Restricted Boltzmann Machines for the Long Range Ising Models

Ken-Ichi Aoki¹,* and Tamao Kobayashi²,†

¹Institute for Theoretical Physics, Kanazawa University, Kanazawa 920-1192, Japan
²National Institute of Technology, Yonago College, Yonago 683-8502, Japan

Abstract

We set up Restricted Boltzmann Machines (RBM) to reproduce the Long Range Ising (LRI) models of the Ohmic type in one dimension. The RBM parameters are tuned by using the standard machine learning procedure with an additional method of Configuration with Probability (CwP). The quality of resultant RBM are evaluated through the susceptibility with respect to the magnetic external field. We compare the results with those by Block Decimation Renormalization Group (BDRG) method, and our RBM clear the test with satisfactory precision.

*Electronic address: aoki@hep.s.kanazawa-u.ac.jp
†Electronic address: kobayasi@yonago-k.ac.jp
I. INTRODUCTION

Quite recently the deep learning machines have drawn much attention since they are very effective for image processing \[1\] and Go game \[2\] etc. The deep learning machines can be regarded as a method of information reduction keeping as much macroscopically important features as possible. This policy or idea resembles to the renormalization group method in physics \[3, 6\], and the intrinsic relationship between them has been argued \[7\], and further investigation is strongly desired from both sides.

Here in this article we make Restricted Boltzmann Machines (RBM) \[8, 9\] to reproduce the Long Range Ising (LRI) models in one dimension. The LRI models have its own long history \[10\], since they work as most simplified models to investigate the quantum dissipation issues which are still unveiled subjects lying in between classical and quantum physics \[11–15\]. The LRI models have a critical point (temperature) to exhibit the spontaneous magnetization \[16, 17\]. The critical point depends on the long range nature determined by the power exponent of the interactions \[18\]. Moreover, functional renormalization group approaches revealed Ising model critical phenomena\[4, 5\]. They organized new framework using the field-theoretic formulation and developed powerful techniques with including higher order diagrams. In this article, however, we are attempting to utilize the finite range scaling method and direct comparison of our results with the above mentioned ones are not possible yet. Here we adopt the Ohmic case where the power exponent is $-2$ and it is known to give a marginal point of bringing about the finite critical temperature ($K_{1c} = 0.657$) \[19\].

We are interested in the procedure of how we can make up appropriate RBM to reproduce the LRI models. We define RBM with link parameters respecting the translational and Parity invariance. We generate sample data set of the LRI models, and make RBM to learn the data by tuning the RBM parameters to reach the maximum likelihood point.

Here we introduce a new method in setting up the input data for RBM learning. We slice out the learning procedures into many small steps, where the sample data set is defined by a set of pair of Configuration with its corresponding Probability (CwP). This method resembles to the multi-canonical ensemble method where a part of the Hamiltonian is moved out of the configuration measure into the physical quantity to be averaged.

Finally we evaluate the total quality of the tuned up RBM. Starting with completely random spins, we produce output set of configurations, step by step, checking the susceptibility
of each set. After the onset of equilibrium, we examine the susceptibility. We compare our
results with those calculated by a renormalization group method called the Block Decimation
Renormalization Group (BDRG) which gives the exact susceptibility numerically [19, 20].
This article is a short report of our work and full analysis will be published elsewhere.

II. RESTRICTED BOLTZMANN MACHINES FOR LONG RANGE ISING MODELS

We introduce the standard RBM consisting of visible variables $v$ and hidden variables $h$.
The total probability distribution is defined by

$$P(v, h) = \frac{1}{Z} e^{-H(v, h)}, \quad Z = \sum_v h e^{-H(v, h)},$$

where $H$ is the Hamiltonian (energy function) and the partition function $Z$ is the total
normalization constant. We integrate out the hidden variables to get the probability distribution function for $v$,

$$P(v) = \sum_h P(v, h).$$

The standard restriction of RBM requires the Hamiltonian to take the following form,

$$H(v, h) = -\sum_{ij} w_{ij} v_i h_j,$$

where we omit the external field terms (linear in $v, h$) here.

