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TEMPERATURE ESTIMATION IN THE TWO-DIMENSIONAL ISING MODEL

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We present two new algorithms for the estimation of the temperature from a realization of a 2-D Ising model. The methods here introduced are based in the maximization of pseudo likelihood and on the minimum mean squared error (MSE) fit of the conditional probability function. We derive the analytical expressions of these estimators and also we include computational results comparing these new techniques with the traditional method. A very good performance in terms of the average absolute error and the average standard deviation is demonstrated through simulations in a 100×100 lattice in the ferromagnetic and antiferromagnetic cases. Summarizing, we have provided two new useful computational tools that allow us to measure the "virtual" temperature of an Ising like system.

Keywords: Ising model; mean squared error; ferromagnet.

1. Introduction

Ising model is one of the most famous tools from the statistical mechanics that have been successfully applied to problems not in the traditional physics scope. For example, in sociophysics, phenomena like "social phase transition",[1] "opinion formation"[2] or "group decision making"[3] can be analyzed through this model. There are also many applications to econophysics[4,5] and engineering problems like "image restoration"[6] and "telecommunication networks".[7] In all these cases the Ising model is capable to model the complex interaction among a huge number of agents like individuals in a social system, pixels in an image, phone cells in a telecommunication network, etc.

The spin behavior in the Ising model is governed by the external magnetic field (if it exist) and by the inner interaction energy which is inversely related to

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the temperature of the system.[8] One desirable tool, when we use this model in computational simulations, is to have a method to estimate the temperature of the system only from the spin state observations, this is the aim of the present paper. The temperature estimation in an Ising model was covered in the past (see Ref. 9 and similar approaches in Refs. 10 and 11). In this paper, we present two new techniques of temperature estimation that exhibit a better performance than the traditional method.

This work is organized as follows: in Sec. 1 the main well known results from the Ising model and the usual method for estimating the temperature are presented; in Sec. 2, we derive the analytical expression of our first method called Maximum Pseudo Likelihood; in Sec. 3, we derive a new estimator called Conditional Probability Function Fit which, as we will show, takes a simpler expression than the previous method; in Sec. 4, we present a large set of simulation results comparing both methods with the traditional method; finally in Sec. 5, the main conclusions of this paper are summarized.

2. Parameter Estimation in the 2-D Ising Model. The Traditional Approach

In the Ising model we have N spins which can assume only two opposite states, $s_i = -1$ or $s_i = +1$. The energy of the Ising system in the configuration specified by $\{s_i\}$ is defined as

$$E_I\{s_i\} = -\sum_{\langle ij\rangle} \epsilon_{ij} s_i s_j - H\sum_{i=1}^{N} s_i \,, \tag{1}$$

where the subscript I stands for Ising and the symbol $\langle ij\rangle$ denotes a nearest-neighbor pair of spins. There is no distinction between $\langle ij\rangle$ and $\langle ji\rangle$. Thus the sum over $\langle ij\rangle$ contains $\gamma N/2$ terms, where γ is the number of nearest neighbors of any given spin and the lattice geometry is described through γ and ϵ_{ij}.

In this work we use the classical two dimensional $L \times L$ Ising lattice ($N = L^2$), with all $\epsilon_{ij} = \epsilon$, $\gamma = 4$ (nearest neighbor structure) and $H = 0$ (no external magnetic field). As usually we impose periodic boundary conditions in both dimensions.

From the statistical point of view, Ising model is a particular case of a Markov Random Field[12] and it gives us a direct way to calculate the probability of a determined configuration of the system by its Gibbs formula $P(\{s_i\}) = 1/Z \exp(-1/kTE_I\{s_i\})$, where Z is the partition function, k is the Boltzmann constant and T is the temperature of the system.

