots, x_d]^\top$, we have:

$$Z := \sum_{\boldsymbol{x} \in \mathbb{R}^d} e^{-\beta E(x)}.$$
 (3)

The coefficient $\beta \geq 0$ is defined as:

$$\beta := \frac{1}{k_{\beta}T} \propto \frac{1}{T},\tag{4}$$

where k_{β} is the Boltzmann constant and $T \geq 0$ is the absolute thermodynamic temperature in Kelvins. If the temperature tends to absolute zero, $T \to 0$, we have $\beta \to \infty$ and $\mathbb{P}(x) \to 0$, meaning that the absolute zero temperature occurs extremely rarely in the universe.

The free energy is defined as:

$$F(\beta) := \frac{-1}{\beta} \ln(Z),\tag{5}$$

where ln(.) is the natural logarithm. The *internal energy* is defined as:

$$U(\beta) := \frac{\partial}{\partial \beta} (\beta F(\beta)). \tag{6}$$

Therefore, we have:

$$U(\beta) = \frac{\partial}{\partial \beta} (-\ln(Z)) = \frac{-1}{Z} \frac{\partial Z}{\partial \beta}$$

$$\stackrel{(3)}{=} \sum_{\boldsymbol{x} \in \mathbb{R}^d} E(x) \frac{e^{-\beta E(x)}}{Z} \stackrel{(2)}{=} \sum_{\boldsymbol{x} \in \mathbb{R}^d} \mathbb{P}(x) E(x). \quad (7)$$

The *entropy* is defined as:

$$H(\beta) := -\sum_{\boldsymbol{x} \in \mathbb{R}^d} \mathbb{P}(x) \ln \left(\mathbb{P}(x) \right)$$

$$\stackrel{(2)}{=} -\sum_{\boldsymbol{x} \in \mathbb{R}^d} \mathbb{P}(x) \left(-\beta E(x) - \ln(Z) \right)$$

$$= \beta \sum_{\boldsymbol{x} \in \mathbb{R}^d} \mathbb{P}(x) E(x) + \ln(Z) \sum_{\boldsymbol{x} \in \mathbb{R}^d} \mathbb{P}(x)$$

$$\stackrel{(a)}{=} -\beta F(\beta) + \beta U(\beta), \tag{8}$$

where (a) is because of Eqs. (7) and (3).

Lemma 1. A physical system prefers to be in low energy; hence, the system always loses energy to have less energy.

Proof. On one hand, according to the second law of thermodynamics, entropy of a physical system always increases by passing time (Carroll, 2010). Entropy is a measure of randomness and disorder in system. On the other hand, when a system loses energy to its surrounding, it becomes less ordered. Hence, by passing time, the energy of system decreases to have more entropy. Q.E.D. □

Corollary 1. According to Eq. (2) and Lemma 1, the probability $\mathbb{P}(x)$ of states in a system tend to increase by passing time.

This corollary makes sense because systems tend to become more probable. This idea is also used in simulated annealing (Kirkpatrick et al., 1983) where the temperature of system is cooled down gradually. Simulated annealing and temperature-based learning have been used in BM models (Passos & Papa, 2018; Alberici et al., 2020; 2021).

2.3.2. ISING MODEL

The Lenz-Ising model (Lenz, 1920; Ising, 1925), also known as Ising model, is a model in which the particles can have -1 or +1 spins (Brush, 1967). Therefore, $x_i \in \{-1,+1\}, \forall i \in \{1,\ldots,d\}$. It uses the Boltzmann distribution, Eq. (2), where the energy function is defined as:

$$E(x) := \mathcal{H}(x) = -\sum_{(i,j)} J_{ij} x_i x_j,$$
 (9)

where $\mathcal{H}(x)$ is called the Hamiltonian, $J_{ij} \in \mathbb{R}$ is the coupling parameter, and the summation is over particles which interact with each other. Note that as energy is proportional to the reciprocal of squared distance, nearby particles are only assumed to be interacting. Therefore, usually the interaction graph of particles is a chain (one dimensional grid), mesh grid (lattice), closed chain (loop), or torus (multi-dimensional loop).

Based on the characteristic of model, the coupling parameter has different values. If for all interacting i and j, we have $J_{ij} \geq 0$ or $J_{ij} < 0$, the models is named ferromagnetic and anti-ferromagnetic, respectively. If J_{ij} can be both positive and negative, the model is called a spin glass. If the coupling parameters are all constant, the model is homogeneous. According to Lemma 1, the energy decreases over time. According to Eq. (9), in ferromagnetic model $(J_{ij} \geq 0)$, the energy of Ising model decreases if interacting x_i and x_j have the same state (spin) because of the negative sign behind summation. Likewise, in antiferromagnetic models, the nearby particles tend to have different spins over time.

According to Eq. (9), in ferromagnetic models, the energy is zero if $J_{ij} = 0$. This results in $\mathbb{P}(x) = 1$ according to Eq. (2). With similar analysis and according to the previous discussion, in ferromagnetic models, $J_{ij} \to \infty$ yields to having the same spins for all particles. This means that we finally have all +1 spins with probability of half or all -1 spins with probability of half. Ising models can be modeled as normal factor graphs. For more information on this, refer to (Molkaraie, 2017; 2020). The BM and RBM are Ising models whose coupling parameters are considered as weights and these weights are learned using maximum likelihood estimation (Hinton, 2007). Hence, we can say that BM and RBM are energy-based learning methods (LeCun et al., 2006).

2.4. Hopfield Network

It was proposed in (Little, 1974) to use the Ising model in a neural network structure. Hopfield extended this idea to model memory by a neural network. The resulting network was the Hopfield network (Hopfield, 1982). This network has some units or neurons denoted by $\{x_i\}_{i=1}^d$. The states or outputs of units are all binary $x_i \in \{-1, +1\}, \forall i$. Let w_{ij} denote the weight of link connecting unit i to unit j. The weights of Hopfield network are learned using the Hebbian learning (Hebb's law of association) (Hebb, 1949):

$$w_{ij} := \begin{cases} x_i \times x_j & \text{if } i \neq j, \\ 0 & \text{otherwise.} \end{cases}$$
 (10)

After training, the outputs of units can be determined for an input if the weighted summation of inputs to unit passes a threshold θ :

$$x_i := \begin{cases} +1 & \text{if } \sum_{j=1}^d w_{ij} x_j \ge \theta, \\ -1 & \text{otherwise.} \end{cases}$$
 (11)

In the original paper of Hopfield network (Hopfield, 1982), the binary states are $x_i \in \{0, 1\}, \forall i$ so the Hebbian learning is $w_{ij} := (2x_i - 1) \times (2x_j - 1), \forall i \neq j$. Hopfield network is an Ising model so it uses Eq. (9) as its energy. This energy is also used in the Boltzmann distribution which is Eq. (2). Note that recently, Hopfield network with continuous states has been proposed (Ramsauer et al., 2020). The BM and RBM models are Hopfield networks whose weights are learned using maximum likelihood estimation and not Hebbian learning.

3. Restricted Boltzmann Machine

3.1. Structure of Restricted Boltzmann Machine

Boltzmann Machine (BM) is a generative model and a Probabilistic Graphical Model (PGM) (Bishop, 2006) which is a building block of many probabilistic models. Its name is because of the Boltzmann distribution (Boltzmann, 1868; Gibbs, 1902) used in this model. It was first introduced to be used in machine learning in (Hinton & Sejnowski, 1983; Ackley et al., 1985) and then in (Hinton, 2002; Welling et al., 2004). A BM consists of an visible (or observation) layer $\boldsymbol{v} = [v_1, \dots, v_d] \in \mathbb{R}^d$ and a hidden layer $h = [h_1, \dots, h_p] \in \mathbb{R}^p$. The visible layer is the layer that we can see; for example, it can be the layer of data. The hidden layer is the layer of latent variables which represent meaningful features or embeddings for the visible data. In other words, there is a meaningful connection between the hidden and visible layers although their dimensionality might differ, i.e., $d \neq p$. In the PGM of BM, there is connection links between elements of v and elements of h. Each of the elements of v and h also have a bias. There are also links between the elements of v as well as between the elements of h (Salakhutdinov & Hinton, 2009a). Let w_{ij} denote the link between v_i and h_j , and l_{ij} be the link between v_i and v_j , and j_{ij} be the link between h_i and h_j , and b_i be the bias link for v_i , and c_i be the bias link for \check{h}_i . The dimensionality of these links are $\boldsymbol{W} = [w_{ij}] \in \mathbb{R}^{d \times p}, \boldsymbol{L} = [l_{ij}] \in \mathbb{R}^{d \times d}, \boldsymbol{J} = [j_{ij}] \in \mathbb{R}^{p \times p},$ $\boldsymbol{b} = [b_1, \dots, b_d] \in \mathbb{R}^d$, and $\boldsymbol{c} = [c_1, \dots, c_p] \in \mathbb{R}^p$. Note that $\hat{\boldsymbol{W}}$ is a symmetric matrix, i.e., $w_{ij} = w_{ji}$. Also, as there is no link from a node to itself, the diagonal elements of L and J are zero, i.e., $l_{ii} = j_{ii} = 0, \forall i$. Restricted Boltzmann Machine (RBM) is BM which does not have links within a layer, i.e., there is no any link between the elements of v and no any link between the elements of h. In other words, the links are restricted in RBM to be L = J = 0. Figure 1 depicts both BM and RBM with their layers and links. In this section, we focus on RBM.