Our target system is one dimensional Ising system and all variables $v, h$ takes +1 or
−1 respectively. The number of hidden variables is exactly half of that of visible variables
and we adopt the periodic boundary condition. The links and their weights are defined
as drawn in Fig. 1. Although other types of linking pattern may be considered, we take
this type since it has a well-defined nearest neighbor solution. We respect the translational
and Parity invariance of the system, and therefore the link weights are all common to each
hidden variables and also are left-right symmetric $k_{-n} = k_n$. Note that precisely speaking,
the translational invariance holds for the hidden sector only, and in the visible sector, odd
and even site spins are not equivalent. Hereafter our RBM are denoted by

$$P(v, h; k),$$

3
where the machine parameter $k$ represents $\{k_0, k_1, \cdots\}$. The RBM visible probability distribution is given similarly,

$$P(v; k) = \sum_h P(v, h; k).$$

(5)

III. THE LONG RANGE ISING MODELS

The LRI model is defined by the following statistical weights,

$$P_{\text{LRI}}(v) = \frac{1}{Z} \exp \left( \sum_n K_n \sum_i v_i v_{i+n} \right),$$

(6)
where \( K_n \) is the coupling constant for range \( n \). We take the Ohmic type of the long range behavior,

\[
K_n = \frac{K_1}{n^2}.
\]  

(7)

Our purpose in this article is to tune the RBM parameter \( k \) so that the RBM visible probability distribution may best reproduce the LRI probability distribution,

\[
P(v; k^*) \simeq P_{\text{LRI}}(v).
\]  

(8)

We divide the LRI Hamiltonian into two parts which are the nearest neighbor base part and other long range part,

\[
P_{\text{LRI}} = \frac{1}{Z} \exp \left( K_1 \sum_i v_i v_{i+1} \right) \exp \left( \sum_{n=2} \sum_i K_n v_i v_{i+n} \right)
\]  

\[
= \frac{1}{Z} \exp(-H_0(v)) \exp(-H_L(v)).
\]  

(9)

We set up the input data for RBM as follows. In this section we omit the Hamiltonian slicing procedure for simplicity, which will be explained in the next section. We generate a set of spin configurations exactly respecting the nearest neighbor part probability distribution. This is done most quickly via the domain wall representation [21] where the domain wall exists with probability,

\[
q = \frac{1}{1 + \exp(2K_1)},
\]  

(10)

and there is no correlation among domain walls. Therefore we can set each domain wall independently, expect for caring the periodic boundary condition. We express this set of configuration by \( \{ v(\mu) \} \) where \( \mu \) denotes discriminator of each configuration.

Then the second part of the weight is considered as the physical quantity side. We calculate the additional probability which should be assigned to each configuration generated above,

\[
v_\mu \rightarrow p_\mu \propto \exp(-H_L(v_\mu)).
\]  

(11)

Now our target probability distribution to be learned by RBM is defined by a set of pair of Configuration with corresponding Probability, CwP:

\[
\{ v(\mu); p_\mu \}.
\]  

(12)
The normalization of the probability is taken to be

$$\sum_{\mu} p_{\mu} = N,$$  (13)

where \( N \) is the total number of configurations.

Now we define the likelihood of RBM to produce the above CwP as follows:

$$L(k) = N \prod_{\mu} p_{\mu} \sum_{\mathbf{h}} P(v^{(\mu)}, \mathbf{h}; k).$$  (14)

Note that the probability \( p_{\mu} \) is included representing the effective number of occurrences of the corresponding configuration. To search for the stationary point of the likelihood, we differentiate the logarithm of likelihood function with respect to \( k \). Using the explicit definition of our RBM, we have the following derivative,

$$\frac{1}{N j_{M}} \frac{\partial \log(L(k))}{\partial k_n} = \frac{1}{N j_{M}} \sum_{\mu} p_{\mu} \sum_{j} v^{(\mu)}_{j+n} \tanh(\lambda_j) - \frac{1}{j_{M}} \sum_{j} E[v_{j+n} h_j; k],$$  (15)

where \( j_{M} \) is the total number of hidden variables \( \mathbf{h} \), \( \lambda_j \) is defined by

$$\lambda_j = \sum_n k_n v^{(\mu)}_{j+n},$$  (16)

and \( E[\cdot] \) denotes the expectation value of operator by the RBM,

$$E[v_{j+n} h_j; k] = \sum_{v, \mathbf{h}} v_{j+n} h_j P(v, \mathbf{h}; k).$$  (17)

Using the derivative above we adopt the steepest descent method to find the maximum likelihood position of RBM parameters. The expectation value part is evaluated by the contrastive divergence method with several times of sample updates [9].