In the traditional approach, the estimation of the β parameter is performed considering the probabilities of having an up spin surrounded with different combinations of neighbor's values.[9] Defining the neighbor's summation $\sigma_i = \sum_j s_j$ with j indexing the neighbors of spin i, we can calculate then the number of up spins with its neighbors summing up to -4, -2, 0, $+2$ and $+4$. More precisely, defining N_α^+ (N_α^-) as the number of up (down) spins whose neighbors sum up to α and, using the usual Gibbs formula, the traditional method allows us to calculate two independent estimates of the parameter β through the following equations:[9]

$$\frac{N^+_{-2}}{N^+_{+2}} \approx \exp(-4\beta) \quad \text{and} \quad \frac{N^+_{-4}}{N^+_{+4}} \approx \exp(-8\beta)\,, \tag{2}$$

In the following sections we present two new alternative methods for the estimation of the parameter β.

3. Method 1: Maximum Pseudo Likelihood

Pseudo Maximum Likelihood estimation is a common technique in Markov Random Fields[12] and have been used for the case of Gaussian random fields by J. Besag in Ref. 14. This criterion states that $\hat{\beta}$ (the estimator of β) is the one which maximizes the following conditional probabilities product.

$$\prod_{i=1}^{N} P(s_i/\sigma_i)\,, \tag{3}$$

where σ_i is the previously defined neighbor's summation. Using the Gibbs formula[12] we can calculate the conditional probability for a fixed spin at position i provided the sum of its neighbors σ_i as follows:

$$P(s_i = s/\sigma_i = \alpha) = \frac{\exp(\beta s \alpha)}{\exp(\beta\alpha) + \exp(-\beta\alpha)}\,, \tag{4}$$

where $\beta = \epsilon/kT$ is the parameter which we want to estimate and it is inversely proportional to the temperature T, $s = \pm 1$ is the state of the spin at position i, and $\sigma_i = \alpha$ is restricted to have the values: 0, +2, −2, −4 and +4 in our nearest neighbor case. The advantage of using the conditional probability is that, as it is a ratio of probabilities, the partition function, which has a complicated dependency on parameter β, is cancelled from numerator and denominator.

Putting equation (4) in (3) and applying natural logarithm to the expression above we reach the following objective function of the parameter β:

$$J(\beta) = \sum_{i=1}^{N} [\beta s_i \sigma_i - \ln(2\cosh(\beta\sigma_i))]\,. \tag{5}$$

In order to maximize this function, we differentiate, respect to β, the above expression and we find out which is the value of β that makes $dJ(\beta)/d\beta = 0$.

$$\frac{dJ(\beta)}{d\beta} = \sum_{i=1}^{N} [s_i\sigma_i - \sigma_i \tanh(\beta\sigma_i)] = 0\,. \tag{6}$$

Defining N_α as the number of sites for which its neighbor summation is equal to α ($N_\alpha = N^+_\alpha + N^-_\alpha$), and noting that $N = N_0 + N_{-2} + N_{+2} + N_{-4} + N_{+4}$, we decompose the sum in equation (6) as follows:

$$\begin{aligned} &\underbrace{-2\sum^{N_{-2}} s_i + 2\sum^{N_{+2}} s_i - 4\sum^{N_{-4}} s_i + 4\sum^{N_{+4}} s_i}_{A} - \underbrace{2(N_{-2}+N_{+2})}_{B}\tanh(2\beta) \\ &\qquad - \underbrace{4(N_{-4}+N_{+4})}_{C}\tanh(4\beta) = 0 \end{aligned}, \tag{7}$$

where the notation $\sum^{N_\alpha} s_i$ means to take a summation of all sites values whose neighbors sum α. Finally, he estimator is obtained as the $\hat{\beta}$ which satisfies:

$$A - B\tanh(2\hat{\beta}) - C\tanh(4\hat{\beta}) = 0\,. \tag{8}$$

Is easy to see that the number A is directly related to the energy of the system $E_I\{s_i\}$ defined by Eq. (1). Summarizing, the numbers A, B and C are calculated as follows:

$$A = -2E_I\{s_i\}\,, \tag{9}$$

$$B = 2(N_{-2} + N_{+2})\,, \tag{10}$$

$$C = 4(N_{-4} + N_{+4})\,. \tag{11}$$

The numbers A, B, and C are quantities that we can easily calculate from the configuration $\{s_i\}$ just counting spins. The estimator $\hat{\beta}$ can be obtained using a zero finding numeric technique like optimal Myller's method.[13]