Recall that RBM is an Ising model. As we saw in Eq. (9),

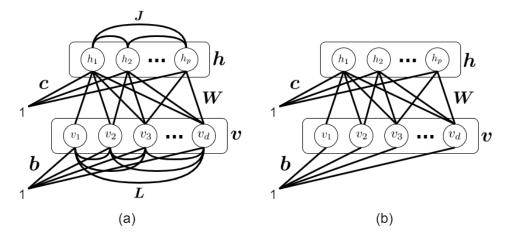


Figure 1. The structures of (a) a Boltzmann machine and (b) a restricted Boltzmann machine.

the energy of an Ising model can be modeled as (Hinton & Sejnowski, 1983; Ackley et al., 1985):

$$\mathbb{R} \ni E(\boldsymbol{v}, \boldsymbol{h}) := -\boldsymbol{b}^{\top} \boldsymbol{v} - \boldsymbol{c}^{\top} \boldsymbol{h} - \boldsymbol{v}^{\top} \boldsymbol{W} \boldsymbol{h}, \tag{12}$$

which is based on interactions between linked units. As introduced in Eq. (2), the visible and hidden variables make a joint Boltzmann distribution (Hinton, 2012):

$$\mathbb{P}(\boldsymbol{v}, \boldsymbol{h}) = \frac{1}{Z} \exp(-E(\boldsymbol{v}, \boldsymbol{h}))$$

$$\stackrel{(12)}{=} \frac{1}{Z} \exp(\boldsymbol{b}^{\top} \boldsymbol{v} + \boldsymbol{c}^{\top} \boldsymbol{h} + \boldsymbol{v}^{\top} \boldsymbol{W} \boldsymbol{h}),$$
(13)

where Z is the partition function:

$$Z := \sum_{\boldsymbol{v} \in \mathbb{R}^d} \sum_{\boldsymbol{h} \in \mathbb{R}^p} \exp(-E(\boldsymbol{v}, \boldsymbol{h})). \tag{14}$$

According to Lemma 1, the BM and RBM try to reduce the energy of model. Training the BM or RBM reduces its energy (Hinton & Sejnowski, 1983; Ackley et al., 1985).

3.2. Conditional Distributions

Proposition 1 (Conditional Independence of Variables). *In RBM, given the visible variables, the hidden variables are conditionally independent. Likewise, given the hidden variables, the visible variables are conditionally independent. This does not hold in BM because of the links within each layer.*

Proof. According to the Bayes rule, we have:

$$\begin{split} & \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}) = \frac{\mathbb{P}(\boldsymbol{h},\boldsymbol{v})}{\mathbb{P}(\boldsymbol{v})} = \frac{\mathbb{P}(\boldsymbol{v},\boldsymbol{h})}{\sum_{\boldsymbol{h}\in\mathbb{R}^p} \mathbb{P}(\boldsymbol{v},\boldsymbol{h})} \\ & \stackrel{(13)}{=} \frac{\frac{1}{Z} \exp(\boldsymbol{b}^{\top}\boldsymbol{v} + \boldsymbol{c}^{\top}\boldsymbol{h} + \boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})}{\sum_{\boldsymbol{h}\in\mathbb{R}^p} \frac{1}{Z} \exp(\boldsymbol{b}^{\top}\boldsymbol{v} + \boldsymbol{c}^{\top}\boldsymbol{h} + \boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})} \\ & = \frac{\frac{1}{Z} \exp(\boldsymbol{b}^{\top}\boldsymbol{v}) \exp(\boldsymbol{c}^{\top}\boldsymbol{h}) \exp(\boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})}{\frac{1}{Z} \sum_{\boldsymbol{h}\in\mathbb{R}^p} \exp(\boldsymbol{b}^{\top}\boldsymbol{v}) \exp(\boldsymbol{c}^{\top}\boldsymbol{h}) \exp(\boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})} \end{split}$$

$$\frac{(a)}{\exp(\boldsymbol{b}^{\top}\boldsymbol{v})\exp(\boldsymbol{c}^{\top}\boldsymbol{h})\exp(\boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})} \\
= \frac{\exp(\boldsymbol{b}^{\top}\boldsymbol{v})\sum_{\boldsymbol{h}\in\mathbb{R}^p}\exp(\boldsymbol{c}^{\top}\boldsymbol{h})\exp(\boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})}{\sum_{\boldsymbol{h}\in\mathbb{R}^p}\exp(\boldsymbol{c}^{\top}\boldsymbol{h})\exp(\boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})},$$

where (a) is because the term $\exp(\boldsymbol{b}^{\top}\boldsymbol{v})$ does not have \boldsymbol{h} in it. Note that $\sum_{\boldsymbol{h}\in\mathbb{R}^p}$ denotes summation over all possible p-dimensional hidden variables for the sake of marginalization. Let $Z' := \sum_{\boldsymbol{h}\in\mathbb{R}^p} \exp(\boldsymbol{c}^{\top}\boldsymbol{h}) \exp(\boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})$. Hence:

$$\mathbb{P}(\boldsymbol{h}|\boldsymbol{v}) = \frac{1}{Z'} \exp(\boldsymbol{c}^{\top}\boldsymbol{h} + \boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h})$$

$$= \frac{1}{Z'} \exp\left(\sum_{j=1}^{p} c_{j}h_{j} + \sum_{j=1}^{p} \boldsymbol{v}^{\top}\boldsymbol{W}_{:j}h_{j}\right)$$

$$= \frac{1}{Z'} \prod_{j=1}^{p} \exp(c_{j}h_{j} + \boldsymbol{v}^{\top}\boldsymbol{W}_{:j}h_{j}), \quad (15)$$

where $W_{:j} \in \mathbb{R}^d$ denotes the *j*-th column of matrix W. The Eq. (15) shows that given the visible variables, the hidden variables are conditionally independent because their joint distribution is the product of every distribution. We can write similar expressions for the probability $\mathbb{P}(v|h)$:

$$\mathbb{P}(\boldsymbol{v}|\boldsymbol{h}) = \frac{1}{Z''} \exp(\boldsymbol{b}^{\top} \boldsymbol{v} + \boldsymbol{v}^{\top} \boldsymbol{W} \boldsymbol{h})$$

$$= \frac{1}{Z''} \exp\left(\sum_{i=1}^{d} b_{i} v_{i} + \sum_{i=1}^{d} v_{i} \boldsymbol{W}_{i:} \boldsymbol{h}\right)$$

$$= \frac{1}{Z''} \prod_{i=1}^{d} \exp(b_{i} v_{i} + v_{i} \boldsymbol{W}_{i:} \boldsymbol{h}), \tag{16}$$

where $\boldsymbol{W}_{i:} \in \mathbb{R}^p$ denotes the *i*-th row of matrix \boldsymbol{W} and $Z'' := \sum_{\boldsymbol{v} \in \mathbb{R}^d} \exp(\boldsymbol{b}^\top \boldsymbol{v}) \exp(\boldsymbol{v}^\top \boldsymbol{W} \boldsymbol{h})$. This equation shows that the given the hidden variables, the visible variables are conditionally independent. Q.E.D.

According to Eq. (15) and considering the rule $\mathbb{P}(h|v) = \mathbb{P}(h,v)/\mathbb{P}(v)$, we have:

$$\mathbb{P}(\boldsymbol{h}|\boldsymbol{v}) = \frac{1}{Z'} \prod_{j=1}^{p} \exp(c_{j}h_{j} + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j}h_{j})$$
$$= \frac{1}{Z'} \prod_{j=1}^{p} \mathbb{P}(h_{j}, \boldsymbol{v})$$

$$\implies \mathbb{P}(h_j, \boldsymbol{v}) = \exp(c_j h_j + \boldsymbol{v}^\top \boldsymbol{W}_{:j} h_j)$$

$$= \exp(c_j h_j + \sum_{i=1}^d v_i w_{ij} h_j). \tag{17}$$

Similarly, according to Eq. (16) and considering the rule $\mathbb{P}(\boldsymbol{v}|\boldsymbol{h}) = \mathbb{P}(\boldsymbol{h},\boldsymbol{v})/\mathbb{P}(\boldsymbol{h})$, we have:

$$\mathbb{P}(\boldsymbol{h}|\boldsymbol{v}) = \frac{1}{Z''} \prod_{i=1}^{d} \exp(b_i v_i + v_i \boldsymbol{W}_{i:} \boldsymbol{h})$$
$$= \frac{1}{Z''} \prod_{i=1}^{d} \mathbb{P}(\boldsymbol{h}, v_i)$$

$$\implies \mathbb{P}(\boldsymbol{h}, v_i) = \exp(b_i v_i + v_i \boldsymbol{W}_i \cdot \boldsymbol{h})$$

$$= \exp(b_i v_i + \sum_{j=1}^p v_i w_{ij} h_j). \tag{18}$$

We will use these equations later.

3.3. Sampling Hidden and Visible Variables

3.3.1. GIBBS SAMPLING

We can use Gibbs sampling for sampling and generating the hidden and visible units. If ν denotes the iteration index of Gibbs sampling, we iteratively sample:

$$\boldsymbol{h}^{(\nu)} \sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}^{(\nu)}),$$
 (19)

$$\boldsymbol{v}^{(\nu+1)} \sim \mathbb{P}(\boldsymbol{v}|\boldsymbol{h}^{(\nu)}),$$
 (20)

until the burn-out convergence. As was explained before, only several iterations of Gibbs sampling are usually sufficient. After the burn-out, the samples are approximately samples from the joint distribution $\mathbb{P}(\boldsymbol{v},\boldsymbol{h})$. As the variables are conditionally independent, this Gibbs sampling can be implemented as in Algorithm 1. In this algorithm, $h_j^{(\nu)} \sim \mathbb{P}(h_j|\boldsymbol{v}^{(\nu)})$ can be implemented as drawing a sample from uniform distribution $u \sim U[0,1]$ and compare it to the value of Probability Density Function (PDF), $\mathbb{P}(h_j|\boldsymbol{v}^{(\nu)})$. If u is less than or equal to this value, we have $h_j=1$; otherwise, we have $h_j=0$. Implementation of sampling v_i has a similar procedure. Alternatively, we can use inverse of Cumulative Distribution Function of these distributions for drawing samples (see (Ghojogh et al., 2020) for more details about sampling).

