Generalized Ising model, approximate calculation method

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Abstract

An approximate solution of the expected value of the direction of an arbitrary electron on the generalized Ising model (Ising model in which the energy with the external magnetic field and the energy of the interaction between the electrons take an arbitrary value) was obtained. Actually, considering application to the information system, we calculated each electron spin state as 0or1 instead of -1or1. As a result, even if the number of each spin increased, the error did not increase and it fell within 2%. If the expected value of the spin state is 0.1 to 0.9, the expected value can be obtained within an error range of 2% regardless of whether the energy value is positive or negative. The calculation amount of the approximate solution is obtained by the calculation amount of the square of N multiplied by 10 times. It can be expected as application of network analysis and the like. We also posted python source code.

1 Introduction

The generalized Ising model (Ising model in which the energy with the external magnetic field and the energy of the interaction between the electrons take an arbitrary value) is useful not only in physics but also in applied fields of information technology. This is because it is a generalizable model that represents network systems in which nodes taking 0 or 1 interact. From analysis of interactive networks such as block chains to Bayesian networks, artificial intelligence, etc. Application fields that can be modeled in the Ising model are diverse. As a result of the interaction, in order to calculate the expected value of the node, it is necessary to add all the states, and the calculation amount is 2 to the power of N. For this reason, it is not realistic to calculate all states steadily. The problem was the discovery of approximate calculation with less error, with practically calculable amount. Here, we present an approximate calculation method in which the error falls within 2% even if the number of nodes in the system increases, and is calculated by the calculation amount of the square of N multiplied by 10. We post python source code, so you can actually check.

2 Theory

2.1 Generalized Ising model

First, check well-known definitions. Hamiltonian can be expressed as follows.

$$H = \sum_{i=1}^{N} -h_i\sigma_i + \sum_{\{i,j\}} -J_{i,j}\sigma_i\sigma_j \tag{1}$$

σ takes 0 or 1, The first term on the right side of equation (1) is the energy when node σ is 1, The second term is the energy of the interaction that works when the nodes are mutually 1. The sum of {ij} takes on all edges (interaction). h and J may be positive or negative. If it is positive, it tends to be 1 because it lowers energy, and if it is minus it raises energy so it is difficult to become 1.
The expected value $\langle\sigma_x\rangle$ of a certain node σ_x is obtained by the following equation.

$$\langle\sigma_x\rangle = \frac{1}{Z}\sum_{\{\sigma\}}\sigma_x\prod_{i=1}^{N}\exp\left(\frac{h_i\sigma_i}{k_BT}\right)\prod_{\{i,j\}}\exp\left(\frac{J_{i,j}\sigma_i\sigma_j}{k_BT}\right) \tag{2}$$

On the right side,

$$\prod_{i=1}^{N}\exp\left(\frac{h_i\sigma_i}{k_BT}\right)\prod_{\{i,j\}}\exp\left(\frac{J_{i,j}\sigma_i\sigma_j}{k_BT}\right) = f \tag{3}$$

That is the probability of a state. Z is the state sum (partition function) of the system, It can be written as follows.

$$Z = \sum_{\{\sigma\}}\prod_{i=1}^{N}\exp\left(\frac{h_i\sigma_i}{k_BT}\right)\prod_{\{i,j\}}\exp\left(\frac{J_{i,j}\sigma_i\sigma_j}{k_BT}\right) \tag{4}$$

The sum of σ is taken in all states, It is the sum of the combinations at all σ (0 or 1).So far, it was confirmation of the well-known definition. Next, an approximate calculation method of the expected value $\langle\sigma_x\rangle$, which is the main argument, will be described.

2.2 Self-referencing approximate expression

The state sum of equation (4) is the sum of combinations when each node σ is 1 and 0. Let's assume that this is divided into the sum when the ith σ is 1 and the sum when it is 0.

$$Z = (Z_{\sigma_x=1} + Z_{\sigma_x=0}) \tag{5}$$

Then, from the equation (2), the expected value $\langle\sigma_x\rangle$ of the node σ_x is found as follows.

$$\langle\sigma_x\rangle = \frac{Z_{\sigma_x=1}}{Z_{\sigma_x=1} + Z_{\sigma_x=0}} \tag{6}$$

Introduce C_x .

$$\langle\sigma_x\rangle = \frac{\exp\left(\frac{h_x}{k_BT}\right)C_x}{\exp\left(\frac{h_x}{k_BT}\right)C_x + 1} \tag{7}$$

$$C_x = \frac{\exp\left(\frac{-h_x}{k_B T}\right) Z_{\sigma_x=1}}{Z_{\sigma_x=0}} \tag{8}$$

The denominator of C_x is the state sum (partition function) of the system from which node x is removed, The molecule removes node x , with the following

$$h_i \longrightarrow h_i + J_{x,i} \tag{9}$$

It is the state sum (partition function) of the system.

$$C_x = \frac{Z_{(\overline{x}, h_i \to h_i + J_{x,i})}}{Z_{(\overline{x})}} \tag{10}$$