**IV. MACHINE LEARNING PROCEDURE AND RESULTS**

Our purpose here is to make appropriate RBM to generate high quality distribution of spin chain for the 1D Ising model with long range interactions. If the interactions among spins are limited to the nearest neighbor type, the model is easily solved exactly and the corresponding RBM solution is also obtained straightforwardly, although the practical machine learning process is not trivial. However if the interactions are not nearest neighbor, the model cannot be solved analytically, and its RBM counterpart is far from trivial.
Our total strategy here is drawn in Fig. 2, although we omit the slicing processes explained below for simplicity. Slicing is necessary since the difference of the probabilities in a set should not be too large. The large deviation of probabilities causes drastic loss of sample quality and the effective size of data set is shrunk. We tune the slicing width so that the averaged probability might be limited by some small size.

Now the slicing procedure is explained in some detail. First of all we prepare sliced Hamiltonians $\Delta H_m (m = 1, 2, \cdots m_{\text{Max}})$ so that they satisfy the following properties:

$$\sum_{m=1}^{M} \Delta H_m(v) = H_M(v), \quad H_M(v)|_{M=m_{\text{Max}}} = H_L(v).$$

At each slicing step ($m$-th step here), the initial input configurations, denoted by

$$\{v^{(\mu)}[m]\},$$

is regarded as satisfying the probability distribution,

$$P_m(v) \propto \exp(-H_0(v)) \exp(-H_{m-1}(v)).$$

FIG. 2: View of RBM learning procedures.
Then we assign additional probability factor given by
\[ p_{\mu}[m] = \frac{N \exp(-\Delta H_m(v^{(\mu)}[m]))}{\sum_{\mu} \exp(-\Delta H_m(v^{(\mu)}[m]))}, \]  
(21)

where \( \Delta H_m \) is a current slice of the remaining part of the Hamiltonian. Using this Configuration with Probability: \( \{ v^{(\mu)}[m], p_{\mu}[m] \} \) as the target data, RBM parameters are tuned up \( (k_m \rightarrow k_{m+1}) \),

\[
\{ v^{(\mu)}[m], p_{\mu}[m] \} \iff \text{RBM}(k_m) \implies \text{RBM}(k_{m+1}) \implies \{ v^{(\mu)}[m+1] \},
\]
(22)

and the output data set \( \{ v^{(\mu)}[m+1] \} \) by RBM \( (k_{m+1}) \) is expected to obey the probability distribution,

\[ P_{m+1}(v) \propto \exp(-H_0(v))\exp(-H_m(v)). \]
(23)

Then this data set works for the input configuration set for the next sliced step and is coupled with probability \( p_{\mu}[m+1] \) defined through \( \Delta H_{m+1} \).

In this serial procedures of learning, the set of configuration is simultaneously updated. The set is updated at each step of the steepest descent move of the machine through the contrastive divergence iteration. At the stationary point of the machine, the final set of configuration is used as the initial set of configuration for the next slice, that is, each configuration is assigned the probability coming from the next sliced Hamiltonian effect.

Actually our slicing order respects the range of interactions as follows. Starting with the nearest neighbor configurations, where the probability of configuration is all 1 (constant), we add the non-nearest neighbor interactions of range 2, but sliced (divided) by some number. We proceed RBM learning slice by slice, to reach the range 2 full interactions. Then we add range 3 interactions, again with a slice. Proceeding this way further, finally we reach the maximum range interactions, which is 9 in this article.