- Input: visible dataset v, (initialization: optional)
 Get initialization or do random initialization of v
 while until burn-out do

Algorithm 1: Gibbs sampling in RBM

3.3.2. GENERATIONS AND EVALUATIONS BY GIBBS SAMPLING

Gibbs sampling for generating both observation and hidden units is used for both training and evaluation phases of RBM. Use of Gibbs sampling in training RBM will be explained in Sections 3.4 and 3.5. After the RBM model is trained, we can generate any number of *p*-dimensional hidden variables as a meaningful representation of the *d*-dimensional observation using Gibbs sampling. Moreover, using Gibbs sampling, we can generate other *d*-dimensional observations in addition to the original dataset. These new generated observations are *d*-dimensional representations for the *p*-dimensional hidden variables. This shows that BM and RBM are generative models.

3.4. Training Restricted Boltzmann Machine by Maximum Likelihood Estimation

The weights of links which are W, b, and c should be learned so that we can use them for sampling/generating the hidden and visible units. Consider a dataset of n visible vectors $\{v_i \in \mathbb{R}^d\}_{i=1}^n$. Note that v_i should not be confused with v_i where the former is the i-th visible data instance and the latter is the i-th visible unit. We denote the j-th dimension of v_i by $v_{i,j}$; in other words, $v_i = [v_{i,1}, \dots, v_{i,d}]^\top$. The log-likelihood of the visible data is:

$$\ell(\boldsymbol{W}, \boldsymbol{b}, \boldsymbol{c}) = \sum_{i=1}^{n} \log(\mathbb{P}(\boldsymbol{v}_{i})) = \sum_{i=1}^{n} \log\left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \mathbb{P}(\boldsymbol{v}_{i}, \boldsymbol{h})\right)$$

$$\stackrel{(13)}{=} \sum_{i=1}^{n} \log\left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \frac{1}{Z} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))\right)$$

$$= \sum_{i=1}^{n} \log\left(\frac{1}{Z} \sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))\right)$$

$$= \sum_{i=1}^{n} \left[\log\left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))\right) - \log Z\right]$$

$$= \sum_{i=1}^{n} \log\left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))\right) - n \log Z$$

$$\stackrel{\text{(14)}}{=} \sum_{i=1}^{n} \log \left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h})) \right) - n \log \sum_{\boldsymbol{v} \in \mathbb{R}^{d}} \sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}, \boldsymbol{h})). \tag{21}$$

We use Maximum Likelihood Estimation (MLE) for finding the parameters $\theta := \{W, b, c\}$. The derivative of log-likelihood with respect to parameter θ is:

$$\nabla_{\theta} \ell(\theta) = \nabla_{\theta} \sum_{i=1}^{n} \log \left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h})) \right) - n \nabla_{\theta} \log \sum_{\boldsymbol{v} \in \mathbb{R}^{d}} \sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}, \boldsymbol{h})).$$
(22)

The first term of this derivative is:

$$\nabla_{\theta} \sum_{i=1}^{n} \log \left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h})) \right)$$

$$= \sum_{i=1}^{n} \nabla_{\theta} \log \left(\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h})) \right)$$

$$= \sum_{i=1}^{n} \frac{\nabla_{\theta} \sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))}{\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))}$$

$$= \sum_{i=1}^{n} \frac{\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h})) \nabla_{\theta}(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))}{\sum_{\boldsymbol{h} \in \mathbb{R}^{p}} \exp(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))}$$

$$\stackrel{(a)}{=} \sum_{i=1}^{n} \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h} | \boldsymbol{v}_{i})} [\nabla_{\theta}(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))], \qquad (23)$$

where (a) is because the definition of expectation is $\mathbb{E}_{\sim \mathbb{P}}[x] := \sum_{i=1} \mathbb{P}(x_i) x_i$. However, if \mathbb{P} is not an actual distribution and does not sum to one, we should normalize it to behave like a distribution in the expectation: $\mathbb{E}_{\sim \mathbb{P}}[x] := (\sum_{i=1} \mathbb{P}(x_i) x_i)/(\sum_{i=1} \mathbb{P}(x_i))$. The second term of the derivative of log-likelihood is:

$$-n\nabla_{\theta}\log \sum_{\boldsymbol{v}\in\mathbb{R}^{d}} \sum_{\boldsymbol{h}\in\mathbb{R}^{p}} \exp(-E(\boldsymbol{v},\boldsymbol{h}))$$

$$=-n\frac{\nabla_{\theta}\sum_{\boldsymbol{v}\in\mathbb{R}^{d}} \sum_{\boldsymbol{h}\in\mathbb{R}^{p}} \exp(-E(\boldsymbol{v},\boldsymbol{h}))}{\sum_{\boldsymbol{v}\in\mathbb{R}^{d}} \sum_{\boldsymbol{h}\in\mathbb{R}^{p}} \exp(-E(\boldsymbol{v},\boldsymbol{h}))}$$

$$=-n\frac{\sum_{\boldsymbol{v}\in\mathbb{R}^{d}} \sum_{\boldsymbol{h}\in\mathbb{R}^{p}} \nabla_{\theta} \exp(-E(\boldsymbol{v},\boldsymbol{h}))}{\sum_{\boldsymbol{v}\in\mathbb{R}^{d}} \sum_{\boldsymbol{h}\in\mathbb{R}^{p}} \exp(-E(\boldsymbol{v},\boldsymbol{h}))}$$

$$=-n\frac{\sum_{\boldsymbol{v}\in\mathbb{R}^{d}} \sum_{\boldsymbol{h}\in\mathbb{R}^{p}} \exp(-E(\boldsymbol{v},\boldsymbol{h}))\nabla_{\theta}(-E(\boldsymbol{v},\boldsymbol{h}))}{\sum_{\boldsymbol{v}\in\mathbb{R}^{d}} \sum_{\boldsymbol{h}\in\mathbb{R}^{p}} \exp(-E(\boldsymbol{v},\boldsymbol{h}))\nabla_{\theta}(-E(\boldsymbol{v},\boldsymbol{h}))}$$

 $\stackrel{(a)}{=} -n \, \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}, \boldsymbol{v})} [\nabla_{\theta} (-E(\boldsymbol{v}, \boldsymbol{h}))], \tag{24}$

where (a) is for the definition of expectation which was already explained. In summary, the derivative of log-likelihood is:

$$\nabla_{\theta} \ell(\theta) = \sum_{i=1}^{n} \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_{i})} [\nabla_{\theta}(-E(\boldsymbol{v}_{i}, \boldsymbol{h}))] - n \, \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}, \boldsymbol{v})} [\nabla_{\theta}(-E(\boldsymbol{v}, \boldsymbol{h}))].$$
(25)

Setting this derivative to zero does not give us a closedform solution. Hence, we should learn the parameters iteratively using gradient ascent for MLE.

Now, consider each of the parameters $\theta = \{W, b, c\}$. The derivative w.r.t. these parameters in Eq. (25) are:

$$\nabla_{\boldsymbol{W}}(-E(\boldsymbol{v},\boldsymbol{h})) \stackrel{(12)}{=} \frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{b}^{\top}\boldsymbol{v} + \boldsymbol{c}^{\top}\boldsymbol{h} + \boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h}) = \boldsymbol{v}\boldsymbol{h}^{\top},$$

$$\nabla_{\boldsymbol{b}}(-E(\boldsymbol{v},\boldsymbol{h})) \stackrel{(12)}{=} \frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{b}^{\top}\boldsymbol{v} + \boldsymbol{c}^{\top}\boldsymbol{h} + \boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h}) = \boldsymbol{v},$$

$$\nabla_{\boldsymbol{c}}(-E(\boldsymbol{v},\boldsymbol{h})) \stackrel{(12)}{=} \frac{\partial}{\partial \boldsymbol{c}}(\boldsymbol{b}^{\top}\boldsymbol{v} + \boldsymbol{c}^{\top}\boldsymbol{h} + \boldsymbol{v}^{\top}\boldsymbol{W}\boldsymbol{h}) = \boldsymbol{h}.$$

Therefore, Eq. (25) for these parameters becomes:

$$\begin{split} \nabla_{\boldsymbol{W}} \ell(\boldsymbol{\theta}) &= \sum_{i=1}^n \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_i)}[\boldsymbol{v}\boldsymbol{h}_i^\top] - n\,\mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h},\boldsymbol{v})}[\boldsymbol{v}\boldsymbol{h}^\top] \\ &= \sum_{i=1}^n \boldsymbol{v}_i\,\mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_i)}[\boldsymbol{h}^\top] - n\,\mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h},\boldsymbol{v})}[\boldsymbol{v}\boldsymbol{h}^\top], \end{split}$$

$$\nabla_{\boldsymbol{b}} \ell(\boldsymbol{\theta}) = \sum_{i=1}^{n} \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_{i})}[\boldsymbol{v}_{i}] - n \, \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h},\boldsymbol{v})}[\boldsymbol{v}]$$
$$= \sum_{i=1}^{n} \boldsymbol{v}_{i} - n \, \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h},\boldsymbol{v})}[\boldsymbol{v}],$$

$$\nabla_{\boldsymbol{c}}\ell(\theta) = \sum_{i=1}^{n} \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_{i})}[\boldsymbol{h}] - n \,\mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h},\boldsymbol{v})}[\boldsymbol{h}].$$

If we define:

$$\widehat{\boldsymbol{h}}_i := \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_i)}[\boldsymbol{h}], \tag{26}$$

we can summarize these derivatives as:

$$\mathbb{R}^{d \times p} \ni \nabla_{\boldsymbol{W}} \ell(\theta) = \sum_{i=1}^{n} \boldsymbol{v}_{i} \widehat{\boldsymbol{h}}_{i}^{\top} - n \, \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}, \boldsymbol{v})}[\boldsymbol{v} \boldsymbol{h}^{\top}], \quad (27)$$

$$\mathbb{R}^{d} \ni \nabla_{\boldsymbol{b}} \ell(\theta) = \sum_{i=1}^{n} \boldsymbol{v}_{i} - n \, \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}, \boldsymbol{v})}[\boldsymbol{v}], \tag{28}$$

$$\mathbb{R}^p \ni \nabla_{\boldsymbol{c}} \ell(\theta) = \sum_{i=1}^n \widehat{\boldsymbol{h}}_i - n \, \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}, \boldsymbol{v})}[\boldsymbol{h}]. \tag{29}$$

Setting these derivatives to zero does not give a closed form solution. Hence, we need to find the solution iteratively using gradient descent where the above gradients are used. In the derivatives of log-likelihood, we have two types of expectation. The conditional expectation $\mathbb{E}_{\sim \mathbb{P}(h|v_i)}[.]$ is based on the observation or data which is v_i . The joint expectation $\mathbb{E}_{\sim \mathbb{P}(h,v)}[.]$, however, has nothing to do with the observation and is merely about the RBM model.