4. Method 2: Conditional Probability Function Fit

Now we introduce another approach to the estimation of β parameter. If we denote the probability to see a center spin up provided the neighborhood is alpha by $p_\alpha^+ = P(s_i = +1|\sigma_i = \alpha)$, from equation (4) we obtain a simple expression of this conditional probability:

$$p_\alpha^+ = \frac{1}{1 + \exp(-2\beta\alpha)}\,. \tag{12}$$

Therefore parameter β must satisfy the following equation:

$$\beta = -\frac{1}{2\alpha}\ln\left(\frac{1 - p_\alpha^+}{p_\alpha^+}\right)\,. \tag{13}$$

Note that we can estimate probabilities $\hat{p}_\alpha^+$ from a configuration $\{s_i\}$ dividing the number of up spins with neighborhood α over the total number of spins with neighborhood α. Also note, that each value of α gives a different estimate of β, so we denote by $\hat{\beta}_\alpha$ to the estimation of the parameter using the class of spins whose neighbors summation is α. Additionally we have a special case for $\alpha = 0$, in this situation, $p_0^+ = 0.5$ and it is independent of the β value (see equation (12)). For this reason we are able to use only the values $\hat{p}_{-2}^+$, $\hat{p}_{+2}^+$, $\hat{p}_{-4}^+$ and $\hat{p}_{+4}^+$ to estimate the parameter. Additionally, if we impose to minimize the Mean Square Error (MSE) of the estimator, we finally obtain $\hat{\beta}$ as the aritmethic mean of $\hat{\beta}_{-2}$, $\hat{\beta}_{+2}$, $\hat{\beta}_{-4}$ and $\hat{\beta}_{+4}$, which is:

$$\hat{\beta} = \frac{1}{4}(\hat{\beta}_{-2} + \hat{\beta}_{+2} + \hat{\beta}_{-4} + \hat{\beta}_{+4})\,. \tag{14}$$

It is important to highlight a relationship between these four estimates of β and the traditional technique of Sec. 1. The probability in equation (12), as we explained before, can be related with experimental counters of spins as follows:

$$\hat{p}^{+}_{\alpha} = \frac{N^{+1}_{\alpha}}{N_{\alpha}}\,. \tag{15}$$

Note that the probability of having an up spin surrounded with α is the same as having a down spin surrounding with $-\alpha$. Therefore, if we use the approximation $N^{-1}_{\alpha} \approx N^{+1}_{-\alpha}$ in equation (15) and using equation (12) we reach to the same formula (2) of the traditional method. In other words, if the approximation $N^{-1}_{\alpha} \approx N^{+1}_{-\alpha}$ is considered as an identity, the number of independent estimates of β is restricted to two.

Anyway, in real life applications, where we have only one realization of the lattice it is better to calculate each one of the numbers N^{+1}_{α} and obtain as many independent estimates of β as posible. From the statistical point of view we should consider all the information available from a realization of the lattice and this includes: N^{+1}_{-4}, N^{+1}_{-4}, N^{+1}_{+2} and N^{+1}_{+4}.

In the next section we present some simulation results comparing the statistics of our estimates of β (method 1 and method 2) against the estimate of β based on the traditional method and showing that our estimates give smaller average absolute error and reduced variance also.