Practical and full analysis of RBM learning procedures are reported in the future full paper and here we show the tuned RBM parameters and its evaluation by checking the susceptibility estimates. The size of the system is 128 spins (the number of visible variables \( v \)). The RBM links contains up to \( k_{12} \), that is, RBM has 13 machine parameters. The total number of configurations for input is 1024. We take 64 random number series to get averaged RBM machine parameters. The initial values of parameters are taken to be normal
TABLE I: Tuned Restricted Boltzmann Machines and their Evaluation.

| $K_1$ | n | $X$(RBM) | $k$(BDRG) | $k_0$ | $k_1$ | $k_2$ | $k_3$ | $k_4$ | $k_5$ | $k_6$ | $k_7$ |
|-------|---|----------|----------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.2   | 2 | 0.266    | 0.269    | 0.897 | 0.294 | 0.037 | -0.003| 0.002 | 0.001 | 0.000 | 0.001 |
|       | 3 | 0.305    | 0.304    | 0.929 | 0.289 | 0.038 | 0.023 | 0.001 | 0.002 | 0.001 | 0.001 |
|       | 4 | 0.327    | 0.326    | 0.922 | 0.291 | 0.037 | 0.026 | 0.008 | 0.001 | 0.000 | 0.000 |
|       | 5 | 0.340    | 0.340    | 0.919 | 0.293 | 0.039 | 0.024 | 0.008 | 0.010 | 0.000 | 0.001 |
|       | 6 | 0.351    | 0.351    | 0.917 | 0.295 | 0.038 | 0.025 | 0.008 | 0.009 | 0.003 | 0.003 |
|       | 7 | 0.357    | 0.359    | 0.922 | 0.296 | 0.037 | 0.024 | 0.008 | 0.009 | 0.002 | 0.009 |
|       | 8 | 0.366    | 0.365    | 0.912 | 0.299 | 0.037 | 0.023 | 0.008 | 0.009 | 0.000 | 0.013 |
|       | 9 | 0.368    | 0.370    | 0.907 | 0.301 | 0.038 | 0.022 | 0.008 | 0.010 | 0.000 | 0.013 |
| 0.4   | 2 | 0.563    | 0.566    | 1.290 | 0.519 | 0.064 | 0.004 | 0.004 | 0.002 | 0.001 | 0.001 |
|       | 3 | 0.662    | 0.663    | 1.339 | 0.509 | 0.064 | 0.045 | 0.000 | 0.004 | 0.001 | 0.000 |
|       | 4 | 0.726    | 0.733    | 1.335 | 0.512 | 0.062 | 0.054 | 0.012 | 0.005 | 0.002 | 0.002 |
|       | 5 | 0.771    | 0.783    | 1.342 | 0.513 | 0.062 | 0.052 | 0.013 | 0.020 | 0.000 | 0.005 |
|       | 6 | 0.809    | 0.823    | 1.343 | 0.517 | 0.063 | 0.050 | 0.012 | 0.023 | 0.006 | 0.001 |
|       | 7 | 0.843    | 0.855    | 1.356 | 0.518 | 0.063 | 0.051 | 0.011 | 0.023 | 0.006 | 0.010 |
|       | 8 | 0.864    | 0.882    | 1.352 | 0.521 | 0.061 | 0.051 | 0.013 | 0.021 | 0.005 | 0.014 |
|       | 9 | 0.892    | 0.904    | 1.347 | 0.525 | 0.063 | 0.050 | 0.013 | 0.021 | 0.004 | 0.014 |
| 0.6   | 2 | 0.878    | 0.875    | 1.648 | 0.756 | 0.088 | 0.004 | 0.005 | 0.004 | 0.001 | 0.002 |
|       | 3 | 1.066    | 1.053    | 1.706 | 0.748 | 0.091 | 0.066 | 0.001 | 0.008 | 0.003 | 0.001 |
|       | 4 | 1.180    | 1.185    | 1.720 | 0.752 | 0.087 | 0.078 | 0.017 | 0.009 | 0.002 | 0.001 |
|       | 5 | 1.303    | 1.288    | 1.726 | 0.756 | 0.087 | 0.077 | 0.019 | 0.030 | 0.001 | 0.003 |
|       | 6 | 1.372    | 1.374    | 1.744 | 0.758 | 0.086 | 0.079 | 0.020 | 0.033 | 0.008 | 0.005 |
|       | 7 | 1.447    | 1.446    | 1.744 | 0.760 | 0.084 | 0.078 | 0.022 | 0.032 | 0.008 | 0.015 |
|       | 8 | 1.522    | 1.509    | 1.745 | 0.761 | 0.087 | 0.076 | 0.023 | 0.034 | 0.004 | 0.020 |
|       | 9 | 1.567    | 1.565    | 1.748 | 0.761 | 0.087 | 0.074 | 0.022 | 0.039 | 0.005 | 0.017 |
| 0.8   | 2 | 1.182    | 1.186    | 1.999 | 1.004 | 0.112 | 0.009 | 0.001 | 0.001 | 0.000 | 0.000 |
|       | 3 | 1.448    | 1.442    | 2.043 | 1.010 | 0.130 | 0.068 | 0.009 | 0.013 | 0.003 | 0.010 |
|       | 4 | 1.638    | 1.634    | 2.066 | 1.023 | 0.130 | 0.081 | 0.036 | 0.001 | 0.001 | 0.010 |
|       | 5 | 1.792    | 1.788    | 2.086 | 1.023 | 0.130 | 0.083 | 0.039 | 0.027 | 0.002 | 0.011 |
|       | 6 | 1.889    | 1.917    | 2.106 | 1.031 | 0.131 | 0.080 | 0.037 | 0.039 | 0.008 | 0.018 |
|       | 7 | 1.900    | 2.027    | 2.121 | 1.041 | 0.136 | 0.074 | 0.034 | 0.045 | 0.008 | 0.023 |
|       | 8 | 2.076    | 2.123    | 2.137 | 1.054 | 0.138 | 0.063 | 0.039 | 0.053 | 0.006 | 0.025 |
|       | 9 | 2.144    | 2.208    | 2.141 | 1.055 | 0.141 | 0.062 | 0.046 | 0.054 | 0.001 | 0.027 |