3.5. Contrastive Divergence

According to Eq. (23), the conditional expectation used in Eq. (26) includes one summation. Moreover, according to Eq. (24), the joint expectations used in Eqs. (27), (28), and (29) are contains two summations. This double-summation makes computation of the joint expectation intractable because it sums over all possible values for both hidden and visible units. Therefore, exact computation of MLE is hard and we should approximate it. One way to approximate computation of joint expectations in MLE is contrastive divergence (Hinton, 2002). Contrastive divergence improves the efficiency and reduces teh variance of estimation in RBM (Hinton, 2002; Welling et al., 2004).

The idea of contrastive divergence is as follows. First, we obtain a point \tilde{v} using Gibbs sampling starting from the observation v_i (see Section 3.3 for Gibbs sampling in RBM). Then, we compute expectation by using only that one point \tilde{v} . The intuitive reason for why contrastive divergence works is explained in the following. We need to minimize the gradients to find the solution of MLE. In the joint expectations in Eqs. (27), (28), and (29), rather than considering all possible values of observations, contrastive divergence considers only one of the data points (observations). If this observation is a wrong belief which we do not wish to see in generation of observations by RBM, contrastive divergence is performing a task which is called negative sampling (Hinton, 2012). In negative sampling, we say rather than training the model to not generate all wrong observations, we train it iteratively but less ambitiously in every iteration. Each iteration tries to teach the model to not generate only one of the wrong outputs. Gradually, the model learns to generate correct observations by avoiding to generate these negative samples.

Let $\tilde{h} = [\tilde{h}_1, \dots, \tilde{h}_m]^{\top}$ be the corresponding sampled h to $\tilde{v} = [\tilde{v}_1, \dots, \tilde{v}_m]^{\top}$ in Gibbs sampling. According to the above explanations, contrastive divergence approximates the joint expectation in the derivative of log-likelihood, Eq. (25), by Monte-Carlo approximation (Ghojogh et al., 2020) evaluated at \tilde{v}_i and \tilde{h}_i for the i-th observation and hidden units where \tilde{v}_i and \tilde{h}_i are found by Gibbs sampling. Hence:

$$\mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}, \boldsymbol{v})} [\nabla_{\theta}(-E(\boldsymbol{v}, \boldsymbol{h}))] \approx \frac{1}{n} \sum_{i=1}^{n} \nabla_{\theta}(-E(\boldsymbol{v}_{i}, \boldsymbol{h}_{i})) \Big|_{\boldsymbol{v}_{i} = \widetilde{\boldsymbol{v}}_{i}, \boldsymbol{h}_{i} = \widetilde{\boldsymbol{h}}_{i}}. \quad (30)$$

Experiments have shown that a small number of iterations in Gibbs sampling suffice for contrastive divergence. Paper (Hinton, 2002) even uses one iteration of Gibbs sampling for this task. This small number of required iterations has the support of literature because Gibbs sampling is a special case of Metropolis-Hastings algorithms (Ghojogh et al., 2020) which are fast (Dwivedi et al., 2018).

By the approximation in Eq. (30), the Eqs. (27), (28), and

```
1 Input: training data \{x_i\}_{i=1}^n
  2 Randomly initialize W, b, c
  3 while not converged do
                     Sample a mini-batch \{oldsymbol{v}_1,\ldots,oldsymbol{v}_m\} from
                         training dataset \{x_i\}_{i=1}^n (n.b. we may set
                     // Gibbs sampling for each data point:
  5
                     Initialize \widehat{\boldsymbol{v}}_i^{(0)} \leftarrow \boldsymbol{v}_i for all i \in \{1, \dots, m\}
   6
                    for i from 1 to m do
   7
                               Algorithm 1 \leftarrow \widehat{\boldsymbol{v}}_i^{(0)} \{h_i\}_{i=1}^p, \{v_i\}_{i=1}^d \leftarrow \text{Last iteration of Algorithm 1}
   8
    9
                              \widetilde{\boldsymbol{h}}_i \leftarrow [h_1, \dots, h_p]^{\top}

\widetilde{\boldsymbol{v}}_i \leftarrow [v_1, \dots, v_d]^{\top}
10
11
                          \widehat{m{h}}_i \leftarrow \mathbb{E}_{\sim \mathbb{P}(m{h} | m{v}_i)}[m{h}]
                     // gradients:
13
                   \begin{split} &\nabla_{\boldsymbol{W}}\ell(\boldsymbol{\theta}) \leftarrow \sum_{i=1}^{m} \boldsymbol{v}_{i} \widehat{\boldsymbol{h}}_{i}^{\top} - \sum_{i=1}^{m} \widetilde{\boldsymbol{h}}_{i} \widetilde{\boldsymbol{v}}_{i}^{\top} \\ &\nabla_{\boldsymbol{b}}\ell(\boldsymbol{\theta}) \leftarrow \sum_{i=1}^{m} \boldsymbol{v}_{i} - \sum_{i=1}^{m} \widetilde{\boldsymbol{v}}_{i} \\ &\nabla_{\boldsymbol{c}}\ell(\boldsymbol{\theta}) \leftarrow \sum_{i=1}^{m} \widehat{\boldsymbol{h}}_{i} - \sum_{i=1}^{m} \widetilde{\boldsymbol{h}}_{i} \\ &\text{ // gradient descent for updating solution:} \end{split}
14
16
17
                     \boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \nabla_{\boldsymbol{W}} \ell(\theta)
18
                    \boldsymbol{b} \leftarrow \boldsymbol{b} - \eta \nabla_{\boldsymbol{b}} \ell(\theta)
19
                    c \leftarrow c - \eta \nabla_c \ell(\theta)
21 Return W, b, c
```

Algorithm 2: Training RBM using contrastive divergence

(29) become:

$$\nabla_{\boldsymbol{W}} \ell(\theta) = \sum_{i=1}^{n} \boldsymbol{v}_{i} \widehat{\boldsymbol{h}}_{i}^{\top} - \sum_{i=1}^{n} \widetilde{\boldsymbol{v}}_{i} \widetilde{\boldsymbol{h}}_{i}^{\top}, \tag{31}$$

$$\nabla_{\boldsymbol{b}}\ell(\theta) = \sum_{i=1}^{n} \boldsymbol{v}_i - \sum_{i=1}^{n} \widetilde{\boldsymbol{v}}_i, \tag{32}$$

$$\nabla_{\mathbf{c}}\ell(\theta) = \sum_{i=1}^{n} \widehat{\mathbf{h}}_{i} - \sum_{i=1}^{n} \widetilde{\mathbf{h}}_{i}.$$
 (33)

These equations make sense because when the observation and hidden variable given the variable become equal to the approximation by Gibbs sampling, the gradient should be zero and the training should stop. Note that some works in the literature restate Eqs. (31), (32), and (33) as (Hinton, 2002; 2012; Taylor et al., 2007):

$$\forall i, j \colon \nabla_{w_{i,i}} \ell(\theta) = \langle v_i h_i \rangle_{\text{data}} - \langle v_i h_i \rangle_{\text{recon.}}, \tag{34}$$

$$\forall i: \quad \nabla_{b_i} \ell(\theta) = \langle v_i \rangle_{\text{data}} - \langle v_i \rangle_{\text{recon.}}, \tag{35}$$

$$\forall j : \quad \nabla_{c_i} \ell(\theta) = \langle h_j \rangle_{\text{data}} - \langle h_j \rangle_{\text{recon.}}, \tag{36}$$

where $\langle . \rangle_{\text{data}}$ and $\langle . \rangle_{\text{recon.}}$ denote expectation over data and reconstruction of data, respectively.

The training algorithm of RBM, using contrastive divergence, can be found in Algorithm 2. In this algorithm, we are using mini-batch gradient descent with the batch size m. If training dataset is not large, one can set m=n to have gradient descent. This algorithm is iterative until convergence where, in every iteration, a mini-batch is sampled where we have an observation $v_i \in \mathbb{R}^d$ and a hidden variable $h_i \in \mathbb{R}^p$ for every i-th training data point. For every data point, we apply Gibbs sampling as shown in Algorithm 1. After Gibbs sampling, gradients are calculated by Eqs. (31), (32), and (33) and then the variables are updated using a gradient descent step.