5. Simulation Results

In order to test and compare these new parameter estimation techniques against the traditional method, we have performed a large set of simulations. We have generated realizations of Ising model with a known β parameter and we have calculated its estimates $\hat{\beta}$ through all the methods: the traditional technique and our two new methods. For the generation of the realizations we have implemented the well known Metropolis algorithm[15] starting from a random configuration of the lattice and performing random flips on spins according to the algorithm rule. As the iteration of the algorithm is increased, the configuration of the system tends to be a sample from the corresponding Gibbs probability distribution of Ising model.[15]

The experiment that we proposed was to calculate the corresponding β parameter estimates for every Metropolis iteration step using the three techniques. This experiment allowed us to compare both methods with the traditional approach and also to analyze how the Metropolis algorithm evolves converging to a valid configuration where the parameter estimate is close to the real known parameter β value.

In our experiment we used a 100×100 lattice ($N = 10000$ spins) with periodic boundary conditions. The starting configuration was generated with random spins states at $+1$ (up) and -1 (down) chosen with probability 0.5 each one. In the initial configuration all spins were independently selected which corresponds to the case of $\beta = 0$.

Regarding the range of the parameter β we note that the estimations make sense when the parameter is in the range of disorder (or non magnetized) ($\beta < 0.44$).[8] Note, for example that, when the whole lattice is magnetized (all spins at the same state), estimation of the parameter using equation (8) gives $\hat{\beta} = \pm\infty$. For this reason we performed Metropolis simulations of Ising model with a known β in the range -0.44 to $+0.44$, negative values correspond to the antiferromagnetic behavior while positive values correspond to ferromagnetic region. We covered this range changing the parameter with a step of 0.0176 reaching to a total of 50 simulations. We have use a total number of iterations of 1 000 000 for each simulation.

In order to apply all the estimation techniques we needed to calculate, at every Metropolis iteration step t, the corresponding parameters $N_0(t)$, $N_{-2}(t)$, $N_{+2}(t)$, $N_{-4}(t)$ and $N_{+4}(t)$ which are the number of spin sites surrounded by 0, -2, $+2$, -4 and $+4$ respectively. Given that the Metropolis algorithm is allowed to flip one spin state by step at most, we perform an adaptive calculation of these parameters reaching to a fast calculation.

For the traditional method (Sec. 1), at every Metropolis step t, we calculated the ratios of equations (2) reaching to two estimates of β that we denote: $\hat{\beta}_{\pm 2}$ and $\hat{\beta}_{\pm 4}$. In order to combine these two estimates in a final estimate we performed the arithmetic mean of these values: $\hat{\beta}(t) = 1/2(\hat{\beta}_{\pm 2}(t) + \hat{\beta}_{\pm 4}(t))$.

For our method 1 (Maximum Pseudo Likelihood), at every Metropolis step t, we used equations (1), (9), (10) and (11) to calculate parameters A, B and C and then we found the solution of equation (8) using the optimal Myller's method,[13] which determines the estimation of parameter $\hat{\beta}(t)$.

For our method 2 (Conditional Probability Function Fit) we estimated, at every Metropolis step, the $\hat{p}^+_{-2}$, $\hat{p}^+_{+2}$, $\hat{p}^+_{-4}$ and $\hat{p}^+_{+4}$ values using following formula.15 Once we have estimated $\hat{p}^+_{\alpha}$ values, we calculated $\hat{\beta}_{\alpha}$ using equation (13), and finally we obtained the parameter $\hat{\beta}(t)$ estimate using equation (14).

In Fig. 1 we show the time evolution of estimates for all the methods: Traditional Method, Maximum Pseudo Likelihood (Method 1) and Conditional Probability Function Fit (Method 2) for five special cases of β (± 0.44, ± 0.288 and 0). Note that in all cases the initial estimate of the parameter is $\hat{\beta} \approx 0$.

In order to make a more complete numerical analysis we calculated the mean and standard deviation of these estimators for each β value. We used the iterations number 800 000 to 1 000 000 (200 000 samples) to calculate the statistics in order to assure that we are in a stationary regime of the Metropolis algorithm.