values $k_0 = 1, k_1 = 1, k_n = 1/n^2$ (for $n > 1$). The total structure of the likelihood function in the multi-dimensional space of $k$ will not be discussed here. In fact, 64 machines give well-converged results and we take averaged machine parameters to define the tuned up RBM in the following results.

Table 1 is the results of the averaged RBM parameters, where $K_1$ is the nearest neighbor coupling constant and $n$ is the maximum rang of the target LRI model interactions. For $n > 7$, optimized $k_n$ are all small numbers and are not listed in the table.

In order to evaluate the quality of tuned RBM, we compare the susceptibility given by RBM with those calculated by the Block Decimation Renormalization Group (BDRG). We
refer to a half of the logarithm of susceptibility $\chi$,

$$X = \log(\chi)/2, \quad \chi = \frac{1}{2jM} \left\langle \left( \sum_i v_i \right)^2 \right\rangle.$$  \hfill (24)

For the nearest neighbor case, $X$ coincides with the coupling constant,

$$X = K_1,$$  \hfill (25)

exactly in the infinite size limit.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{RBM_iteration.png}
\caption{RBM iteration of output data.}
\end{figure}

Starting with a set of 1024 perfectly random spin configurations (high temperature limit ensemble), we operate the tuned up RBM. We evaluate the susceptibility, step by step, which is seen in Fig. 3 as an example, where the target system is $K_1 = 0.6$ and $n = 9$. The value $X$ starts from the vanishing value of random spins and it increases rather quickly. Finally it slowly approaches towards the target value (1.565 in this case) which is drawn by a straight line. After the equilibrium, the thermal fluctuation is observed, whose size will be argued in a separate paper. After the onset of thermalized equilibrium, we read out the parameter $X$ of the RBM by averaging over 100 iterations.

The results are listed in Table 1 and are shown in Fig. 4, where all data of four $K$ values are plotted ($K = 0.2, 0.4, 0.6, 0.8$ from bottom to top). The coincidence looks very good and our tuned RBM well reproduce the LRI model results for the wide range of parameter values of $K$ and $n$. As for large susceptibility region, however, there appears small differences,
some part of which might come from the fact that our system is finite, periodic 128 spins, and shortage of the number of input configurations and/or iteration sets of learning and evaluation. These will be discussed in a separate paper.

It should be noted here that the susceptibility is just one physical quantity though it is most important, and we will investigate the RBM output configurations in detail to further check the total equivalence or quality of probability distribution. Also we will clarify the intimate relation between RBM and renormalization group method through multi-layer RBM systems, which will give us a new viewpoint to understand the physical features of LRI models.

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FIG. 4: Evaluation of RBM by comparing with BDRG.

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