3.6. Boltzmann Machine

So far, we introduced and explained RBM. BM has more links compared to RBM (Salakhutdinov & Hinton, 2009a). Here, in parentheses, we briefly introduce training of BM. Its structure is depicted in Fig. 1. As was explained in Section 3.1, BM has additional links $\boldsymbol{L} = [l_{ij}] \in \mathbb{R}^{d \times d}$ and $\boldsymbol{J} = [j_{ij}] \in \mathbb{R}^{p \times p}$. The weights $\boldsymbol{W} \in \mathbb{R}^{d \times p}$ and biases $\boldsymbol{b} \in \mathbb{R}^d$ and $\boldsymbol{c} \in \mathbb{R}^p$ are trained by gradient descent using the gradients in Eqs. (31), (32), and (33). The additional weights \boldsymbol{L} and \boldsymbol{J} are updated similarly using the following gradients (Salakhutdinov & Hinton, 2009a):

$$\nabla_{\boldsymbol{L}}\ell(\theta) = \sum_{i=1}^{n} \boldsymbol{v}_{i} \boldsymbol{v}_{i}^{\top} - \sum_{i=1}^{n} \widetilde{\boldsymbol{v}}_{i} \widetilde{\boldsymbol{v}}_{i}^{\top}, \tag{37}$$

$$\nabla_{\boldsymbol{J}}\ell(\theta) = \sum_{i=1}^{n} \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_{i})}[\boldsymbol{h}\boldsymbol{h}^{\top}] - \sum_{i=1}^{n} \widetilde{\boldsymbol{h}}_{i}\widetilde{\boldsymbol{h}}_{i}^{\top}.$$
 (38)

These equations can be restated as:

$$\forall i, j \colon \nabla_{l_{i,i}} \ell(\theta) = \langle v_i v_i \rangle_{\text{data}} - \langle v_i v_i \rangle_{\text{recon.}}, \tag{39}$$

$$\forall i, j \colon \nabla_{j_{ij}} \ell(\theta) = \langle h_i h_j \rangle_{\text{data}} - \langle h_i h_j \rangle_{\text{recon.}}, \tag{40}$$

where $\langle . \rangle_{data}$ and $\langle . \rangle_{recon.}$ denote expectation over data and reconstruction of data, respectively.

4. Distributions of Visible and Hidden Variables

4.1. Modeling with Exponential Family Distributions

According to Proposition 1, the units $v \in \mathbb{R}^d$ and $h \in \mathbb{R}^p$ have conditional independence so their distribution is the product of each conditional distribution. We can choose distributions from exponential family for the visible and hidden variables (Welling et al., 2004):

$$\mathbb{P}(\boldsymbol{v}) = \prod_{i=1}^{d} r_i(v_i) \exp\left(\sum_{a} \theta_{ia} f_{ia}(v_i) - A_i(\{\theta_{ia}\})\right),$$
(41)

$$\mathbb{P}(\boldsymbol{h}) = \prod_{j=1}^{p} s_j(h_j) \exp\left(\sum_{b} \lambda_{jb} g_{jb}(h_j) - B_j(\{\lambda_{jb}\})\right),$$
(42)

where $\{f_{ia}(v_i),g_{jb}(h_j)\}$ are the sufficient statistics, $\{\theta_i,\lambda_j\}$ are the canonical parameters of the models, $\{A_i,B_j\}$ are the log-normalization factors, and $\{r_i(v_i),s_j(h_j)\}$ are the normalization factors which are some additional features multiplied by some constants. We can ignore the log-normalization factors because they are hard to compute.

For the joint distribution of visible and hidden variables, we should introduce a quadratic term for their cross-interaction (Welling et al., 2004):

$$\mathbb{P}(\boldsymbol{v}, \boldsymbol{h}) \propto \exp\Big(\sum_{i=1}^{d} \sum_{a} \theta_{ia} f_{ia}(v_i) + \sum_{j=1}^{p} \sum_{b} \lambda_{jb} g_{jb}(h_j) + \sum_{i=1}^{d} \sum_{j=1}^{p} \sum_{a} \sum_{b} \boldsymbol{W}_{ia}^{jb} f_{ia}(v_i) g_{jb}(h_j)\Big). \tag{43}$$

According to Proposition 1, the visible and hidden units have conditional independence. Therefore, the conditional distributions can be written as multiplication of exponential family distributions (Welling et al., 2004):

$$\mathbb{P}(\boldsymbol{v}|\boldsymbol{h}) = \prod_{i=1}^{d} \exp\left(\sum_{a} \widehat{\theta}_{ia} f_{ia}(v_i) - A_i(\{\widehat{\theta}_{ia}\})\right), \quad (44)$$

$$\mathbb{P}(\boldsymbol{h}|\boldsymbol{v}) = \prod_{j=1}^{p} \exp\left(\sum_{b} \widehat{\lambda}_{jb} g_{jb}(h_{j}) - B_{j}(\{\widehat{\lambda}_{jb}\})\right), (45)$$

where:

$$\widehat{\theta}_{ia} := \theta_{ia} + \sum_{j=1}^{p} \sum_{h} W_{ia}^{jb} g_{jb}(h_j), \tag{46}$$

$$\widehat{\lambda}_{jb} := \lambda_{jb} + \sum_{i=1}^{d} \sum_{a} \boldsymbol{W}_{ia}^{jb} f_{ia}(v_i). \tag{47}$$

Therefore, we can choose one of the distributions in the exponential family for the conditional distributions of visible and hidden variables. In the following, we introduce different cases where the units can have either discrete or continuous values. In all cases, the distributions are from exponential families.

4.2. Binary States

The hidden and visible variables can have discrete number of values, also called states. Most often, inspired by the Hopfield network, BM and RBM have binary states. In this case, the hidden and visible units can have binary states, i.e., $v_i, h_j \in \{0,1\}, \forall i,j$. Hence, we can say:

$$\mathbb{P}(h_j = 1 | \boldsymbol{v}) = \frac{\mathbb{P}(h_j = 1, \boldsymbol{v})}{\mathbb{P}(h_j = 0, \boldsymbol{v}) + \mathbb{P}(h_j = 1, \boldsymbol{v})}.$$
 (48)

In binary states, the joint probability in Eq. (17) is simplified to:

$$\mathbb{P}(h_j = 0, \boldsymbol{v}) = \exp(c_j \times 0 + \boldsymbol{v}^\top \boldsymbol{W}_{:j} \times 0)$$

$$= \exp(0) = 1,$$

$$\mathbb{P}(h_j = 1, \boldsymbol{v}) = \exp(c_j \times 1 + \boldsymbol{v}^\top \boldsymbol{W}_{:j} \times 1)$$

$$= \exp(c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:j}).$$

Hence, Eq. (48) becomes:

$$\mathbb{P}(h_j = 1 | \boldsymbol{v}) = \frac{\exp(c_j + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j})}{1 + \exp(c_j + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j})}$$
$$= \frac{1}{1 + \exp(-(c_j + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j}))} = \sigma(c_j + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j}),$$
(49)

where:

$$\sigma(x) := \frac{\exp(x)}{1 + \exp(x)} = \frac{1}{1 + \exp(-x)},$$

is the sigmoid (or logistic) function and $W_{:j} \in \mathbb{R}^d$ denotes the j-th column of matrix W. If the visible units also have binary states, we will similarly have:

$$\mathbb{P}(v_i = 1|\boldsymbol{h}) = \sigma(b_i + \boldsymbol{W}_{i:}\boldsymbol{h}), \tag{50}$$

where $W_{i:} \in \mathbb{R}^p$ denotes the *i*-th row of matrix W. As we have only two states $\{0,1\}$, from Eqs. (49) and (50), we have:

$$\mathbb{P}(h_j|\boldsymbol{v}) = \sigma(c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:j}) = \sigma(c_j + \sum_{i=1}^d v_i w_{ij}), \quad (51)$$

$$\mathbb{P}(v_i|\boldsymbol{h}) = \sigma(b_i + \boldsymbol{W}_{i:}\boldsymbol{h}) = \sigma(b_i + \sum_{i=1}^p w_{ij} h_j). \quad (52)$$

According to Proposition 1, the units have conditional independence so their distribution is the product of each conditional distribution:

$$\mathbb{P}(\boldsymbol{h}|\boldsymbol{v}) = \prod_{j=1}^{p} \mathbb{P}(h_{j}|\boldsymbol{v}) = \prod_{j=1}^{p} \sigma(c_{j} + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j}), \quad (53)$$

$$\mathbb{P}(\boldsymbol{v}|\boldsymbol{h}) = \prod_{i=1}^{d} \mathbb{P}(v_i|\boldsymbol{h}) = \prod_{i=1}^{d} \sigma(b_i + \boldsymbol{W}_{i:}\boldsymbol{h}).$$
 (54)

Therefore, in Gibbs sampling of Algorithm 1, we sample from the distributions of Eqs. (51) and (52). Note that the sigmoid function is between zero and one so we can use the uniform distribution $u \sim U[0,1]$ for sampling from it. This was explained in Section 3.3. Moreover, for binary states, we have $\mathbb{E}_{\sim \mathbb{P}(h_j|\boldsymbol{v})}[h_j] = \sigma(c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:j})$. Hence, if we apply the sigmoid function element-wise on elements of $\hat{\boldsymbol{h}}_i \in \mathbb{R}^p$, we can have this for Eq. (26) in training binary-state RBM:

$$\widehat{\boldsymbol{h}}_i = \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_i)}[\boldsymbol{h}] = \sigma(\boldsymbol{c} + \boldsymbol{v}_i^{\top} \boldsymbol{W}).$$
 (55)

This equation is also used in Algorithm 2.