To evaluate the accuracy of these methods we needed to look at the mean value and standard deviation of these estimators. In Fig. 2, a comparison of mean values of estimators are shown. We ploted the mean ratio $\hat{\beta}/\beta$ versus the real parameter

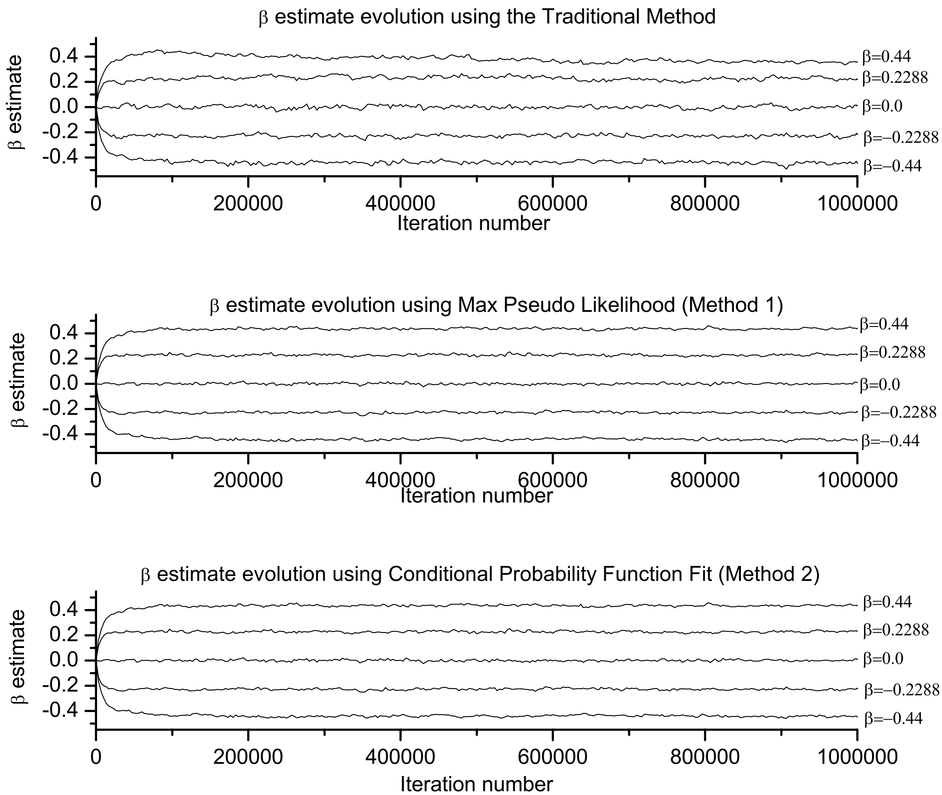

Fig. 1. Time evolution of estimator $\hat{\beta}$ during Metropolis algorithm progress for traditional method (top), method 1 (middle) and method 2 (bottom).

Table 1. Comparison of the estimator's statistics.

	Traditional Method	Method 1	Method 2
Average absolute error (%)	2.62%	0.83%	0.85%
Average standard deviation	0.0119	0.0069	0.0070

β for the three estimators. In Fig. 3, a plot of the standard deviation of estimators versus the real parameter β is presented for all the methods.

As can be observed in Figs. 2 and 3 our methods 2 and method 3 have similar statistics and are better than the traditional method. More specifically, if we calculate their average absolute error and their standard deviation we obtain the results displayed in Table 1 where the advantage of using method 1 or 2 over traditional method is noticeable.