Here we consider approximating C_x . When the equation (4) is expressed using the expected value $\langle \sigma_x \rangle$

$$C_x = \frac{\prod_{i=1}^{N} \exp\left(\frac{(h_i + J_{x,i})\langle \sigma_i \rangle}{k_B T}\right) \prod_{\{i,j\}} \exp\left(\frac{J_{i,j}\langle \sigma_i \rangle \langle \sigma_j \rangle}{k_B T}\right)}{\prod_{i=1}^{N} \exp\left(\frac{h_i \langle \sigma_i \rangle}{k_B T}\right) \prod_{\{i,j\}} \exp\left(\frac{J_{i,j}\langle \sigma_i \rangle \langle \sigma_j \rangle}{k_B T}\right)} \tag{11}$$

In the end,

$$C_x = \prod_{i=1}^{N} \exp\left(\frac{J_{x,i}\langle \sigma_i \rangle}{k_B T}\right) \tag{12}$$

To summarize the approximate expressions for obtaining the expected value $\langle \sigma_x \rangle$

$$\langle \sigma_x \rangle = \frac{\exp\left(\frac{h_x}{k_B T}\right) C_x}{\exp\left(\frac{h_x}{k_B T}\right) C_x + 1} \tag{13}$$

$$C_x = \prod_{i=1}^{N} \exp\left(\frac{J_{x,i}\langle \sigma_i \rangle}{k_B T}\right) \tag{14}$$

And $\langle \sigma_x \rangle$ can be written as an expression that refers to itself.

2.3 Calculation method

Include numbers and calculate. Expected value $\langle \sigma_x \rangle$ is expressed as self-referencing by equations (23), (24) and (25) It changes according to the following parameters.

$$\frac{1}{k_B T} \tag{15}$$

Therefore, we successfully take parameter (26) into the following range, Each $\langle \sigma_x \rangle$ successfully entered between 0.1 and 0.9, It was also found that the value of $\langle \sigma_x \rangle$ can be obtained with high accuracy.

$$-\frac{8}{N} < \left\{ \frac{h_i}{k_B T}, \frac{J_{i,j}}{k_B T} \right\} < \frac{8}{N} \tag{16}$$

Suppose now that the target system has the following values after adjustment by parameters

$$\frac{h_i}{k_B T} = \hat{h_i}, \frac{J_{i,j}}{k_B T} = \hat{J_{i,j}} \tag{17}$$

I want to find the expected value $\langle \sigma \rangle$, but since it is self-referencing, an initial value is necessary. In case of (18) it is (19).

$$\hat{h_i} = 0, \hat{J_{i,j}} = 0 \tag{18}$$

$$\langle \sigma_x \rangle = \frac{1}{2} \tag{19}$$

We will make this the initial value. As follows

$$\hat{h_i} t, \hat{J_{i,j}} t \tag{20}$$

While moving t to the condition t = 1 to be found from t = 0 corresponding to the initial value, While gradually repeating calculation and reference, Calculate by the method of obtaining the desired $\langle \sigma \rangle$. The number of times to approach is 10 times, and it can be taken with sufficient accuracy. As a result, the expected value $\langle \sigma \rangle$ of all the nodes can be obtained with a calculation amount of 10 × N × N.

The source code for obtaining expected value $\langle \sigma \rangle$ by python is presented below.

Listing 1 python3

```
import math
import numpy as np
N=8
h = np.random.rand(N)*2*8/N-8/N
J = [np.random.rand(N)*2*8/N-8/N for i in range(N)]
m = [0.5 for i in range(N)]
t=0.0
for a in range(10):
    t+=0.1
    for i in range(N):
        Ci = pow(math.exp(-h[i]), t)
        for j in range(N):
            if i!=j:
                if i<j:
                    Ci *= pow(math.exp(-J[i][j]), t*m[j])
                else:
                    Ci *= pow(math.exp(-J[j][i]), t*m[j])
        m[i] = (Ci) / (Ci + 1)
print(m)
```

The energy value was randomly determined under the condition (16), and the result of the subtraction of the approximate calculated expected value $\langle \sigma \rangle$ and the exact solution is as follows. (100 attempts)

Table1 Random h, J, 100 times trial

	Maximum difference	Average difference
N=8	0.031577966075	0.014093268382
N=12	0.026096346206	0.008297652209
N=16	0.0156324302932	0.0061926475208

3 Results

An approximate solution of the expected value of the direction of an arbitrary electron on the generalized Ising model (Ising model in which the energy with the external magnetic field and the energy of the interaction between the electrons take an arbitrary value) was obtained. As a result, even if the number of each spin increases, the error does not increase, Approximate calculation with error less than 2% could be performed. If the expected value of the spin state takes a value between 0.1 and 0.9, the expected value can be found within an error range within 2%, regardless of whether the value of each energy is plus or minus. The calculation amount of the approximate solution is obtained by the calculation amount of the square of N multiplied by 10 times. Further, if modeling with higher accuracy is performed in the equation (14), the accuracy of the expected value is expected to improve.

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