4.3. Continuous Values

In some cases, we set the hidden units to have continuous values as continuous representations for the visible unit. According to the definition of conditional probability, we have:

$$\mathbb{P}(v_i = 1 | \boldsymbol{h}) = \frac{\mathbb{P}(v_i = 1, \boldsymbol{h})}{\sum_{v_i \in \mathbb{R}^d} \mathbb{P}(\boldsymbol{h}, v_i)}.$$
 (56)

According to Eq. (18), we have:

$$\mathbb{P}(\boldsymbol{h}, v_i = 1) = \exp(b_i \times 1 + 1 \times \boldsymbol{W}_{i:} \boldsymbol{h})$$
$$= \exp(b_i + \boldsymbol{W}_{i:} \boldsymbol{h}). \tag{57}$$

Hence, Eq. (56) becomes:

$$\mathbb{P}(v_i = 1 | \boldsymbol{h}) = \frac{\exp(b_i + \boldsymbol{W}_{i:} \boldsymbol{h})}{\sum_{v_i \in \mathbb{R}^d} \mathbb{P}(\boldsymbol{h}, v_i)}.$$
 (58)

This is a softmax function which can approximate a Gaussian (normal) distribution and it sums to one. Therefore, we can write is as the normal distribution with variance one:

$$\mathbb{P}(v_i|\boldsymbol{h}) = \mathcal{N}(b_i + \boldsymbol{W}_i; \boldsymbol{h}, 1) = \mathcal{N}(b_i + \sum_{j=1}^p w_{ij}h_j, 1).$$
(59)

According to Proposition 1, the units have conditional independence so their distribution is the product of each conditional distribution:

$$\mathbb{P}(\boldsymbol{v}|\boldsymbol{h}) = \prod_{i=1}^{d} \mathbb{P}(v_i|\boldsymbol{h}) = \prod_{i=1}^{d} \mathcal{N}(b_i + \boldsymbol{W}_{i:}\boldsymbol{h}, 1). \quad (60)$$

Usually, when the hidden units have continuous values, the visible units have binary states (Welling et al., 2004; Mohamed & Hinton, 2010). In this case, the conditional distribution $\mathbb{P}(\boldsymbol{h}|\boldsymbol{v})$ is obtained by Eq. (53). If the visible units have continuous values, their distribution can be similarly calculated as:

$$\mathbb{P}(\boldsymbol{h}|\boldsymbol{v}) = \prod_{j=1}^{p} \mathbb{P}(h_{j}|\boldsymbol{v}) = \prod_{j=1}^{p} \mathcal{N}(c_{j} + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j}, 1). \quad (61)$$

These normal distributions can be used for sampling in Gibbs sampling of Algorithm 1. In this case, Eq. (26), used in Algorithm 2 for training RBM, is:

$$\widehat{\boldsymbol{h}}_i = \mathbb{E}_{\sim \mathbb{P}(\boldsymbol{h}|\boldsymbol{v}_i)}[\boldsymbol{h}] = \mathcal{N}(\boldsymbol{c} + \boldsymbol{v}_i^\top \boldsymbol{W}, \boldsymbol{I}_{p \times p}), \quad (62)$$

where I denotes the identity matrix.

4.4. Discrete Poisson States

In some cases, the units have discrete states but with more than two values which was discussed in Section 4.2. In this case, we can use the well-known Poisson distribution for discrete random variables:

$$Ps(t,\lambda) = \frac{e^{-\lambda}\lambda^t}{t!}.$$

Assume every visible unit can have a value $t \in \{0, 1, 2, 3, \dots\}$. If we consider the conditional Poisson distribution for the visible units, we have (Salakhutdinov & Hinton, 2009b):

$$\mathbb{P}(v_i = t | \boldsymbol{h}) = \operatorname{Ps}(t, \frac{\exp(b_i + \boldsymbol{W}_{i:} \boldsymbol{h})}{\sum_{k=1}^{d} \exp(b_k + \boldsymbol{W}_{k:} \boldsymbol{h})}).$$
(63)

Similarly, if we have discrete states for the hidden units, we can have:

$$\mathbb{P}(h_j = t | \boldsymbol{v}) = \operatorname{Ps}(t, \frac{\exp(c_j + \boldsymbol{v}^{\top} \boldsymbol{W}_{:j})}{\sum_{k=1}^{p} \exp(c_k + \boldsymbol{v}^{\top} \boldsymbol{W}_{:k})}), \quad (64)$$

These Poisson distributions can be used for sampling in Gibbs sampling of Algorithm 1. In this case, Eq. (26), used in Algorithm 2 for training RBM, can be calculated using a multivariate Poisson distribution (Edwards, 1962). It is noteworthy that RBM has been used for *semantic hashing* where the hidden variables are used as a hashing representation of data (Salakhutdinov & Hinton, 2009b). Semantic hashing uses Poisson distribution and sigmoid function for the conditional visible and hidden variables, respectively.

5. Conditional Restricted Boltzmann Machine

If data are a time-series, RBM does not include its temporal (time) information. In other words, RBM is suitable for static data. Conditional RBM (CRBM), proposed in (Taylor et al., 2007), incorporates the temporal information into the configuration of RBM. It considers visible variables of previous time steps as conditional variables. CRBM adds two sets of directed links to RBM. The first set of directed links is the autoregressive links from the past \mathcal{T}_1 visible units to the visible units of current time step. The second set of directed links is the links from the past τ_2 visible units to the hidden units of the current time step. In general, \mathcal{T}_1 is not necessarily equal to \mathcal{T}_2 but for simplicity, we usually set $\mathcal{T}_1 = \mathcal{T}_2 = \mathcal{T}$ (Taylor et al., 2007). We denote the links from the visible units at time $t-\tau$ to visible units at current time by $G^{(t-\tau)} = [g_{ij}] \in \mathbb{R}^{d \times d}$. We also denote the links from the visible units at time $t-\tau$ to hidden units at current time by $\mathbf{Q}^{(t-\tau)}=[q_{ij}]\in\mathbb{R}^{d\times p}$. The structure of CRBM is shown in Fig. 2. Note that each arrow in this figure is a set of links representing a matrix or vector of weights.

The updating rule for the weights W and biases b and c are the same as in Eqs. (31), (32), and (33). We consider the directed links from the previous visible units to current visible units and current hidden units as dynamically changing biases. Recall that for updating the biases b and c, we used

Eqs. (32) and (33). Similarly, for updating the added links from τ previous time steps, we have:

$$\forall i : \mathbb{R}^d \ni \nabla_{\boldsymbol{G}_{i:}^{(t-\tau)}} \ell(\theta) = v_i^{(t-\tau)} \Big(\sum_{k=1}^n \boldsymbol{v}_k^{(t)} - \sum_{k=1}^n \widetilde{\boldsymbol{v}}_k^{(t)} \Big), \tag{65}$$

$$\forall i : \mathbb{R}^p \ni \nabla_{\boldsymbol{Q}_{i:}^{(t-\tau)}} \ell(\theta) = v_i^{(t-\tau)} \Big(\sum_{k=1}^n \widehat{\boldsymbol{h}}_k - \sum_{k=1}^n \widetilde{\boldsymbol{h}}_k \Big), \tag{66}$$

where $i \in \{1,\ldots,d\}$, $\tau \in \{1,2,\ldots,\mathcal{T}\}$, $\boldsymbol{G}_{i:}^{(t-\tau)}$ denotes the i-th row of $\boldsymbol{G}^{(t-\tau)}$, and $\boldsymbol{Q}_{i:}^{(t-\tau)}$ denotes the i-th row of $\boldsymbol{Q}^{(t-\tau)}$. These equations are similar to Eqs. (32) and (33) but they are multiplied by the visible values in previous time steps. This is because RBM multiplies biases with one (see Fig. 1) while these newly introduced biases have previous visible values instead of one (see Fig. 2). These equations can be restated as (Taylor et al., 2007):

$$\forall i,j \colon \nabla_{g_{ij}^{(t-\tau)}} \ell(\theta) = v_i^{(t-\tau)} \Big(\langle v_i^{(t)} \rangle_{\text{data}} - \langle v_i^{(t)} \rangle_{\text{recon.}} \Big), \tag{67}$$

$$\forall i,j \colon \nabla_{q_{ij}^{(t-\tau)}} \ell(\theta) = v_i^{(t-\tau)} \Big(\langle h_j^{(t)} \rangle_{\text{data}} - \langle h_j^{(t)} \rangle_{\text{recon.}} \Big), \tag{68}$$

where $\langle . \rangle_{data}$ and $\langle . \rangle_{recon.}$ denote expectation over data and reconstruction of data, respectively. In addition to the weights and biases of RBM, the additional links are learned by gradient descent using the above gradients. Algorithm 2 can be used for training CRBM if learning the added links is also included in the algorithm.

Interpolating CRBM (ICRBM) (Mohamed & Hinton, 2010) is an improvement over the CRBM where some links have been added from visible variables in the future. Figure 2 depicts the structure of ICRBM. Its training and formulation is similar but we do not cover its theory in this paper for the sake of brevity. Note that CRBM has been used in various time-series applications such as action recognition (Taylor et al., 2007) and acoustics (Mohamed & Hinton, 2010).

6. Deep Belief Network

6.1. Stacking RBM Models

We can train a neural network using RBM training (Hinton & Salakhutdinov, 2006; Hinton et al., 2006). Training neural network using RBM training can result in very good initialization of weights for training network using backpropagation. Before the development of ReLu (Glorot et al., 2011) and dropout (Srivastava et al., 2014), multiplayer perceptron networks could not become deep for the problem of vanishing gradients. This was because random initial weights were not suitable enough for starting optimization in backpropagation, especially in deep networks.