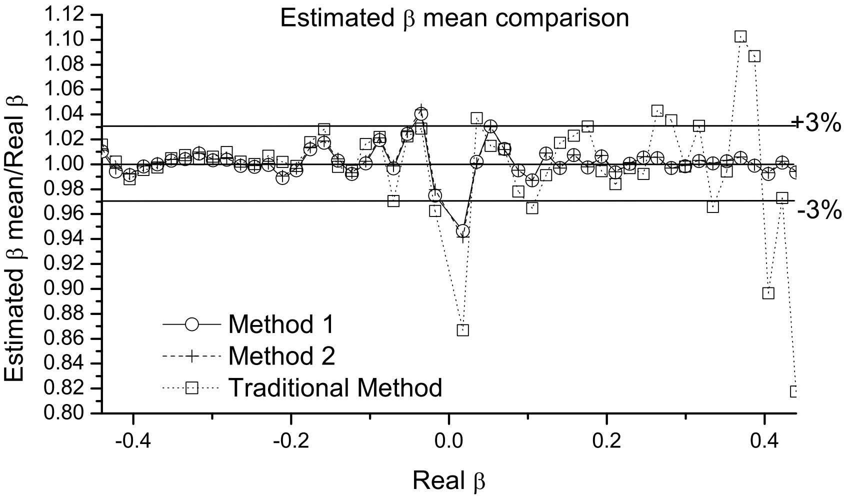

Fig. 2. Means of $\hat{\beta}$ estimators divided by real β comparison. Means were calculated over 200 000 samples for each known parameter β.

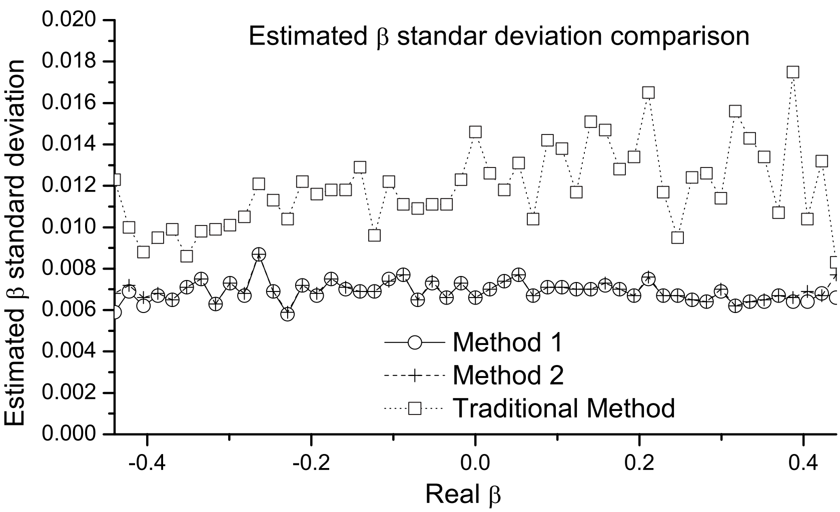

Fig. 3. Standard deviations of $\hat{\beta}$ estimators calculated over 200 000 samples for each known parameter β.

6. Conclusions

We have presented two new methods for the estimation of β parameter in 2-D Ising models which is equivalent to estimate the temperature of the system. The methods here presented are based on two different estimation criteria: one is based on the maximization of the Pseudo Likelihood and the other is based on the minimum Mean Squared Error (MSE) fit of the conditional probability function. Even though these methods came from different approaches it was observed that both methods provide very similar results (see figures).

These methods showed to be very efficient for the estimation of β (or temperature) in Ising models in the ferromagnetic ($\beta > 0$) and antiferromagnetic ($\beta < 0$) regions and for the range of the parameter where magnetization is not present, it means, below the critical value of the parameter ($|\beta| < 0.44$). We have made simulations for a 100×100 lattice for which the accuracy of the proposed methods is higher than the one obtained with the traditional approach in terms of average absolute error and average standard deviation (see Table 1).

We note that the method 2 (minimum Mean Squared Error fit of conditional probability function) is simpler than method 1 (maximum Pseudo Likelihood). Method 1 requires to solve a zero finding numerical algorithm like optimal Myller's method,[13] on the other hand, method 2 provides a direct calculation of the parameter which is simpler.

In this way we have provided two new useful tools for the study of complex systems using Ising model because, following these methods, one can measure the "virtual" temperature of a system.

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