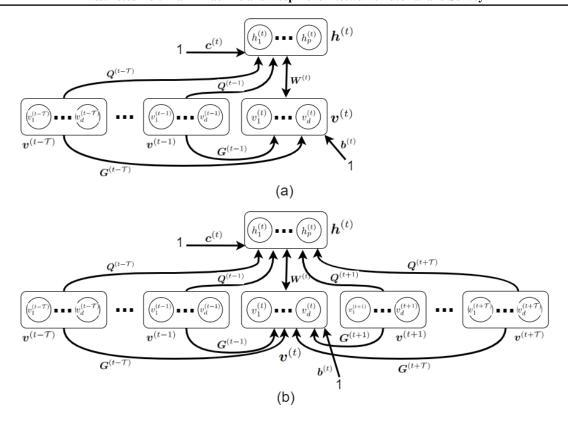


Figure 2. The structures of (a) a conditional Boltzmann machine and (b) an interpolating conditional restricted Boltzmann machine. Note that each arrow in this figure represents a set of links.

Therefore, a method was proposed for pre-training neural networks which initializes network to a suitable set of weights and then the pre-trained weights are fine-tuned using backpropagation (Hinton & Salakhutdinov, 2006; Hinton et al., 2006).

A neural network consists of several layers. Let ℓ denote the number of layers, where the first layer gets the input data, and let p_{ℓ} be the number of neurons in the ℓ -th layer. By convention, we have $p_1 = d$. We can consider every two successive layers as one RBM. This is shown in Fig. 3. We start from the first pair of layers as an RBM and we introduce training dataset $\{x_i \in \mathbb{R}^d\}_{i=1}^n$ as the visible variable $\{v_i\}_{i=1}^n$ of the first pair of layers. We train the weights and biases of this first layer as an RBM using Algorithm 2. After training this RBM, we generate n p_2 -dimensional hidden variables using Gibbs sampling in Algorithm 1. Now, we consider the hidden variables of the first RBM as the visible variables for the second RBM (the second pair of layers). Again, this RBM is trained by Algorithm 2 and, then, hidden variables are generated using Gibbs sampling in Algorithm 1. This procedure is repeated until all pairs of layers are trained using RBM training. This layer-wise training of neural network has a greedy approach (Bengio et al., 2007). This greedy training of layers prepares good initialized weights and biases for the whole neural network. Now, we fine-tune the weights and biases using backpropagation (Rumelhart et al., 1986).

The explained training algorithm was first proposed in (Hinton & Salakhutdinov, 2006; Hinton et al., 2006) and was used for dimensionality reduction. By increasing ℓ to any large number, the network becomes large and deep. As layers are trained one by one as RBM models, we can make the network as deep as we want without being worried for vanishing gradients because weights are initialized well for backpropagation. As this network can get deep and is pretrained by belief propagation (RBM training), it is referred to as the *Deep Belief Network* (DBN) (Hinton et al., 2006; Hinton, 2009). DBN can be seen as a stack of RBM models. The pre-training of a DBN using RBM training is depicted in Fig. 3. This algorithm is summarized in Algorithm 3. In this algorithm, $\boldsymbol{W}_l \in \mathbb{R}^{p_l \times p_{l+1}}$ denotes the weights connecting layer l to layer (l+1) and $\boldsymbol{b}_l \in \mathbb{R}^{p_l}$ denotes the biases of the layer l. Note that as weights are between every two layers, the sets of weights are $\{\boldsymbol{W}_l\}_{l=1}^{\ell-1}$. Note that pre-training of DBN is an unsupervised task because RBM training is unsupervised. Fine-tuning of DBN can be either unsupervised or supervised depending on the loss function for backpropagation. If the DBN is an autoencoder with a low-dimensional middle layer in the network, both its pre-training and fine-tuning stages are un-

```
1 Input: training data \{x_i\}_{i=1}^n
 2 // pre-training:
 3 for l from 1 to \ell-1 do
              if l=1 then
                     \{v_i\}_{i=1}^n \leftarrow \{x_i\}_{i=1}^n
 5
 6
                     // generate n hidden variables of previous
 7
                     \begin{aligned} &\{\boldsymbol{h}_i\}_{i=1}^n \leftarrow \text{Algorithm 1 for } (l-1)\text{-th} \\ &\text{RBM} \leftarrow \{\boldsymbol{v}_i\}_{i=1}^n \\ &\{\boldsymbol{v}_i\}_{i=1}^n \leftarrow \{\boldsymbol{h}_i\}_{i=1}^n \end{aligned}
 8
              \boldsymbol{W}_{l}, \boldsymbol{b}_{l}, \boldsymbol{b}_{l+1} \leftarrow \text{Algorithm 2 for } l\text{-th RBM}
10
                 \leftarrow \{\boldsymbol{v}_i\}_{i=1}^n
11 // fine-tuning using backpropagation:
12 Initialize network with weights \{oldsymbol{W}_l\}_{l=1}^{\ell-1} and
        biases \{\boldsymbol{b}_l\}_{l=2}^{\ell}.
13 \{ oldsymbol{W}_l \}_{l=1}^{\ell-1}, \{ oldsymbol{b}_l \}_{l=1}^{\ell} \leftarrow 	ext{Backpropagate the error}
        of loss fro several epochs.
```

Algorithm 3: Training a deep belief network

supervised because the loss function of backpropagation is also a mean squared error. This DBN autoencoder can learn a low-dimensional embedding or representation of data and can be used for dimensionality reduction (Hinton & Salakhutdinov, 2006). The DBN autoencoder has also been used for hashing (Salakhutdinov & Hinton, 2009b). The structure of this network is depicted in Fig. 4.

6.2. Other Improvements over RBM and DBN

Some improvements over DBN are convolutional DBN (Krizhevsky & Hinton, 2010) and use of DBN for hashing (Salakhutdinov & Hinton, 2009b). Greedy training of DBN using RBM training has been used in training the t-SNE network for general degree of freedom (Van Der Maaten, 2009). In addition to CRBM (Taylor et al., 2007), recurrent RBM (Sutskever et al., 2009) has been proposed to handle the temporal information of data. Also, note that there exist some other energy-based models in addition to BM; Helmholtz machine (Dayan et al., 1995) is an example.

There also exists Deep Boltzmann Machine (DBM) which is slightly different from DBN. For the sake of brevity, we do not cover it here and refer the interested reader to (Salakhutdinov & Hinton, 2009a). Various efficient training algorithms have been proposed for DBM (Salakhutdinov & Larochelle, 2010; Salakhutdinov, 2010; Salakhutdinov, 2010; Salakhutdinov & Hinton, 2012; Srivastava & Salakhutdinov, 2012; Hinton & Salakhutdinov, 2012; Montavon & Müller, 2012; Goodfellow et al., 2013; Srivastava & Salakhutdinov, 2014; Melchior et al., 2016). Some of the applications of DBM are document processing (Srivastava et al., 2013), face modeling (Nhan Duong et al., 2015)

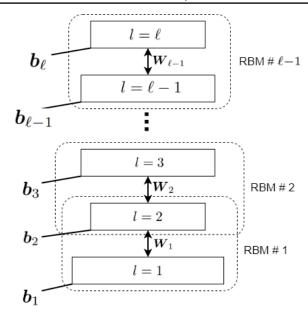


Figure 3. Pre-training a deep belief network by considering every pair of layers as an RBM.

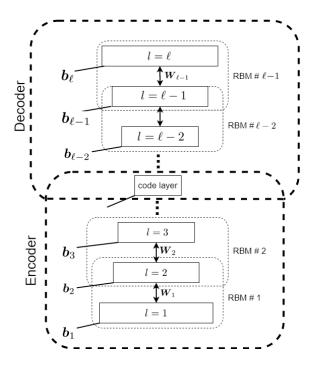


Figure 4. A DBN autoencoder where the number of neurons in the corresponding layers of encoder and decoder are usually set to be equal. The coder layer is a low-dimensional embedding for representation of data.

7. Conclusion

This was a tutorial paper on BM, RBM, and DBN. After some background, we covered the structure of BM and RBM, Gibbs sampling in RBM for generating visible and

hidden variables, training RBM using contrastive divergence, and training BM. Then, we introduced various cases for states of visible and hidden units. Thereafter, CRBM and DBN were explained in detail.

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References

- Ackley, David H, Hinton, Geoffrey E, and Sejnowski, Terrence J. A learning algorithm for Boltzmann machines. *Cognitive science*, 9(1):147–169, 1985.
- Alberici, Diego, Barra, Adriano, Contucci, Pierluigi, and Mingione, Emanuele. Annealing and replica-symmetry in deep Boltzmann machines. *Journal of Statistical Physics*, 180(1):665–677, 2020.
- Alberici, Diego, Contucci, Pierluigi, and Mingione, Emanuele. Deep Boltzmann machines: rigorous results at arbitrary depth. In *Annales Henri Poincaré*, pp. 1–24. Springer, 2021.
- Bengio, Yoshua, Lamblin, Pascal, Popovici, Dan, and Larochelle, Hugo. Greedy layer-wise training of deep networks. In *Advances in neural information processing systems*, pp. 153–160, 2007.
- Bishop, Christopher M. Pattern recognition. *Machine learning*, 128(9), 2006.
- Boltzmann, Ludwig. Studien uber das gleichgewicht der lebenden kraft. *Wissenschafiliche Abhandlungen*, 1:49–96, 1868.
- Boser, Bernhard E, Guyon, Isabelle M, and Vapnik, Vladimir N. A training algorithm for optimal margin classifiers. In *Proceedings of the fifth annual workshop on Computational learning theory*, pp. 144–152, 1992.
- Brush, Stephen G. History of the Lenz-Ising model. *Reviews of modern physics*, 39(4):883, 1967.
- Carroll, Sean. From eternity to here: the quest for the ultimate theory of time. Penguin, 2010.
- Dayan, Peter, Hinton, Geoffrey E, Neal, Radford M, and Zemel, Richard S. The Helmholtz machine. *Neural computation*, 7(5):889–904, 1995.
- Dwivedi, Raaz, Chen, Yuansi, Wainwright, Martin J, and Yu, Bin. Log-concave sampling: Metropolis-Hastings algorithms are fast! In *Conference on learning theory*, pp. 793–797. PMLR, 2018.

- Edwards, Carol Bates. *Multivariate and multiple Poisson distributions*. Iowa State University, 1962.
- Geman, Stuart and Geman, Donald. Stochastic relaxation, Gibbs distributions, and the Bayesian restoration of images. *IEEE Transactions on pattern analysis and machine intelligence*, PAMI-6(6):721–741, 1984.
- Ghojogh, Benyamin and Crowley, Mark. The theory behind overfitting, cross validation, regularization, bagging, and boosting: tutorial. *arXiv* preprint *arXiv*:1905.12787, 2019.
- Ghojogh, Benyamin, Nekoei, Hadi, Ghojogh, Aydin, Karray, Fakhri, and Crowley, Mark. Sampling algorithms, from survey sampling to Monte Carlo methods: Tutorial and literature review. *arXiv preprint arXiv:2011.00901*, 2020.
- Gibbs, J Willard. *Elementary principles in statistical mechanics*. Courier Corporation, 1902.
- Glorot, Xavier, Bordes, Antoine, and Bengio, Yoshua. Deep sparse rectifier neural networks. In *Proceedings of the fourteenth international conference on artificial intelligence and statistics*, pp. 315–323. JMLR Workshop and Conference Proceedings, 2011.
- Goodfellow, Ian, Mirza, Mehdi, Courville, Aaron, and Bengio, Yoshua. Multi-prediction deep Boltzmann machines. *Advances in Neural Information Processing Systems*, 26:548–556, 2013.
- Hebb, Donald. *The Organization of Behavior*. Wiley & Sons, New York, 1949.
- Hinton, Geoffrey E. Training products of experts by minimizing contrastive divergence. *Neural computation*, 14 (8):1771–1800, 2002.
- Hinton, Geoffrey E. Boltzmann machine. *Scholarpedia*, 2 (5):1668, 2007.
- Hinton, Geoffrey E. Deep belief networks. *Scholarpedia*, 4(5):5947, 2009.
- Hinton, Geoffrey E. A practical guide to training restricted Boltzmann machines. In *Neural networks: Tricks of the trade*, pp. 599–619. Springer, 2012.
- Hinton, Geoffrey E and Salakhutdinov, Ruslan R. Reducing the dimensionality of data with neural networks. *Science*, 313(5786):504–507, 2006.
- Hinton, Geoffrey E and Salakhutdinov, Russ R. A better way to pretrain deep Boltzmann machines. *Advances in Neural Information Processing Systems*, 25:2447–2455, 2012.

- Hinton, Geoffrey E and Sejnowski, Terrence J. Optimal perceptual inference. In *Proceedings of the IEEE conference on Computer Vision and Pattern Recognition*, volume 448. IEEE, 1983.
- Hinton, Geoffrey E, Osindero, Simon, and Teh, Yee-Whye. A fast learning algorithm for deep belief nets. *Neural computation*, 18(7):1527–1554, 2006.
- Hopfield, John J. Neural networks and physical systems with emergent collective computational abilities. *Proceedings of the national academy of sciences*, 79(8): 2554–2558, 1982.
- Huang, Kerson. Statistical Mechanics. John Wiley & Sons, 1987.
- Ising, Ernst. Beitrag zur theorie des ferromagnetismus. Zeitschrift für Physik, 31(1):253–258, 1925.
- Karpathy, Andrej and Fei-Fei, Li. Deep visual-semantic alignments for generating image descriptions. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 3128–3137, 2015.
- Kirkpatrick, Scott, Gelatt, C Daniel, and Vecchi, Mario P. Optimization by simulated annealing. *science*, 220 (4598):671–680, 1983.
- Koller, Daphne and Friedman, Nir. *Probabilistic graphical models: principles and techniques*. MIT press, 2009.
- Krizhevsky, Alex and Hinton, Geoff. Convolutional deep belief networks on CIFAR-10. *Unpublished manuscript*, 40(7):1–9, 2010.
- LeCun, Yann, Chopra, Sumit, Hadsell, Raia, Ranzato, M, and Huang, F. A tutorial on energy-based learning. *Predicting structured data*, 1, 2006.
- LeCun, Yann, Bengio, Yoshua, and Hinton, Geoffrey. Deep learning. *nature*, 521(7553):436–444, 2015.
- Lenz, Wilhelm. Beitršge zum verstšndnis der magnetischen eigenschaften in festen kšrpern. *Physikalische Z*, 21:613–615, 1920.
- Little, William A. The existence of persistent states in the brain. *Mathematical biosciences*, 19(1-2):101–120, 1974.
- Melchior, Jan, Fischer, Asja, and Wiskott, Laurenz. How to center deep Boltzmann machines. *The Journal of Machine Learning Research*, 17(1):3387–3447, 2016.
- Mohamed, Abdel-rahman and Hinton, Geoffrey. Phone recognition using restricted Boltzmann machines. In 2010 IEEE International Conference on Acoustics, Speech and Signal Processing, pp. 4354–4357. IEEE, 2010.

- Mohamed, Abdel-rahman, Dahl, George, Hinton, Geoffrey, et al. Deep belief networks for phone recognition. In *Nips workshop on deep learning for speech recognition and related applications*, volume 1, pp. 39. Vancouver, Canada, 2009.
- Mohamed, Abdel-rahman, Dahl, George E, and Hinton, Geoffrey. Acoustic modeling using deep belief networks. *IEEE transactions on audio, speech, and language processing*, 20(1):14–22, 2011.
- Molkaraie, Mehdi. The primal versus the dual ising model. In 2017 55th Annual Allerton Conference on Communication, Control, and Computing (Allerton), pp. 53–60. IEEE, 2017.
- Molkaraie, Mehdi. Marginal densities, factor graph duality, and high-temperature series expansions. In *International Conference on Artificial Intelligence and Statistics*, pp. 256–265, 2020.
- Montavon, Grégoire and Müller, Klaus-Robert. Deep Boltzmann machines and the centering trick. In *Neural networks: tricks of the trade*, pp. 621–637. Springer, 2012.
- Nhan Duong, Chi, Luu, Khoa, Gia Quach, Kha, and Bui, Tien D. Beyond principal components: Deep Boltzmann machines for face modeling. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recogni*tion, pp. 4786–4794, 2015.
- Passos, Leandro Aparecido and Papa, Joao Paulo. Temperature-based deep Boltzmann machines. *Neural Processing Letters*, 48(1):95–107, 2018.
- Ramsauer, Hubert, Schäfl, Bernhard, Lehner, Johannes, Seidl, Philipp, Widrich, Michael, Adler, Thomas, Gruber, Lukas, Holzleitner, Markus, Pavlović, Milena, Sandve, Geir Kjetil, et al. Hopfield networks is all you need. *arXiv preprint arXiv:2008.02217*, 2020.
- Rumelhart, David E, Hinton, Geoffrey E, and Williams, Ronald J. Learning representations by back-propagating errors. *Nature*, 323(6088):533–536, 1986.
- Salakhutdinov, Ruslan. Learning deep boltzmann machines using adaptive mcmc. In *Proceedings of the 27th International Conference on Machine Learning*, pp. 943–950, 2010.
- Salakhutdinov, Ruslan and Hinton, Geoffrey. Deep Boltzmann machines. In *Artificial intelligence and statistics*, pp. 448–455. PMLR, 2009a.
- Salakhutdinov, Ruslan and Hinton, Geoffrey. Semantic hashing. *International Journal of Approximate Reasoning*, 50(7):969–978, 2009b.

- Salakhutdinov, Ruslan and Hinton, Geoffrey. An efficient learning procedure for deep Boltzmann machines. *Neural computation*, 24(8):1967–2006, 2012.
- Salakhutdinov, Ruslan and Larochelle, Hugo. Efficient learning of deep Boltzmann machines. In *Proceedings of the thirteenth international conference on artificial intelligence and statistics*, pp. 693–700. JMLR Workshop and Conference Proceedings, 2010.
- Srivastava, Nitish and Salakhutdinov, Ruslan. Multimodal learning with deep Boltzmann machines. In *Advances in neural information processing systems*, volume 1, pp. 2, 2012.
- Srivastava, Nitish and Salakhutdinov, Ruslan. Multimodal learning with deep Boltzmann machines. *Journal of Machine Learning Research*, 15(1):2949–2980, 2014.
- Srivastava, Nitish, Salakhutdinov, Ruslan R, and Hinton, Geoffrey E. Modeling documents with deep Boltzmann machines. *arXiv* preprint arXiv:1309.6865, 2013.
- Srivastava, Nitish, Hinton, Geoffrey, Krizhevsky, Alex, Sutskever, Ilya, and Salakhutdinov, Ruslan. Dropout: a simple way to prevent neural networks from overfitting. *The journal of machine learning research*, 15(1):1929–1958, 2014.
- Sutskever, Ilya, Hinton, Geoffrey E, and Taylor, Graham W. The recurrent temporal restricted Boltzmann machine. In *Advances in neural information processing systems*, pp. 1601–1608, 2009.
- Taylor, Graham W, Hinton, Geoffrey E, and Roweis, Sam T. Modeling human motion using binary latent variables. In *Advances in neural information processing systems*, pp. 1345–1352, 2007.
- Van Der Maaten, Laurens. Learning a parametric embedding by preserving local structure. In *Artificial Intelligence and Statistics*, pp. 384–391, 2009.
- Welling, Max, Rosen-Zvi, Michal, and Hinton, Geoffrey E. Exponential family harmoniums with an application to information retrieval. In *Advances in neural information processing systems*, volume 4, pp. 1481–1488, 2004.